Full wwPDB NMR Structure Validation Report (i)

Jun 24, 2024 – 11:25 AM EDT

PDB ID	:	6W4E
BMRB ID	:	30734
Title	:	NMR-driven structure of KRAS4B-GTP homodimer on a lipid bilayer nanodisc
Authors	:	Lee, K.; Fang, Z.; Enomoto, M.; Gasmi-Seabrook, G.M.; Zheng, L.; Marshall, C.B.; Ikura, M.
Deposited on	:	2020-03-10

This is a Full wwPDB NMR Structure Validation Report for a publicly released PDB entry.

We welcome your comments at *validation@mail.wwpdb.org*
A user guide is available at
https://www.wwpdb.org/validation/2017/NMRValidationReportHelp
with specific help available everywhere you see the (i) symbol.

The types of validation reports are described at
http://www.wwpdb.org/validation/2017/FAQs#types.

The following versions of software and data (see references (i)) were used in the production of this report:

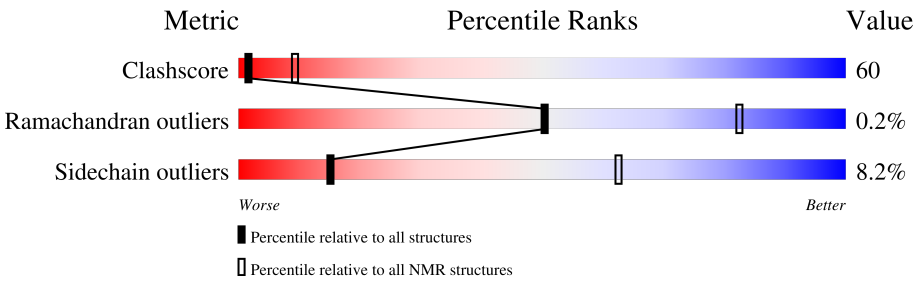
MolProbity	:	4.02b-467
Mogul	:	2022.3.0, CSD as543be (2022)
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
wwPDB-RCI	:	v_1n_11_5_13_A (Berjanski et al., 2005)
PANAV	:	Wang et al. (2010)
wwPDB-ShiftChecker	:	v1.2
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.37.1

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
SOLUTION NMR

The overall completeness of chemical shifts assignment is 1%.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	NMR archive (#Entries)
Clashscore	158937	12864
Ramachandran outliers	154571	11451
Sidechain outliers	154315	11428

The table below summarises the geometric issues observed across the polymeric chains and their fit to the experimental data. The red, orange, yellow and green segments indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria. A cyan segment indicates the fraction of residues that are not part of the well-defined cores, and a grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=5%

Mol	Chain	Length	Quality of chain
1	A	200	86% 12% ••
1	D	200	87% 12% •
2	B	185	78% 11% 10% •
2	C	185	74% 16% 9% •

2 Ensemble composition and analysis (i)

This entry contains 20 models. Model 15 is the overall representative, medoid model (most similar to other models). The authors have identified model 1 as representative, based on the following criterion: *lowest energy*.

The following residues are included in the computation of the global validation metrics.

Well-defined (core) protein residues			
Well-defined core	**Residue range (total)**	**Backbone RMSD (Å)**	**Medoid model**
1	A:202-A:398, D:399-D:596 (395)	0.33	15
2	B:1-B:165, C:1-C:167 (332)	0.69	16

Ill-defined regions of proteins are excluded from the global statistics.

Ligands and non-protein polymers are included in the analysis.

The models can be grouped into 2 clusters and 1 single-model cluster was found.

Cluster number	Models
1	1, 2, 3, 4, 5, 6, 7, 8, 9, 12, 13, 14, 15, 16, 18, 19
2	10, 11, 20
Single-model clusters	17

3 Entry composition (i)

There are 6 unique types of molecules in this entry. The entry contains 12112 atoms, of which 1536 are hydrogens and 0 are deuteriums.

- Molecule 1 is a protein called Apolipoprotein A-I.

Mol	Chain	Residues	Atoms						Trace
			Total	C	H	N	O	S	
1	A	198	2004	1019	381	287	314	3	0
1	D	198	2002	1019	379	287	314	3	0

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	199	GLY	-	expression tag	UNP P02647
A	200	PRO	-	expression tag	UNP P02647
D	397	GLY	-	expression tag	UNP P02647
D	398	PRO	-	expression tag	UNP P02647

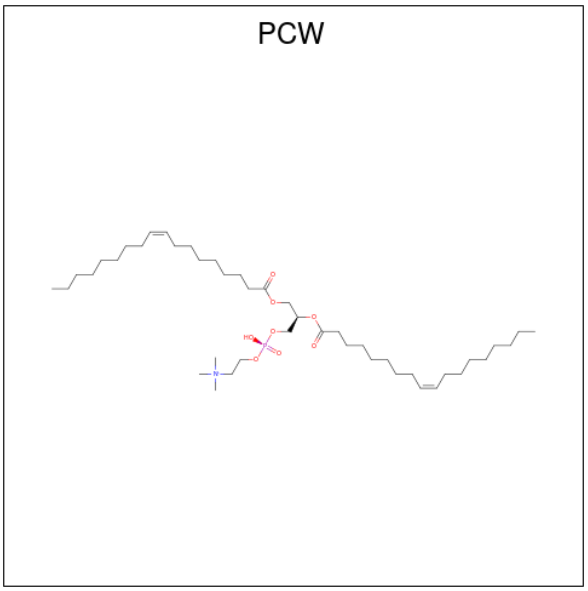
- Molecule 2 is a protein called GTPase KRas.

Mol	Chain	Residues	Atoms						Trace
			Total	C	H	N	O	S	
2	B	184	1830	920	358	256	289	7	0
2	C	184	1830	920	358	256	289	7	0

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	1	SER	-	expression tag	UNP P01116
B	12	ASP	GLY	conflict	UNP P01116
C	1	SER	-	expression tag	UNP P01116
C	12	ASP	GLY	conflict	UNP P01116

- Molecule 3 is 1,2-DIOLEOYL-SN-GLYCERO-3-PHOSPHOCHOLINE (three-letter code: PCW) (formula: $C_{44}H_{85}NO_8P$).



Mol	Chain	Residues	Atoms				
			Total	C	N	O	P
3	A	1	54	44	1	8	1
			Total	C	N	O	P
3	A	1	54	44	1	8	1
			Total	C	N	O	P
3	A	1	54	44	1	8	1
			Total	C	N	O	P
3	A	1	54	44	1	8	1
			Total	C	N	O	P
3	A	1	54	44	1	8	1
			Total	C	N	O	P
3	A	1	54	44	1	8	1
			Total	C	N	O	P
3	A	1	54	44	1	8	1
			Total	C	N	O	P
3	A	1	54	44	1	8	1
			Total	C	N	O	P
3	A	1	54	44	1	8	1
			Total	C	N	O	P
3	A	1	54	44	1	8	1
			Total	C	N	O	P
3	A	1	54	44	1	8	1
			Total	C	N	O	P
3	A	1	54	44	1	8	1
			Total	C	N	O	P
3	A	1	54	44	1	8	1

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Mol	Chain	Residues	Atoms				
3	A	1	Total	C	N	O	P
			54	44	1	8	1
3	A	1	Total	C	N	O	P
			54	44	1	8	1
3	A	1	Total	C	N	O	P
			54	44	1	8	1
3	A	1	Total	C	N	O	P
			54	44	1	8	1
3	A	1	Total	C	N	O	P
			54	44	1	8	1
3	D	1	Total	C	N	O	P
			54	44	1	8	1
3	D	1	Total	C	N	O	P
			54	44	1	8	1
3	D	1	Total	C	N	O	P
			54	44	1	8	1
3	D	1	Total	C	N	O	P
			54	44	1	8	1
3	D	1	Total	C	N	O	P
			54	44	1	8	1
3	D	1	Total	C	N	O	P
			54	44	1	8	1
3	D	1	Total	C	N	O	P
			54	44	1	8	1
3	D	1	Total	C	N	O	P
			54	44	1	8	1
3	D	1	Total	C	N	O	P
			54	44	1	8	1
3	D	1	Total	C	N	O	P
			54	44	1	8	1
3	D	1	Total	C	N	O	P
			54	44	1	8	1
3	D	1	Total	C	N	O	P
			54	44	1	8	1
3	D	1	Total	C	N	O	P
			54	44	1	8	1
3	D	1	Total	C	N	O	P
			54	44	1	8	1

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Mol	Chain	Residues	Atoms				
			Total	C	N	O	P
3	D	1	54	44	1	8	1
			Total	C	N	O	P
3	D	1	54	44	1	8	1
			Total	C	N	O	P
3	D	1	54	44	1	8	1
			Total	C	N	O	P
3	D	1	54	44	1	8	1
			Total	C	N	O	P
3	D	1	54	44	1	8	1
			Total	C	N	O	P
3	D	1	54	44	1	8	1
			Total	C	N	O	P
3	D	1	54	44	1	8	1
			Total	C	N	O	P
3	D	1	54	44	1	8	1
			Total	C	N	O	P
3	D	1	54	44	1	8	1
			Total	C	N	O	P
3	D	1	54	44	1	8	1
			Total	C	N	O	P
3	D	1	54	44	1	8	1
			Total	C	N	O	P
3	B	1	54	44	1	8	1
			Total	C	N	O	P
3	B	1	54	44	1	8	1
			Total	C	N	O	P
3	B	1	54	44	1	8	1
			Total	C	N	O	P
3	B	1	54	44	1	8	1
			Total	C	N	O	P
3	B	1	54	44	1	8	1
			Total	C	N	O	P
3	B	1	54	44	1	8	1
			Total	C	N	O	P
3	C	1	54	44	1	8	1
			Total	C	N	O	P
3	C	1	54	44	1	8	1
			Total	C	N	O	P
3	C	1	54	44	1	8	1
			Total	C	N	O	P
3	C	1	54	44	1	8	1

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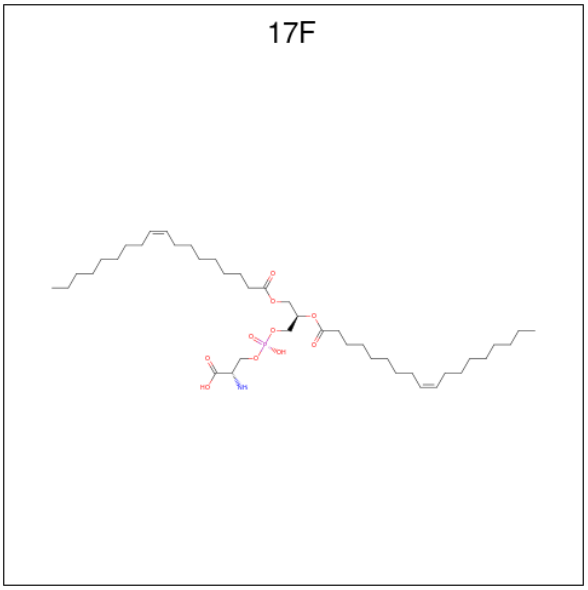
Mol	Chain	Residues	Atoms				
			Total	C	N	O	P
3	C	1	54	44	1	8	1
			Total	C	N	O	P
3	C	1	54	44	1	8	1
			Total	C	N	O	P
3	C	1	54	44	1	8	1
			Total	C	N	O	P
3	C	1	54	44	1	8	1
			Total	C	N	O	P
3	C	1	54	44	1	8	1
			Total	C	N	O	P
3	C	1	54	44	1	8	1
			Total	C	N	O	P
3	C	1	54	44	1	8	1
			Total	C	N	O	P
3	C	1	54	44	1	8	1

- Molecule 4 is O-[(S)-({(2R)-2,3-bis[(9Z)-octadec-9-enoyloxy]propyl}oxy)(hydroxy)phosphoryl]-L-serine (three-letter code: 17F) (formula: $C_{42}H_{78}NO_{10}P$).



Mol	Chain	Residues	Atoms					
			Total	C	H	N	O	P
4	A	1	57	42	3	1	10	1
			Total	C	H	N	O	P
4	A	1	57	42	3	1	10	1
			Total	C	H	N	O	P
4	A	1	57	42	3	1	10	1

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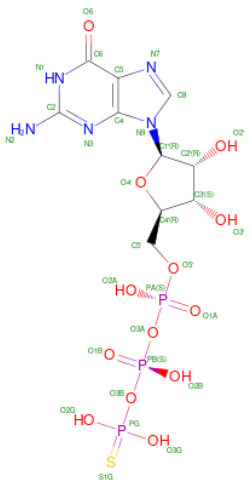
Mol	Chain	Residues	Atoms					
			Total	C	H	N	O	P
4	D	1	57	42	3	1	10	1
			Total	C	H	N	O	P
4	D	1	57	42	3	1	10	1
			Total	C	H	N	O	P
4	D	1	57	42	3	1	10	1
			Total	C	H	N	O	P
4	D	1	57	42	3	1	10	1
			Total	C	H	N	O	P
4	D	1	57	42	3	1	10	1
			Total	C	H	N	O	P
4	B	1	57	42	3	1	10	1
			Total	C	H	N	O	P
4	B	1	57	42	3	1	10	1
			Total	C	H	N	O	P
4	B	1	57	42	3	1	10	1
			Total	C	H	N	O	P
4	C	1	57	42	3	1	10	1
			Total	C	H	N	O	P
4	C	1	57	42	3	1	10	1
			Total	C	H	N	O	P
4	C	1	57	42	3	1	10	1
			Total	C	H	N	O	P
4	C	1	57	42	3	1	10	1
			Total	C	H	N	O	P
4	C	1	57	42	3	1	10	1

- Molecule 5 is 5'-GUANOSINE-DIPHOSPHATE-MONOTHIOPHOSPHATE (three-letter code: GSP) (formula: $C_{10}H_{16}N_5O_{13}P_3S$).

GSP



Mol	Chain	Residues	Atoms						
			Total	C	H	N	O	P	S
5	B	1	38	10	6	5	13	3	1
			Total	C	H	N	O	P	S
5	C	1	38	10	6	5	13	3	1

- Molecule 6 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms	
			Total	Mg
6	B	1	1	1
			Total	Mg
6	C	1	1	1

4 Residue-property plots (i)

4.1 Average score per residue in the NMR ensemble

These plots are provided for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic is the same as shown in the summary in section 1 of this report. The second graphic shows the sequence where residues are colour-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. Stretches of 2 or more consecutive residues without any outliers are shown as green connectors. Residues which are classified as ill-defined in the NMR ensemble, are shown in cyan with an underline colour-coded according to the previous scheme. Residues which were present in the experimental sample, but not modelled in the final structure are shown in grey.

• Molecule 1: Apolipoprotein A-I

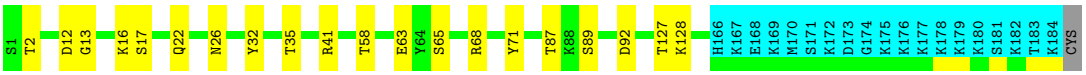
Chain A:

• Molecule 1: Apolipoprotein A-I

Chain D:

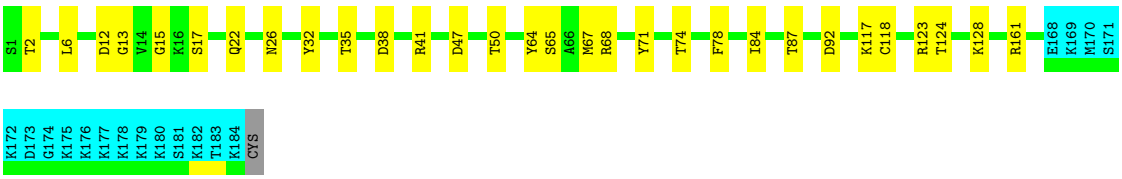
• Molecule 2: GTPase KRas

Chain B:



• Molecule 2: GTPase KRas

Chain C:



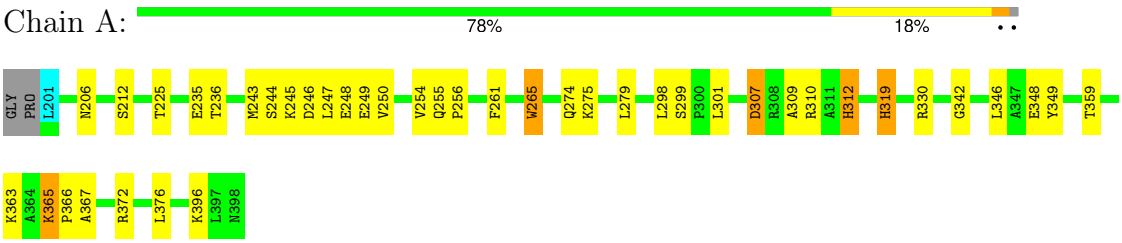
4.2 Scores per residue for each member of the ensemble

Colouring as in section 4.1 above.

4.2.1 Score per residue for model 1

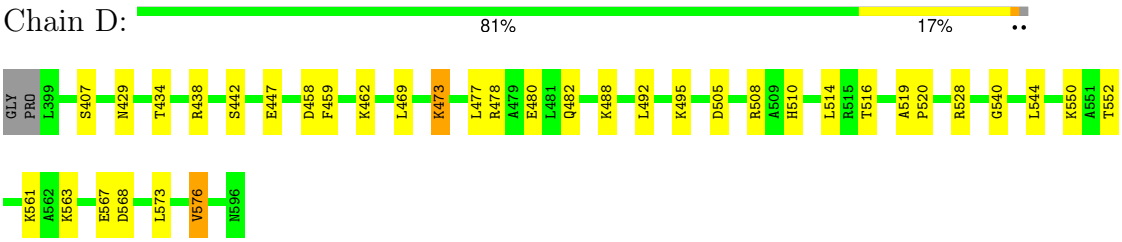
- Molecule 1: Apolipoprotein A-I

Chain A:



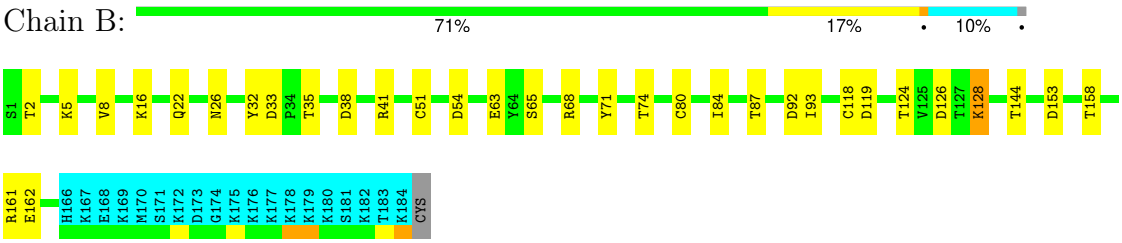
- Molecule 1: Apolipoprotein A-I

Chain D:



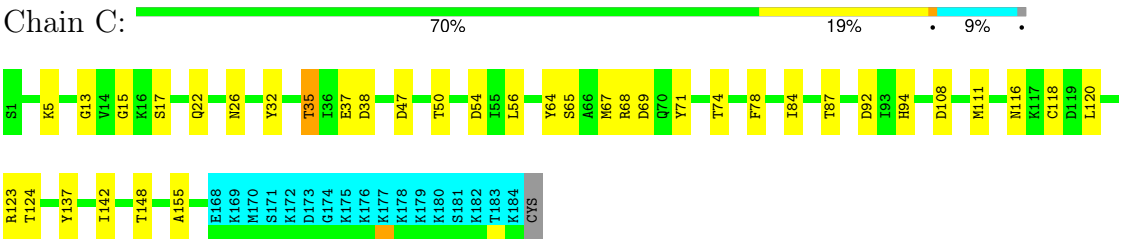
- Molecule 2: GTPase KRas

Chain B:



- Molecule 2: GTPase KRas

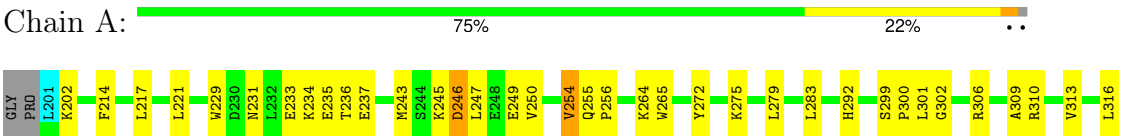
Chain C:



4.2.2 Score per residue for model 2

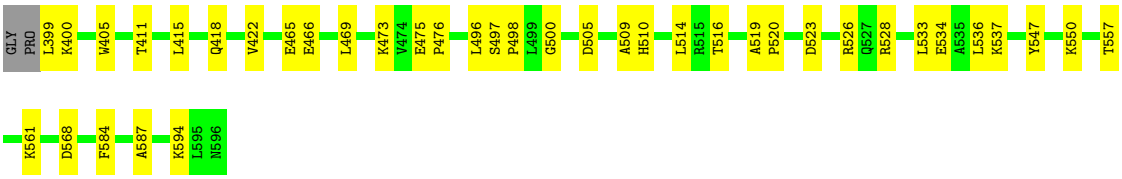
- Molecule 1: Apolipoprotein A-I

Chain A:



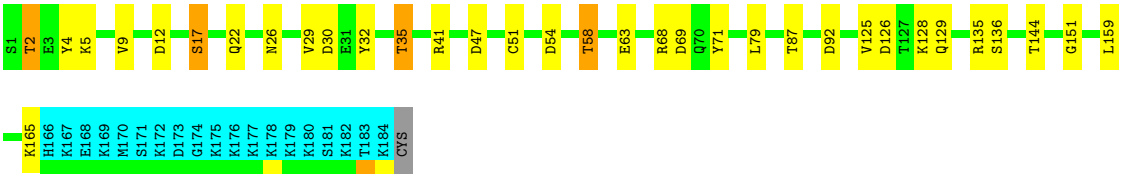
• Molecule 1: Apolipoprotein A-I

Chain D:



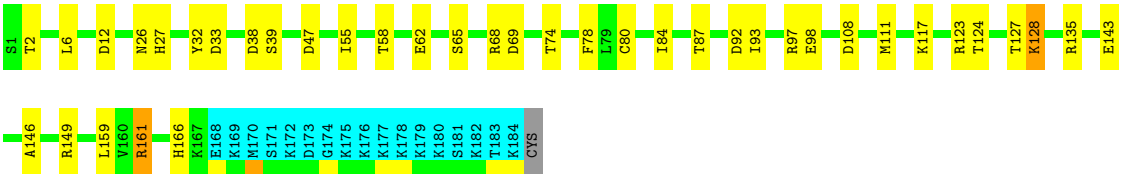
• Molecule 2: GTPase KRas

Chain B:



• Molecule 2: GTPase KRas

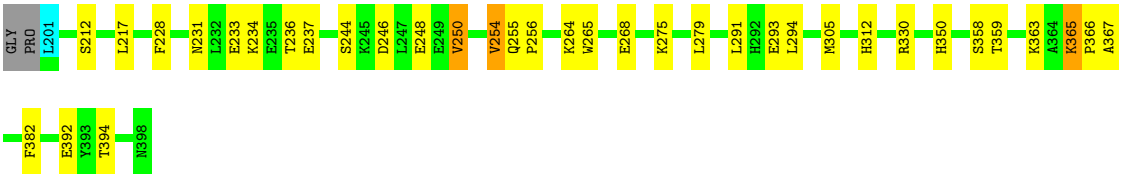
Chain C:



4.2.3 Score per residue for model 3

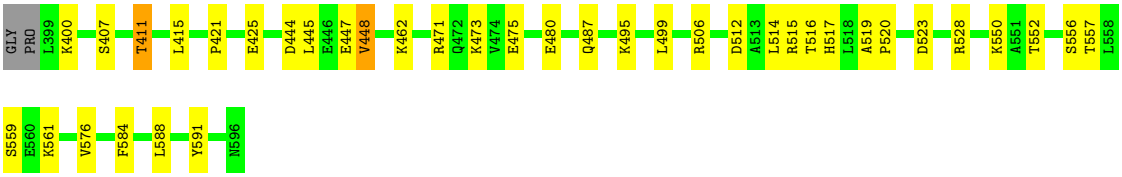
• Molecule 1: Apolipoprotein A-I

Chain A:



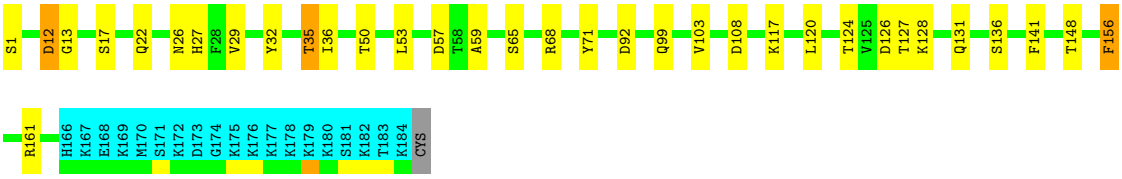
• Molecule 1: Apolipoprotein A-I

Chain D:



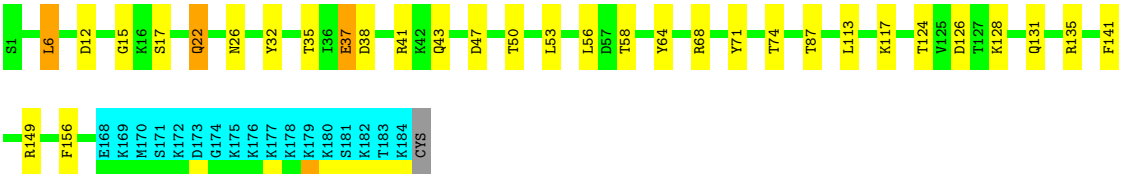
• Molecule 2: GTPase KRas

Chain B:



• Molecule 2: GTPase KRas

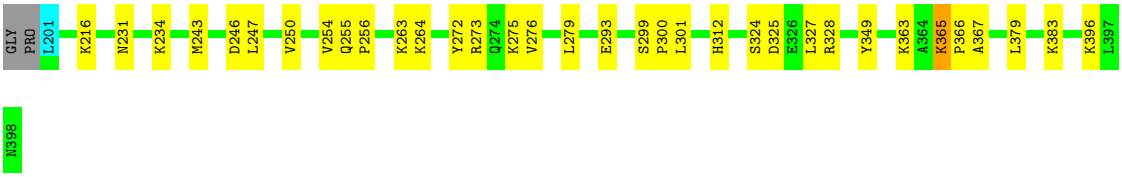
Chain C:



4.2.4 Score per residue for model 4

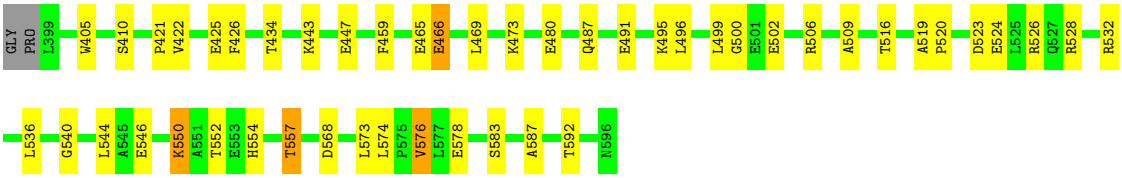
• Molecule 1: Apolipoprotein A-I

Chain A:



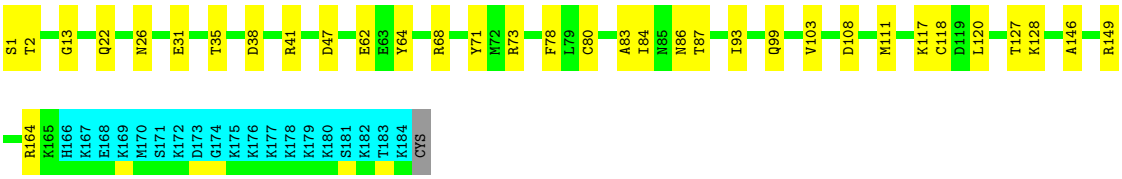
• Molecule 1: Apolipoprotein A-I

Chain D:



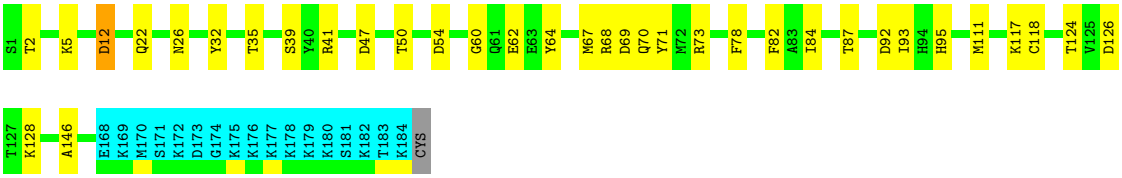
• Molecule 2: GTPase KRas

Chain B: 71% 18% 10%



• Molecule 2: GTPase KRas

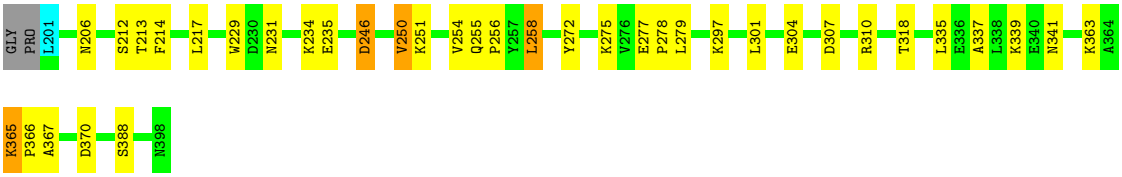
Chain C: 71% 18% • 9% •



4.2.5 Score per residue for model 5

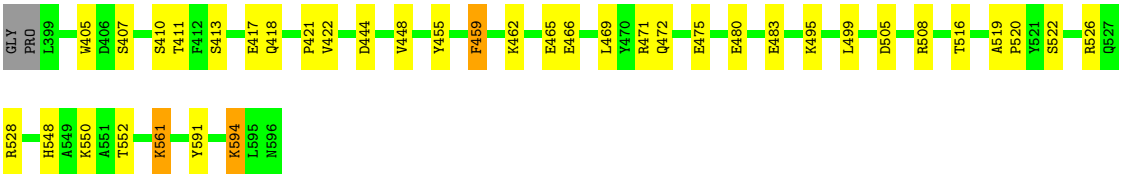
• Molecule 1: Apolipoprotein A-I

Chain A: 80% 16% • •



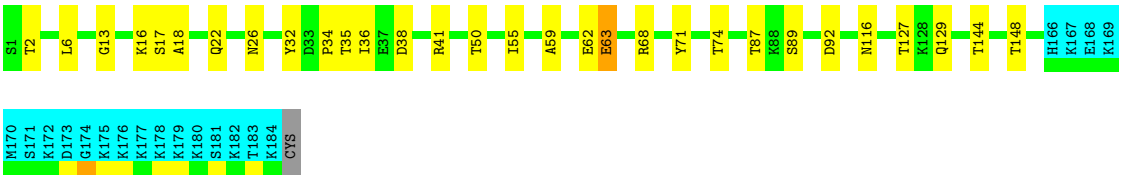
• Molecule 1: Apolipoprotein A-I

Chain D: 80% 18% • •



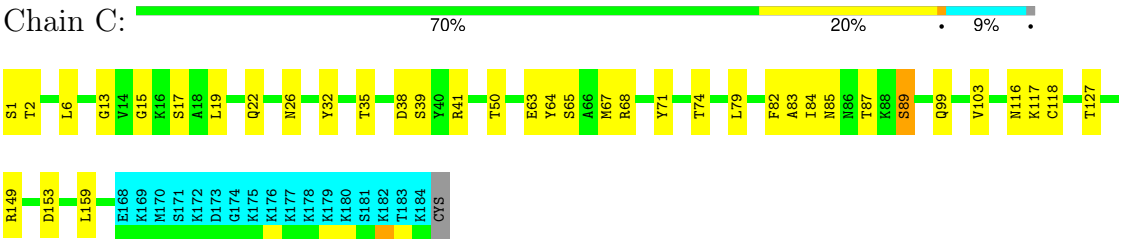
• Molecule 2: GTPase KRas

Chain B: 73% 16% • 10% •



• Molecule 2: GTPase KRas

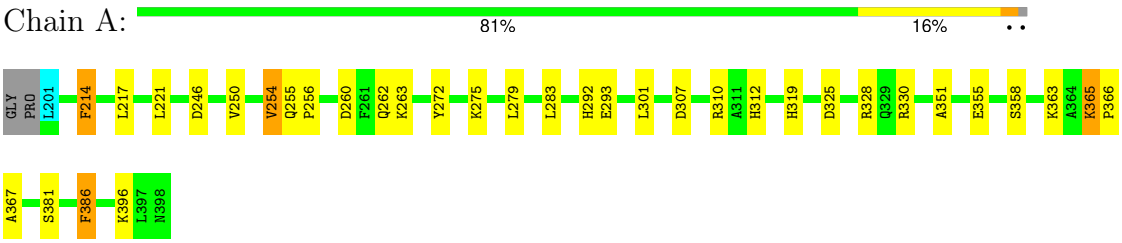
Chain C:



4.2.6 Score per residue for model 6

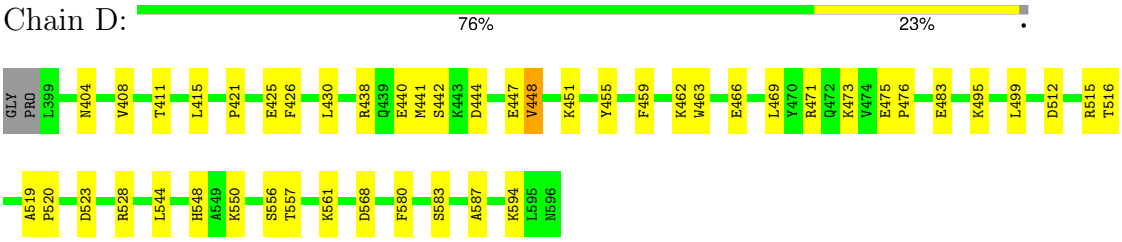
• Molecule 1: Apolipoprotein A-I

Chain A:



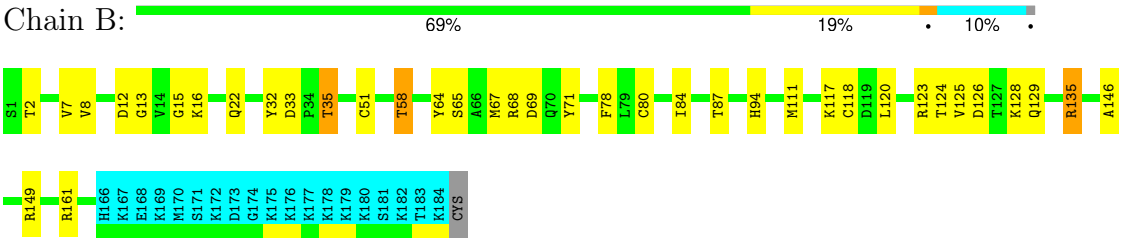
• Molecule 1: Apolipoprotein A-I

Chain D:



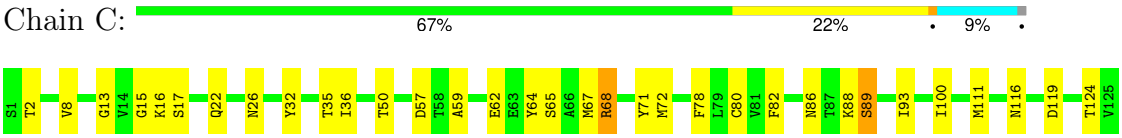
• Molecule 2: GTPase KRas

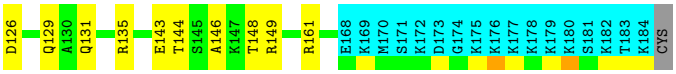
Chain B:



• Molecule 2: GTPase KRas

Chain C:





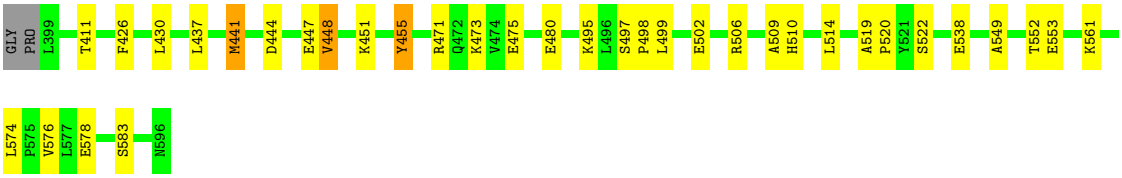
4.2.7 Score per residue for model 7

- Molecule 1: Apolipoprotein A-I

Chain A:

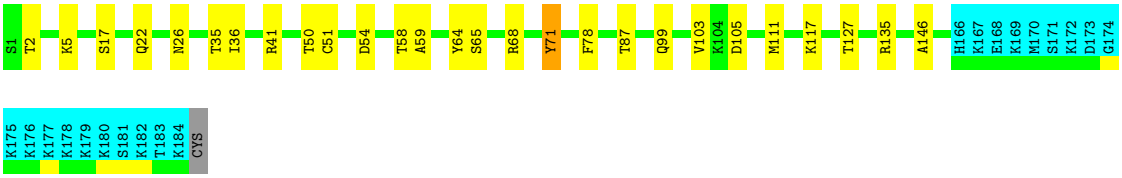
- Molecule 1: Apolipoprotein A-I

Chain D:



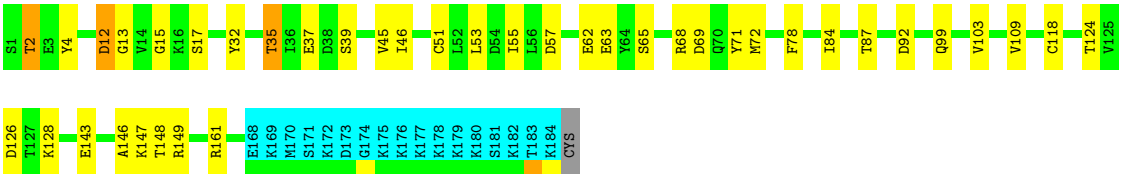
- Molecule 2: GTPase KRas

Chain B:



- Molecule 2: GTPase KRas

Chain C:



4.2.8 Score per residue for model 8

- Molecule 1: Apolipoprotein A-I

Chain A: 76% 20%

GLY PRO L201 S209 L217 L221 W229 D230 N231 K234 E235 M243 L247 V250 V254 Q255 P256 D259 K263 K264 Y272 K275 L279 R288 H292 E293 L301 D307 R310 H319 D325 R330 L331 R334 L335 L360

K363 A364 K365 P366 A367 L368 E369 D370 L371 L375 F386 L387 E391 K396 L397 N398

• Molecule 1: Apolipoprotein A-I

Chain D: 82% 16%

GLY PRO L399 T411 L415 P421 E425 D444 L445 E446 E447 V448 F459 K462 K473 E480 K495 L496 G500 D505 R508 A509 H510 L514 R515 T516 A519 P520 L525 K550 A551 T552 T557 K561 D568 L574 E578

A587 L588 E589 K593 N596

• Molecule 2: GTPase KRas

Chain B: 69% 18% 10%

S1 T2 E3 Y4 G13 V14 G15 K16 S17 Q22 N26 T35 I36 E37 D38 S39 T50 I55 L56 D57 T58 E63 Y64 S65 A66 M67 R68 D69 T74 F78 F82 A83 I84 T87 K88 S89 D92 D108 M111 C118 R123 T124 V125 D126

S145 F156 R161 H166 K167 E168 K169 M170 S171 K172 D173 G174 K175 K176 K177 K178 K179 K180 S181 K182 T183 K184 CYS

• Molecule 2: GTPase KRas

Chain C: 74% 15% 9%

S1 L6 G13 V14 G15 K16 S17 Q22 N26 Y32 D33 P34 T35 I36 E37 D38 S39 Y40 R41 D54 I55 A59 Y64 S65 A66 M67 R68 D69 I84 D92 N116 K117 C118 R123 D126 A146 K147 T148 T158 R161 E168 K169 M170

S171 K172 D173 G174 K175 K176 K177 K178 K179 K180 S181 K182 T183 K184 CYS

4.2.9 Score per residue for model 9

• Molecule 1: Apolipoprotein A-I

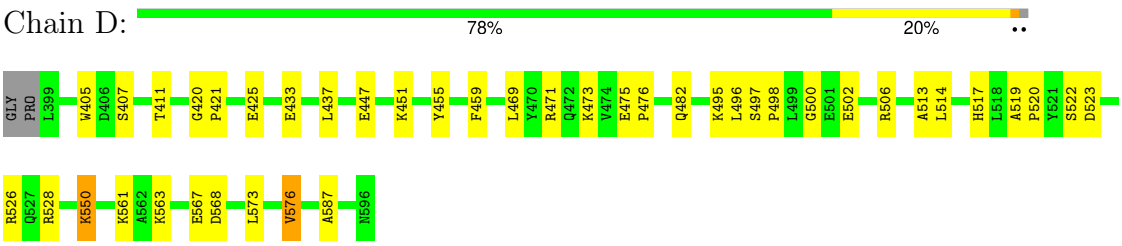
Chain A: 76% 20%

GLY PRO L201 N206 S209 T213 F214 L217 V224 N231 K234 E235 M243 D246 L247 V250 V254 Q255 P256 Q262 K263 K264 Y272 K275 L279 L298 S299 P300 L301 G302 R308 H312 D325 E326 L327 R328 Q329 R330 L335

K339 T359 E362 K363 A364 K365 P366 A367 S381 F382 S385 K396 L397 N398

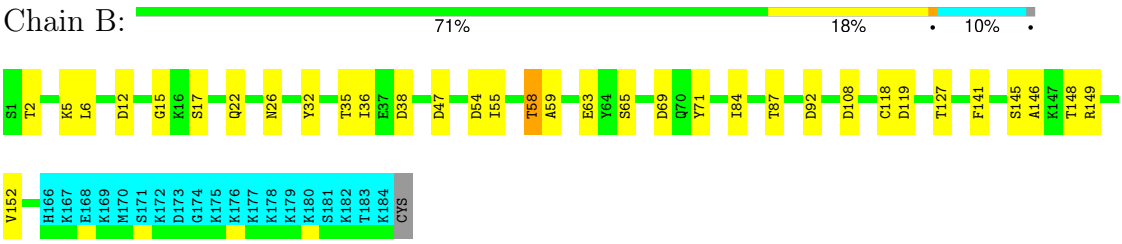
• Molecule 1: Apolipoprotein A-I

Chain D:



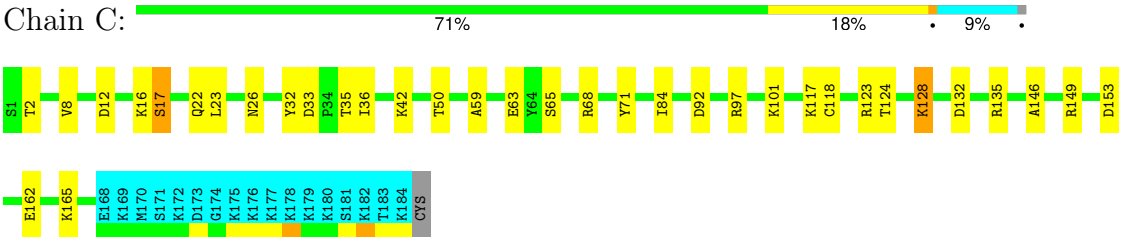
• Molecule 2: GTPase KRas

Chain B:



• Molecule 2: GTPase KRas

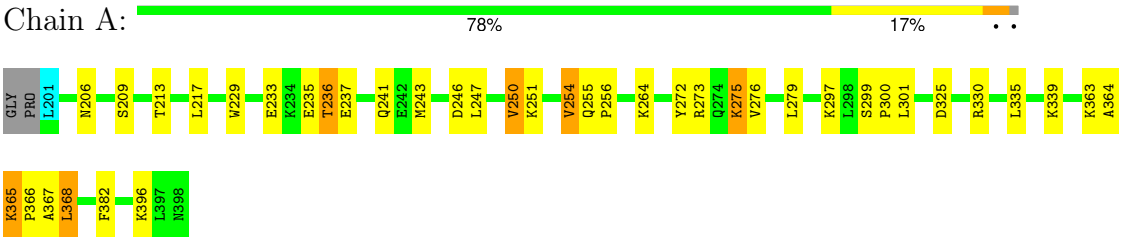
Chain C:



4.2.10 Score per residue for model 10

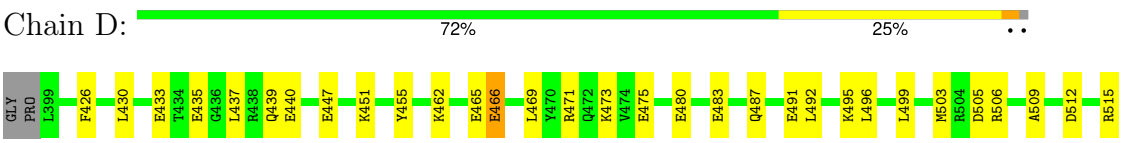
• Molecule 1: Apolipoprotein A-I

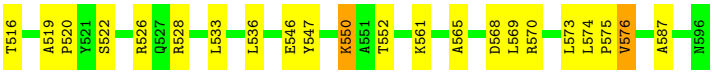
Chain A:



• Molecule 1: Apolipoprotein A-I

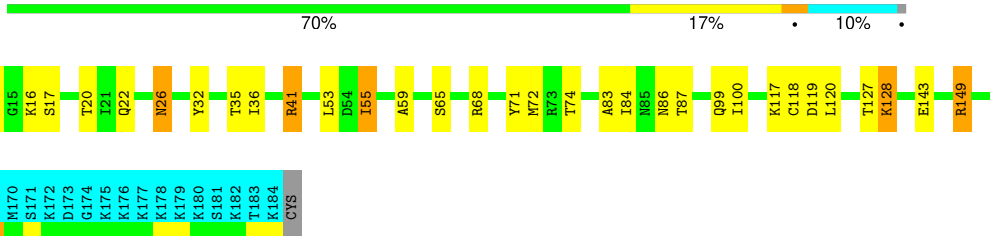
Chain D:





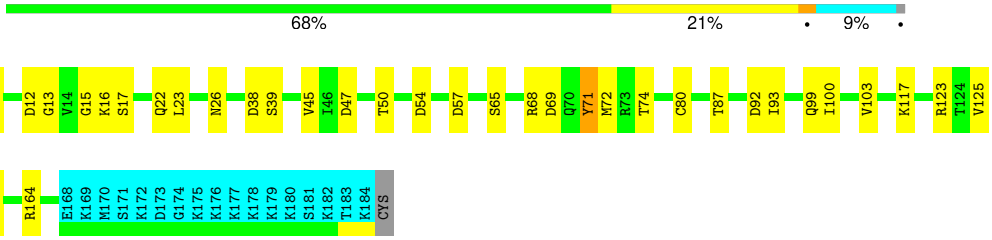
• Molecule 2: GTPase KRas

Chain B:



• Molecule 2: GTPase KRas

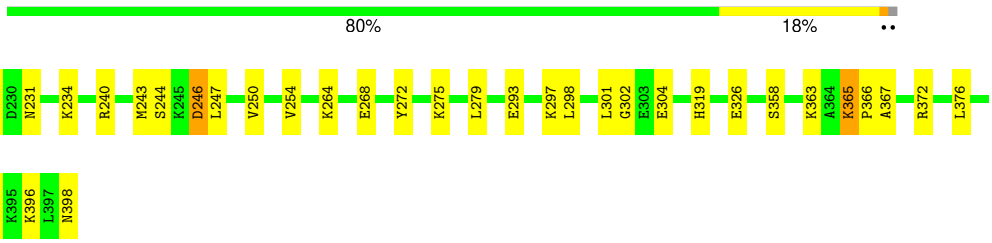
Chain C:



4.2.11 Score per residue for model 11

• Molecule 1: Apolipoprotein A-I

Chain A:

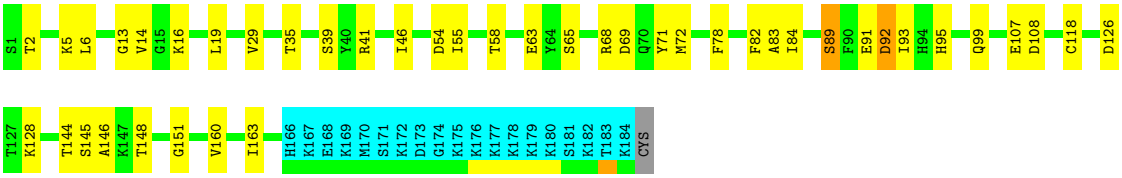


• Molecule 1: Apolipoprotein A-I

Chain D:

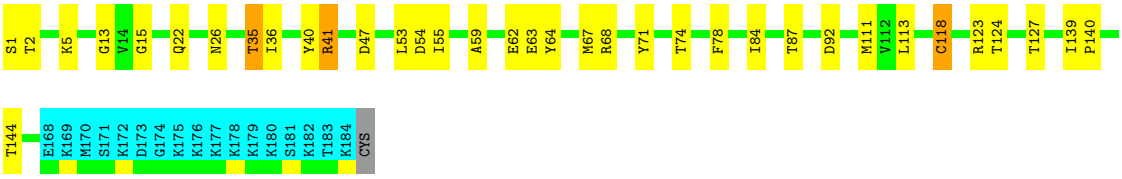
• Molecule 2: GTPase KRas

Chain B:



- Molecule 2: GTPase KRas

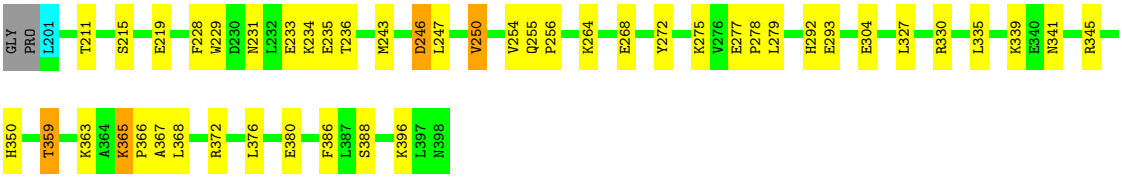
Chain C:



4.2.12 Score per residue for model 12

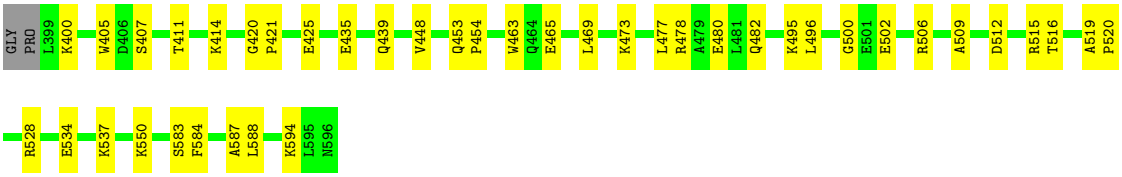
- Molecule 1: Apolipoprotein A-I

Chain A:



- Molecule 1: Apolipoprotein A-I

Chain D:

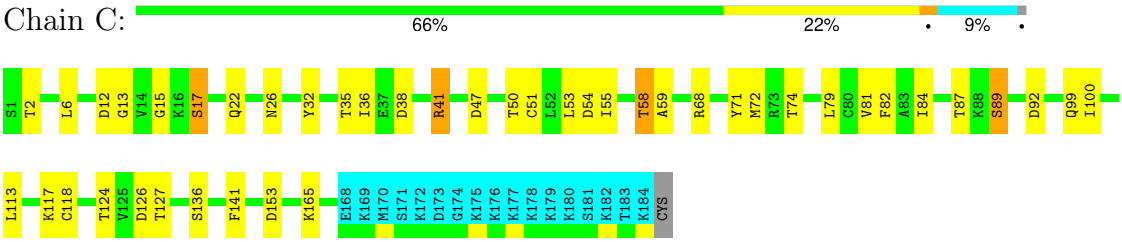


- Molecule 2: GTPase KRas

Chain B:

- Molecule 2: GTPase KRas

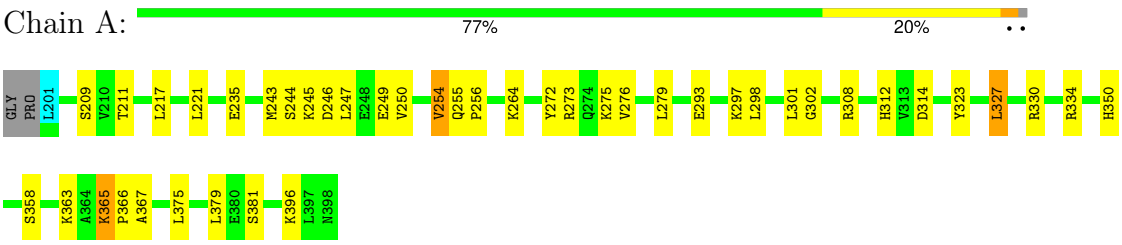
Chain C:



4.2.13 Score per residue for model 13

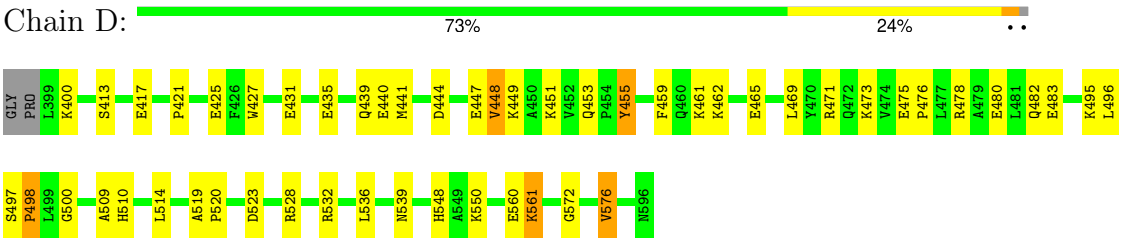
- Molecule 1: Apolipoprotein A-I

Chain A:



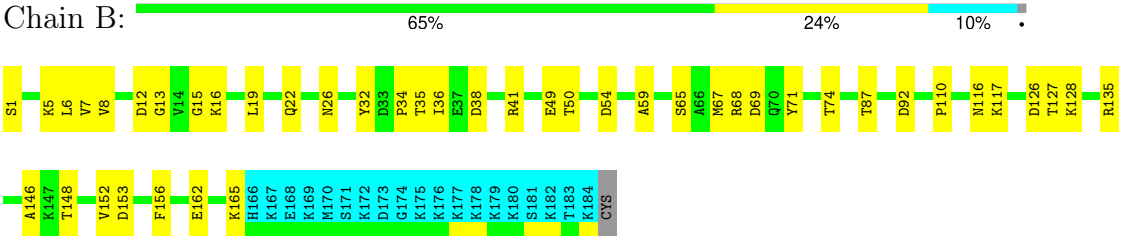
- Molecule 1: Apolipoprotein A-I

Chain D:



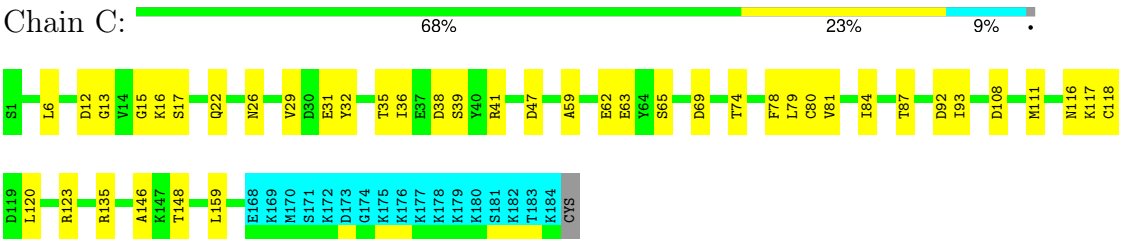
- Molecule 2: GTPase KRas

Chain B:



- Molecule 2: GTPase KRas

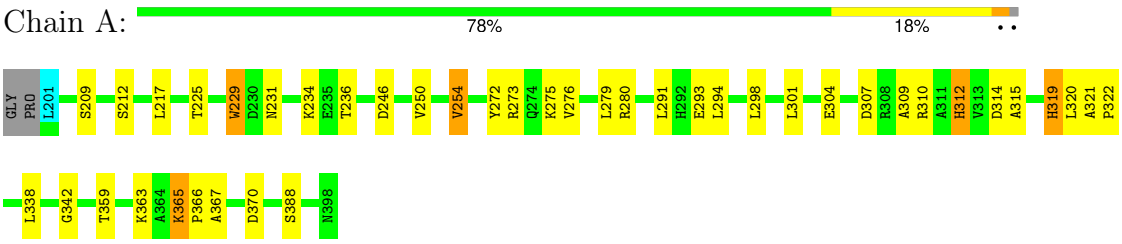
Chain C:



4.2.14 Score per residue for model 14

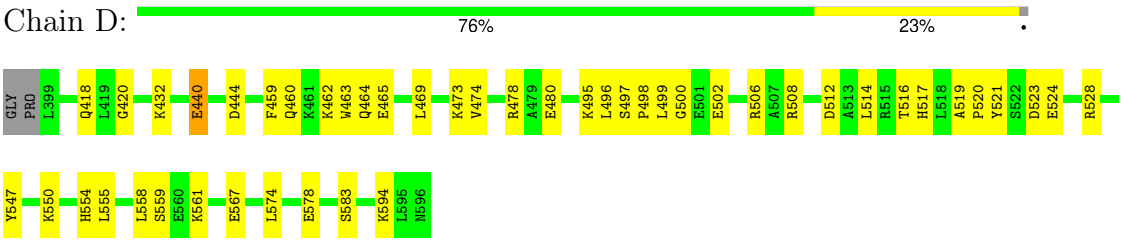
- Molecule 1: Apolipoprotein A-I

Chain A:



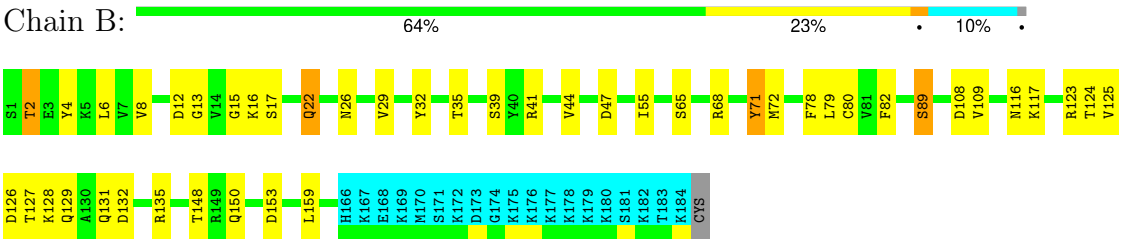
- Molecule 1: Apolipoprotein A-I

Chain D:



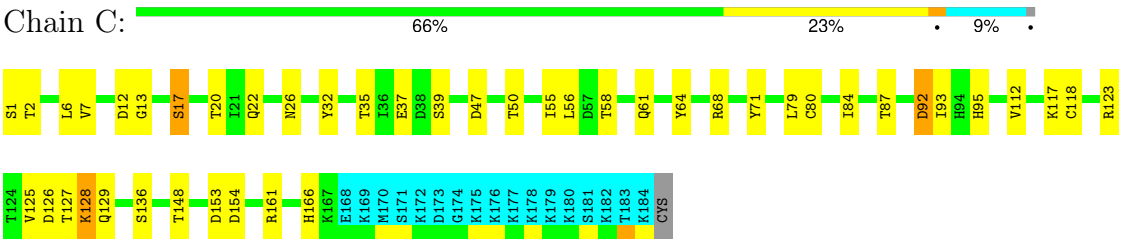
- Molecule 2: GTPase KRas

Chain B:



- Molecule 2: GTPase KRas

Chain C:



4.2.15 Score per residue for model 15 (medoid)

- Molecule 1: Apolipoprotein A-I

Chain A:

F382 F386 L387 E391 K396 L397 N398

• Molecule 1: Apolipoprotein A-I

Chain D: 76% 22% ••

GLY PRO L399 W405 D406 S407 K414 L415 L419 F426 L430 T434 E435 Q439 E440 D444 V448 K451 Y455 K462 W463 Q464 E465 E466 L469 R478 Q482 L489 K495 L499 D505 A509 H510 L514 R515 T516 H517 L518 A519

P520 Y521 S522 R526 Q527 R528 R532 L536 A549 K550 E553 K561 D568 V576 A587 N596

• Molecule 2: GTPase KRas

Chain B: 68% 21% • 10% •

S1 T2 V8 D12 G13 V14 G15 K16 L19 I24 D33 P34 T35 I36 E37 I46 D47 T50 C51 L56 D57 T58 E63 Y64 S65 R68 D69 Q70 Y71 T74 A83 N86 T87 D92 V114 G115 N116 T127 K128 I142 E143 T144 S145

A146 K147 T148 R149 D153 D154 Y157 R161 H166 K167 E168 K169 M170 S171 K172 D173 G174 K175 K176 K177 K178 K179 K180 S181 K182 T183 K184 CYS

• Molecule 2: GTPase KRas

Chain C: 75% 15% 9% •

S1 T2 L6 G15 K16 S17 T20 F28 Y32 T35 I36 R41 D47 T50 C51 A59 Y64 M67 R68 Y71 T87 K88 S89 K128 Q131 R135 S136 Y137 G138 I139 P140 F141 D153 R161 E168 K169 M170 S171 K172 D173

G174 K175 K176 K177 K178 K179 K180 S181 K182 T183 K184 CYS

4.2.16 Score per residue for model 16

• Molecule 1: Apolipoprotein A-I

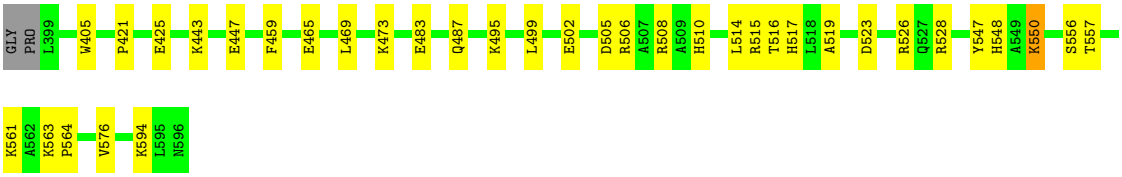
Chain A: 78% 20% ••

GLY PRO L201 V224 E235 M243 S244 K245 D246 L247 E248 E249 V250 V254 Q262 W265 Q266 E267 E268 Y272 R273 Q274 K275 V276 L279 E285 R288 H292 E293 K297 L298 L301 G302 D307 R310 H319 E326 L327 R330 E348

K352 H356 K363 A364 K365 P366 A367 S388 N398

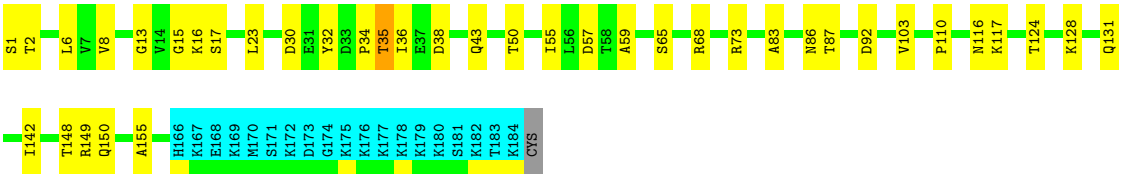
• Molecule 1: Apolipoprotein A-I

Chain D: 81% 18% •



• Molecule 2: GTPase KRas

Chain B:



• Molecule 2: GTPase KRas

Chain C:

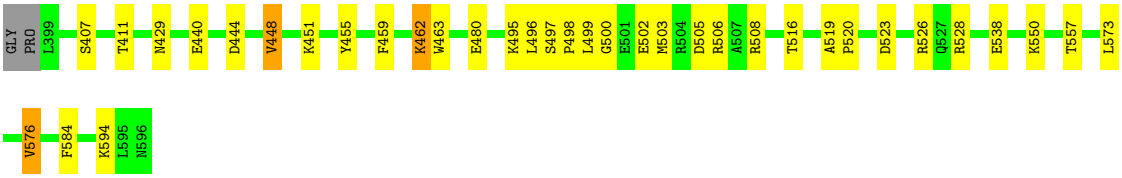
4.2.17 Score per residue for model 17

• Molecule 1: Apolipoprotein A-I

Chain A:

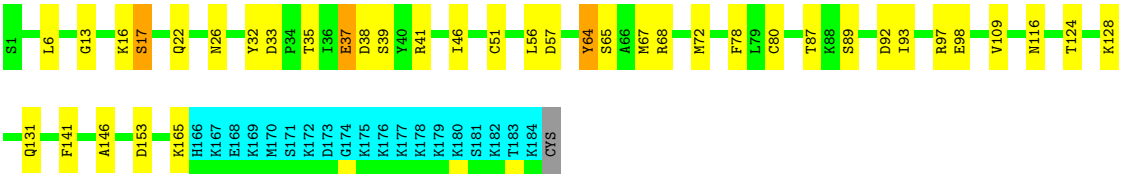
• Molecule 1: Apolipoprotein A-I

Chain D:



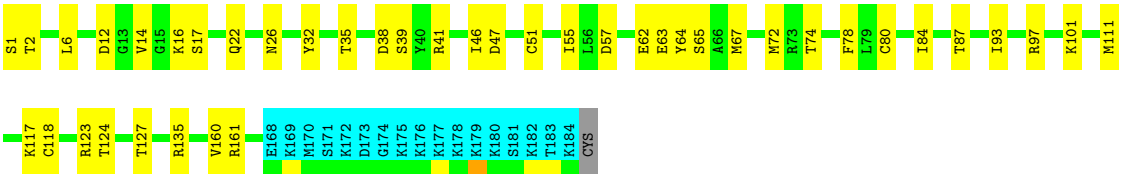
• Molecule 2: GTPase KRas

Chain B:



• Molecule 2: GTPase KRas

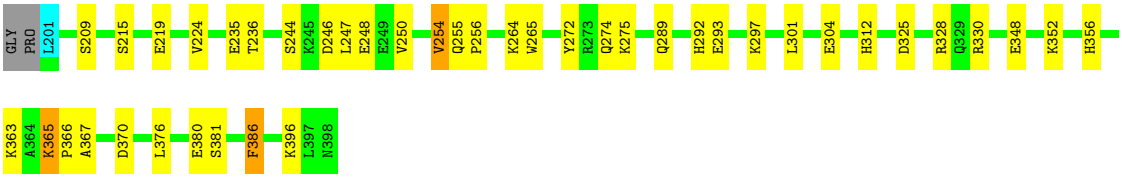
Chain C:



4.2.18 Score per residue for model 18

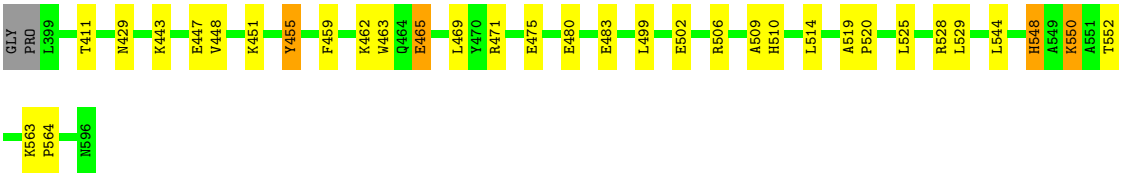
• Molecule 1: Apolipoprotein A-I

Chain A:



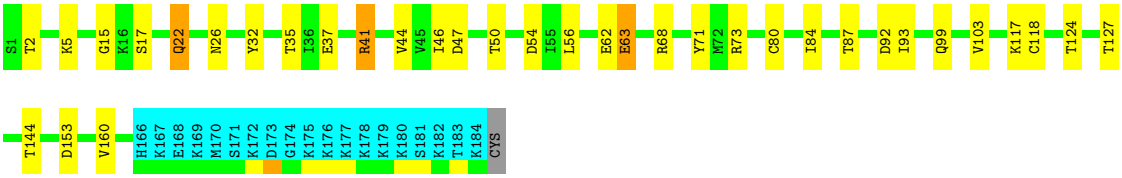
• Molecule 1: Apolipoprotein A-I

Chain D:



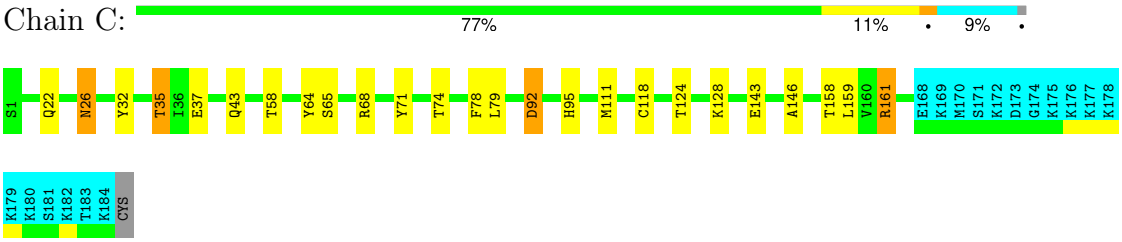
• Molecule 2: GTPase KRas

Chain B:



• Molecule 2: GTPase KRas

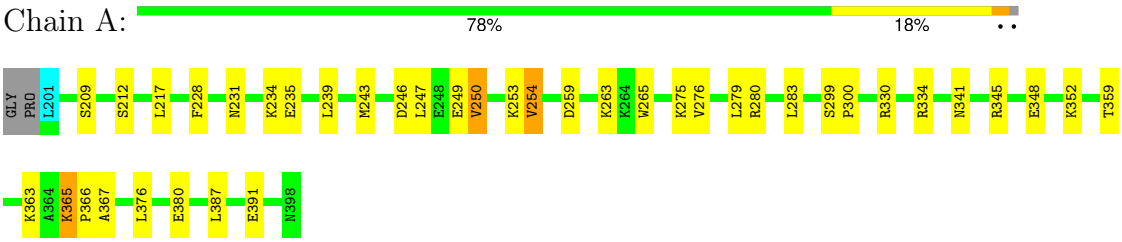
Chain C:



4.2.19 Score per residue for model 19

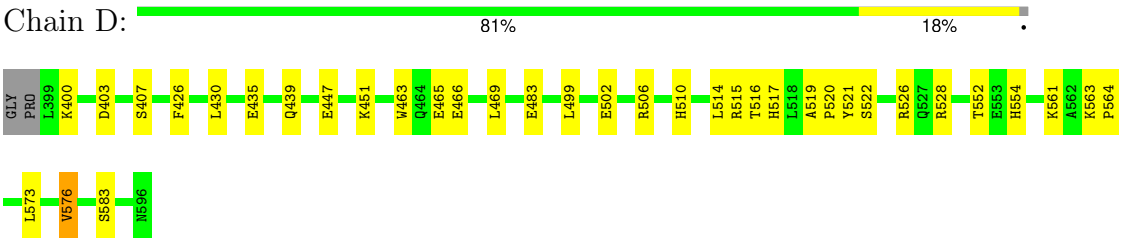
- Molecule 1: Apolipoprotein A-I

Chain A:



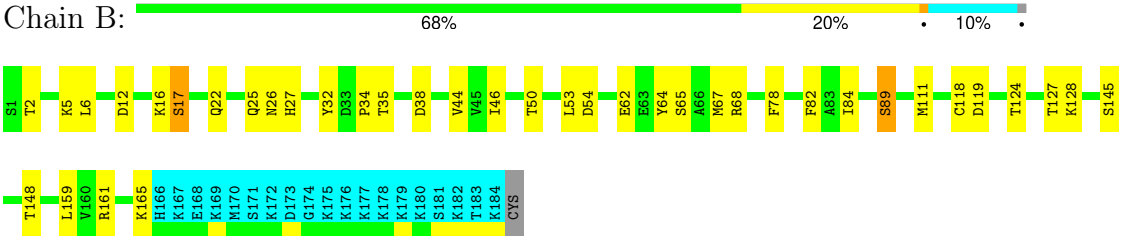
- Molecule 1: Apolipoprotein A-I

Chain D:



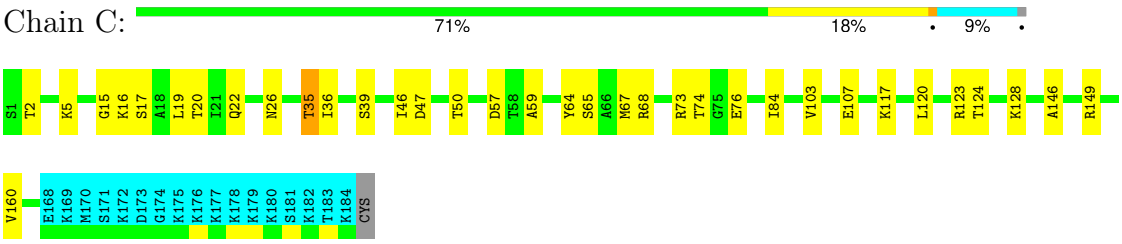
- Molecule 2: GTPase KRas

Chain B:



- Molecule 2: GTPase KRas

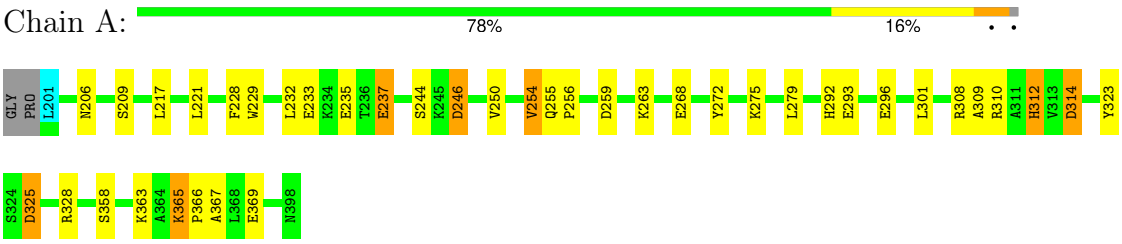
Chain C:



4.2.20 Score per residue for model 20

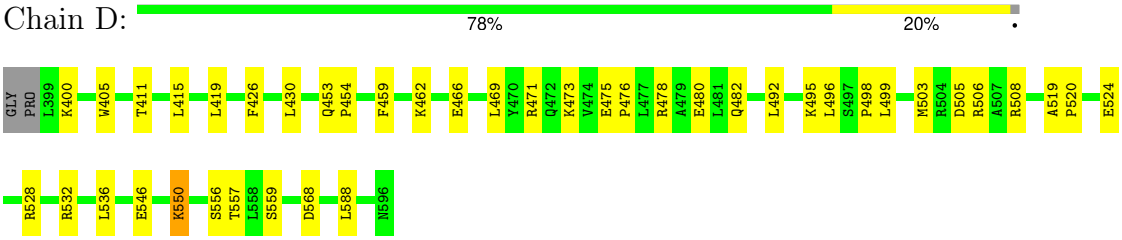
- Molecule 1: Apolipoprotein A-I

Chain A:



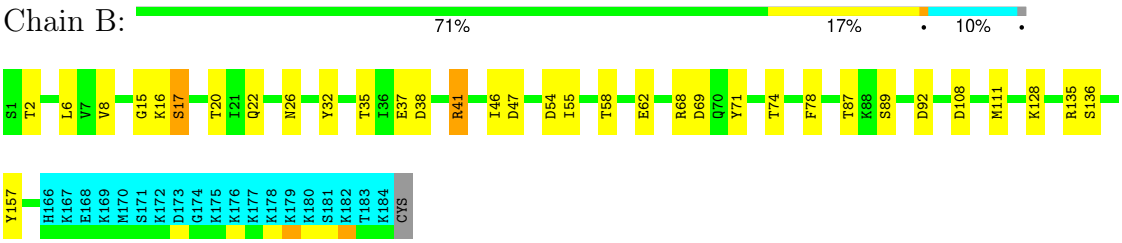
- Molecule 1: Apolipoprotein A-I

Chain D:



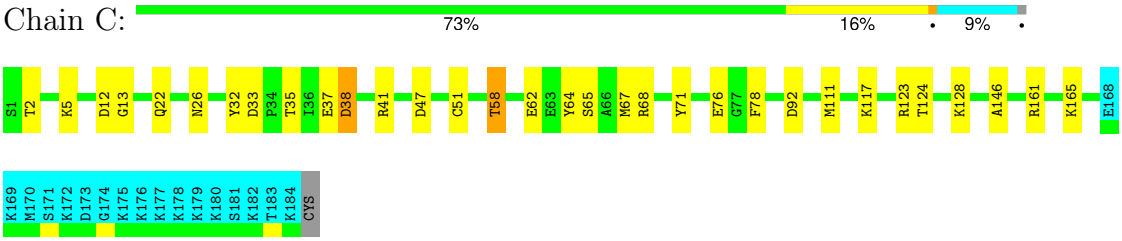
- Molecule 2: GTPase KRas

Chain B:



- Molecule 2: GTPase KRas

Chain C:



5 Refinement protocol and experimental data overview (i)

The models were refined using the following method: *simulated annealing*.

Of the 3000 calculated structures, 20 were deposited, based on the following criterion: *structures with the lowest energy*.

The following table shows the software used for structure solution, optimisation and refinement.

Software name	Classification	Version
HADDOCK	refinement	
HADDOCK	structure calculation	

The following table shows chemical shift validation statistics as aggregates over all chemical shift files. Detailed validation can be found in section 7 of this report.

Chemical shift file(s)	working_cs.cif
Number of chemical shift lists	1
Total number of shifts	154
Number of shifts mapped to atoms	61
Number of unparsed shifts	0
Number of shifts with mapping errors	93
Number of shifts with mapping warnings	0
Assignment completeness (well-defined parts)	1%

6 Model quality (i)

6.1 Standard geometry (i)

Bond lengths and bond angles in the following residue types are not validated in this section: 17F, MG, PCW, GSP

There are no covalent bond-length or bond-angle outliers.

There are no bond-length outliers.

There are no bond-angle outliers.

There are no chirality outliers.

There are no planarity outliers.

6.2 Too-close contacts (i)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in each chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes averaged over the ensemble.

Mol	Chain	Non-H	H(model)	H(added)	Clashes
1	A	1615	380	1616	24±4
1	D	1623	379	1626	21±4
2	B	1315	302	1290	18±4
2	C	1334	308	1310	20±3
3	A	1026	0	1520	362±21
3	B	324	0	480	159±15
3	C	648	0	960	324±22
3	D	1458	0	2160	557±21
4	A	162	9	228	62±11
4	B	162	9	228	69±10
4	C	270	15	380	109±13
4	D	270	15	380	106±15
5	B	32	6	12	9±3
5	C	32	6	12	9±2
6	B	1	0	0	1±0
6	C	1	0	0	1±0
All	All	205460	28580	244046	27079

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 60.

All unique clashes are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
3:D:626:PCW:C20	3:D:626:PCW:H251	1.20	1.67	15	1
3:A:414:PCW:H472	3:A:414:PCW:H432	1.16	1.18	16	20
3:A:409:PCW:C19	3:A:409:PCW:H142	1.15	1.72	14	20
3:A:420:PCW:H372	3:D:618:PCW:H431	1.15	1.16	18	18
3:D:624:PCW:H20	3:D:624:PCW:H241	1.15	1.17	10	20
3:D:606:PCW:H172	3:D:606:PCW:H212	1.15	1.16	20	19
3:D:615:PCW:H461	3:D:615:PCW:H421	1.15	1.16	16	20
3:C:203:PCW:H252	3:C:203:PCW:H212	1.14	1.19	15	20
4:B:210:17F:H12	4:B:210:17F:H41	1.14	1.16	10	8
3:D:606:PCW:H422	3:D:609:PCW:H31	1.14	1.20	19	4
3:B:208:PCW:H472	3:B:208:PCW:H432	1.14	1.20	15	20
3:C:204:PCW:H461	3:C:204:PCW:H421	1.14	1.19	10	20
3:C:209:PCW:H472	3:C:209:PCW:H432	1.14	1.20	19	19
3:D:617:PCW:H39	3:D:619:PCW:H142	1.14	1.14	1	13
3:D:613:PCW:C17	3:D:613:PCW:H212	1.14	1.73	6	1
3:C:206:PCW:H182	3:C:208:PCW:H172	1.14	1.16	6	2
3:A:407:PCW:H212	3:A:407:PCW:C17	1.13	1.72	17	19
3:D:601:PCW:H461	3:D:601:PCW:H421	1.13	1.17	18	18
3:D:607:PCW:H432	3:D:626:PCW:H472	1.13	1.21	17	6
3:D:612:PCW:C32	3:D:623:PCW:H352	1.13	1.73	10	16
3:D:618:PCW:H272	3:D:618:PCW:H232	1.13	1.18	10	20
3:C:210:PCW:H261	3:C:210:PCW:H221	1.13	1.19	16	20
3:C:212:PCW:H20	3:C:212:PCW:H241	1.13	1.20	16	20
3:A:418:PCW:H422	3:D:613:PCW:H231	1.13	1.21	2	17
3:C:209:PCW:H262	3:C:209:PCW:H222	1.13	1.19	17	20
3:A:413:PCW:H341	3:A:413:PCW:H132	1.13	1.15	10	16
3:D:617:PCW:H451	3:C:204:PCW:H472	1.13	1.21	9	5
3:A:420:PCW:H422	3:D:617:PCW:H232	1.13	1.18	5	9
4:C:218:17F:H18A	4:C:218:17F:O7	1.13	1.44	5	18
4:A:422:17F:H4A	3:D:622:PCW:H132	1.12	1.15	15	18
4:A:422:17F:H6	3:D:622:PCW:H141	1.12	1.13	3	18
3:D:612:PCW:H39	3:D:623:PCW:H462	1.12	1.21	1	16
3:D:614:PCW:H251	4:B:209:17F:H47	1.12	1.17	18	10
3:D:626:PCW:H231	3:D:626:PCW:H271	1.12	1.16	8	19
4:D:628:17F:H57	4:D:628:17F:H19A	1.12	1.18	14	20
3:A:403:PCW:H282	3:A:403:PCW:C23	1.12	1.72	3	3
3:D:606:PCW:H161	4:C:218:17F:H11A	1.12	1.18	9	15
3:C:203:PCW:H422	3:C:204:PCW:H161	1.12	1.16	19	3
3:A:401:PCW:H62	3:B:207:PCW:H11	1.12	1.12	7	2
3:D:606:PCW:H182	3:D:606:PCW:H142	1.12	1.18	20	20
3:B:205:PCW:H251	3:B:205:PCW:H211	1.12	1.15	18	16
3:B:207:PCW:H31	3:B:207:PCW:H41	1.12	1.14	20	18

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
3:A:418:PCW:H332	3:D:613:PCW:H132	1.11	1.18	15	6
3:A:420:PCW:H451	3:D:611:PCW:H211	1.11	1.22	2	14
3:A:403:PCW:H231	3:A:403:PCW:C28	1.11	1.74	3	3
3:D:614:PCW:H20	4:B:209:17F:H43	1.11	1.19	7	1
3:A:403:PCW:H362	3:A:403:PCW:C31	1.11	1.75	8	7
3:A:404:PCW:H161	3:A:404:PCW:H421	1.11	1.18	14	10
3:A:405:PCW:H361	3:A:411:PCW:H441	1.11	1.13	4	12
3:D:603:PCW:H2	3:D:603:PCW:H41	1.11	1.12	20	19
3:C:210:PCW:H121	3:C:210:PCW:H371	1.11	1.20	17	15
3:B:204:PCW:H272	3:B:204:PCW:H231	1.11	1.21	8	13
3:C:206:PCW:H181	3:C:208:PCW:H171	1.11	1.22	18	4
3:A:413:PCW:H422	3:C:210:PCW:H452	1.11	1.22	5	1
3:B:206:PCW:H212	3:C:209:PCW:H321	1.11	1.12	14	1
3:D:607:PCW:H31	3:D:626:PCW:H381	1.11	1.13	15	1
3:A:418:PCW:H431	3:D:613:PCW:H172	1.10	1.14	4	8
3:D:613:PCW:H172	3:D:613:PCW:H212	1.10	1.19	18	16
3:C:217:PCW:H141	4:C:219:17F:H33	1.10	1.18	18	7
3:D:603:PCW:H412	3:D:603:PCW:H371	1.10	1.20	6	19
3:A:407:PCW:H82	3:A:410:PCW:H351	1.10	1.13	3	7
3:B:204:PCW:H211	3:B:204:PCW:H171	1.10	1.20	2	3
3:B:205:PCW:H331	3:B:208:PCW:H121	1.10	1.21	5	3
3:D:604:PCW:H451	3:D:606:PCW:H181	1.10	1.24	5	11
3:A:406:PCW:H242	3:A:411:PCW:H472	1.10	1.12	13	8
3:C:206:PCW:H241	3:C:206:PCW:H282	1.10	1.22	18	5
3:A:414:PCW:H31	3:A:414:PCW:H371	1.10	1.23	20	11
3:D:624:PCW:H242	3:C:217:PCW:H242	1.10	1.23	20	16
3:A:418:PCW:H341	3:D:613:PCW:H132	1.10	1.21	8	7
3:C:207:PCW:H231	3:C:207:PCW:H283	1.10	1.11	18	1
3:D:602:PCW:H172	3:D:602:PCW:H212	1.10	1.21	18	17
3:D:602:PCW:H142	3:D:602:PCW:H381	1.10	1.17	5	7
3:A:408:PCW:H351	3:A:413:PCW:H162	1.09	1.14	13	7
3:D:608:PCW:H19	4:D:629:17F:H46	1.09	1.20	15	13
3:A:403:PCW:H472	3:A:404:PCW:H283	1.09	1.20	18	6
3:A:404:PCW:H352	3:A:404:PCW:H62	1.09	1.17	11	2
3:B:206:PCW:H42	3:B:206:PCW:H31	1.09	1.21	15	5
3:A:414:PCW:H341	4:A:415:17F:H57	1.09	1.15	15	13
3:A:404:PCW:H182	3:A:404:PCW:H221	1.09	1.15	17	12
3:D:604:PCW:H461	3:D:626:PCW:H282	1.09	1.23	18	12
3:A:411:PCW:H262	3:B:205:PCW:H252	1.09	1.19	20	4
3:C:206:PCW:H141	3:C:208:PCW:H321	1.09	1.24	20	5
3:A:406:PCW:H351	4:B:211:17F:H8A	1.09	1.22	4	2

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
3:A:408:PCW:H152	3:A:411:PCW:H211	1.09	1.23	11	9
4:B:209:17F:H57	4:B:209:17F:H19A	1.09	1.18	1	19
3:A:408:PCW:H42	3:A:413:PCW:H32	1.09	1.16	12	4
3:B:206:PCW:H231	3:C:205:PCW:H151	1.09	1.15	14	8
3:C:207:PCW:H283	3:C:207:PCW:C23	1.09	1.76	18	1
3:A:411:PCW:H172	3:A:411:PCW:H211	1.09	1.18	2	2
3:D:612:PCW:H51	3:D:623:PCW:H342	1.08	1.19	4	10
3:A:414:PCW:H141	4:A:415:17F:H62	1.08	1.22	6	6
3:A:406:PCW:H39	3:B:205:PCW:H152	1.08	1.26	4	10
3:C:212:PCW:H142	4:C:215:17F:H9A	1.08	1.21	11	4
4:A:422:17F:H29	4:C:218:17F:H71	1.08	1.15	18	3
3:D:625:PCW:H412	3:D:626:PCW:H412	1.08	1.22	7	13
3:C:217:PCW:H141	4:C:219:17F:H32	1.08	1.24	11	11
3:C:216:PCW:H462	4:C:218:17F:H76	1.08	1.08	15	4
3:A:401:PCW:H452	3:D:612:PCW:H271	1.08	1.22	5	6
3:D:616:PCW:H221	3:C:208:PCW:H232	1.08	1.11	14	1
3:C:207:PCW:H231	3:C:207:PCW:C28	1.08	1.77	18	1
3:D:627:PCW:H20	3:C:217:PCW:H352	1.08	1.24	7	12
3:A:401:PCW:H442	3:D:615:PCW:H262	1.08	1.24	15	6
3:B:203:PCW:H222	4:B:209:17F:H32	1.08	1.18	10	2
3:A:404:PCW:H351	3:A:404:PCW:O31	1.08	1.48	18	17
3:D:607:PCW:H12	3:D:626:PCW:H372	1.08	1.23	5	15
3:D:619:PCW:H241	3:C:204:PCW:H442	1.08	1.19	20	6
3:C:217:PCW:H121	4:C:219:17F:H33	1.08	1.24	19	9
3:A:401:PCW:H62	3:B:207:PCW:H2	1.08	1.08	19	6
3:A:407:PCW:H321	3:A:410:PCW:H372	1.08	1.19	17	17
3:C:211:PCW:H12	3:C:211:PCW:H51	1.08	1.17	3	15
3:D:617:PCW:H371	3:D:619:PCW:H142	1.08	1.14	4	7
3:C:205:PCW:H132	3:C:209:PCW:H131	1.08	1.23	4	5
3:B:208:PCW:H40	3:C:216:PCW:H283	1.08	1.23	8	5
3:B:203:PCW:H361	3:C:211:PCW:H40	1.08	1.16	5	1
3:C:216:PCW:H241	3:C:216:PCW:H282	1.08	1.22	7	1
3:A:403:PCW:H19	3:A:404:PCW:H142	1.08	1.09	20	1
4:A:422:17F:H62	3:D:622:PCW:H421	1.07	1.23	6	19
3:A:403:PCW:H281	3:A:414:PCW:H211	1.07	1.23	2	1
3:C:206:PCW:H63	3:C:212:PCW:H321	1.07	1.19	19	7
3:A:407:PCW:H51	3:A:410:PCW:H351	1.07	1.24	12	8
3:A:414:PCW:H121	4:A:415:17F:H20	1.07	1.17	14	1
3:D:627:PCW:H421	3:D:627:PCW:H381	1.07	1.09	18	9
3:C:206:PCW:H241	3:C:208:PCW:H411	1.07	1.23	16	7
3:C:206:PCW:H222	3:C:208:PCW:H431	1.07	1.21	17	6

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
3:B:206:PCW:H241	3:B:206:PCW:H282	1.07	1.19	8	1
3:A:401:PCW:H381	3:B:204:PCW:H172	1.07	1.25	16	1
3:D:612:PCW:H321	3:D:623:PCW:H352	1.07	1.11	19	20
3:B:208:PCW:H471	3:C:203:PCW:H161	1.07	1.21	6	2
3:A:417:PCW:H452	3:A:421:PCW:H421	1.07	1.27	20	1
3:A:414:PCW:H181	3:A:414:PCW:H221	1.07	1.20	6	15
3:D:621:PCW:H121	4:D:632:17F:H4A	1.07	1.27	9	8
3:A:403:PCW:H171	3:A:404:PCW:H122	1.07	1.18	14	5
3:A:407:PCW:H171	3:A:407:PCW:H212	1.07	1.13	10	9
3:B:208:PCW:H321	3:C:211:PCW:H63	1.07	1.27	20	6
3:D:607:PCW:H12	3:D:626:PCW:H371	1.07	1.27	10	2
3:D:612:PCW:H63	3:D:623:PCW:H321	1.07	1.18	10	17
3:D:623:PCW:H362	3:D:623:PCW:H322	1.07	1.07	13	6
3:B:206:PCW:H131	3:C:209:PCW:H331	1.07	1.09	14	1
3:D:622:PCW:H412	4:D:632:17F:H77	1.06	1.11	8	2
3:A:405:PCW:H281	3:A:418:PCW:H221	1.06	1.25	2	11
3:A:408:PCW:H262	3:A:411:PCW:H252	1.06	1.22	4	1
3:D:601:PCW:H472	3:D:601:PCW:H432	1.06	1.24	14	2
3:D:603:PCW:H222	3:D:611:PCW:H351	1.06	1.24	12	18
3:D:615:PCW:H42	3:D:625:PCW:H42	1.06	1.18	1	3
3:A:406:PCW:H351	4:B:211:17F:H9	1.06	1.24	6	3
3:A:413:PCW:H422	3:C:210:PCW:H442	1.06	1.18	14	1
3:B:208:PCW:H2	3:B:208:PCW:H42	1.06	1.25	15	1
3:D:612:PCW:H321	3:D:623:PCW:C35	1.06	1.80	10	13
3:D:608:PCW:H42	3:D:626:PCW:H242	1.06	1.26	9	3
3:A:406:PCW:H351	4:B:211:17F:C8	1.06	1.79	4	7
3:A:403:PCW:H332	3:A:406:PCW:H11	1.06	1.18	5	7
3:D:604:PCW:H251	4:C:215:17F:H76	1.06	1.24	2	5
3:D:619:PCW:H381	3:D:627:PCW:H161	1.06	1.12	19	18
3:D:619:PCW:H412	4:D:631:17F:H45	1.06	1.20	17	8
3:D:607:PCW:H361	3:D:626:PCW:H431	1.06	1.16	10	5
3:A:402:PCW:H162	3:A:407:PCW:H211	1.06	1.18	3	11
3:C:203:PCW:H171	3:C:203:PCW:H132	1.06	1.28	7	19
3:C:204:PCW:H272	3:C:217:PCW:H441	1.06	1.25	6	7
3:C:207:PCW:O1P	3:C:207:PCW:H31	1.06	1.51	15	12
3:C:211:PCW:H283	4:C:215:17F:H55	1.06	1.23	8	1
3:B:208:PCW:H362	3:C:203:PCW:H151	1.06	1.23	20	1
3:A:414:PCW:H141	3:A:414:PCW:H182	1.05	1.27	9	3
3:A:421:PCW:H162	4:D:630:17F:H57	1.05	1.22	15	19
3:D:608:PCW:H431	4:D:628:17F:H34	1.05	1.26	9	17
3:A:406:PCW:H381	3:C:204:PCW:H321	1.05	1.18	10	3

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
4:A:416:17F:H65	3:B:204:PCW:H272	1.05	1.18	18	2
3:D:606:PCW:H252	4:C:218:17F:H38	1.05	1.12	16	13
3:D:609:PCW:H483	3:C:208:PCW:H472	1.05	1.21	20	11
3:D:610:PCW:H63	4:D:631:17F:H6A	1.05	1.23	13	8
3:C:212:PCW:H182	3:C:212:PCW:H452	1.05	1.22	2	1
3:A:404:PCW:H421	3:A:404:PCW:C16	1.05	1.82	7	9
3:D:605:PCW:H451	3:D:624:PCW:H441	1.05	1.22	20	9
3:C:206:PCW:H251	3:C:206:PCW:H211	1.05	1.24	17	5
3:D:612:PCW:H221	3:D:620:PCW:H482	1.05	1.22	5	3
3:D:604:PCW:H411	4:C:218:17F:H36	1.05	1.22	6	1
3:C:206:PCW:H182	3:C:208:PCW:C17	1.05	1.80	6	4
3:B:207:PCW:H19	4:B:210:17F:H19A	1.05	1.29	10	4
3:D:604:PCW:H482	3:D:626:PCW:H282	1.05	1.25	17	13
4:D:632:17F:H52	3:C:208:PCW:H181	1.05	1.23	16	9
3:B:203:PCW:H51	3:C:211:PCW:H331	1.05	1.29	8	6
3:D:611:PCW:H462	3:B:208:PCW:H261	1.05	1.24	11	10
3:C:206:PCW:H82	3:C:212:PCW:H321	1.05	1.17	8	1
3:C:208:PCW:H61	4:C:213:17F:H1A	1.05	1.24	11	4
3:A:420:PCW:H31	3:D:618:PCW:H421	1.05	1.28	20	7
3:A:406:PCW:H39	3:B:205:PCW:H121	1.05	1.24	17	5
3:B:206:PCW:H241	3:C:209:PCW:H122	1.05	1.27	11	2
3:A:403:PCW:H161	3:A:404:PCW:H322	1.05	1.21	13	3
3:B:203:PCW:H222	4:B:209:17F:H56	1.05	1.28	17	2
3:D:607:PCW:H352	3:D:626:PCW:H372	1.05	1.24	19	1
3:B:207:PCW:H332	3:B:207:PCW:H132	1.05	1.13	1	11
3:A:414:PCW:H471	4:B:209:17F:H12A	1.05	1.26	15	3
3:B:203:PCW:H242	4:B:209:17F:H19	1.05	1.28	11	2
3:D:602:PCW:H362	4:C:214:17F:H67	1.04	1.13	17	8
3:D:603:PCW:O11	3:D:604:PCW:H61	1.04	1.52	13	5
3:C:209:PCW:H442	3:C:212:PCW:H262	1.04	1.25	14	4
4:C:218:17F:H46	4:C:219:17F:H73	1.04	1.29	5	11
2:B:13:GLY:HA2	5:B:201:GSP:H5'1	1.04	1.24	14	9
4:B:211:17F:H12	4:B:211:17F:H65	1.04	1.28	18	3
3:D:604:PCW:H231	4:C:215:17F:H53	1.04	1.29	8	1
3:A:418:PCW:H411	3:D:613:PCW:H152	1.04	1.28	1	1
3:D:608:PCW:H181	4:D:629:17F:H11	1.04	1.25	8	14
3:D:627:PCW:H2	3:D:627:PCW:H42	1.04	1.14	2	9
4:B:210:17F:C12	4:B:210:17F:H41	1.04	1.83	16	6
3:C:216:PCW:H442	3:C:217:PCW:H341	1.04	1.24	16	12
3:D:606:PCW:H161	4:C:218:17F:H30	1.04	1.15	15	7
3:D:606:PCW:H73	3:D:626:PCW:H19	1.04	1.26	17	12

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
3:A:403:PCW:H322	3:A:403:PCW:C36	1.04	1.81	9	1
3:C:203:PCW:H73	3:C:207:PCW:H11	1.04	1.27	14	1
3:A:408:PCW:H12	3:A:411:PCW:H141	1.04	1.22	6	2
3:C:206:PCW:H73	4:C:213:17F:O1	1.04	1.51	10	7
3:A:421:PCW:H122	4:D:630:17F:H9	1.04	1.21	7	12
3:D:625:PCW:H12	3:D:626:PCW:H12	1.04	1.14	19	10
3:D:607:PCW:H241	3:B:206:PCW:H481	1.04	1.30	3	1
4:A:422:17F:H29	4:C:218:17F:H69	1.04	1.13	16	1
3:D:616:PCW:H451	4:C:214:17F:H55	1.04	1.28	13	3
3:A:404:PCW:H73	3:B:205:PCW:H40	1.04	1.24	17	2
3:D:609:PCW:H271	4:D:628:17F:H73	1.04	1.10	17	8
3:C:204:PCW:H232	3:C:210:PCW:H20	1.04	1.18	5	8
3:C:207:PCW:H162	4:C:213:17F:H60	1.04	1.12	20	3
3:A:417:PCW:H451	3:D:618:PCW:H242	1.04	1.19	16	12
3:A:417:PCW:H19	3:A:420:PCW:H431	1.04	1.11	18	8
3:D:613:PCW:H321	3:D:619:PCW:H132	1.04	1.23	5	14
3:A:418:PCW:H411	3:A:418:PCW:H371	1.04	1.27	4	6
3:D:627:PCW:C20	3:C:217:PCW:H352	1.04	1.83	9	17
3:C:205:PCW:H141	3:C:209:PCW:H342	1.04	1.17	17	4
3:A:418:PCW:H422	3:D:613:PCW:H212	1.03	1.29	1	1
3:A:419:PCW:H40	3:D:625:PCW:H441	1.03	1.12	16	17
3:C:206:PCW:H171	3:C:208:PCW:H362	1.03	1.28	17	7
3:A:403:PCW:H282	3:A:403:PCW:H231	1.03	1.04	3	3
4:A:416:17F:H64	3:B:204:PCW:H283	1.03	1.29	16	2
3:A:418:PCW:H341	3:D:613:PCW:C13	1.03	1.83	13	6
3:D:616:PCW:H452	3:C:208:PCW:H241	1.03	1.21	7	9
3:D:627:PCW:C4	3:D:627:PCW:H2	1.03	1.84	14	2
3:B:207:PCW:H132	3:B:207:PCW:C33	1.03	1.83	6	8
3:D:619:PCW:H131	3:D:627:PCW:H151	1.03	1.30	11	14
4:B:210:17F:H41	4:B:210:17F:H12	1.03	1.11	16	5
3:C:212:PCW:H421	4:C:215:17F:H12	1.03	1.11	13	6
3:A:408:PCW:H152	3:A:411:PCW:H232	1.03	1.27	6	6
3:C:206:PCW:H162	3:C:208:PCW:H362	1.03	1.25	18	2
3:D:617:PCW:H483	3:B:205:PCW:H221	1.03	1.26	8	2
4:B:211:17F:H56	4:B:211:17F:H62	1.03	1.25	13	1
3:D:622:PCW:H171	4:D:631:17F:H5	1.03	1.30	16	2
3:A:421:PCW:H122	4:D:630:17F:H11	1.03	1.27	17	13
3:D:623:PCW:H322	3:D:623:PCW:C36	1.03	1.82	8	17
4:D:629:17F:H19A	4:D:629:17F:H9A	1.03	1.28	10	4
3:D:607:PCW:H431	3:D:625:PCW:H471	1.03	1.17	6	9
3:C:209:PCW:H431	3:C:212:PCW:H262	1.03	1.29	4	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
3:C:206:PCW:H142	3:C:208:PCW:H151	1.03	1.29	6	2
3:C:205:PCW:H421	3:C:212:PCW:H261	1.03	1.31	18	1
3:A:407:PCW:H212	3:A:407:PCW:H171	1.03	1.10	3	10
3:A:420:PCW:H11	3:D:618:PCW:H411	1.03	1.21	19	16
3:D:606:PCW:H212	3:D:606:PCW:C17	1.03	1.83	15	20
3:B:208:PCW:H11	3:C:211:PCW:H342	1.03	1.19	9	3
3:A:406:PCW:H321	3:B:205:PCW:H362	1.03	1.20	17	8
3:C:203:PCW:H442	3:C:204:PCW:H212	1.03	1.21	18	3
3:A:411:PCW:H283	3:C:210:PCW:H222	1.03	1.29	8	1
3:C:209:PCW:H442	3:C:212:PCW:H283	1.03	1.20	18	1
3:C:217:PCW:H141	4:C:219:17F:C1Z	1.03	1.83	18	14
3:A:419:PCW:H462	3:C:212:PCW:H283	1.03	1.28	13	1
3:C:203:PCW:H2	3:C:211:PCW:H62	1.03	1.24	18	2
3:C:217:PCW:H122	4:C:218:17F:H67	1.03	1.31	16	1
4:C:218:17F:H47	4:C:219:17F:H39	1.02	1.17	11	19
3:D:603:PCW:H182	3:D:624:PCW:H222	1.02	1.28	19	7
3:D:627:PCW:H20	3:C:217:PCW:C35	1.02	1.83	4	18
3:C:203:PCW:H442	3:C:204:PCW:H181	1.02	1.26	4	8
4:A:416:17F:H65	3:B:204:PCW:H252	1.02	1.23	6	3
3:B:205:PCW:H20	3:C:204:PCW:H132	1.02	1.30	1	1
3:A:403:PCW:H41	3:A:403:PCW:H31	1.02	1.28	5	13
3:D:617:PCW:H19	3:D:618:PCW:H461	1.02	1.32	17	8
3:A:407:PCW:H162	3:A:407:PCW:H212	1.02	1.26	8	1
3:C:206:PCW:H52	4:C:214:17F:H37	1.02	1.21	8	2
3:C:212:PCW:H442	4:C:215:17F:H36	1.02	1.25	12	1
3:A:405:PCW:H241	3:A:418:PCW:H262	1.02	1.24	13	2
3:A:417:PCW:H161	3:A:420:PCW:H331	1.02	1.27	3	10
4:A:422:17F:H4A	3:D:622:PCW:C13	1.02	1.84	18	13
3:D:619:PCW:H151	3:D:627:PCW:H142	1.02	1.31	8	12
3:D:623:PCW:H421	3:D:625:PCW:H261	1.02	1.26	15	17
3:D:608:PCW:H42	3:D:626:PCW:H222	1.02	1.10	4	6
3:D:605:PCW:O1P	3:D:614:PCW:H52	1.02	1.53	12	13
3:A:401:PCW:H272	3:D:615:PCW:H281	1.02	1.23	6	3
3:D:602:PCW:H362	4:C:214:17F:H61	1.02	1.24	9	7
3:D:604:PCW:H381	4:C:218:17F:H36	1.02	1.14	10	10
3:D:612:PCW:H172	3:D:612:PCW:H351	1.02	1.17	12	11
3:C:203:PCW:H461	3:C:204:PCW:H161	1.02	1.29	1	2
3:D:622:PCW:H283	3:C:217:PCW:H61	1.02	1.24	6	8
3:A:408:PCW:H241	3:C:210:PCW:H242	1.02	1.30	10	4
3:A:409:PCW:H2	4:B:210:17F:H33	1.02	1.16	7	2
3:D:604:PCW:H2	3:D:606:PCW:H82	1.02	1.08	4	12

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
3:D:607:PCW:H31	3:D:626:PCW:H372	1.02	1.26	16	12
3:D:616:PCW:H472	3:C:208:PCW:H222	1.02	1.05	17	10
3:C:207:PCW:H151	4:C:213:17F:H20A	1.02	1.31	1	1
3:D:621:PCW:H2	3:D:621:PCW:H41	1.02	1.31	2	5
3:D:608:PCW:H41	3:D:626:PCW:H222	1.02	1.21	3	10
3:A:414:PCW:H321	4:A:415:17F:H32	1.02	1.32	15	7
4:A:415:17F:H61	4:B:209:17F:H37	1.02	1.28	8	5
3:A:420:PCW:H382	3:D:611:PCW:H161	1.02	1.22	4	5
3:A:420:PCW:C37	3:D:618:PCW:H431	1.01	1.84	9	17
4:A:422:17F:H11	4:C:218:17F:H69	1.01	1.27	3	8
3:C:205:PCW:H142	3:C:209:PCW:H362	1.01	1.09	4	1
3:D:623:PCW:C36	3:D:623:PCW:H322	1.01	1.85	5	3
3:D:613:PCW:H212	3:D:613:PCW:H172	1.01	1.25	6	1
3:C:205:PCW:H361	3:C:212:PCW:H252	1.01	1.29	7	1
3:A:408:PCW:H242	3:A:411:PCW:H221	1.01	1.25	11	4
3:C:209:PCW:O4P	3:C:209:PCW:H32	1.01	1.52	13	15
3:C:210:PCW:H352	3:C:210:PCW:O31	1.01	1.55	12	19
3:A:406:PCW:H381	3:C:204:PCW:H342	1.01	1.29	17	5
3:B:205:PCW:H132	3:C:204:PCW:H11	1.01	1.31	14	3
3:C:203:PCW:H341	3:C:204:PCW:H122	1.01	1.32	2	8
3:D:613:PCW:H232	3:D:613:PCW:H471	1.01	1.30	8	9
3:D:627:PCW:H222	3:C:217:PCW:H352	1.01	1.26	14	3
3:B:203:PCW:H211	4:B:209:17F:H18	1.01	1.31	8	2
3:A:414:PCW:H252	4:A:415:17F:H59	1.01	1.27	14	3
3:D:608:PCW:H261	4:D:629:17F:H62	1.01	1.32	14	6
3:D:607:PCW:C1	3:D:626:PCW:H372	1.01	1.84	5	15
3:C:216:PCW:H152	3:C:217:PCW:H162	1.01	1.33	8	10
3:D:613:PCW:H212	3:D:613:PCW:C17	1.01	1.85	16	16
4:A:422:17F:H8A	4:C:218:17F:H65	1.01	1.26	14	6
3:D:627:PCW:H52	3:D:627:PCW:H2	1.01	1.30	4	3
3:C:204:PCW:H231	3:C:210:PCW:H282	1.01	1.22	11	9
3:C:207:PCW:H63	3:C:207:PCW:H322	1.01	1.30	15	4
3:B:204:PCW:H172	3:B:204:PCW:H211	1.01	1.13	15	1
3:A:414:PCW:O2	3:A:414:PCW:H351	1.01	1.55	18	1
3:A:403:PCW:H362	3:A:403:PCW:C32	1.01	1.85	9	8
4:A:422:17F:H6	3:D:622:PCW:C14	1.01	1.85	2	17
3:D:623:PCW:H362	3:D:623:PCW:C32	1.01	1.85	8	20
3:B:205:PCW:H181	3:B:205:PCW:H222	1.01	1.27	19	2
3:B:206:PCW:H422	3:C:209:PCW:H39	1.01	1.26	6	4
3:C:206:PCW:H19	3:C:207:PCW:H242	1.01	1.22	2	1
3:B:208:PCW:H161	3:C:203:PCW:H261	1.01	1.27	4	3

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
3:B:206:PCW:H252	3:C:205:PCW:H171	1.01	1.25	9	8
3:A:406:PCW:H432	4:B:211:17F:H12	1.01	1.27	17	4
3:A:401:PCW:H322	3:B:207:PCW:H382	1.01	1.06	4	10
3:A:406:PCW:H451	4:B:211:17F:H57	1.01	1.26	2	1
3:D:622:PCW:H20	3:C:217:PCW:H82	1.01	1.32	3	9
4:B:211:17F:H47	3:C:204:PCW:H422	1.01	1.33	2	6
3:D:609:PCW:H452	3:C:208:PCW:H20	1.01	1.33	15	6
3:D:624:PCW:H321	3:D:624:PCW:H73	1.01	1.28	13	4
3:C:212:PCW:H422	4:C:215:17F:H40	1.01	1.31	8	1
3:D:619:PCW:H322	3:D:627:PCW:H152	1.01	1.31	16	3
3:A:402:PCW:H411	3:C:208:PCW:H361	1.00	1.23	8	8
3:A:420:PCW:H432	3:D:611:PCW:H211	1.00	1.22	1	14
3:D:623:PCW:H322	3:D:623:PCW:H362	1.00	1.05	14	14
3:D:619:PCW:H251	3:C:204:PCW:H451	1.00	1.27	2	2
3:A:402:PCW:H421	3:C:208:PCW:H132	1.00	1.25	16	8
3:D:618:PCW:H471	3:D:618:PCW:H431	1.00	1.14	3	1
3:D:622:PCW:H222	4:D:631:17F:H19A	1.00	1.28	6	7
3:B:207:PCW:H332	3:B:207:PCW:C13	1.00	1.85	6	6
3:A:418:PCW:H351	3:D:613:PCW:H152	1.00	1.33	4	7
4:D:628:17F:H36	4:D:629:17F:H70	1.00	1.31	3	7
3:A:420:PCW:H242	3:A:420:PCW:H20	1.00	1.25	5	1
3:C:209:PCW:H431	3:C:209:PCW:H472	1.00	1.22	15	1
3:A:414:PCW:H122	4:A:415:17F:H67	1.00	1.26	17	1
3:D:605:PCW:H211	3:D:614:PCW:H382	1.00	1.31	17	17
3:B:203:PCW:H451	3:C:211:PCW:H232	1.00	1.27	4	4
3:A:419:PCW:H63	3:D:626:PCW:H2	1.00	1.33	13	2
3:A:414:PCW:H162	4:A:415:17F:H20	1.00	1.34	11	1
3:A:404:PCW:C16	3:A:404:PCW:H421	1.00	1.84	17	3
3:C:207:PCW:H151	4:C:213:17F:H56	1.00	1.32	3	5
3:A:401:PCW:H252	3:D:615:PCW:H281	1.00	1.31	11	6
3:A:414:PCW:H232	4:A:415:17F:H34	1.00	1.28	14	1
3:A:417:PCW:H283	3:A:420:PCW:H251	1.00	1.32	17	8
4:C:218:17F:H43	4:C:219:17F:H69	1.00	1.32	7	4
3:A:414:PCW:H422	4:A:415:17F:H69	1.00	1.26	12	1
3:C:206:PCW:H242	3:C:208:PCW:H411	1.00	1.26	7	7
3:C:203:PCW:H321	3:C:207:PCW:H351	1.00	1.33	14	1
3:D:622:PCW:H181	3:D:622:PCW:H142	0.99	1.30	11	20
3:D:601:PCW:H39	3:D:602:PCW:H151	0.99	1.28	5	2
4:C:213:17F:H77	4:C:219:17F:H49	0.99	1.26	16	1
3:B:205:PCW:H31	3:B:205:PCW:O1P	0.99	1.56	15	5
3:B:205:PCW:H12	3:B:205:PCW:H42	0.99	1.32	2	2

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
4:C:219:17F:H9	4:C:219:17F:C18	0.99	1.87	5	1
3:C:203:PCW:H472	3:C:204:PCW:H232	0.99	1.34	8	1
3:B:207:PCW:H31	3:B:207:PCW:C4	0.99	1.87	14	17
3:A:406:PCW:H441	3:C:204:PCW:H442	0.99	1.27	2	2
3:A:418:PCW:H361	3:D:613:PCW:H131	0.99	1.31	19	4
3:A:420:PCW:H362	3:D:618:PCW:H412	0.99	1.27	20	17
3:D:603:PCW:H271	3:D:611:PCW:H212	0.99	1.34	7	9
3:C:206:PCW:H172	3:C:208:PCW:H151	0.99	1.28	18	3
3:C:206:PCW:H151	3:C:208:PCW:H151	0.99	1.34	10	6
3:A:404:PCW:H421	3:A:404:PCW:H161	0.99	1.29	17	3
3:C:209:PCW:H51	3:C:209:PCW:O11	0.99	1.58	13	15
3:A:421:PCW:C12	4:D:630:17F:H9	0.99	1.87	19	12
3:D:623:PCW:H122	3:D:624:PCW:H332	0.99	1.33	1	11
3:B:206:PCW:H31	3:B:206:PCW:C4	0.99	1.87	12	7
3:B:205:PCW:H231	3:C:210:PCW:H241	0.99	1.35	15	6
4:A:422:17F:H11	4:C:218:17F:H68	0.99	1.01	9	7
3:D:605:PCW:H472	3:D:620:PCW:H432	0.99	1.29	20	10
4:C:219:17F:H18A	4:C:219:17F:C9	0.99	1.88	5	1
3:C:207:PCW:H441	4:C:213:17F:H33	0.99	1.31	9	5
3:A:405:PCW:H262	3:A:418:PCW:H241	0.99	1.31	13	1
4:A:422:17F:H39	4:C:219:17F:H67	0.99	1.33	4	13
3:C:216:PCW:H462	3:C:217:PCW:H361	0.99	1.32	6	7
3:A:410:PCW:H39	3:A:412:PCW:H371	0.98	1.35	20	12
3:B:206:PCW:H272	3:C:205:PCW:H19	0.98	1.34	18	8
3:B:204:PCW:H211	3:B:204:PCW:C17	0.98	1.86	15	5
3:D:604:PCW:H41	3:D:604:PCW:H31	0.98	1.33	8	5
3:C:208:PCW:H271	3:C:208:PCW:H232	0.98	1.25	8	1
3:A:408:PCW:H242	3:A:411:PCW:H231	0.98	1.31	7	10
3:A:420:PCW:H372	3:D:618:PCW:C43	0.98	1.87	9	19
3:B:205:PCW:H31	3:B:205:PCW:P	0.98	1.99	1	5
3:B:208:PCW:H161	3:C:203:PCW:H283	0.98	1.31	11	3
3:C:207:PCW:H42	3:C:207:PCW:H31	0.98	1.27	8	2
3:A:407:PCW:H212	3:A:407:PCW:C16	0.98	1.87	8	1
3:C:207:PCW:H161	4:C:213:17F:H60	0.98	1.34	12	1
3:A:421:PCW:H372	3:D:618:PCW:H141	0.98	0.99	18	3
3:D:627:PCW:H241	3:C:216:PCW:H451	0.98	1.32	19	8
3:A:402:PCW:H352	3:A:402:PCW:O31	0.98	1.58	4	18
3:D:624:PCW:H19	3:B:208:PCW:H271	0.98	1.36	1	1
3:D:622:PCW:H231	3:C:217:PCW:H82	0.98	1.35	13	9
3:A:419:PCW:O1P	3:D:615:PCW:H41	0.98	1.59	7	7
3:B:206:PCW:H411	3:C:209:PCW:H39	0.98	1.34	9	2

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
3:B:208:PCW:H351	3:C:203:PCW:H20	0.98	1.34	17	2
3:D:614:PCW:H121	3:D:620:PCW:H382	0.98	1.35	14	4
3:D:617:PCW:O4P	3:D:617:PCW:H31	0.98	1.58	10	5
3:C:211:PCW:P	3:C:211:PCW:H62	0.98	1.99	4	1
3:D:625:PCW:C41	3:D:626:PCW:H412	0.98	1.89	19	13
3:A:406:PCW:H472	3:B:205:PCW:H262	0.98	1.35	6	4
3:A:420:PCW:H372	3:D:618:PCW:H422	0.98	1.34	10	2
3:A:414:PCW:H122	4:A:415:17F:H66	0.98	1.35	8	6
3:B:205:PCW:O11	3:C:204:PCW:H51	0.98	1.58	11	3
3:A:406:PCW:H451	4:B:211:17F:H58	0.98	1.34	13	5
3:C:207:PCW:H19	4:C:213:17F:H57	0.98	1.30	12	2
3:A:408:PCW:H41	3:A:413:PCW:H11	0.98	1.33	10	3
3:C:206:PCW:H152	3:C:207:PCW:H221	0.97	1.36	5	2
3:C:206:PCW:H242	3:C:208:PCW:H431	0.97	1.32	18	1
3:A:409:PCW:H371	4:B:210:17F:H65	0.97	1.32	1	2
3:D:625:PCW:H151	3:D:625:PCW:H19	0.97	1.32	10	20
3:B:207:PCW:C19	4:B:210:17F:H19	0.97	1.89	15	1
4:D:631:17F:H53	3:C:210:PCW:H252	0.97	1.36	3	6
3:C:206:PCW:C20	3:C:208:PCW:H19	0.97	1.89	1	3
3:D:624:PCW:H471	4:B:209:17F:H55	0.97	1.32	7	3
3:C:212:PCW:H452	3:C:212:PCW:C18	0.97	1.89	2	1
3:D:606:PCW:H61	3:D:626:PCW:H281	0.97	1.28	7	13
3:B:205:PCW:H232	3:C:210:PCW:H262	0.97	1.35	5	1
3:C:206:PCW:H171	3:C:207:PCW:H222	0.97	1.31	9	4
3:C:212:PCW:H122	4:C:215:17F:H20	0.97	1.34	1	1
3:A:414:PCW:H162	4:A:415:17F:H59	0.97	1.33	15	8
3:A:413:PCW:H442	3:C:210:PCW:H472	0.97	1.33	5	1
3:D:621:PCW:H283	4:D:632:17F:H37	0.97	1.34	14	5
3:D:612:PCW:H222	3:D:620:PCW:H442	0.97	1.35	9	2
3:C:203:PCW:H452	3:C:204:PCW:H232	0.97	1.30	11	8
3:B:206:PCW:H212	3:C:209:PCW:C32	0.97	1.90	14	3
3:C:204:PCW:H241	3:C:210:PCW:H282	0.97	1.34	9	7
3:D:612:PCW:H2	3:D:620:PCW:H63	0.97	1.29	6	14
3:D:615:PCW:H442	3:D:620:PCW:H20	0.97	1.02	13	8
3:A:403:PCW:H141	3:A:404:PCW:H322	0.97	1.30	14	8
3:D:603:PCW:H261	3:D:611:PCW:H171	0.97	1.32	16	10
3:B:203:PCW:C5	3:C:211:PCW:H331	0.97	1.90	17	4
3:A:421:PCW:H372	3:D:618:PCW:C14	0.97	1.89	18	2
3:D:617:PCW:H451	3:C:204:PCW:H452	0.97	1.35	5	9
3:D:612:PCW:H63	3:D:623:PCW:C32	0.97	1.89	18	9
3:A:408:PCW:H32	3:A:411:PCW:H152	0.97	1.36	16	4

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
3:D:608:PCW:H452	4:D:628:17F:H60	0.97	1.37	11	8
3:D:609:PCW:H2	3:D:616:PCW:H61	0.96	1.36	15	14
3:D:608:PCW:H151	3:D:608:PCW:H19	0.96	1.32	18	2
3:D:621:PCW:H412	3:D:621:PCW:H372	0.96	1.36	16	15
3:D:621:PCW:H152	4:D:632:17F:H18	0.96	1.32	18	9
3:A:418:PCW:H422	3:D:613:PCW:C23	0.96	1.90	4	17
3:D:622:PCW:H412	4:D:632:17F:H75	0.96	1.36	18	6
3:A:406:PCW:H271	3:A:406:PCW:H483	0.96	1.34	9	4
3:C:205:PCW:C13	3:C:209:PCW:H131	0.96	1.91	3	2
3:B:205:PCW:C13	3:C:204:PCW:H41	0.96	1.90	14	1
3:B:207:PCW:H20	4:B:210:17F:H31	0.96	1.37	15	1
3:D:603:PCW:H2	3:D:603:PCW:C4	0.96	1.89	15	15
3:D:619:PCW:H351	3:D:627:PCW:H341	0.96	1.38	16	3
4:C:219:17F:H59	4:C:219:17F:H12A	0.96	1.38	6	17
3:A:405:PCW:H371	3:A:411:PCW:H461	0.96	1.34	2	2
4:A:416:17F:H65	3:B:204:PCW:H262	0.96	1.35	15	3
3:C:204:PCW:H32	3:C:204:PCW:O1P	0.96	1.60	17	7
3:D:617:PCW:H39	3:D:619:PCW:C14	0.96	1.89	15	11
3:C:216:PCW:H172	3:C:217:PCW:H162	0.96	1.36	16	12
3:D:605:PCW:H371	3:D:612:PCW:H322	0.96	1.35	10	4
3:B:206:PCW:C23	3:C:205:PCW:H151	0.96	1.90	13	7
4:B:211:17F:H50	3:C:216:PCW:H212	0.96	1.37	20	2
3:D:606:PCW:H212	3:D:606:PCW:H172	0.96	0.99	15	1
3:D:608:PCW:C19	4:D:629:17F:H46	0.96	1.89	15	17
3:D:607:PCW:H12	3:D:626:PCW:C37	0.96	1.90	10	16
3:A:401:PCW:H12	3:B:207:PCW:H342	0.96	1.37	6	1
3:A:407:PCW:H63	3:A:410:PCW:H371	0.96	1.36	4	14
3:A:409:PCW:H142	3:A:409:PCW:H19	0.96	1.33	19	4
3:C:207:PCW:H412	4:C:213:17F:H12	0.96	1.34	11	4
3:A:413:PCW:H422	3:C:210:PCW:H462	0.96	1.35	15	7
3:D:617:PCW:H441	3:D:627:PCW:H232	0.96	1.34	9	5
3:A:403:PCW:H472	3:A:404:PCW:H281	0.96	1.37	17	4
3:C:203:PCW:H272	3:C:211:PCW:H471	0.96	1.33	5	2
3:A:417:PCW:H452	3:A:421:PCW:C42	0.96	1.91	20	1
3:A:406:PCW:H39	3:B:205:PCW:H161	0.95	1.36	1	1
3:D:616:PCW:H451	4:C:214:17F:H54	0.95	1.37	16	1
3:D:614:PCW:H272	4:B:209:17F:H50	0.95	1.37	20	6
3:D:617:PCW:C34	3:C:216:PCW:H341	0.95	1.90	4	16
3:D:621:PCW:O1P	3:D:622:PCW:H52	0.95	1.59	11	12
3:B:203:PCW:H51	3:C:211:PCW:C33	0.95	1.90	17	5
3:A:403:PCW:H321	3:A:406:PCW:H51	0.95	1.32	14	3

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
3:A:408:PCW:H222	4:D:631:17F:H54	0.95	1.35	10	5
4:B:210:17F:H41	4:B:210:17F:C12	0.95	1.90	20	8
3:C:209:PCW:H42	4:C:214:17F:H4	0.95	1.38	17	1
3:D:625:PCW:H451	3:D:626:PCW:H482	0.95	1.35	1	9
3:A:417:PCW:H411	3:D:618:PCW:H152	0.95	1.36	7	1
3:A:401:PCW:H431	3:D:615:PCW:H262	0.95	1.31	17	1
3:C:209:PCW:H162	4:C:214:17F:H8	0.95	1.39	1	8
3:A:414:PCW:H372	4:A:415:17F:H69	0.95	1.36	4	5
3:D:616:PCW:H221	3:C:208:PCW:H251	0.95	1.37	16	4
4:A:422:17F:C6	3:D:622:PCW:H141	0.95	1.90	12	15
3:D:615:PCW:C44	3:D:620:PCW:H20	0.95	1.92	13	9
3:A:404:PCW:H182	3:A:404:PCW:C22	0.95	1.91	17	11
3:A:404:PCW:H441	3:A:414:PCW:H272	0.95	1.38	16	5
3:C:212:PCW:H352	4:C:213:17F:H9	0.95	1.33	4	1
3:A:404:PCW:H39	3:B:205:PCW:H451	0.95	1.38	10	3
4:D:632:17F:H53	3:C:208:PCW:H161	0.95	1.36	1	10
3:A:414:PCW:C34	4:A:415:17F:H57	0.95	1.92	15	13
3:A:406:PCW:H122	4:B:211:17F:H6A	0.95	1.36	11	3
3:A:406:PCW:H471	4:B:211:17F:H58	0.95	1.36	8	2
5:B:201:GSP:H3'	5:B:201:GSP:O2A	0.95	1.61	13	2
3:D:627:PCW:H2	3:D:627:PCW:H41	0.95	1.35	18	2
3:D:617:PCW:H341	3:C:216:PCW:H341	0.95	1.36	4	13
3:D:619:PCW:H451	4:D:631:17F:H55	0.95	1.39	11	7
3:D:609:PCW:H241	3:D:616:PCW:H381	0.95	1.36	3	8
3:C:209:PCW:H141	4:C:214:17F:O9	0.95	1.61	19	3
3:D:605:PCW:H171	3:D:614:PCW:H342	0.95	1.34	7	13
3:D:604:PCW:H482	3:D:626:PCW:C28	0.95	1.92	13	17
3:D:605:PCW:H182	3:D:614:PCW:H362	0.95	1.38	18	20
3:C:207:PCW:H421	4:C:213:17F:H32	0.95	1.34	2	3
3:A:409:PCW:H19	3:A:409:PCW:C14	0.95	1.91	19	2
3:D:619:PCW:H422	3:D:627:PCW:H261	0.95	1.32	10	8
4:A:416:17F:H53	3:D:614:PCW:H441	0.95	1.35	3	4
3:C:206:PCW:H141	3:C:208:PCW:H342	0.95	1.37	10	6
4:A:416:17F:H57	3:B:204:PCW:H151	0.95	1.36	6	1
3:A:402:PCW:H181	3:A:407:PCW:H211	0.94	1.35	19	6
3:A:418:PCW:C42	3:D:613:PCW:H231	0.94	1.92	20	15
3:D:625:PCW:H412	3:D:626:PCW:C41	0.94	1.92	19	11
4:A:422:17F:C11	4:C:218:17F:H68	0.94	1.92	9	2
3:A:419:PCW:C40	3:D:625:PCW:H441	0.94	1.92	11	20
3:C:211:PCW:H12	3:C:211:PCW:C5	0.94	1.92	19	7
3:D:614:PCW:H482	3:D:620:PCW:H211	0.94	1.36	3	15

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
3:D:602:PCW:H321	4:C:214:17F:H60	0.94	1.35	5	3
3:C:205:PCW:H32	3:C:209:PCW:H152	0.94	1.39	8	10
3:A:421:PCW:H122	4:D:630:17F:C11	0.94	1.91	14	15
3:A:401:PCW:H252	3:D:615:PCW:C28	0.94	1.92	20	3
3:C:212:PCW:H421	4:C:215:17F:H10	0.94	1.39	14	2
3:D:625:PCW:H41	3:D:625:PCW:O31	0.94	1.62	6	10
3:C:212:PCW:H412	4:C:215:17F:H59	0.94	1.34	2	1
3:D:624:PCW:H481	4:B:209:17F:H55	0.94	1.36	12	6
3:A:408:PCW:H162	3:A:411:PCW:H232	0.94	1.39	20	9
3:B:206:PCW:H231	3:C:205:PCW:C15	0.94	1.91	13	5
3:A:404:PCW:C18	3:A:404:PCW:H221	0.94	1.89	12	1
3:C:211:PCW:H282	4:C:215:17F:H78	0.94	1.36	17	1
3:D:606:PCW:C6	3:D:626:PCW:H281	0.94	1.92	7	13
3:D:618:PCW:H2	3:D:618:PCW:H41	0.94	1.38	18	3
3:B:208:PCW:H40	3:C:216:PCW:H271	0.94	1.34	19	1
3:A:402:PCW:C8	3:A:407:PCW:H32	0.94	1.92	15	17
3:A:404:PCW:O2P	3:A:406:PCW:H52	0.94	1.62	2	5
3:D:606:PCW:H152	4:C:218:17F:H8	0.94	1.37	2	2
3:D:617:PCW:H432	3:D:627:PCW:H232	0.94	1.38	4	6
3:C:208:PCW:H2	3:C:208:PCW:H42	0.94	1.36	12	1
3:D:605:PCW:C18	3:D:614:PCW:H362	0.94	1.91	3	20
4:A:422:17F:H35	4:C:218:17F:C42	0.94	1.91	4	1
3:C:209:PCW:H171	4:C:214:17F:H30	0.94	1.35	16	3
3:A:413:PCW:H431	3:C:210:PCW:H232	0.94	1.36	19	10
3:D:617:PCW:C39	3:D:619:PCW:H142	0.94	1.93	1	8
3:D:624:PCW:H242	3:C:217:PCW:C24	0.94	1.92	9	13
3:D:608:PCW:H20	4:D:628:17F:H18	0.94	1.40	18	2
3:A:407:PCW:C6	3:A:410:PCW:H371	0.94	1.93	15	10
3:A:401:PCW:H182	3:A:401:PCW:H221	0.94	1.40	5	7
3:D:625:PCW:H12	3:D:626:PCW:H32	0.94	1.32	15	2
3:C:211:PCW:H181	3:C:211:PCW:H221	0.94	1.37	11	8
3:D:607:PCW:H431	3:D:626:PCW:H472	0.94	1.38	8	5
3:B:204:PCW:H422	3:B:207:PCW:H431	0.94	1.38	7	1
3:A:421:PCW:H362	4:D:630:17F:H8A	0.94	1.36	10	1
3:D:626:PCW:H231	3:D:626:PCW:C27	0.94	1.92	11	19
3:A:414:PCW:H341	4:A:415:17F:H32	0.94	1.39	2	5
3:B:207:PCW:C11	3:B:207:PCW:H73	0.94	1.92	5	14
3:A:409:PCW:H142	3:A:409:PCW:C20	0.94	1.92	18	14
3:A:421:PCW:O2P	3:D:618:PCW:H42	0.94	1.60	7	8
3:C:206:PCW:H131	3:C:208:PCW:H321	0.94	1.37	18	1
3:D:621:PCW:H272	4:D:632:17F:H35	0.94	1.38	20	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
3:D:624:PCW:H20	3:D:624:PCW:C24	0.93	1.93	14	20
3:A:412:PCW:H451	3:C:210:PCW:H182	0.93	1.41	13	8
3:D:612:PCW:C22	3:D:620:PCW:H452	0.93	1.92	10	1
3:B:207:PCW:H182	3:B:207:PCW:H341	0.93	1.40	7	6
3:D:623:PCW:H20	3:B:203:PCW:H481	0.93	1.40	2	1
3:A:401:PCW:C25	3:D:615:PCW:H281	0.93	1.93	20	2
3:C:207:PCW:H282	3:C:207:PCW:H471	0.93	1.37	19	2
3:A:405:PCW:H361	3:A:411:PCW:H461	0.93	1.35	17	3
3:D:623:PCW:H39	3:D:623:PCW:H131	0.93	1.38	8	3
3:A:411:PCW:H322	3:A:411:PCW:H42	0.93	1.39	17	14
3:A:404:PCW:H221	3:A:404:PCW:C18	0.93	1.93	17	11
3:D:605:PCW:H172	3:D:614:PCW:H132	0.93	1.36	3	7
3:D:611:PCW:H483	3:B:208:PCW:H241	0.93	1.37	18	2
3:D:617:PCW:H482	3:C:210:PCW:H271	0.93	1.40	8	4
3:A:401:PCW:H482	3:D:612:PCW:H461	0.93	1.40	16	1
3:D:602:PCW:H483	4:D:629:17F:H43	0.93	1.36	7	1
3:B:208:PCW:O2P	3:B:208:PCW:H32	0.93	1.63	8	2
3:C:209:PCW:H422	3:C:212:PCW:H271	0.93	1.40	17	1
3:D:613:PCW:C32	3:D:619:PCW:H132	0.93	1.92	5	17
3:C:216:PCW:H372	3:C:216:PCW:H142	0.93	1.37	18	6
3:B:203:PCW:H332	4:B:210:17F:H35	0.93	1.41	20	3
3:B:206:PCW:C13	3:C:209:PCW:H331	0.93	1.92	14	1
3:D:605:PCW:O31	3:D:614:PCW:H61	0.93	1.63	2	2
3:C:212:PCW:H122	4:C:215:17F:H9A	0.93	1.40	8	1
3:A:414:PCW:H162	4:A:415:17F:H34	0.93	1.38	4	4
3:C:205:PCW:H421	3:C:212:PCW:H252	0.93	1.39	4	2
3:A:408:PCW:C35	3:A:413:PCW:H162	0.93	1.94	13	14
3:D:612:PCW:C6	3:D:623:PCW:H321	0.93	1.92	18	12
4:A:422:17F:H11	4:C:218:17F:C38	0.93	1.94	14	10
3:C:217:PCW:H172	4:C:219:17F:H34	0.93	1.41	6	9
3:A:404:PCW:H411	4:A:415:17F:H40	0.93	1.37	5	1
3:D:617:PCW:H452	3:C:204:PCW:H472	0.93	1.39	1	7
3:B:206:PCW:H42	3:B:206:PCW:C3	0.93	1.94	12	6
3:C:204:PCW:H482	3:C:216:PCW:H232	0.93	1.41	6	2
3:C:205:PCW:H2	3:C:209:PCW:H32	0.93	1.40	12	1
3:D:608:PCW:H232	4:D:628:17F:H10A	0.93	1.40	17	2
3:A:420:PCW:C36	3:D:618:PCW:H412	0.92	1.94	16	17
4:C:218:17F:C7	4:C:218:17F:H18A	0.92	1.93	14	3
3:C:206:PCW:H61	4:C:213:17F:H9	0.92	1.41	5	1
3:A:410:PCW:H462	3:A:412:PCW:H432	0.92	1.41	8	1
3:C:205:PCW:H471	4:C:215:17F:H38	0.92	1.36	17	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
3:D:602:PCW:H52	4:C:214:17F:O10	0.92	1.64	1	2
3:A:419:PCW:H40	3:D:625:PCW:H461	0.92	1.41	3	9
3:A:402:PCW:H82	3:A:407:PCW:H32	0.92	1.39	15	10
3:A:421:PCW:H61	4:D:630:17F:H4	0.92	1.41	6	5
3:A:404:PCW:H161	3:A:404:PCW:C42	0.92	1.94	9	13
3:D:605:PCW:O31	3:D:614:PCW:H82	0.92	1.63	3	4
3:A:406:PCW:H40	3:B:205:PCW:H172	0.92	1.40	12	5
3:A:409:PCW:H322	3:B:206:PCW:H341	0.92	1.38	8	5
3:A:413:PCW:H451	3:C:210:PCW:H232	0.92	1.40	8	5
4:A:415:17F:H49	3:B:208:PCW:H231	0.92	1.39	4	3
3:D:607:PCW:H471	3:C:209:PCW:H483	0.92	1.42	20	2
3:D:608:PCW:C20	4:D:629:17F:H46	0.92	1.95	11	13
3:D:610:PCW:H63	4:D:631:17F:O1	0.92	1.64	4	3
4:A:415:17F:H49	3:B:208:PCW:C23	0.92	1.93	13	3
3:D:617:PCW:H11	3:C:216:PCW:H342	0.92	1.40	10	5
3:D:614:PCW:H283	4:B:209:17F:H69	0.92	1.41	9	1
4:A:422:17F:H65	4:D:632:17F:H70	0.92	1.36	10	3
3:D:603:PCW:H212	3:D:603:PCW:H441	0.92	1.39	10	13
3:D:605:PCW:H39	3:D:612:PCW:H341	0.92	1.41	13	15
3:D:617:PCW:H39	3:D:619:PCW:H162	0.92	1.37	17	7
3:B:204:PCW:H442	3:C:205:PCW:H462	0.92	1.38	17	2
3:A:411:PCW:H51	4:B:211:17F:H1A	0.92	1.37	14	7
4:B:211:17F:H69	4:B:211:17F:H11	0.92	1.40	10	5
3:A:406:PCW:H31	4:B:211:17F:H77	0.92	1.41	19	1
3:A:407:PCW:H321	3:A:410:PCW:C37	0.92	1.94	6	14
3:D:604:PCW:C8	4:C:219:17F:H4A	0.92	1.95	4	5
4:B:211:17F:H47	3:C:204:PCW:H39	0.92	1.39	8	1
3:C:204:PCW:H242	3:C:210:PCW:H20	0.92	1.42	15	4
3:B:206:PCW:H241	3:C:205:PCW:H171	0.92	1.38	4	1
4:C:219:17F:H9	4:C:219:17F:H18A	0.92	0.95	5	1
3:C:206:PCW:H371	3:C:208:PCW:H141	0.92	1.40	17	1
3:D:617:PCW:H281	3:D:619:PCW:H283	0.92	1.42	18	6
3:B:208:PCW:H321	3:C:211:PCW:H82	0.92	1.36	2	3
3:A:407:PCW:C12	3:A:410:PCW:H331	0.92	1.95	18	7
3:D:603:PCW:H41	3:D:603:PCW:C2	0.91	1.93	15	17
3:B:207:PCW:H41	3:B:207:PCW:C3	0.91	1.95	14	14
3:C:206:PCW:C15	3:C:208:PCW:H151	0.91	1.95	10	6
3:D:608:PCW:H461	4:D:628:17F:H61	0.91	1.40	16	15
3:D:616:PCW:H51	4:D:632:17F:O5	0.91	1.64	9	3
3:D:616:PCW:H262	4:C:214:17F:H72	0.91	1.40	6	1
3:D:602:PCW:H221	3:D:602:PCW:H172	0.91	1.38	17	3

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
3:A:419:PCW:H40	3:D:625:PCW:C44	0.91	1.95	16	3
4:A:416:17F:H57	3:B:204:PCW:H211	0.91	1.42	12	5
3:D:608:PCW:H41	3:D:626:PCW:C22	0.91	1.94	3	7
3:C:205:PCW:H132	3:C:209:PCW:C13	0.91	1.95	4	2
3:D:608:PCW:H261	4:D:629:17F:C35	0.91	1.95	14	4
3:D:621:PCW:H141	4:D:632:17F:O9	0.91	1.65	8	16
3:B:204:PCW:H431	4:B:210:17F:H10A	0.91	1.40	1	1
3:C:210:PCW:H121	3:C:210:PCW:C37	0.91	1.95	16	13
3:A:421:PCW:H122	4:D:630:17F:C9	0.91	1.95	7	17
3:D:612:PCW:H2	3:D:620:PCW:C6	0.91	1.94	6	12
4:D:631:17F:H8	3:C:217:PCW:C7	0.91	1.96	13	11
3:A:408:PCW:H231	3:A:411:PCW:H231	0.91	1.38	3	3
3:A:404:PCW:H152	3:B:205:PCW:H451	0.91	1.43	18	5
3:C:203:PCW:H442	3:C:204:PCW:H161	0.91	1.43	13	5
3:C:205:PCW:C14	3:C:209:PCW:H362	0.91	1.95	4	2
3:A:406:PCW:H351	4:B:211:17F:C9	0.91	1.95	6	3
3:A:414:PCW:H172	3:A:414:PCW:H212	0.91	1.39	20	2
3:A:409:PCW:H181	3:A:409:PCW:H222	0.91	1.41	15	2
3:A:420:PCW:C35	3:D:618:PCW:H412	0.91	1.95	6	8
3:A:418:PCW:H431	3:D:613:PCW:C17	0.91	1.94	4	10
3:D:615:PCW:H442	3:D:620:PCW:C20	0.91	1.95	13	8
3:C:205:PCW:H221	3:C:209:PCW:H242	0.91	1.42	6	5
4:B:210:17F:H60	3:C:205:PCW:H441	0.91	1.42	12	1
4:A:415:17F:H50	3:B:208:PCW:H232	0.91	1.41	9	4
3:B:204:PCW:H12	3:B:207:PCW:H322	0.91	1.42	11	3
3:A:405:PCW:C36	3:A:411:PCW:H441	0.91	1.95	3	7
3:A:403:PCW:H31	3:A:403:PCW:O4P	0.91	1.65	11	5
3:A:408:PCW:H151	3:A:413:PCW:H352	0.91	1.40	3	1
3:A:404:PCW:H352	3:A:404:PCW:C6	0.91	1.94	11	2
3:B:205:PCW:H482	3:B:208:PCW:H19	0.91	1.43	16	3
3:A:414:PCW:H462	3:D:614:PCW:H231	0.91	1.42	12	4
3:A:404:PCW:H141	3:A:404:PCW:H382	0.91	1.40	9	5
3:C:208:PCW:C6	4:C:213:17F:H1A	0.91	1.95	11	3
3:B:206:PCW:H152	3:C:205:PCW:H261	0.91	1.42	16	1
4:B:211:17F:H65	4:B:211:17F:H29	0.91	1.42	19	1
3:B:205:PCW:H332	3:B:208:PCW:H73	0.91	1.38	20	1
3:B:205:PCW:H131	3:C:204:PCW:H41	0.91	1.41	14	2
3:A:420:PCW:O2P	3:A:420:PCW:H32	0.91	1.66	5	1
3:A:410:PCW:H122	3:C:207:PCW:H152	0.91	1.42	8	1
3:B:204:PCW:H483	4:B:210:17F:H56	0.91	1.42	11	1
4:A:422:17F:H39	4:C:219:17F:H71	0.91	1.42	15	3

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
3:A:417:PCW:H141	3:A:420:PCW:H341	0.91	1.42	16	14
3:D:602:PCW:H462	4:D:628:17F:H65	0.91	1.43	7	14
3:C:205:PCW:H411	4:C:215:17F:H4A	0.91	1.39	1	1
3:A:418:PCW:H471	3:D:613:PCW:H271	0.91	1.41	4	9
3:A:406:PCW:C38	3:C:204:PCW:H342	0.91	1.95	17	6
3:D:603:PCW:H451	3:D:611:PCW:H432	0.91	1.42	10	3
3:A:404:PCW:H472	4:A:415:17F:H54	0.91	1.40	6	1
3:A:405:PCW:H82	4:B:211:17F:H5	0.91	1.43	9	1
3:A:403:PCW:H52	3:A:403:PCW:O11	0.91	1.66	11	1
3:B:207:PCW:H361	3:B:207:PCW:H232	0.91	1.43	14	1
3:D:606:PCW:H172	3:D:606:PCW:C21	0.90	1.94	15	20
3:A:403:PCW:H332	3:A:406:PCW:C1	0.90	1.95	5	6
3:D:603:PCW:H242	3:D:611:PCW:H352	0.90	1.43	18	10
3:C:205:PCW:H432	3:C:212:PCW:H231	0.90	1.42	10	1
3:A:411:PCW:H282	3:B:205:PCW:H212	0.90	1.43	17	1
3:A:414:PCW:H141	4:A:415:17F:H33	0.90	1.39	20	1
3:D:606:PCW:C16	4:C:218:17F:H11A	0.90	1.96	5	8
3:A:411:PCW:H211	3:A:411:PCW:C17	0.90	1.96	2	2
3:D:608:PCW:H141	3:D:609:PCW:H171	0.90	1.43	5	12
4:A:422:17F:H49	4:C:218:17F:H10	0.90	1.43	18	8
3:C:212:PCW:H371	4:C:215:17F:H20A	0.90	1.43	9	1
3:A:407:PCW:C32	3:A:410:PCW:H372	0.90	1.95	6	10
3:A:421:PCW:C37	3:D:618:PCW:H141	0.90	1.94	18	3
3:C:205:PCW:H172	3:C:205:PCW:H212	0.90	1.44	4	3
3:C:203:PCW:H452	3:C:204:PCW:H212	0.90	1.42	20	4
3:C:211:PCW:H62	3:C:211:PCW:O3P	0.90	1.66	4	1
3:C:212:PCW:H352	4:C:213:17F:C9	0.90	1.95	4	1
3:D:602:PCW:H321	4:C:214:17F:C33	0.90	1.95	5	2
3:D:616:PCW:H432	3:C:208:PCW:H262	0.90	1.41	9	7
3:D:616:PCW:H211	4:D:632:17F:H41	0.90	1.39	13	9
3:C:212:PCW:H20	3:C:212:PCW:C24	0.90	1.95	18	18
3:D:609:PCW:H442	3:D:616:PCW:H472	0.90	1.39	8	3
3:A:418:PCW:H382	3:D:613:PCW:H151	0.90	1.41	17	1
3:D:612:PCW:H222	3:D:620:PCW:H461	0.90	1.40	20	2
3:A:402:PCW:H431	3:C:206:PCW:H251	0.90	1.42	9	3
3:D:614:PCW:H251	4:B:209:17F:C27	0.90	1.96	18	7
3:D:627:PCW:H42	3:D:627:PCW:C2	0.90	1.93	14	7
3:A:403:PCW:H452	3:A:404:PCW:H282	0.90	1.41	2	1
3:B:204:PCW:C21	3:B:204:PCW:H171	0.90	1.96	14	12
3:A:408:PCW:C4	3:A:413:PCW:H32	0.90	1.96	13	7
3:A:407:PCW:H122	3:A:410:PCW:H331	0.90	1.43	1	9

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
3:D:604:PCW:H31	3:D:604:PCW:O4P	0.90	1.66	13	13
3:A:403:PCW:C11	3:A:403:PCW:H73	0.90	1.96	20	10
3:D:616:PCW:H262	4:C:214:17F:H71	0.90	1.40	9	1
3:B:208:PCW:H331	3:C:203:PCW:H20	0.90	1.41	14	2
3:C:203:PCW:H282	3:C:211:PCW:H451	0.90	1.41	13	1
3:C:209:PCW:C4	4:C:214:17F:H4	0.90	1.97	17	1
3:C:211:PCW:H371	3:C:211:PCW:H412	0.90	1.42	16	11
3:C:203:PCW:H451	3:C:210:PCW:C20	0.90	1.97	4	5
3:B:208:PCW:H351	3:C:203:PCW:H221	0.90	1.43	13	3
3:A:401:PCW:H472	3:D:612:PCW:H251	0.90	1.44	15	3
3:B:208:PCW:H41	3:B:208:PCW:O31	0.90	1.67	14	7
3:A:403:PCW:H322	3:A:403:PCW:H362	0.90	0.95	9	1
3:D:627:PCW:H381	3:D:627:PCW:C42	0.90	1.93	18	9
3:D:605:PCW:O31	3:D:614:PCW:H51	0.90	1.67	7	2
3:D:615:PCW:H432	3:D:620:PCW:H222	0.90	1.44	10	1
3:D:621:PCW:H461	3:C:208:PCW:H471	0.90	1.42	14	1
3:D:627:PCW:H2	3:D:627:PCW:C4	0.89	1.94	3	10
3:C:217:PCW:C14	4:C:219:17F:H33	0.89	1.97	18	8
3:D:612:PCW:H222	3:D:620:PCW:C48	0.89	1.97	11	1
3:A:414:PCW:H132	4:A:415:17F:H33	0.89	1.42	18	1
3:B:208:PCW:C36	3:C:203:PCW:H151	0.89	1.96	20	1
3:D:608:PCW:O1P	3:D:626:PCW:H221	0.89	1.65	10	15
3:A:412:PCW:H483	3:C:204:PCW:H271	0.89	1.41	18	4
3:D:607:PCW:C43	3:D:626:PCW:H472	0.89	1.96	17	6
3:D:616:PCW:H272	4:D:632:17F:H41	0.89	1.44	5	3
3:D:607:PCW:C35	3:D:626:PCW:H372	0.89	1.96	19	1
3:D:624:PCW:C24	3:C:217:PCW:H242	0.89	1.97	9	11
4:A:422:17F:H29	4:C:218:17F:C39	0.89	1.95	18	3
4:A:422:17F:H65	4:D:632:17F:C39	0.89	1.98	17	7
3:D:603:PCW:H231	3:D:603:PCW:H441	0.89	1.42	6	1
3:B:208:PCW:C47	3:C:203:PCW:H161	0.89	1.96	6	1
3:C:206:PCW:H442	4:C:214:17F:H75	0.89	1.44	19	2
3:D:616:PCW:H282	4:D:632:17F:H46	0.89	1.45	1	4
3:D:627:PCW:H42	3:D:627:PCW:O31	0.89	1.66	1	4
3:A:406:PCW:H131	4:B:211:17F:H71	0.89	1.41	9	2
3:A:408:PCW:H351	3:A:413:PCW:C16	0.89	1.98	13	7
3:C:205:PCW:H11	3:C:209:PCW:H152	0.89	1.43	7	1
3:C:207:PCW:H19	4:C:213:17F:H31	0.89	1.42	19	1
3:D:608:PCW:H19	4:D:629:17F:H50	0.89	1.40	17	8
3:D:617:PCW:O2P	3:C:216:PCW:H51	0.89	1.67	17	4
3:C:207:PCW:C42	4:C:213:17F:H32	0.89	1.98	2	3

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
3:C:206:PCW:H221	3:C:208:PCW:H172	0.89	1.42	19	2
3:C:216:PCW:H461	4:C:218:17F:H76	0.89	1.44	9	3
3:A:417:PCW:H472	3:D:618:PCW:H252	0.89	1.41	5	8
3:D:603:PCW:H261	3:D:611:PCW:H142	0.89	1.44	18	11
3:D:616:PCW:H141	4:D:632:17F:H9A	0.89	1.44	12	4
3:C:212:PCW:C42	4:C:215:17F:H12	0.89	1.97	13	5
3:A:409:PCW:H2	4:B:210:17F:H20A	0.89	1.40	8	1
4:C:218:17F:H19	4:C:218:17F:H5	0.89	1.43	5	7
3:A:402:PCW:O2P	3:A:410:PCW:H73	0.89	1.67	13	7
3:D:621:PCW:H121	4:D:632:17F:C17	0.89	1.98	16	1
3:A:410:PCW:H242	4:A:422:17F:H74	0.89	1.42	17	1
3:D:607:PCW:H31	3:D:626:PCW:C37	0.89	1.97	16	8
3:D:614:PCW:C20	4:B:209:17F:H47	0.89	1.97	15	3
3:C:205:PCW:H411	4:C:215:17F:H8	0.89	1.45	13	1
3:D:602:PCW:H422	4:D:628:17F:H41	0.89	1.40	15	2
3:A:401:PCW:C38	3:B:204:PCW:H172	0.89	1.97	16	1
3:C:210:PCW:H371	3:C:210:PCW:C12	0.89	1.97	16	14
3:A:418:PCW:H351	3:D:613:PCW:C15	0.89	1.98	2	8
3:A:406:PCW:H222	4:B:211:17F:H31	0.89	1.45	17	5
3:A:419:PCW:C39	3:D:625:PCW:H441	0.89	1.97	5	10
3:C:207:PCW:H31	3:C:207:PCW:C4	0.89	1.98	8	2
3:B:204:PCW:C40	3:B:207:PCW:H63	0.89	1.98	15	2
3:C:205:PCW:H412	3:C:212:PCW:H231	0.89	1.45	18	1
3:D:627:PCW:H20	3:C:217:PCW:H351	0.88	1.44	8	13
3:B:206:PCW:O4P	3:B:206:PCW:H31	0.88	1.67	2	6
3:D:603:PCW:H62	3:C:216:PCW:O2P	0.88	1.66	20	7
3:C:207:PCW:H31	3:C:207:PCW:O4P	0.88	1.67	18	2
3:A:420:PCW:H11	3:D:618:PCW:C39	0.88	1.97	3	1
3:B:208:PCW:H40	3:C:216:PCW:H262	0.88	1.44	9	2
3:A:410:PCW:H251	4:A:422:17F:H74	0.88	1.44	8	1
3:A:420:PCW:H422	3:D:617:PCW:C23	0.88	1.99	14	10
3:D:623:PCW:O31	3:D:624:PCW:H322	0.88	1.66	16	10
3:C:205:PCW:H432	4:C:215:17F:H6	0.88	1.44	1	1
3:D:618:PCW:H62	3:D:618:PCW:H2	0.88	1.46	12	6
3:C:207:PCW:H322	3:C:207:PCW:C6	0.88	1.99	15	7
3:B:208:PCW:H31	3:C:211:PCW:H432	0.88	1.45	7	5
3:A:405:PCW:H342	3:A:406:PCW:H212	0.88	1.44	6	1
3:D:624:PCW:H282	3:C:217:PCW:H262	0.88	1.45	19	3
3:C:209:PCW:H432	3:C:209:PCW:C47	0.88	1.98	6	19
3:A:414:PCW:C14	4:A:415:17F:H62	0.88	1.99	2	5
3:A:420:PCW:H372	3:D:618:PCW:C42	0.88	1.98	10	2

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
3:D:611:PCW:H483	3:B:208:PCW:C24	0.88	1.97	18	4
3:B:206:PCW:H242	3:C:209:PCW:H122	0.88	1.45	14	9
3:D:626:PCW:H251	3:D:626:PCW:C19	0.88	1.98	15	1
3:A:407:PCW:H171	3:A:407:PCW:C21	0.88	1.94	17	19
3:D:607:PCW:H31	3:D:626:PCW:C38	0.88	1.99	15	7
3:D:627:PCW:H2	3:D:627:PCW:C5	0.88	1.98	10	3
3:D:625:PCW:C1	3:D:626:PCW:H12	0.88	1.99	19	5
4:D:632:17F:H55	3:C:206:PCW:H39	0.88	1.45	8	1
3:C:207:PCW:H252	3:C:208:PCW:H19	0.88	1.45	8	1
3:C:211:PCW:H161	4:C:215:17F:H62	0.88	1.45	15	1
3:D:602:PCW:H73	4:C:214:17F:H19A	0.88	1.42	17	1
3:A:403:PCW:H31	3:A:403:PCW:O1P	0.88	1.67	1	14
3:A:406:PCW:H20	4:B:211:17F:H31	0.88	1.44	18	7
3:D:621:PCW:H283	4:D:632:17F:H35	0.88	1.46	17	8
3:C:203:PCW:H141	4:C:213:17F:C21	0.88	1.99	15	4
3:D:606:PCW:C16	4:C:218:17F:H30	0.88	1.99	3	8
3:B:207:PCW:H342	3:B:207:PCW:H182	0.88	1.46	16	5
3:C:208:PCW:H262	4:C:214:17F:H53	0.88	1.42	12	1
3:C:209:PCW:H52	3:C:209:PCW:O11	0.88	1.68	17	1
3:D:618:PCW:H232	3:D:618:PCW:C27	0.88	1.98	2	20
3:C:211:PCW:H51	3:C:211:PCW:C1	0.88	1.99	19	11
3:A:406:PCW:H471	4:B:211:17F:H57	0.88	1.43	9	9
4:A:416:17F:H73	3:D:614:PCW:H241	0.88	1.45	9	1
3:C:203:PCW:H52	3:C:207:PCW:O31	0.88	1.68	9	2
3:A:414:PCW:C12	4:A:415:17F:H67	0.88	1.98	17	1
3:C:206:PCW:H161	3:C:207:PCW:H222	0.88	1.45	2	1
3:A:406:PCW:H382	3:C:204:PCW:H342	0.88	1.46	11	5
3:A:414:PCW:H121	4:A:415:17F:C20	0.88	1.98	14	1
3:D:617:PCW:C37	3:D:619:PCW:H142	0.88	1.98	7	7
3:D:609:PCW:H483	3:C:208:PCW:H451	0.88	1.44	3	3
3:D:609:PCW:H422	3:D:616:PCW:H461	0.88	1.41	3	3
3:D:627:PCW:H52	3:D:627:PCW:O31	0.88	1.69	4	4
3:C:206:PCW:H182	3:C:208:PCW:H171	0.88	1.43	5	7
3:D:612:PCW:H222	3:D:620:PCW:H482	0.88	1.42	11	3
1:A:365:LYS:HB2	1:A:366:PRO:HD3	0.88	1.46	11	20
3:A:414:PCW:H371	3:A:414:PCW:C3	0.88	1.99	1	9
3:D:601:PCW:H421	3:D:601:PCW:C46	0.88	1.98	4	18
3:D:617:PCW:C45	3:C:204:PCW:H452	0.88	1.99	5	2
3:A:409:PCW:H82	3:B:206:PCW:O31	0.88	1.69	8	1
3:D:611:PCW:O11	3:D:617:PCW:H62	0.88	1.69	19	3
4:A:415:17F:H61	4:B:209:17F:H30	0.88	1.46	14	2

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
3:D:607:PCW:C3	3:D:626:PCW:H372	0.87	1.98	8	13
2:C:32:TYR:CE1	5:C:201:GSP:H5'2	0.87	2.05	18	6
3:C:207:PCW:H142	4:C:213:17F:H20A	0.87	1.44	19	4
3:B:208:PCW:H342	3:C:203:PCW:C17	0.87	1.99	11	2
3:A:409:PCW:H171	3:B:207:PCW:H211	0.87	1.42	6	1
3:D:614:PCW:H352	3:D:620:PCW:H351	0.87	1.43	6	1
3:C:203:PCW:H322	3:C:204:PCW:H122	0.87	1.45	20	2
3:C:208:PCW:C26	4:C:214:17F:H53	0.87	1.99	12	1
3:C:205:PCW:H141	3:C:209:PCW:C34	0.87	1.99	17	1
3:A:411:PCW:H271	3:A:413:PCW:H39	0.87	1.42	2	3
3:A:408:PCW:H31	3:A:413:PCW:O3	0.87	1.68	17	5
3:C:206:PCW:C18	3:C:208:PCW:H171	0.87	1.99	16	8
3:A:418:PCW:H39	3:D:613:PCW:H432	0.87	1.46	9	5
3:D:615:PCW:H421	3:D:615:PCW:C46	0.87	1.99	14	20
3:D:617:PCW:C39	3:D:619:PCW:H162	0.87	1.97	16	13
3:B:203:PCW:C4	3:C:211:PCW:H331	0.87	1.99	4	5
3:A:407:PCW:H221	3:C:206:PCW:H271	0.87	1.43	20	3
3:D:608:PCW:H20	4:D:629:17F:H46	0.87	1.47	11	5
3:C:204:PCW:H482	3:C:216:PCW:C23	0.87	2.00	12	4
3:D:625:PCW:H39	3:D:626:PCW:H141	0.87	1.46	11	6
3:B:203:PCW:H211	4:B:209:17F:H19	0.87	1.45	18	1
3:D:603:PCW:H242	3:D:611:PCW:C35	0.87	2.00	18	8
3:A:408:PCW:H121	3:A:413:PCW:H121	0.87	1.47	3	3
3:A:402:PCW:H451	4:D:632:17F:H51	0.87	1.47	8	8
3:A:401:PCW:H461	3:D:612:PCW:H251	0.87	1.47	12	3
3:A:421:PCW:H362	4:D:630:17F:H10A	0.87	1.44	20	1
3:A:404:PCW:H442	3:A:404:PCW:H161	0.87	1.47	10	2
3:A:405:PCW:H361	3:A:411:PCW:C44	0.87	1.99	14	10
3:A:408:PCW:C24	3:A:411:PCW:H231	0.87	2.00	7	9
3:D:602:PCW:H212	3:D:602:PCW:C17	0.87	1.99	6	16
3:D:603:PCW:C22	3:D:611:PCW:H351	0.87	1.99	3	12
3:D:608:PCW:C19	4:D:629:17F:H50	0.87	1.98	2	6
3:A:404:PCW:H471	4:A:415:17F:H53	0.87	1.46	13	3
3:D:614:PCW:H282	4:B:209:17F:H35	0.87	1.46	5	2
3:D:603:PCW:H212	3:D:603:PCW:H472	0.87	1.45	1	4
3:B:205:PCW:H211	3:B:205:PCW:C25	0.87	2.00	18	16
3:A:409:PCW:H412	3:A:419:PCW:H251	0.87	1.46	9	4
3:D:608:PCW:H63	3:D:626:PCW:H242	0.87	1.44	6	6
3:D:618:PCW:H431	3:D:618:PCW:C47	0.87	2.00	3	1
3:A:417:PCW:H161	3:A:420:PCW:H341	0.87	1.44	5	2
3:A:408:PCW:H31	3:A:413:PCW:H31	0.87	1.46	8	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
3:A:414:PCW:C12	4:A:415:17F:H66	0.87	1.98	8	2
3:C:209:PCW:O2P	4:C:214:17F:H1A	0.87	1.70	12	2
3:A:419:PCW:H63	3:D:626:PCW:C31	0.87	1.98	20	13
3:D:624:PCW:H242	3:C:217:PCW:C23	0.87	2.00	18	4
3:D:605:PCW:H462	4:B:209:17F:H53	0.87	1.46	15	4
3:B:203:PCW:H12	3:C:211:PCW:H372	0.87	1.43	2	2
3:A:406:PCW:H122	4:B:211:17F:C6	0.87	1.99	11	7
3:D:608:PCW:H431	4:D:628:17F:C1Z	0.87	2.00	15	10
3:D:609:PCW:H462	3:C:208:PCW:H451	0.87	1.43	14	6
3:C:206:PCW:H162	3:C:208:PCW:H342	0.87	1.47	17	2
3:A:413:PCW:H442	3:C:210:PCW:H462	0.87	1.44	14	1
3:D:626:PCW:H271	3:D:626:PCW:C23	0.86	2.00	11	19
4:D:632:17F:C29	3:C:208:PCW:H181	0.86	2.00	1	2
3:B:207:PCW:H442	4:B:210:17F:H55	0.86	1.42	4	1
3:A:401:PCW:H472	3:D:612:PCW:H262	0.86	1.43	5	2
3:D:624:PCW:H261	3:C:217:PCW:H242	0.86	1.44	18	2
4:D:629:17F:H1	4:D:629:17F:H4	0.86	1.42	7	2
3:B:203:PCW:H222	4:B:209:17F:C1Y	0.86	2.00	10	1
3:C:212:PCW:H421	4:C:215:17F:C12	0.86	1.99	13	2
3:D:610:PCW:C11	4:D:631:17F:H18	0.86	2.00	18	15
3:D:619:PCW:H361	3:D:627:PCW:H172	0.86	1.45	13	8
3:B:207:PCW:H73	3:B:207:PCW:O11	0.86	1.70	4	10
3:D:606:PCW:H161	4:C:218:17F:C1X	0.86	2.00	15	4
3:B:204:PCW:H441	4:B:210:17F:H44	0.86	1.46	4	3
3:A:406:PCW:O1P	3:B:205:PCW:H372	0.86	1.70	12	8
3:A:406:PCW:C38	3:C:204:PCW:H321	0.86	2.00	10	1
4:A:422:17F:H33	3:D:622:PCW:H351	0.86	1.45	2	12
3:D:618:PCW:H272	3:D:618:PCW:C23	0.86	2.00	2	20
3:C:209:PCW:H451	3:C:212:PCW:H262	0.86	1.47	11	3
4:A:422:17F:H4A	3:D:622:PCW:H151	0.86	1.45	19	4
3:A:408:PCW:C27	3:D:619:PCW:H462	0.86	1.99	10	4
4:C:215:17F:H77	4:C:215:17F:H47	0.86	1.43	8	1
4:C:213:17F:H40	4:C:215:17F:H58	0.86	1.47	9	1
3:D:616:PCW:C22	3:C:208:PCW:H232	0.86	2.00	14	1
3:A:406:PCW:C39	3:B:205:PCW:H161	0.86	1.99	1	1
3:C:206:PCW:H61	3:C:212:PCW:O2P	0.86	1.69	1	2
3:A:414:PCW:H181	3:A:414:PCW:C22	0.86	2.00	6	15
3:D:625:PCW:H31	3:D:626:PCW:H32	0.86	1.46	17	10
3:A:404:PCW:H121	3:A:404:PCW:H371	0.86	1.46	13	6
3:C:207:PCW:H161	4:C:213:17F:H20A	0.86	1.44	18	5
3:C:209:PCW:H162	4:C:214:17F:H11A	0.86	1.44	14	4

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
3:D:625:PCW:H471	3:D:626:PCW:H482	0.86	1.46	16	2
4:A:416:17F:C40	3:D:614:PCW:H241	0.86	2.00	9	1
3:C:209:PCW:H382	3:C:209:PCW:H422	0.86	1.47	11	2
3:C:209:PCW:H41	3:C:209:PCW:O31	0.86	1.68	12	1
3:A:420:PCW:H432	3:D:611:PCW:C21	0.86	2.00	1	9
3:D:604:PCW:C48	3:D:626:PCW:H282	0.86	2.01	2	6
3:B:204:PCW:H171	3:B:204:PCW:C21	0.86	2.00	2	1
3:A:409:PCW:H272	3:A:409:PCW:H472	0.86	1.44	11	7
3:C:203:PCW:H12	3:C:211:PCW:H62	0.86	1.46	16	4
3:B:207:PCW:H19	4:B:210:17F:H19	0.86	1.46	15	2
3:A:411:PCW:H41	3:A:411:PCW:H322	0.86	1.47	6	3
4:B:211:17F:H62	4:B:211:17F:H12	0.86	1.47	1	1
4:A:415:17F:H42	4:B:209:17F:H33	0.86	1.45	2	1
3:D:613:PCW:H172	3:D:613:PCW:C21	0.86	1.99	19	16
3:C:205:PCW:H231	3:C:209:PCW:H261	0.86	1.45	2	2
3:C:216:PCW:C46	4:C:218:17F:H76	0.86	1.99	10	5
3:D:604:PCW:H412	3:D:606:PCW:H232	0.86	1.48	3	2
3:A:401:PCW:H411	3:B:204:PCW:H282	0.86	1.45	11	2
4:B:210:17F:H64	3:C:212:PCW:H281	0.86	1.48	14	1
3:D:624:PCW:C47	4:B:209:17F:H54	0.86	1.99	15	1
3:C:211:PCW:H211	4:C:215:17F:H69	0.86	1.48	17	1
3:D:608:PCW:C14	3:D:609:PCW:H171	0.86	2.01	18	6
4:B:210:17F:H1A	4:C:215:17F:C7	0.86	2.00	2	1
3:B:208:PCW:H351	3:C:203:PCW:H222	0.86	1.47	19	3
3:A:414:PCW:H471	4:A:415:17F:H68	0.86	1.45	14	1
3:D:608:PCW:H262	4:D:629:17F:C2X	0.86	2.00	19	13
3:C:209:PCW:H121	4:C:214:17F:O7	0.86	1.69	2	1
3:D:603:PCW:H11	3:D:624:PCW:H32	0.86	1.48	12	3
3:B:205:PCW:H332	3:B:208:PCW:C8	0.86	2.00	9	6
3:D:603:PCW:H222	3:D:611:PCW:H331	0.86	1.45	16	4
3:A:404:PCW:H221	3:A:404:PCW:H182	0.86	1.48	12	1
3:B:203:PCW:H461	4:C:215:17F:H51	0.86	1.47	19	1
3:D:616:PCW:H51	4:D:632:17F:C3	0.86	2.01	18	11
3:C:209:PCW:H262	3:C:209:PCW:C22	0.86	2.01	16	20
3:A:403:PCW:H132	3:A:404:PCW:H12	0.86	1.47	2	1
3:A:403:PCW:H322	3:A:404:PCW:H11	0.86	1.46	2	1
3:A:414:PCW:H221	3:A:414:PCW:C18	0.86	1.98	17	8
3:D:603:PCW:H261	3:D:611:PCW:C14	0.86	2.01	2	12
3:A:421:PCW:H381	3:D:618:PCW:H151	0.86	1.43	16	2
3:D:612:PCW:H162	3:D:620:PCW:H19	0.86	1.46	7	2
3:D:606:PCW:H252	4:C:218:17F:C22	0.86	1.98	9	13

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
4:B:209:17F:H57	4:B:209:17F:C19	0.86	2.00	9	19
3:C:204:PCW:H461	3:C:204:PCW:C42	0.86	2.00	8	20
3:B:207:PCW:O4P	3:B:207:PCW:H31	0.86	1.71	3	1
3:D:605:PCW:O31	3:D:614:PCW:H52	0.86	1.70	11	3
3:A:406:PCW:H281	3:D:619:PCW:H261	0.86	1.46	20	4
3:A:406:PCW:H39	3:B:205:PCW:H172	0.86	1.46	11	2
2:B:32:TYR:HD1	5:B:201:GSP:H5'2	0.85	1.29	12	7
3:C:204:PCW:H421	3:C:204:PCW:C46	0.85	2.01	19	20
3:C:212:PCW:H432	3:C:212:PCW:H181	0.85	1.45	7	2
3:A:421:PCW:H372	3:D:618:PCW:H151	0.85	1.47	9	2
3:C:212:PCW:H171	3:C:212:PCW:H381	0.85	1.46	8	6
3:A:413:PCW:H461	3:C:204:PCW:H283	0.85	1.44	15	1
3:D:622:PCW:H19	4:D:631:17F:H5	0.85	1.48	15	15
3:C:207:PCW:H421	3:C:207:PCW:H372	0.85	1.46	4	5
3:C:205:PCW:H181	3:C:209:PCW:H221	0.85	1.48	6	7
3:D:611:PCW:H483	3:B:208:PCW:H242	0.85	1.48	17	6
3:D:615:PCW:H52	3:D:625:PCW:O1P	0.85	1.71	3	15
3:A:406:PCW:C35	4:B:211:17F:H8A	0.85	2.00	4	2
3:A:414:PCW:H422	4:A:415:17F:H70	0.85	1.46	9	1
3:A:409:PCW:H321	3:B:206:PCW:H332	0.85	1.46	20	1
3:D:605:PCW:H421	3:D:620:PCW:H141	0.85	1.46	4	13
3:C:217:PCW:H141	4:C:219:17F:C1Y	0.85	2.00	11	9
3:D:608:PCW:H182	4:D:629:17F:H46	0.85	1.47	2	2
3:D:606:PCW:H372	4:C:218:17F:O8	0.85	1.71	6	9
2:B:15:GLY:HA3	5:B:201:GSP:H8	0.85	1.29	13	1
4:A:422:17F:H4A	3:D:622:PCW:H141	0.85	1.46	16	1
3:D:605:PCW:H442	3:D:620:PCW:H483	0.85	1.47	2	6
4:B:210:17F:H58	3:C:212:PCW:H232	0.85	1.45	2	1
3:B:208:PCW:H471	3:C:203:PCW:C16	0.85	1.99	6	1
3:C:203:PCW:O1P	3:C:211:PCW:H73	0.85	1.70	15	5
3:C:205:PCW:H122	3:C:209:PCW:H481	0.85	1.45	12	1
3:A:418:PCW:H141	3:D:618:PCW:H483	0.85	1.46	1	1
3:B:204:PCW:H52	3:B:204:PCW:O31	0.85	1.71	13	5
4:C:218:17F:H42	4:C:219:17F:H73	0.85	1.45	2	4
4:D:628:17F:H36	4:D:629:17F:H74	0.85	1.46	15	2
3:D:611:PCW:H483	3:B:208:PCW:H232	0.85	1.48	14	1
4:D:629:17F:H19A	4:D:629:17F:C9	0.85	2.01	1	3
3:C:203:PCW:H212	3:C:203:PCW:C25	0.85	2.00	18	20
3:C:212:PCW:H122	4:C:215:17F:O8	0.85	1.70	10	3
3:D:612:PCW:H283	3:D:620:PCW:H272	0.85	1.46	7	1
3:B:208:PCW:H51	3:B:208:PCW:O11	0.85	1.70	14	3

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
3:A:403:PCW:H31	3:A:403:PCW:C4	0.85	2.02	5	12
3:B:203:PCW:H482	4:C:215:17F:H55	0.85	1.48	17	2
3:D:604:PCW:C41	4:C:218:17F:H36	0.85	2.00	6	1
4:B:210:17F:H78	3:C:209:PCW:H441	0.85	1.47	6	2
3:A:421:PCW:H141	4:D:630:17F:H11	0.85	1.46	11	1
4:B:211:17F:H59	4:B:211:17F:H12	0.85	1.46	16	2
3:D:603:PCW:H421	3:D:611:PCW:H362	0.85	1.49	17	12
3:C:209:PCW:H32	3:C:209:PCW:P	0.85	2.11	3	17
3:D:617:PCW:C48	3:B:205:PCW:H221	0.85	2.01	8	4
3:C:203:PCW:H442	3:C:204:PCW:C18	0.85	2.01	4	1
3:C:207:PCW:H162	4:C:213:17F:H56	0.85	1.49	15	3
3:B:204:PCW:H32	3:B:207:PCW:H371	0.85	1.48	7	1
3:A:406:PCW:H483	3:D:619:PCW:H261	0.85	1.49	8	1
3:A:404:PCW:C47	4:A:415:17F:H53	0.85	2.02	13	2
3:A:414:PCW:H371	3:A:414:PCW:O3	0.85	1.72	16	1
3:D:612:PCW:C5	3:D:623:PCW:H342	0.85	2.02	11	8
3:D:603:PCW:H62	3:C:216:PCW:P	0.85	2.12	13	8
3:D:624:PCW:H282	3:C:217:PCW:H283	0.85	1.47	2	7
3:C:206:PCW:H181	3:C:208:PCW:C17	0.85	2.00	16	4
3:C:216:PCW:H481	3:C:217:PCW:H431	0.85	1.48	18	4
3:C:207:PCW:H142	4:C:213:17F:C31	0.85	2.02	14	2
3:D:601:PCW:H472	3:D:601:PCW:C43	0.85	2.02	6	2
3:B:203:PCW:H461	4:C:215:17F:H73	0.85	1.46	7	1
3:A:408:PCW:H271	3:D:619:PCW:H462	0.85	1.46	8	2
3:A:410:PCW:H12	3:C:207:PCW:H61	0.85	1.47	16	1
3:C:206:PCW:H232	3:C:208:PCW:H431	0.85	1.48	16	1
3:A:418:PCW:H2	3:A:418:PCW:H42	0.84	1.50	10	4
4:B:209:17F:H19A	4:B:209:17F:C31	0.84	2.01	15	16
3:C:210:PCW:H261	3:C:210:PCW:C22	0.84	2.02	6	20
3:C:210:PCW:H221	3:C:210:PCW:C26	0.84	2.02	2	20
3:A:407:PCW:H51	3:A:410:PCW:H321	0.84	1.46	2	3
3:D:615:PCW:H452	3:D:620:PCW:H222	0.84	1.49	17	8
3:A:421:PCW:H122	4:D:630:17F:H9A	0.84	1.47	10	4
3:C:203:PCW:H39	4:C:213:17F:H68	0.84	1.47	3	1
3:D:625:PCW:H12	3:D:626:PCW:C1	0.84	2.02	19	4
3:B:205:PCW:H2	3:C:204:PCW:H62	0.84	1.46	10	1
3:C:211:PCW:H132	4:C:215:17F:H56	0.84	1.47	10	2
3:D:603:PCW:H222	3:D:611:PCW:C35	0.84	2.01	9	16
3:D:604:PCW:C2	3:D:606:PCW:H82	0.84	1.99	4	4
3:B:207:PCW:H19	4:B:210:17F:C19	0.84	2.02	10	5
3:A:406:PCW:H442	4:B:211:17F:H33	0.84	1.47	11	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
3:D:606:PCW:H152	4:C:218:17F:H11A	0.84	1.46	14	1
3:D:621:PCW:O2P	3:D:622:PCW:H51	0.84	1.71	15	1
3:A:414:PCW:H131	4:A:415:17F:H33	0.84	1.49	1	1
3:D:607:PCW:H432	3:D:626:PCW:C47	0.84	2.01	17	5
3:D:617:PCW:H31	3:D:617:PCW:P	0.84	2.12	15	11
3:C:204:PCW:C23	3:C:210:PCW:H20	0.84	2.01	5	10
3:A:418:PCW:H431	3:D:613:PCW:H162	0.84	1.49	19	3
3:A:401:PCW:H181	3:A:401:PCW:H221	0.84	1.46	12	2
3:A:408:PCW:C4	3:A:413:PCW:H11	0.84	2.02	20	4
3:A:411:PCW:C4	3:A:411:PCW:H322	0.84	2.02	19	5
3:B:207:PCW:H361	3:B:207:PCW:C23	0.84	2.02	14	1
3:A:406:PCW:H432	4:B:211:17F:H12A	0.84	1.46	16	1
3:A:414:PCW:H432	3:A:414:PCW:C47	0.84	2.02	19	20
3:D:619:PCW:H351	3:D:627:PCW:H342	0.84	1.46	4	3
4:A:416:17F:H69	3:B:204:PCW:H262	0.84	1.49	6	1
3:D:604:PCW:C46	3:D:626:PCW:H282	0.84	2.03	11	9
4:A:415:17F:H47	4:A:416:17F:H71	0.84	1.49	10	1
3:D:610:PCW:H42	4:D:631:17F:O8	0.84	1.72	1	15
3:A:408:PCW:H351	3:A:413:PCW:H152	0.84	1.48	10	7
4:A:422:17F:C4	3:D:622:PCW:H132	0.84	1.99	20	12
3:D:605:PCW:H2	3:D:614:PCW:H62	0.84	1.47	6	2
3:B:206:PCW:H271	3:C:205:PCW:H19	0.84	1.46	11	1
3:D:619:PCW:H461	3:B:205:PCW:H232	0.84	1.49	16	1
3:B:203:PCW:C34	4:B:210:17F:H37	0.84	2.02	19	2
3:A:406:PCW:H361	3:B:205:PCW:H322	0.84	1.46	19	1
3:B:204:PCW:H451	3:B:207:PCW:H20	0.84	1.46	4	6
3:B:204:PCW:C7	3:B:204:PCW:H132	0.84	2.02	13	4
3:A:401:PCW:H411	3:B:204:PCW:H262	0.84	1.48	12	3
3:A:409:PCW:C32	3:B:206:PCW:H341	0.84	2.01	4	5
3:D:608:PCW:H42	3:D:626:PCW:C22	0.84	2.02	4	5
3:B:208:PCW:H52	3:B:208:PCW:H2	0.84	1.45	6	1
3:D:623:PCW:H421	3:D:625:PCW:H262	0.84	1.50	9	1
3:D:606:PCW:H142	3:D:606:PCW:C18	0.84	2.01	1	20
3:D:625:PCW:H19	3:D:625:PCW:C15	0.84	2.01	10	20
2:C:13:GLY:HA2	5:C:201:GSP:H5'1	0.84	1.50	11	11
3:A:406:PCW:H341	3:B:205:PCW:H321	0.84	1.49	7	2
4:A:422:17F:H48	4:C:218:17F:H10	0.84	1.46	5	3
4:B:211:17F:C28	3:C:204:PCW:H462	0.84	2.03	5	1
3:D:614:PCW:H471	3:D:620:PCW:H431	0.84	1.49	18	2
4:A:416:17F:H65	3:B:204:PCW:H271	0.84	1.49	1	1
3:D:606:PCW:H161	4:C:218:17F:C11	0.84	2.03	5	10

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
3:D:615:PCW:H461	3:D:615:PCW:C42	0.84	2.03	17	20
3:D:616:PCW:H51	4:D:632:17F:O4	0.84	1.71	2	10
3:C:203:PCW:H252	3:C:203:PCW:C21	0.84	2.02	17	20
3:D:603:PCW:H222	3:D:611:PCW:C33	0.84	2.03	16	8
3:D:614:PCW:H411	3:D:620:PCW:H39	0.84	1.47	12	5
4:D:628:17F:H58	4:D:629:17F:H51	0.84	1.49	6	4
3:D:607:PCW:H12	3:D:626:PCW:H351	0.84	1.50	15	2
3:D:613:PCW:H52	3:D:619:PCW:O11	0.84	1.73	1	3
3:A:408:PCW:H131	3:A:411:PCW:H231	0.84	1.48	2	1
3:D:622:PCW:H262	3:C:217:PCW:H61	0.84	1.48	16	5
3:B:203:PCW:H382	3:C:211:PCW:H182	0.84	1.48	3	2
3:B:208:PCW:C40	3:C:216:PCW:H281	0.84	2.03	11	1
3:A:408:PCW:H181	3:A:413:PCW:C26	0.84	2.03	16	6
3:A:420:PCW:O2	3:D:618:PCW:H411	0.84	1.73	11	13
3:D:601:PCW:H461	3:D:601:PCW:C42	0.84	2.01	4	18
3:D:605:PCW:C31	3:D:614:PCW:H62	0.84	2.03	16	8
3:A:408:PCW:H31	3:A:413:PCW:C3	0.84	2.03	8	1
4:A:416:17F:H65	3:B:204:PCW:C27	0.83	2.03	1	2
3:A:417:PCW:H19	3:A:420:PCW:C43	0.83	2.02	9	5
3:D:606:PCW:H341	3:D:606:PCW:H132	0.83	1.48	4	12
3:D:619:PCW:H341	4:D:631:17F:H36	0.83	1.48	3	6
3:A:413:PCW:H82	3:C:210:PCW:O2P	0.83	1.72	17	6
4:A:422:17F:H66	3:D:622:PCW:H422	0.83	1.49	15	8
3:D:603:PCW:H172	3:D:603:PCW:H211	0.83	1.50	13	13
3:D:624:PCW:H282	3:C:217:PCW:H272	0.83	1.49	4	2
3:D:612:PCW:H221	3:D:620:PCW:C48	0.83	2.03	5	2
3:A:409:PCW:C2	4:B:210:17F:H33	0.83	2.02	7	1
3:C:209:PCW:H442	3:C:212:PCW:C28	0.83	2.03	18	1
4:A:422:17F:H62	3:D:622:PCW:C42	0.83	2.03	4	16
3:D:615:PCW:H42	3:D:625:PCW:C4	0.83	2.00	1	2
3:B:204:PCW:H231	3:B:204:PCW:C27	0.83	2.01	2	13
3:B:208:PCW:H432	3:B:208:PCW:C47	0.83	2.01	11	20
3:C:209:PCW:H451	3:C:212:PCW:H452	0.83	1.50	1	2
3:A:414:PCW:C16	4:A:415:17F:H34	0.83	2.02	4	5
3:A:419:PCW:H63	3:D:626:PCW:C2	0.83	2.02	13	2
3:A:403:PCW:C47	3:A:404:PCW:H281	0.83	2.03	17	2
4:D:628:17F:H19A	4:D:628:17F:C31	0.83	2.02	14	20
3:C:210:PCW:H461	3:C:210:PCW:H181	0.83	1.49	1	6
3:C:203:PCW:O1P	3:C:211:PCW:H62	0.83	1.73	7	2
2:B:128:LYS:HB3	2:C:47:ASP:HA	0.83	1.48	3	7
3:A:411:PCW:H283	3:B:205:PCW:H252	0.83	1.47	5	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
4:B:210:17F:H48	3:C:205:PCW:H481	0.83	1.50	11	3
3:D:608:PCW:C17	4:D:629:17F:H18	0.83	2.02	10	1
3:C:204:PCW:H40	3:C:216:PCW:H251	0.83	1.47	13	3
3:C:207:PCW:H122	4:C:213:17F:C17	0.83	2.03	16	1
3:A:417:PCW:H451	3:D:618:PCW:C24	0.83	2.04	16	10
3:D:619:PCW:H131	3:D:627:PCW:C15	0.83	2.03	11	9
4:C:215:17F:O6	4:C:215:17F:H18A	0.83	1.71	9	12
3:A:402:PCW:H73	3:A:410:PCW:O2P	0.83	1.73	3	5
3:A:405:PCW:H242	3:A:418:PCW:H262	0.83	1.48	4	8
3:A:404:PCW:H39	3:B:205:PCW:H441	0.83	1.49	6	5
3:A:412:PCW:H451	3:C:210:PCW:H19	0.83	1.50	18	3
3:D:601:PCW:C39	3:D:602:PCW:H151	0.83	2.02	5	1
3:C:209:PCW:H121	4:C:214:17F:O9	0.83	1.73	10	5
3:A:413:PCW:H431	3:C:210:PCW:C23	0.83	2.03	18	10
3:D:625:PCW:H432	3:D:626:PCW:H432	0.83	1.47	3	6
4:B:210:17F:H44	3:C:205:PCW:H481	0.83	1.48	8	1
3:A:421:PCW:C36	4:D:630:17F:H8A	0.83	2.03	10	1
3:D:604:PCW:C38	4:C:218:17F:H36	0.83	2.02	10	2
3:A:402:PCW:C41	3:C:208:PCW:H381	0.83	2.02	2	3
3:A:409:PCW:C14	3:A:409:PCW:H19	0.83	2.04	12	4
3:D:601:PCW:C39	4:D:628:17F:H52	0.83	2.03	10	10
3:B:205:PCW:H251	3:B:205:PCW:C21	0.83	2.03	13	16
4:A:422:17F:H65	4:D:632:17F:H71	0.83	1.48	19	10
3:D:618:PCW:H471	3:D:618:PCW:C43	0.83	2.03	3	1
3:A:403:PCW:C17	3:A:404:PCW:H122	0.83	2.04	5	3
3:D:602:PCW:H73	4:C:214:17F:H19	0.83	1.48	18	2
3:A:403:PCW:C19	3:A:404:PCW:H142	0.83	1.99	20	1
3:A:406:PCW:H122	4:B:211:17F:O7	0.83	1.72	9	3
3:A:421:PCW:O1P	3:D:618:PCW:H42	0.83	1.72	6	6
3:C:206:PCW:H282	3:C:206:PCW:C24	0.83	2.04	8	5
3:D:602:PCW:H483	4:D:629:17F:H47	0.83	1.47	6	4
3:D:602:PCW:H261	4:D:629:17F:H76	0.83	1.49	9	3
3:B:203:PCW:H381	3:C:211:PCW:H441	0.83	1.48	11	3
3:B:206:PCW:H441	3:C:209:PCW:H40	0.83	1.50	3	2
3:C:207:PCW:H161	4:C:213:17F:H56	0.83	1.51	2	4
3:A:418:PCW:H441	3:D:613:PCW:H272	0.83	1.50	10	7
3:D:604:PCW:H322	3:D:606:PCW:H122	0.83	1.50	19	5
3:A:414:PCW:O3	3:A:414:PCW:H351	0.83	1.74	3	13
3:D:609:PCW:H182	3:D:616:PCW:H352	0.83	1.50	3	11
3:A:404:PCW:C18	3:A:404:PCW:C22	0.83	2.53	12	9
3:C:205:PCW:H2	4:C:214:17F:C6	0.83	2.04	4	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
3:A:414:PCW:H162	4:A:415:17F:C32	0.83	2.03	8	4
3:A:402:PCW:H82	3:A:407:PCW:O11	0.83	1.73	8	1
3:A:413:PCW:H51	3:C:210:PCW:O2P	0.83	1.73	13	12
3:C:212:PCW:H121	4:C:215:17F:O1	0.83	1.74	1	1
3:A:418:PCW:C33	3:D:613:PCW:H132	0.83	2.03	17	10
3:D:621:PCW:H2	3:D:621:PCW:C4	0.83	2.03	14	5
3:A:409:PCW:C8	3:B:206:PCW:H11	0.83	2.04	8	3
3:A:414:PCW:H372	3:A:414:PCW:H411	0.83	1.49	5	1
4:A:416:17F:H74	4:B:209:17F:H74	0.83	1.50	9	1
3:C:216:PCW:C48	3:C:217:PCW:H431	0.83	2.03	9	3
3:D:619:PCW:H331	3:D:627:PCW:H172	0.83	1.50	16	3
4:B:210:17F:H1A	3:C:205:PCW:H371	0.83	1.49	18	1
3:A:406:PCW:H40	3:B:205:PCW:H242	0.82	1.49	1	1
3:D:614:PCW:H483	3:D:620:PCW:H411	0.82	1.49	1	5
3:B:208:PCW:C1	3:C:211:PCW:H342	0.82	2.03	2	5
3:C:212:PCW:H73	4:C:213:17F:P1	0.82	2.14	15	2
3:A:406:PCW:H331	4:B:211:17F:O8	0.82	1.74	18	2
3:C:205:PCW:H11	4:C:214:17F:H8A	0.82	1.51	6	5
3:A:408:PCW:H242	3:A:411:PCW:C22	0.82	2.04	11	6
3:D:601:PCW:H371	3:D:602:PCW:H121	0.82	1.50	8	1
3:B:206:PCW:C24	3:C:209:PCW:H122	0.82	2.04	18	7
3:B:206:PCW:C21	3:C:209:PCW:H321	0.82	2.02	14	1
3:A:403:PCW:H182	3:A:403:PCW:C23	0.82	2.05	1	2
3:D:622:PCW:C41	4:D:632:17F:H77	0.82	2.02	8	2
3:C:212:PCW:H241	3:C:212:PCW:C20	0.82	2.05	14	20
3:A:420:PCW:C45	3:D:611:PCW:H211	0.82	2.04	2	11
3:A:418:PCW:H361	3:D:613:PCW:C15	0.82	2.03	15	2
3:A:414:PCW:H422	4:A:415:17F:C38	0.82	2.04	12	3
3:C:206:PCW:H82	3:C:212:PCW:C32	0.82	2.03	8	1
3:A:402:PCW:H51	3:A:402:PCW:H322	0.82	1.50	9	2
4:A:422:17F:H65	4:D:632:17F:H67	0.82	1.49	13	1
4:D:628:17F:H78	4:C:214:17F:H53	0.82	1.48	18	1
4:A:422:17F:H29	4:C:218:17F:C38	0.82	2.02	16	6
3:D:606:PCW:H73	3:D:626:PCW:H281	0.82	1.51	14	2
4:A:422:17F:C8	4:C:218:17F:H65	0.82	2.04	14	4
3:D:621:PCW:C27	4:D:632:17F:H35	0.82	2.03	20	1
3:A:419:PCW:H431	3:D:625:PCW:C44	0.82	2.04	6	5
3:D:604:PCW:C45	3:D:606:PCW:H181	0.82	2.04	3	10
3:B:203:PCW:H211	4:B:209:17F:H18A	0.82	1.52	1	1
3:A:401:PCW:H472	3:D:612:PCW:H271	0.82	1.48	14	4
3:C:212:PCW:H142	4:C:215:17F:C9	0.82	2.03	11	3

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
3:B:208:PCW:H481	3:C:203:PCW:H161	0.82	1.51	8	1
3:C:209:PCW:H141	4:C:214:17F:O7	0.82	1.72	9	1
3:A:408:PCW:H171	3:A:411:PCW:H232	0.82	1.52	1	3
3:A:408:PCW:H122	3:A:413:PCW:H352	0.82	1.50	2	5
3:D:622:PCW:H20	3:C:217:PCW:C8	0.82	2.05	9	6
3:C:206:PCW:C17	3:C:208:PCW:H362	0.82	2.04	11	8
3:A:406:PCW:H381	3:C:204:PCW:H332	0.82	1.50	20	2
3:A:421:PCW:H62	4:D:630:17F:O8	0.82	1.73	5	2
3:D:621:PCW:H461	3:C:208:PCW:H481	0.82	1.50	12	3
3:C:205:PCW:C15	3:C:209:PCW:H321	0.82	2.05	17	1
3:D:624:PCW:H272	3:B:208:PCW:H272	0.82	1.52	1	1
3:A:403:PCW:H62	3:A:403:PCW:O11	0.82	1.75	6	2
3:D:604:PCW:H2	3:D:606:PCW:C8	0.82	2.01	4	8
3:D:609:PCW:H122	3:D:616:PCW:C7	0.82	2.05	10	13
3:D:612:PCW:C39	3:D:623:PCW:H462	0.82	2.04	14	10
4:D:628:17F:H57	4:D:629:17F:H51	0.82	1.51	9	10
3:B:208:PCW:H472	3:B:208:PCW:C43	0.82	2.05	5	19
3:A:413:PCW:H40	3:C:210:PCW:H231	0.82	1.50	3	8
3:C:209:PCW:H272	3:C:209:PCW:H471	0.82	1.51	11	11
3:C:206:PCW:H372	3:C:208:PCW:H142	0.82	1.48	8	1
3:D:608:PCW:H42	3:D:626:PCW:C24	0.82	2.05	9	1
3:A:405:PCW:H281	3:A:418:PCW:H241	0.82	1.50	20	2
3:D:605:PCW:H482	3:D:620:PCW:H471	0.82	1.52	15	1
4:A:416:17F:H56	3:B:204:PCW:H151	0.82	1.52	4	5
3:D:608:PCW:H262	4:D:629:17F:H35	0.82	1.51	13	8
3:C:207:PCW:H483	3:C:207:PCW:H251	0.82	1.51	2	1
4:C:219:17F:H36	4:C:219:17F:H65	0.82	1.50	9	10
3:A:406:PCW:H451	4:B:211:17F:H33	0.82	1.51	3	4
3:A:408:PCW:C16	3:A:411:PCW:H232	0.82	2.05	5	12
3:C:204:PCW:H482	3:C:216:PCW:H231	0.82	1.50	12	5
1:D:462:LYS:HD2	3:D:602:PCW:H283	0.82	1.50	14	4
3:C:209:PCW:H121	4:C:214:17F:H6	0.82	1.48	9	1
3:A:414:PCW:H472	3:A:414:PCW:C43	0.82	2.04	20	20
4:D:628:17F:H57	4:D:628:17F:C19	0.82	2.04	17	20
3:A:403:PCW:H472	3:A:404:PCW:C28	0.82	2.05	15	5
3:A:418:PCW:H421	3:D:613:PCW:H251	0.82	1.51	10	5
3:A:411:PCW:H271	3:C:210:PCW:H231	0.82	1.51	6	1
3:C:206:PCW:C18	3:C:208:PCW:H172	0.82	2.01	6	3
3:A:406:PCW:H11	3:A:406:PCW:H42	0.82	1.51	20	3
3:C:211:PCW:H142	3:C:211:PCW:H482	0.82	1.50	3	2
3:D:608:PCW:H482	4:D:628:17F:H61	0.82	1.52	10	4

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
3:A:421:PCW:C6	4:D:630:17F:H6A	0.82	2.05	6	1
4:A:416:17F:C42	4:B:209:17F:H70	0.82	2.05	17	1
3:C:211:PCW:H152	4:C:215:17F:H64	0.82	1.48	18	1
3:D:606:PCW:H471	4:D:632:17F:H31	0.81	1.48	9	2
3:D:603:PCW:H162	3:D:624:PCW:C22	0.81	2.05	5	9
3:C:210:PCW:H172	3:C:210:PCW:H211	0.81	1.51	2	2
3:D:602:PCW:H261	4:D:629:17F:H78	0.81	1.51	3	4
3:D:607:PCW:H31	3:D:626:PCW:C39	0.81	2.05	3	10
3:A:417:PCW:C45	3:D:618:PCW:H242	0.81	2.03	20	6
4:A:415:17F:H2	4:A:415:17F:O1	0.81	1.74	14	13
3:A:421:PCW:O3	4:D:630:17F:H9	0.81	1.74	12	6
3:C:205:PCW:H63	4:C:214:17F:O8	0.81	1.74	7	5
3:A:405:PCW:C36	3:A:411:PCW:H461	0.81	2.05	7	6
3:A:411:PCW:H172	3:A:411:PCW:C21	0.81	2.05	14	2
3:D:609:PCW:H381	3:C:208:PCW:H283	0.81	1.50	9	5
3:D:619:PCW:C24	3:C:204:PCW:H451	0.81	2.04	9	1
3:D:624:PCW:H221	3:C:217:PCW:H232	0.81	1.52	16	2
3:B:203:PCW:C33	4:B:210:17F:H37	0.81	2.05	15	3
3:C:203:PCW:H42	3:C:211:PCW:O1P	0.81	1.75	16	2
3:A:418:PCW:H411	3:D:613:PCW:C15	0.81	2.05	1	1
3:D:622:PCW:H142	3:D:622:PCW:C18	0.81	2.05	11	20
4:C:218:17F:H52	4:C:219:17F:H43	0.81	1.49	6	4
3:D:617:PCW:H39	3:D:619:PCW:C16	0.81	2.05	8	7
3:B:204:PCW:H2	3:B:204:PCW:H62	0.81	1.51	2	1
3:A:408:PCW:H231	3:A:411:PCW:C23	0.81	2.04	3	1
3:D:603:PCW:H231	3:D:603:PCW:H472	0.81	1.50	3	7
3:C:203:PCW:H19	3:C:211:PCW:H31	0.81	1.52	5	1
3:D:609:PCW:H2	3:D:616:PCW:C6	0.81	2.05	15	6
3:D:612:PCW:C22	3:D:620:PCW:H442	0.81	2.05	9	2
3:C:209:PCW:H121	4:C:214:17F:C17	0.81	2.05	16	4
3:D:617:PCW:H483	3:B:205:PCW:C22	0.81	2.05	8	1
3:D:617:PCW:H431	3:C:204:PCW:H472	0.81	1.52	19	3
3:D:619:PCW:H242	3:C:204:PCW:H451	0.81	1.52	9	2
4:A:415:17F:H61	4:B:209:17F:C1X	0.81	2.05	12	2
3:A:403:PCW:O11	3:A:403:PCW:H41	0.81	1.74	15	1
4:B:210:17F:H30	4:C:215:17F:H11	0.81	1.50	15	1
3:C:207:PCW:H19	4:C:213:17F:H19	0.81	1.51	18	1
3:C:212:PCW:H371	4:C:215:17F:H10	0.81	1.51	18	1
3:A:411:PCW:H322	3:A:411:PCW:C4	0.81	2.06	5	12
3:D:615:PCW:C4	3:D:625:PCW:H42	0.81	2.05	1	2
3:A:406:PCW:H361	3:B:205:PCW:H321	0.81	1.50	9	5

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
3:B:204:PCW:H2	3:B:204:PCW:C7	0.81	2.05	4	6
3:C:204:PCW:H171	3:C:216:PCW:H281	0.81	1.51	16	1
3:D:613:PCW:C17	3:D:613:PCW:C21	0.81	2.55	6	17
3:A:420:PCW:H351	3:D:618:PCW:H422	0.81	1.52	17	6
3:B:205:PCW:H332	3:B:208:PCW:H82	0.81	1.50	9	2
3:B:205:PCW:H31	4:B:211:17F:O8	0.81	1.76	6	1
4:A:415:17F:H10	4:B:209:17F:H11A	0.81	1.52	10	1
3:B:203:PCW:H472	3:C:211:PCW:H271	0.81	1.50	20	3
3:A:411:PCW:O2P	4:B:211:17F:H1A	0.81	1.75	16	1
3:A:420:PCW:C43	3:D:611:PCW:H211	0.81	2.05	1	10
3:D:606:PCW:H63	3:D:606:PCW:O11	0.81	1.75	4	12
3:D:624:PCW:H241	3:D:624:PCW:C20	0.81	2.06	7	20
3:D:612:PCW:H471	3:B:203:PCW:H281	0.81	1.52	9	2
3:A:405:PCW:O1P	3:A:406:PCW:H171	0.81	1.75	17	6
3:A:408:PCW:H42	3:A:413:PCW:C3	0.81	2.03	13	5
3:A:409:PCW:H39	4:B:210:17F:H65	0.81	1.53	13	2
4:A:422:17F:H29	4:C:218:17F:H68	0.81	1.49	5	7
3:A:420:PCW:H11	3:D:618:PCW:C41	0.81	2.06	10	4
3:C:206:PCW:H152	3:C:207:PCW:C20	0.81	2.06	11	2
3:C:205:PCW:H2	3:C:209:PCW:C3	0.81	2.05	12	1
3:C:203:PCW:H321	3:C:207:PCW:C35	0.81	2.06	14	1
3:A:414:PCW:H361	4:B:209:17F:H11	0.81	1.52	20	1
3:A:418:PCW:H371	3:A:418:PCW:C41	0.81	2.05	4	7
4:B:211:17F:H10	4:B:211:17F:H66	0.81	1.50	3	1
3:A:401:PCW:C6	3:B:207:PCW:H2	0.81	2.02	19	3
3:D:627:PCW:H20	3:C:217:PCW:H331	0.81	1.53	18	3
3:A:409:PCW:C19	3:A:409:PCW:C14	0.81	2.58	2	20
4:A:422:17F:H36	4:C:219:17F:H62	0.81	1.50	8	4
3:C:206:PCW:H241	3:C:206:PCW:C28	0.81	2.04	17	5
3:D:627:PCW:H421	3:D:627:PCW:C38	0.81	2.02	18	7
3:B:204:PCW:H272	3:B:204:PCW:C23	0.81	2.05	13	13
3:B:206:PCW:H422	3:C:209:PCW:C39	0.81	2.05	6	4
3:A:420:PCW:H351	3:D:618:PCW:C42	0.81	2.06	3	10
3:D:619:PCW:H322	3:D:627:PCW:H121	0.81	1.52	9	8
3:C:203:PCW:H12	3:C:211:PCW:H73	0.81	1.51	3	4
3:C:208:PCW:H232	4:C:214:17F:H55	0.81	1.52	4	1
3:D:607:PCW:H361	3:D:626:PCW:C43	0.81	2.02	10	6
3:C:208:PCW:H61	4:C:213:17F:C1	0.81	2.05	11	2
3:A:407:PCW:H332	3:A:410:PCW:H351	0.81	1.52	14	1
3:D:616:PCW:C47	3:C:208:PCW:H222	0.81	1.99	17	8
3:A:404:PCW:H121	3:B:205:PCW:H442	0.81	1.53	2	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
3:A:414:PCW:H321	4:A:415:17F:H19A	0.81	1.53	6	2
3:D:623:PCW:H232	3:B:203:PCW:H481	0.81	1.52	11	5
3:C:206:PCW:H251	3:C:206:PCW:C21	0.81	2.06	8	5
3:A:408:PCW:H152	3:A:411:PCW:C21	0.81	2.04	11	4
3:D:612:PCW:H221	3:D:620:PCW:H452	0.81	1.49	10	1
3:A:414:PCW:O31	3:A:414:PCW:H351	0.81	1.75	16	1
3:D:610:PCW:H62	4:D:631:17F:P1	0.81	2.15	18	2
3:A:401:PCW:H62	3:B:207:PCW:O31	0.80	1.76	10	12
3:C:205:PCW:H2	3:C:209:PCW:H152	0.80	1.51	9	2
3:A:406:PCW:H451	4:B:211:17F:C31	0.80	2.06	2	1
2:B:128:LYS:HB2	2:C:47:ASP:HA	0.80	1.51	19	6
3:C:203:PCW:C44	3:C:204:PCW:H181	0.80	2.06	4	1
3:A:420:PCW:H242	3:A:420:PCW:C20	0.80	2.06	5	1
3:D:614:PCW:C28	4:B:209:17F:H35	0.80	2.05	5	3
3:C:206:PCW:H61	3:C:212:PCW:H321	0.80	1.52	15	1
3:D:607:PCW:H451	3:D:625:PCW:H471	0.80	1.51	1	1
3:D:616:PCW:H2	3:D:616:PCW:H42	0.80	1.52	9	11
3:D:619:PCW:H431	3:D:627:PCW:H282	0.80	1.52	1	5
3:A:421:PCW:P	3:D:618:PCW:H42	0.80	2.17	20	12
3:D:602:PCW:H341	4:C:214:17F:H63	0.80	1.52	12	1
3:A:418:PCW:H331	3:D:613:PCW:H132	0.80	1.54	18	7
3:D:605:PCW:C17	3:D:614:PCW:H342	0.80	2.06	7	9
3:D:610:PCW:H172	4:D:631:17F:H61	0.80	1.53	6	8
4:B:211:17F:H12	4:B:211:17F:C36	0.80	2.06	9	4
3:D:617:PCW:H342	3:C:216:PCW:H341	0.80	1.49	9	2
3:C:206:PCW:H211	3:C:206:PCW:C25	0.80	2.03	8	5
3:A:403:PCW:P	3:A:403:PCW:H31	0.80	2.16	19	2
3:C:209:PCW:H73	4:C:214:17F:O2	0.80	1.76	14	1
3:D:626:PCW:C20	3:D:626:PCW:C25	0.80	2.57	15	1
3:C:207:PCW:H162	4:C:213:17F:C33	0.80	2.04	20	1
3:A:403:PCW:C31	3:A:403:PCW:C36	0.80	2.59	6	7
3:A:421:PCW:H351	3:D:618:PCW:H151	0.80	1.50	17	9
3:A:419:PCW:H472	3:D:625:PCW:H483	0.80	1.51	19	8
3:D:624:PCW:H321	3:D:624:PCW:C7	0.80	2.07	4	9
3:D:623:PCW:H211	3:B:203:PCW:H481	0.80	1.52	3	1
3:C:207:PCW:H122	4:C:213:17F:O10	0.80	1.75	3	2
3:B:203:PCW:H431	3:C:211:PCW:C22	0.80	2.07	10	4
3:A:411:PCW:H51	4:B:211:17F:O4	0.80	1.75	5	6
3:A:408:PCW:H42	3:A:413:PCW:H11	0.80	1.51	20	2
3:A:417:PCW:C41	3:D:618:PCW:H152	0.80	2.05	7	1
4:C:213:17F:H50	4:C:215:17F:H70	0.80	1.52	11	2

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
4:A:415:17F:H49	3:B:208:PCW:H232	0.80	1.52	13	1
3:A:401:PCW:C32	3:B:207:PCW:H382	0.80	2.01	4	4
3:D:622:PCW:C22	4:D:631:17F:H31	0.80	2.06	13	13
4:A:422:17F:C35	3:D:622:PCW:H421	0.80	2.06	2	13
3:C:205:PCW:H411	4:C:215:17F:H12A	0.80	1.52	2	1
3:A:405:PCW:H52	3:A:406:PCW:H121	0.80	1.52	4	8
3:B:204:PCW:H441	3:C:205:PCW:H483	0.80	1.52	9	2
3:D:618:PCW:H2	3:D:618:PCW:C4	0.80	2.05	18	3
3:A:419:PCW:H2	3:A:419:PCW:O2P	0.80	1.76	13	4
3:B:203:PCW:H472	3:C:211:PCW:H251	0.80	1.50	16	3
3:C:203:PCW:H281	3:C:211:PCW:H431	0.80	1.51	12	1
3:A:401:PCW:H82	3:B:204:PCW:O2P	0.80	1.76	16	1
3:C:206:PCW:H131	3:C:207:PCW:H19	0.80	1.52	20	1
3:A:420:PCW:C37	3:D:618:PCW:H422	0.80	2.06	3	2
3:A:407:PCW:C33	3:A:410:PCW:H351	0.80	2.06	14	1
3:D:627:PCW:C31	3:D:627:PCW:H63	0.80	2.07	14	1
3:A:411:PCW:H262	3:C:210:PCW:H241	0.80	1.53	17	1
3:D:605:PCW:H181	3:D:614:PCW:H362	0.80	1.54	19	11
3:D:606:PCW:H182	3:D:606:PCW:C14	0.80	2.05	10	20
3:B:206:PCW:C42	3:C:209:PCW:H39	0.80	2.07	6	5
3:A:404:PCW:H432	3:A:414:PCW:H251	0.80	1.52	16	5
3:C:204:PCW:H272	3:C:217:PCW:H421	0.80	1.53	20	5
3:B:204:PCW:H31	3:B:207:PCW:H351	0.80	1.54	4	2
3:A:413:PCW:H82	3:C:210:PCW:H2	0.80	1.53	9	2
3:C:203:PCW:O11	3:C:211:PCW:H32	0.80	1.76	5	1
3:C:206:PCW:H171	3:C:207:PCW:H182	0.80	1.53	12	1
3:A:401:PCW:H322	3:B:207:PCW:C39	0.80	2.06	5	5
3:C:204:PCW:H252	3:C:217:PCW:H472	0.80	1.52	17	5
3:A:421:PCW:H321	3:D:618:PCW:H52	0.80	1.53	4	5
3:D:627:PCW:H282	4:D:631:17F:H51	0.80	1.52	2	8
3:B:203:PCW:H73	3:C:211:PCW:O31	0.80	1.76	4	7
3:D:607:PCW:H241	3:B:206:PCW:C48	0.80	2.06	3	2
3:B:205:PCW:C33	3:B:208:PCW:H121	0.80	2.05	3	1
3:B:207:PCW:H232	3:B:207:PCW:H382	0.80	1.51	9	4
3:A:408:PCW:C23	3:A:411:PCW:H231	0.80	2.07	12	7
3:D:607:PCW:H31	3:D:626:PCW:H411	0.80	1.53	6	3
3:B:205:PCW:H182	3:C:203:PCW:C48	0.80	2.06	12	4
3:C:217:PCW:H181	4:C:219:17F:H37	0.80	1.52	16	2
3:A:408:PCW:C22	4:D:631:17F:H54	0.80	2.07	10	1
3:B:205:PCW:O11	3:C:204:PCW:H52	0.80	1.76	20	2
3:B:207:PCW:H451	3:B:207:PCW:H232	0.80	1.54	13	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:279:LEU:HD22	1:D:495:LYS:HE3	0.80	1.52	17	13
3:A:408:PCW:H371	3:A:413:PCW:H182	0.80	1.53	4	2
3:A:420:PCW:C42	3:D:617:PCW:H232	0.80	2.06	14	11
3:A:408:PCW:H262	3:A:411:PCW:C25	0.80	2.06	4	2
3:A:408:PCW:H171	3:A:411:PCW:H222	0.80	1.54	18	8
3:C:206:PCW:H62	4:C:213:17F:O8	0.80	1.77	7	1
3:D:619:PCW:H131	3:D:627:PCW:H132	0.80	1.50	8	1
3:B:203:PCW:H381	3:C:211:PCW:H421	0.80	1.52	13	1
4:A:416:17F:C30	3:D:614:PCW:H441	0.80	2.06	15	2
3:D:610:PCW:H12	4:D:631:17F:H6	0.80	1.51	20	2
3:D:617:PCW:H31	3:D:617:PCW:C4	0.80	2.07	10	4
3:A:401:PCW:H322	3:B:207:PCW:H39	0.80	1.53	5	3
3:D:624:PCW:H242	3:C:217:PCW:H232	0.80	1.54	5	2
3:D:623:PCW:H281	3:D:624:PCW:C46	0.80	2.05	17	4
3:C:217:PCW:H362	4:C:218:17F:H76	0.80	1.53	13	4
4:A:422:17F:C23	4:C:219:17F:H67	0.79	2.07	12	11
3:D:622:PCW:H283	4:D:631:17F:H30	0.79	1.55	10	6
3:D:602:PCW:H252	4:D:629:17F:H76	0.79	1.54	18	4
4:A:416:17F:C36	3:B:204:PCW:H272	0.79	2.06	18	4
4:B:210:17F:C25	3:C:205:PCW:H481	0.79	2.07	8	2
3:C:203:PCW:H372	4:C:213:17F:H75	0.79	1.54	9	2
3:A:404:PCW:H152	3:B:205:PCW:H472	0.79	1.54	13	2
3:A:414:PCW:H31	3:A:414:PCW:C37	0.79	2.04	5	4
3:A:414:PCW:H141	4:A:415:17F:H58	0.79	1.51	6	4
3:A:414:PCW:H341	4:A:415:17F:C31	0.79	2.04	15	10
3:A:414:PCW:H122	4:A:415:17F:C37	0.79	2.07	17	2
3:D:617:PCW:H451	3:C:204:PCW:H481	0.79	1.52	2	1
3:A:403:PCW:H73	3:A:404:PCW:O2P	0.79	1.76	3	1
3:A:407:PCW:H121	3:A:410:PCW:H331	0.79	1.54	18	5
4:B:211:17F:H46	3:C:204:PCW:H422	0.79	1.51	4	1
3:C:209:PCW:H472	3:C:209:PCW:H271	0.79	1.53	4	1
3:D:605:PCW:H412	3:D:620:PCW:H121	0.79	1.53	6	1
3:B:208:PCW:H481	3:C:203:PCW:H211	0.79	1.54	6	1
3:A:402:PCW:C41	3:C:208:PCW:H361	0.79	2.07	15	5
3:A:406:PCW:H331	4:B:211:17F:H8	0.79	1.52	7	1
3:D:617:PCW:C38	3:D:619:PCW:H142	0.79	2.07	14	5
3:C:206:PCW:H31	4:C:214:17F:H35	0.79	1.54	12	1
4:B:210:17F:H60	3:C:205:PCW:H462	0.79	1.54	16	1
3:D:624:PCW:H451	4:B:209:17F:C42	0.79	2.08	19	2
3:C:209:PCW:H472	3:C:209:PCW:C43	0.79	2.06	12	19
3:D:604:PCW:H412	3:D:606:PCW:H241	0.79	1.52	4	8

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
3:A:404:PCW:H152	3:B:205:PCW:C45	0.79	2.07	4	4
3:D:615:PCW:H63	3:D:625:PCW:O1P	0.79	1.77	7	11
3:C:217:PCW:H121	4:C:219:17F:C1Z	0.79	2.06	19	3
3:D:617:PCW:O2P	3:D:617:PCW:H31	0.79	1.76	9	4
3:D:622:PCW:H31	3:D:622:PCW:O1P	0.79	1.75	5	1
3:C:206:PCW:H52	4:C:214:17F:H35	0.79	1.53	6	1
3:A:414:PCW:H422	4:A:415:17F:H68	0.79	1.52	18	3
3:C:212:PCW:H421	4:C:215:17F:H36	0.79	1.54	10	1
4:A:422:17F:H12	3:D:622:PCW:H481	0.79	1.51	19	3
3:D:627:PCW:C22	3:C:217:PCW:H352	0.79	2.07	14	2
4:B:211:17F:H65	4:B:211:17F:H30	0.79	1.53	17	2
3:D:604:PCW:H341	4:C:219:17F:H8	0.79	1.52	14	1
3:D:621:PCW:C12	4:D:632:17F:H4A	0.79	2.07	4	3
3:A:408:PCW:H162	3:A:413:PCW:C41	0.79	2.07	5	1
3:A:402:PCW:H322	3:A:402:PCW:C5	0.79	2.06	9	2
4:C:213:17F:H29	4:C:215:17F:C31	0.79	2.07	9	1
3:A:413:PCW:H382	3:C:210:PCW:H141	0.79	1.55	10	10
4:B:211:17F:H66	4:B:211:17F:H12	0.79	1.54	2	1
3:A:409:PCW:H152	4:B:210:17F:H31	0.79	1.51	4	1
4:B:211:17F:H54	3:C:204:PCW:H483	0.79	1.51	4	1
3:A:417:PCW:H161	3:A:420:PCW:C34	0.79	2.07	5	5
3:A:417:PCW:H121	3:D:618:PCW:H331	0.79	1.54	16	3
3:D:627:PCW:H42	3:D:627:PCW:H32	0.79	1.52	5	1
3:A:401:PCW:H62	3:B:207:PCW:C1	0.79	2.04	7	1
3:D:609:PCW:H211	3:D:616:PCW:H372	0.79	1.53	9	3
3:A:414:PCW:H182	3:A:414:PCW:C14	0.79	2.08	1	3
3:C:209:PCW:H222	3:C:209:PCW:C26	0.79	2.06	2	20
3:A:405:PCW:C37	3:A:411:PCW:H461	0.79	2.07	2	3
4:B:210:17F:H12	4:B:210:17F:C24	0.79	2.06	20	6
3:C:206:PCW:C6	3:C:212:PCW:H321	0.79	2.07	7	6
3:A:406:PCW:C35	4:B:211:17F:H9	0.79	2.07	16	2
3:A:407:PCW:H82	3:A:410:PCW:H362	0.79	1.55	7	5
3:D:616:PCW:H142	4:D:632:17F:H9A	0.79	1.54	16	3
3:A:405:PCW:H361	3:A:411:PCW:H421	0.79	1.55	15	2
3:D:617:PCW:H482	3:C:210:PCW:H283	0.79	1.52	2	4
3:D:624:PCW:C47	4:B:209:17F:H55	0.79	2.06	2	4
3:D:603:PCW:C46	3:D:611:PCW:H432	0.79	2.08	20	5
3:A:403:PCW:H171	3:A:404:PCW:C12	0.79	2.06	14	5
3:A:407:PCW:H82	3:A:410:PCW:C36	0.79	2.07	7	5
3:D:608:PCW:H282	4:D:629:17F:H65	0.79	1.52	7	1
3:A:403:PCW:C33	3:A:406:PCW:H11	0.79	2.04	5	5

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
3:A:408:PCW:H232	3:A:411:PCW:H222	0.79	1.52	20	7
3:B:206:PCW:H282	3:B:206:PCW:C24	0.79	2.05	8	1
3:C:206:PCW:C8	3:C:212:PCW:H321	0.79	2.06	8	1
3:C:206:PCW:C14	3:C:208:PCW:H321	0.79	2.05	20	2
3:C:203:PCW:H251	3:C:211:PCW:H471	0.79	1.53	13	1
3:C:209:PCW:H2	3:C:209:PCW:H42	0.79	1.53	15	1
3:C:203:PCW:H361	3:C:204:PCW:H142	0.79	1.53	17	2
2:B:32:TYR:CD1	5:B:201:GSP:H5'2	0.79	2.13	14	10
3:B:203:PCW:C21	4:B:209:17F:H18A	0.79	2.08	1	1
3:D:617:PCW:H451	3:C:204:PCW:C48	0.79	2.07	2	1
3:B:205:PCW:H51	3:C:204:PCW:H62	0.79	1.53	12	2
3:C:206:PCW:H222	3:C:208:PCW:H411	0.79	1.54	5	1
3:A:420:PCW:H482	3:D:619:PCW:H281	0.79	1.54	7	2
3:A:401:PCW:H322	3:B:207:PCW:C38	0.79	2.01	4	11
3:B:205:PCW:O1P	3:B:205:PCW:H51	0.79	1.78	1	2
3:D:612:PCW:O2P	3:D:620:PCW:H41	0.79	1.78	2	7
1:D:471:ARG:HA	1:D:475:GLU:HG3	0.79	1.55	11	9
3:A:404:PCW:H441	3:A:414:PCW:H251	0.79	1.55	19	3
3:A:418:PCW:H332	3:D:613:PCW:C13	0.79	2.05	15	3
3:D:617:PCW:H12	3:D:617:PCW:H41	0.79	1.54	8	1
3:D:604:PCW:H381	4:C:218:17F:C2X	0.79	2.04	10	2
3:A:402:PCW:H422	3:C:208:PCW:H152	0.79	1.55	17	1
3:A:402:PCW:O2P	3:A:410:PCW:H41	0.78	1.77	1	11
3:D:603:PCW:H162	3:D:624:PCW:H211	0.78	1.54	7	5
3:A:409:PCW:H82	3:B:206:PCW:C1	0.78	2.09	4	1
3:A:418:PCW:H352	3:D:613:PCW:H182	0.78	1.55	5	1
3:A:406:PCW:H381	3:C:204:PCW:C32	0.78	2.07	10	1
3:A:404:PCW:H161	3:A:404:PCW:C44	0.78	2.08	1	1
3:D:608:PCW:C4	3:D:626:PCW:H222	0.78	2.04	4	5
3:D:614:PCW:H221	4:B:209:17F:H47	0.78	1.54	1	7
3:A:406:PCW:C45	4:B:211:17F:H57	0.78	2.07	2	1
3:A:401:PCW:H381	3:B:204:PCW:H232	0.78	1.54	3	1
3:D:610:PCW:H63	4:D:631:17F:C6	0.78	2.08	12	5
3:C:203:PCW:H411	3:C:204:PCW:H141	0.78	1.54	6	2
4:B:211:17F:H55	3:C:216:PCW:H182	0.78	1.51	20	3
3:B:205:PCW:H182	3:C:203:PCW:H482	0.78	1.55	12	2
3:D:617:PCW:H271	3:D:619:PCW:H282	0.78	1.54	16	1
3:D:603:PCW:H62	3:C:216:PCW:O3P	0.78	1.79	6	3
3:D:605:PCW:O31	3:D:614:PCW:H62	0.78	1.78	9	8
3:A:403:PCW:H41	3:A:403:PCW:O11	0.78	1.79	20	11
3:A:403:PCW:C31	3:A:403:PCW:H351	0.78	2.07	19	12

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
3:A:413:PCW:H132	3:A:413:PCW:C34	0.78	2.07	11	11
3:D:602:PCW:H172	3:D:602:PCW:C21	0.78	2.08	12	14
3:D:606:PCW:H442	3:D:609:PCW:O2	0.78	1.78	2	3
3:D:608:PCW:C20	4:D:628:17F:H18	0.78	2.08	18	2
3:B:203:PCW:H431	3:C:211:PCW:H232	0.78	1.55	2	2
4:B:210:17F:H43	3:C:205:PCW:H481	0.78	1.56	6	3
3:D:611:PCW:H462	3:B:208:PCW:C26	0.78	2.08	16	8
3:D:621:PCW:H121	4:D:632:17F:C4	0.78	2.08	9	4
3:D:625:PCW:C45	3:D:626:PCW:H482	0.78	2.07	4	9
3:B:205:PCW:H322	3:C:204:PCW:H332	0.78	1.55	3	1
3:A:406:PCW:H272	4:B:211:17F:H60	0.78	1.53	14	4
3:D:607:PCW:C26	3:B:206:PCW:H481	0.78	2.08	20	5
3:A:407:PCW:O3P	3:A:412:PCW:H11	0.78	1.78	16	4
3:D:612:PCW:C8	3:D:625:PCW:H141	0.78	2.08	6	7
4:B:210:17F:H72	3:C:209:PCW:H421	0.78	1.55	7	2
3:A:406:PCW:H451	4:B:211:17F:H30	0.78	1.54	12	2
3:D:617:PCW:H371	3:D:617:PCW:H412	0.78	1.52	14	1
3:A:418:PCW:H422	3:D:613:PCW:H251	0.78	1.54	18	1
3:B:208:PCW:H452	4:C:218:17F:H49	0.78	1.55	19	1
3:A:401:PCW:H221	3:A:401:PCW:C18	0.78	2.09	20	14
4:A:416:17F:C36	3:B:204:PCW:H262	0.78	2.07	15	2
3:B:205:PCW:H151	3:C:204:PCW:O2	0.78	1.77	14	2
3:C:204:PCW:C23	3:C:210:PCW:H282	0.78	2.08	4	10
4:B:211:17F:H11A	4:B:211:17F:H69	0.78	1.53	6	3
3:C:204:PCW:H11	3:C:204:PCW:H41	0.78	1.53	17	4
3:A:420:PCW:H441	3:D:617:PCW:H232	0.78	1.56	10	1
3:A:405:PCW:H73	3:A:406:PCW:O11	0.78	1.78	11	1
3:C:207:PCW:H372	4:C:213:17F:H34	0.78	1.54	14	2
3:C:203:PCW:C1	3:C:211:PCW:H62	0.78	2.08	15	3
1:A:239:LEU:HD13	3:A:408:PCW:H441	0.78	1.55	19	1
3:D:608:PCW:H252	4:D:629:17F:H33	0.78	1.54	1	1
2:C:32:TYR:CD1	5:C:201:GSP:H5'2	0.78	2.13	1	16
4:A:422:17F:H35	4:C:218:17F:H78	0.78	1.54	4	1
3:A:408:PCW:C15	3:A:411:PCW:H232	0.78	2.08	18	7
3:C:207:PCW:H19	4:C:213:17F:H20A	0.78	1.54	17	2
3:C:217:PCW:H362	4:C:218:17F:C42	0.78	2.08	13	4
4:D:632:17F:H52	3:C:208:PCW:H161	0.78	1.53	8	2
3:C:206:PCW:H152	3:C:207:PCW:C19	0.78	2.08	11	2
3:A:407:PCW:H51	3:A:410:PCW:C35	0.78	2.06	12	1
3:A:418:PCW:H431	3:D:613:PCW:H151	0.78	1.55	1	1
3:A:419:PCW:H431	3:D:625:PCW:C46	0.78	2.08	15	16

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
3:D:605:PCW:H171	3:D:614:PCW:C34	0.78	2.09	7	12
3:D:611:PCW:H151	3:D:617:PCW:O11	0.78	1.79	17	7
3:B:203:PCW:C1	3:C:211:PCW:H372	0.78	2.07	2	3
4:A:422:17F:H49	4:C:218:17F:H12	0.78	1.53	3	3
3:B:203:PCW:H222	4:B:209:17F:C18	0.78	2.08	12	2
3:D:624:PCW:H481	4:B:209:17F:H54	0.78	1.53	6	1
3:C:216:PCW:H282	3:C:216:PCW:C24	0.78	2.09	7	1
3:A:407:PCW:H162	3:A:407:PCW:C21	0.78	2.09	8	1
3:A:410:PCW:H252	4:A:422:17F:H74	0.78	1.56	9	3
3:D:613:PCW:H352	3:D:627:PCW:O11	0.78	1.79	14	2
3:B:208:PCW:H452	4:C:218:17F:H54	0.78	1.53	10	3
3:A:401:PCW:H452	3:D:612:PCW:C27	0.78	2.06	5	4
3:B:206:PCW:H231	3:C:205:PCW:H171	0.78	1.53	5	3
3:D:607:PCW:H431	3:D:626:PCW:C47	0.78	2.09	20	2
3:A:409:PCW:C32	3:B:206:PCW:H322	0.78	2.09	13	1
3:B:206:PCW:H131	3:C:209:PCW:C33	0.78	2.03	14	1
3:D:610:PCW:H283	4:D:631:17F:H68	0.78	1.54	16	5
3:B:206:PCW:H31	3:B:206:PCW:P	0.78	2.19	20	11
3:A:420:PCW:H121	3:D:618:PCW:H451	0.78	1.54	3	1
3:B:206:PCW:H61	4:B:210:17F:O1	0.78	1.79	4	1
3:A:406:PCW:C44	4:B:211:17F:H33	0.78	2.08	11	1
3:C:216:PCW:C32	3:C:216:PCW:H52	0.78	2.09	17	6
3:D:619:PCW:H382	4:D:631:17F:H41	0.78	1.52	20	7
3:D:623:PCW:H382	3:D:625:PCW:H171	0.78	1.55	13	7
3:D:627:PCW:H20	3:C:217:PCW:C33	0.78	2.09	18	5
4:D:628:17F:H66	4:D:629:17F:H52	0.78	1.53	5	1
3:D:616:PCW:H262	4:C:214:17F:C40	0.78	2.09	6	1
3:D:621:PCW:H11	3:D:621:PCW:C7	0.78	2.09	15	4
3:B:207:PCW:H132	3:B:207:PCW:H332	0.78	0.91	6	1
3:D:614:PCW:H132	3:D:620:PCW:H382	0.78	1.56	13	3
3:C:212:PCW:H171	3:C:212:PCW:H411	0.78	1.56	19	2
3:D:617:PCW:C44	3:D:627:PCW:H232	0.78	2.07	17	3
3:A:401:PCW:H252	3:D:615:PCW:H271	0.78	1.56	10	1
3:A:406:PCW:O1P	3:B:205:PCW:H381	0.78	1.78	10	1
3:A:403:PCW:H322	3:A:404:PCW:H12	0.78	1.54	13	3
3:D:624:PCW:H73	3:D:624:PCW:C32	0.78	2.09	13	1
3:A:403:PCW:H472	3:A:404:PCW:H271	0.78	1.56	14	1
4:A:422:17F:C1X	4:C:218:17F:H69	0.78	2.06	16	1
3:B:208:PCW:H31	3:C:211:PCW:H431	0.78	1.56	16	1
4:B:210:17F:H47	3:C:205:PCW:H483	0.78	1.55	17	1
4:A:416:17F:H71	3:B:203:PCW:H272	0.78	1.54	3	2

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
3:A:417:PCW:H283	3:A:420:PCW:C25	0.78	2.08	17	6
3:D:610:PCW:C20	3:D:610:PCW:H241	0.78	2.09	6	19
3:A:411:PCW:H42	3:A:411:PCW:C32	0.78	2.08	17	6
3:B:208:PCW:H12	3:C:211:PCW:H321	0.78	1.54	9	5
3:C:205:PCW:H251	3:C:209:PCW:H283	0.78	1.53	2	1
3:A:407:PCW:C32	3:A:410:PCW:H352	0.78	2.09	11	5
3:C:206:PCW:C26	3:C:208:PCW:H381	0.78	2.09	4	2
4:B:210:17F:C27	3:C:205:PCW:H481	0.78	2.09	5	1
3:C:205:PCW:C3	3:C:209:PCW:H152	0.78	2.08	8	4
3:A:421:PCW:P	3:D:618:PCW:H52	0.78	2.19	8	1
3:A:403:PCW:H271	3:A:414:PCW:H20	0.78	1.54	17	1
4:A:415:17F:H55	3:B:208:PCW:H232	0.78	1.55	19	1
3:A:404:PCW:H351	3:A:404:PCW:C31	0.77	2.08	5	4
3:A:418:PCW:H2	3:A:418:PCW:C4	0.77	2.09	10	4
3:D:618:PCW:H41	3:D:618:PCW:O31	0.77	1.79	1	1
3:D:603:PCW:H82	3:D:603:PCW:O31	0.77	1.78	5	6
3:A:401:PCW:H381	3:B:204:PCW:H231	0.77	1.56	20	3
3:A:419:PCW:H431	3:D:625:PCW:H441	0.77	1.53	6	2
3:D:614:PCW:H262	4:B:209:17F:H50	0.77	1.55	9	2
3:B:205:PCW:H241	3:C:210:PCW:H262	0.77	1.54	10	1
3:A:407:PCW:H461	3:A:410:PCW:C26	0.77	2.09	12	1
3:C:208:PCW:H61	4:C:213:17F:O4	0.77	1.79	16	1
3:A:406:PCW:C37	4:B:211:17F:H8A	0.77	2.08	17	1
3:D:612:PCW:C16	3:D:620:PCW:H171	0.77	2.09	2	8
3:C:209:PCW:H32	3:C:209:PCW:O4P	0.77	1.78	7	2
3:C:206:PCW:H151	3:C:207:PCW:H242	0.77	1.52	8	2
3:B:207:PCW:C19	4:B:210:17F:H19A	0.77	2.09	10	3
3:C:205:PCW:H32	3:C:209:PCW:H132	0.77	1.54	14	2
4:D:632:17F:C30	3:C:208:PCW:H141	0.77	2.09	14	1
3:A:411:PCW:H272	3:A:413:PCW:H39	0.77	1.53	18	1
3:A:406:PCW:H321	3:B:205:PCW:H321	0.77	1.55	1	1
3:A:417:PCW:H451	3:D:618:PCW:C25	0.77	2.09	11	11
3:D:604:PCW:H372	3:D:604:PCW:H422	0.77	1.54	7	17
3:C:210:PCW:H52	3:C:210:PCW:H321	0.77	1.55	19	9
3:A:404:PCW:H442	3:A:404:PCW:H172	0.77	1.53	2	5
4:C:215:17F:H30	4:C:215:17F:H63	0.77	1.56	3	2
3:D:605:PCW:H212	3:D:614:PCW:H152	0.77	1.55	4	2
3:B:208:PCW:H41	3:C:211:PCW:C8	0.77	2.09	4	1
3:D:627:PCW:H281	4:D:631:17F:H46	0.77	1.56	10	3
3:B:203:PCW:H482	4:C:215:17F:H51	0.77	1.54	10	1
3:C:209:PCW:H422	3:C:209:PCW:C38	0.77	2.10	11	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
3:A:406:PCW:H31	4:B:211:17F:H75	0.77	1.56	12	1
3:C:203:PCW:C2	3:C:211:PCW:H62	0.77	2.07	18	1
3:D:610:PCW:H62	4:D:631:17F:O1	0.77	1.79	12	7
3:D:610:PCW:O3	4:D:631:17F:H18	0.77	1.80	6	2
3:C:209:PCW:H52	4:C:214:17F:C4	0.77	2.08	8	4
3:B:208:PCW:H11	3:C:211:PCW:C34	0.77	2.07	9	1
3:A:406:PCW:H40	3:B:205:PCW:H152	0.77	1.55	20	1
3:D:605:PCW:H152	3:D:614:PCW:O2	0.77	1.80	2	15
3:D:608:PCW:C18	4:D:629:17F:H11	0.77	2.08	8	7
3:C:206:PCW:C18	3:C:208:PCW:H151	0.77	2.09	17	4
3:A:408:PCW:H162	3:A:413:PCW:H372	0.77	1.56	3	1
3:A:409:PCW:H322	3:B:206:PCW:H322	0.77	1.57	3	1
3:A:418:PCW:H483	3:D:613:PCW:H281	0.77	1.53	6	5
3:D:619:PCW:C38	3:D:627:PCW:H161	0.77	2.05	19	10
3:D:608:PCW:O1P	3:D:626:PCW:H241	0.77	1.80	13	3
3:C:208:PCW:H271	3:C:208:PCW:C23	0.77	2.09	8	1
3:D:619:PCW:H271	3:C:204:PCW:H442	0.77	1.54	10	1
3:A:417:PCW:H362	3:A:421:PCW:H371	0.77	1.54	11	3
3:D:614:PCW:H251	4:B:209:17F:H46	0.77	1.56	15	2
3:D:607:PCW:H361	3:D:626:PCW:H381	0.77	1.56	19	1
3:A:403:PCW:H182	3:A:403:PCW:H232	0.77	1.56	1	2
3:A:404:PCW:C35	3:A:404:PCW:H51	0.77	2.10	11	2
3:D:612:PCW:H20	3:D:612:PCW:H432	0.77	1.56	4	7
3:A:408:PCW:H352	3:A:413:PCW:H162	0.77	1.56	11	11
3:D:621:PCW:H141	4:D:632:17F:C17	0.77	2.08	17	7
3:A:419:PCW:H82	3:D:626:PCW:H331	0.77	1.57	5	6
3:A:408:PCW:C26	3:A:411:PCW:H252	0.77	2.07	4	1
3:A:414:PCW:H162	4:A:415:17F:C1Z	0.77	2.09	4	4
2:C:12:ASP:HA	5:C:201:GSP:S1G	0.77	2.20	4	1
3:B:203:PCW:C21	4:B:209:17F:H18	0.77	2.08	8	2
3:D:602:PCW:H462	4:D:628:17F:H64	0.77	1.56	19	2
3:A:411:PCW:O1P	3:C:204:PCW:H73	0.77	1.78	17	2
3:D:611:PCW:H462	3:B:208:PCW:H262	0.77	1.55	17	1
3:C:207:PCW:C44	4:C:213:17F:H33	0.77	2.09	20	1
3:A:404:PCW:C39	3:B:205:PCW:H421	0.77	2.08	1	1
3:D:605:PCW:O2P	3:D:624:PCW:H82	0.77	1.79	3	10
3:C:206:PCW:H262	3:C:208:PCW:H381	0.77	1.57	4	2
3:D:617:PCW:H461	3:D:627:PCW:H262	0.77	1.53	5	3
3:B:206:PCW:H241	3:B:206:PCW:C28	0.77	2.05	8	1
3:B:205:PCW:H42	3:C:204:PCW:C6	0.77	2.09	20	1
3:A:410:PCW:H241	4:A:422:17F:H74	0.77	1.55	1	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
3:D:603:PCW:H412	3:D:603:PCW:C37	0.77	2.03	12	18
3:D:605:PCW:H332	3:D:624:PCW:C7	0.77	2.10	6	9
3:D:616:PCW:C28	4:D:632:17F:H46	0.77	2.08	1	5
3:B:203:PCW:H42	3:C:211:PCW:H331	0.77	1.55	15	5
3:C:203:PCW:C45	3:C:204:PCW:H232	0.77	2.10	11	5
3:D:602:PCW:H461	3:D:608:PCW:C48	0.77	2.09	5	1
3:A:408:PCW:H12	3:A:411:PCW:C14	0.77	2.08	6	1
3:A:406:PCW:H351	4:B:211:17F:H8	0.77	1.55	14	4
3:B:203:PCW:H381	3:C:211:PCW:H442	0.77	1.55	7	1
3:A:401:PCW:H422	3:B:207:PCW:H472	0.77	1.55	8	1
3:B:203:PCW:H211	4:B:209:17F:C18	0.77	2.08	8	1
3:A:407:PCW:H461	3:A:410:PCW:H262	0.77	1.57	12	1
3:A:420:PCW:C1	3:D:618:PCW:H411	0.77	2.07	19	17
4:A:422:17F:O8	3:D:622:PCW:H141	0.77	1.78	17	5
3:D:605:PCW:O31	3:D:605:PCW:P	0.77	2.43	18	20
4:C:219:17F:H12A	4:C:219:17F:C32	0.77	2.09	18	16
3:D:617:PCW:H451	3:C:204:PCW:C47	0.77	2.07	9	5
5:C:201:GSP:S1G	5:C:201:GSP:O2A	0.77	2.43	9	7
3:D:603:PCW:H442	3:D:611:PCW:H371	0.77	1.56	11	11
3:C:205:PCW:O11	3:C:209:PCW:H152	0.77	1.80	11	4
3:A:401:PCW:H472	3:D:612:PCW:C25	0.77	2.10	6	2
3:D:601:PCW:H422	4:D:628:17F:H52	0.77	1.57	6	1
3:D:609:PCW:H422	3:D:616:PCW:H452	0.77	1.55	8	2
3:D:627:PCW:H262	3:C:210:PCW:H271	0.77	1.57	6	1
3:A:404:PCW:C17	3:A:404:PCW:H442	0.77	2.10	8	1
3:A:408:PCW:C24	3:C:210:PCW:H242	0.77	2.10	10	3
4:B:211:17F:H62	4:B:211:17F:C31	0.77	2.06	13	1
3:D:612:PCW:H61	3:D:625:PCW:H141	0.77	1.55	14	1
3:A:407:PCW:C17	3:A:407:PCW:C21	0.77	2.53	1	14
3:A:417:PCW:C19	3:A:420:PCW:H431	0.77	2.09	9	6
3:D:619:PCW:C15	3:D:627:PCW:H142	0.77	2.09	16	9
3:D:623:PCW:C23	3:B:203:PCW:H481	0.77	2.10	4	6
3:B:204:PCW:H431	4:B:210:17F:H9A	0.77	1.55	20	3
3:A:411:PCW:C28	3:C:210:PCW:H222	0.77	2.08	8	1
3:C:212:PCW:H61	4:C:213:17F:C3	0.77	2.10	18	1
3:A:418:PCW:H361	3:D:613:PCW:C13	0.76	2.10	19	3
3:D:617:PCW:H31	3:D:617:PCW:O2P	0.76	1.78	1	5
3:D:619:PCW:H381	3:D:627:PCW:H181	0.76	1.57	12	9
3:D:622:PCW:H222	4:D:631:17F:H31	0.76	1.57	12	8
3:B:205:PCW:O1P	3:B:205:PCW:C3	0.76	2.34	15	5
3:B:207:PCW:C23	3:B:207:PCW:H381	0.76	2.10	1	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
3:D:627:PCW:C28	4:D:631:17F:H51	0.76	2.10	20	14
3:B:203:PCW:C32	4:B:210:17F:H29	0.76	2.11	2	1
3:D:603:PCW:H371	3:D:611:PCW:H342	0.76	1.57	4	2
3:D:606:PCW:H51	3:D:606:PCW:O11	0.76	1.79	6	4
3:B:208:PCW:H421	3:C:216:PCW:C27	0.76	2.10	9	3
3:B:206:PCW:C23	3:C:205:PCW:H19	0.76	2.10	15	1
3:C:209:PCW:H431	3:C:209:PCW:C47	0.76	2.08	15	1
3:D:616:PCW:H451	4:C:214:17F:C30	0.76	2.10	13	4
3:D:619:PCW:H362	4:D:631:17F:C22	0.76	2.10	20	11
4:C:218:17F:O7	4:C:218:17F:C18	0.76	2.33	5	17
3:D:617:PCW:H482	3:C:210:PCW:C28	0.76	2.10	2	6
3:B:207:PCW:H62	3:B:207:PCW:H121	0.76	1.55	2	1
3:D:610:PCW:H20	3:D:610:PCW:H241	0.76	1.55	3	1
3:B:204:PCW:H40	4:B:210:17F:H10A	0.76	1.56	11	5
3:A:401:PCW:H411	3:B:204:PCW:C26	0.76	2.09	12	3
3:D:603:PCW:H271	3:D:611:PCW:H182	0.76	1.57	1	8
3:D:609:PCW:H251	4:D:628:17F:H70	0.76	1.57	20	13
3:D:617:PCW:C43	3:D:627:PCW:H232	0.76	2.08	4	4
3:B:205:PCW:H352	3:B:208:PCW:C7	0.76	2.09	5	1
3:A:420:PCW:C3	3:D:618:PCW:H421	0.76	2.06	20	2
3:A:406:PCW:H411	3:C:204:PCW:H341	0.76	1.56	19	1
3:C:204:PCW:H40	3:C:216:PCW:H242	0.76	1.54	19	1
3:A:421:PCW:C16	4:D:630:17F:H57	0.76	2.08	15	12
3:D:608:PCW:H212	4:D:629:17F:C1X	0.76	2.11	9	11
4:D:632:17F:O10	4:D:632:17F:H6	0.76	1.79	11	20
3:A:402:PCW:C44	3:C:208:PCW:H152	0.76	2.11	13	4
3:D:615:PCW:O1P	3:D:625:PCW:H62	0.76	1.80	17	4
3:A:404:PCW:H132	3:B:205:PCW:H452	0.76	1.57	16	4
3:B:204:PCW:H171	3:B:204:PCW:H212	0.76	1.56	4	11
3:A:404:PCW:C39	3:A:404:PCW:H141	0.76	2.11	17	4
3:C:207:PCW:H142	4:C:213:17F:H56	0.76	1.56	14	3
3:D:607:PCW:H31	3:D:626:PCW:C40	0.76	2.11	9	2
3:C:206:PCW:C1	4:C:214:17F:H12A	0.76	2.10	12	1
3:B:203:PCW:H342	4:B:210:17F:H37	0.76	1.54	19	2
2:C:32:TYR:HE1	5:C:201:GSP:H5'2	0.76	1.40	18	1
3:C:206:PCW:H261	3:C:208:PCW:H411	0.76	1.57	18	1
3:A:401:PCW:H451	3:D:615:PCW:H262	0.76	1.56	1	2
3:A:418:PCW:C8	3:D:618:PCW:H40	0.76	2.11	1	3
3:D:601:PCW:H39	4:D:628:17F:H52	0.76	1.57	2	2
3:D:617:PCW:C45	3:C:204:PCW:H472	0.76	2.08	16	9
3:A:402:PCW:H352	3:A:402:PCW:C31	0.76	2.11	12	16

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
3:A:404:PCW:H141	3:B:205:PCW:C45	0.76	2.11	8	2
3:A:408:PCW:H351	3:A:413:PCW:C15	0.76	2.10	6	12
3:C:211:PCW:C3	4:C:215:17F:H31	0.76	2.10	2	1
3:B:208:PCW:H471	3:C:203:PCW:H152	0.76	1.57	5	1
3:B:208:PCW:O2P	3:C:211:PCW:H362	0.76	1.80	14	1
3:C:203:PCW:H432	3:C:210:PCW:H19	0.76	1.56	17	1
3:A:401:PCW:H272	3:D:615:PCW:C28	0.76	2.11	1	1
4:D:631:17F:H11A	3:C:217:PCW:C7	0.76	2.10	5	9
3:B:204:PCW:H39	4:B:210:17F:H10A	0.76	1.57	2	1
3:D:618:PCW:H12	3:D:618:PCW:O31	0.76	1.80	9	12
3:B:203:PCW:H212	4:B:209:17F:H19	0.76	1.55	5	1
3:B:204:PCW:H73	3:B:204:PCW:O3P	0.76	1.80	17	4
3:D:602:PCW:H351	4:C:214:17F:H73	0.76	1.57	11	2
4:C:213:17F:H55	4:C:215:17F:H71	0.76	1.54	11	1
3:D:612:PCW:H62	3:D:623:PCW:H321	0.76	1.56	14	1
3:A:420:PCW:H482	3:D:617:PCW:H271	0.76	1.58	15	3
3:D:627:PCW:H241	3:C:216:PCW:H431	0.76	1.56	5	4
4:A:415:17F:H46	4:B:209:17F:H59	0.76	1.56	2	1
3:A:406:PCW:H242	3:A:411:PCW:C47	0.76	2.11	12	5
4:A:422:17F:H40	4:A:422:17F:H30	0.76	1.56	4	6
3:D:627:PCW:H211	3:C:217:PCW:H372	0.76	1.55	13	6
3:A:413:PCW:H431	3:C:210:PCW:H231	0.76	1.57	18	3
4:A:416:17F:O5	3:B:204:PCW:H51	0.76	1.79	5	4
3:D:603:PCW:H162	3:D:624:PCW:H222	0.76	1.57	4	3
3:B:205:PCW:C5	3:C:204:PCW:H62	0.76	2.10	12	3
3:B:206:PCW:P	3:B:206:PCW:H31	0.76	2.21	5	7
3:D:602:PCW:H462	4:D:628:17F:C36	0.76	2.10	19	8
3:C:203:PCW:H82	3:C:211:PCW:H11	0.76	1.55	16	1
3:A:406:PCW:H142	4:B:211:17F:H63	0.76	1.55	1	1
3:D:602:PCW:C5	4:C:214:17F:H19	0.76	2.11	5	2
3:B:205:PCW:H181	3:B:205:PCW:C22	0.76	2.05	19	2
3:A:420:PCW:H12	3:D:618:PCW:H351	0.76	1.55	7	2
3:D:605:PCW:H231	3:D:614:PCW:H382	0.76	1.55	7	3
3:A:410:PCW:H222	4:A:422:17F:H74	0.76	1.56	11	1
3:D:613:PCW:H332	3:D:627:PCW:H131	0.76	1.55	13	6
4:B:211:17F:C27	3:C:204:PCW:H422	0.76	2.10	2	2
3:A:419:PCW:H40	3:D:625:PCW:C46	0.76	2.10	3	3
3:A:410:PCW:C39	3:A:412:PCW:H371	0.76	2.09	20	7
3:D:604:PCW:H461	3:D:626:PCW:C28	0.76	2.08	18	5
4:B:211:17F:H49	3:C:203:PCW:H242	0.76	1.57	7	1
3:D:617:PCW:O2P	3:C:216:PCW:H42	0.76	1.81	8	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
3:C:206:PCW:H62	4:C:213:17F:O6	0.76	1.80	8	1
3:B:205:PCW:O11	3:C:204:PCW:H62	0.76	1.81	20	2
3:D:624:PCW:H472	4:B:209:17F:H54	0.76	1.53	15	1
3:A:402:PCW:O31	3:A:402:PCW:C35	0.76	2.34	4	6
3:D:611:PCW:H462	3:B:208:PCW:C15	0.76	2.11	1	1
3:D:614:PCW:H31	3:D:620:PCW:H2	0.76	1.58	19	10
3:D:603:PCW:H73	3:C:216:PCW:H31	0.76	1.58	13	9
3:C:205:PCW:C18	3:C:209:PCW:H221	0.76	2.10	6	4
3:D:604:PCW:C23	4:C:215:17F:H53	0.76	2.09	8	1
3:D:612:PCW:H131	3:D:620:PCW:H171	0.76	1.57	10	1
3:D:605:PCW:H382	3:D:612:PCW:O2	0.75	1.81	15	16
3:A:421:PCW:H63	3:A:421:PCW:O11	0.75	1.81	3	2
3:B:207:PCW:C4	3:B:207:PCW:H31	0.75	2.11	2	2
3:C:203:PCW:C34	3:C:204:PCW:H122	0.75	2.11	2	4
3:B:208:PCW:H161	3:C:203:PCW:C26	0.75	2.10	4	3
3:B:206:PCW:C41	3:C:209:PCW:H39	0.75	2.10	9	5
4:A:422:17F:H6	3:D:622:PCW:C13	0.75	2.10	11	2
3:C:212:PCW:H432	3:C:212:PCW:H212	0.75	1.56	8	2
3:D:616:PCW:H63	4:D:632:17F:H2	0.75	1.56	17	2
3:D:623:PCW:H281	3:D:624:PCW:H431	0.75	1.57	10	1
3:D:624:PCW:H242	3:C:217:PCW:H231	0.75	1.58	10	2
3:D:614:PCW:H431	3:D:620:PCW:H39	0.75	1.58	17	3
3:A:417:PCW:O11	3:D:618:PCW:H341	0.75	1.81	18	1
3:A:412:PCW:H411	3:C:210:PCW:H362	0.75	1.56	2	2
4:A:422:17F:H67	3:D:622:PCW:H451	0.75	1.57	2	5
3:D:618:PCW:H62	3:D:618:PCW:O31	0.75	1.81	14	4
3:B:207:PCW:H221	3:B:207:PCW:H361	0.75	1.58	6	6
3:A:408:PCW:H32	3:A:411:PCW:C15	0.75	2.11	9	4
3:B:208:PCW:O1P	3:C:211:PCW:H82	0.75	1.81	4	2
3:D:602:PCW:H461	3:D:608:PCW:H482	0.75	1.56	5	1
5:C:201:GSP:O1B	5:C:201:GSP:S1G	0.75	2.45	15	5
3:C:211:PCW:H241	4:C:215:17F:H73	0.75	1.57	9	4
4:A:422:17F:C1X	4:C:218:17F:H71	0.75	2.05	18	1
3:B:208:PCW:H362	3:C:203:PCW:C15	0.75	2.07	20	1
3:D:623:PCW:H421	3:D:625:PCW:C26	0.75	2.11	4	11
3:D:625:PCW:H151	3:D:625:PCW:C19	0.75	2.10	1	20
3:C:206:PCW:C24	3:C:208:PCW:H411	0.75	2.09	16	9
3:A:403:PCW:O3P	3:A:406:PCW:H61	0.75	1.81	3	2
3:C:205:PCW:C14	3:C:209:PCW:H342	0.75	2.11	3	2
3:A:406:PCW:H242	3:A:411:PCW:H482	0.75	1.57	11	3
3:D:617:PCW:H441	3:D:627:PCW:C23	0.75	2.11	20	2

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
3:C:205:PCW:O3P	4:C:214:17F:H8A	0.75	1.81	9	1
3:B:206:PCW:H20	3:C:209:PCW:H321	0.75	1.57	12	1
3:A:404:PCW:O2P	3:A:406:PCW:H62	0.75	1.81	15	1
3:B:208:PCW:H121	3:B:208:PCW:C7	0.75	2.12	15	1
3:C:207:PCW:H211	4:C:213:17F:H57	0.75	1.57	20	1
3:D:608:PCW:H212	4:D:629:17F:H29	0.75	1.55	11	10
3:A:410:PCW:H131	3:C:207:PCW:H171	0.75	1.58	2	1
4:C:214:17F:H36	4:C:214:17F:H42	0.75	1.57	9	3
3:D:614:PCW:H212	4:B:209:17F:H51	0.75	1.57	6	5
3:B:206:PCW:C25	3:C:205:PCW:H171	0.75	2.11	10	6
3:A:417:PCW:H472	3:D:618:PCW:H251	0.75	1.57	10	2
3:B:208:PCW:C42	3:C:204:PCW:H171	0.75	2.11	8	1
3:A:411:PCW:H262	3:B:205:PCW:C25	0.75	2.11	12	1
3:C:203:PCW:C28	3:C:211:PCW:H451	0.75	2.12	13	3
3:D:617:PCW:H481	3:B:205:PCW:C22	0.75	2.10	14	1
3:D:622:PCW:P	3:D:622:PCW:H32	0.75	2.22	16	1
3:C:205:PCW:C42	3:C:212:PCW:H261	0.75	2.11	18	1
2:C:59:ALA:HA	5:C:201:GSP:S1G	0.75	2.22	19	1
3:A:406:PCW:H32	4:B:211:17F:H75	0.75	1.57	1	1
3:D:601:PCW:H382	4:D:628:17F:H52	0.75	1.58	13	2
3:B:206:PCW:H441	3:C:209:PCW:C40	0.75	2.11	3	2
3:D:612:PCW:O2P	3:D:620:PCW:H63	0.75	1.81	2	8
3:D:622:PCW:C20	3:C:217:PCW:H82	0.75	2.11	16	6
3:A:420:PCW:H20	3:A:420:PCW:C24	0.75	2.11	5	1
3:B:204:PCW:H421	3:B:207:PCW:H232	0.75	1.58	5	1
3:C:216:PCW:C16	3:C:217:PCW:H162	0.75	2.12	18	6
3:B:208:PCW:H421	3:C:216:PCW:H271	0.75	1.55	13	2
1:A:250:VAL:O	1:A:254:VAL:HB	0.75	1.81	7	19
3:A:413:PCW:C42	3:C:210:PCW:H462	0.75	2.11	15	4
3:D:611:PCW:H462	3:B:208:PCW:H151	0.75	1.57	1	1
3:A:418:PCW:H471	3:D:613:PCW:C27	0.75	2.11	2	3
3:A:421:PCW:C32	3:D:618:PCW:H52	0.75	2.11	4	3
3:A:410:PCW:H281	4:D:631:17F:H78	0.75	1.54	4	1
3:A:409:PCW:H12	4:B:210:17F:O1	0.75	1.82	13	1
3:A:402:PCW:H381	3:C:208:PCW:H31	0.75	1.59	19	1
3:A:410:PCW:C22	4:A:422:17F:H76	0.75	2.12	20	1
3:D:606:PCW:H321	3:D:608:PCW:C8	0.75	2.11	1	2
4:D:628:17F:C32	4:D:629:17F:H51	0.75	2.12	6	6
3:C:207:PCW:H421	4:C:213:17F:C1Y	0.75	2.11	2	1
3:C:205:PCW:H32	3:C:209:PCW:C15	0.75	2.11	18	4
3:A:418:PCW:C33	3:D:613:PCW:H152	0.75	2.12	12	2

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
3:A:414:PCW:H262	4:A:415:17F:H61	0.75	1.58	17	2
3:D:624:PCW:H442	4:B:209:17F:H76	0.75	1.59	14	1
3:D:608:PCW:H151	3:D:608:PCW:C19	0.75	2.11	18	1
3:A:404:PCW:H132	3:B:205:PCW:H471	0.75	1.59	19	1
3:A:408:PCW:C12	3:A:413:PCW:H352	0.75	2.12	2	6
3:A:401:PCW:C44	3:D:615:PCW:H262	0.75	2.09	15	7
3:A:420:PCW:H11	3:D:618:PCW:C38	0.75	2.11	3	1
3:D:602:PCW:H461	3:D:608:PCW:H472	0.75	1.59	3	6
3:B:208:PCW:H31	3:C:211:PCW:C43	0.75	2.12	16	5
3:D:619:PCW:C35	3:D:627:PCW:H342	0.75	2.11	12	3
2:C:32:TYR:HD1	5:C:201:GSP:H5'2	0.75	1.42	20	6
3:C:211:PCW:H262	4:C:215:17F:H50	0.75	1.57	8	1
3:C:212:PCW:H39	4:C:213:17F:H50	0.75	1.59	13	1
3:B:206:PCW:C4	3:B:206:PCW:H31	0.75	2.12	17	1
3:A:404:PCW:H62	3:A:404:PCW:C35	0.75	2.08	11	2
3:A:401:PCW:H342	3:B:207:PCW:H39	0.75	1.59	6	4
3:D:604:PCW:H73	3:D:604:PCW:O11	0.75	1.80	7	3
4:B:210:17F:O6	4:B:210:17F:H18A	0.74	1.81	13	9
3:C:217:PCW:C12	4:C:219:17F:H33	0.74	2.10	19	5
3:A:406:PCW:H39	3:B:205:PCW:C15	0.74	2.08	8	6
3:B:203:PCW:H361	3:C:211:PCW:C40	0.74	2.08	5	1
3:D:621:PCW:H283	4:D:632:17F:C21	0.74	2.12	6	6
3:C:207:PCW:H441	4:C:213:17F:H32	0.74	1.59	15	3
3:D:622:PCW:H372	3:D:622:PCW:H411	0.74	1.57	15	1
4:A:422:17F:H55	3:D:606:PCW:H411	0.74	1.56	20	2
1:A:363:LYS:HA	1:A:367:ALA:HB3	0.74	1.60	19	20
3:A:403:PCW:O1P	3:A:403:PCW:C3	0.74	2.35	1	2
3:D:618:PCW:C1	3:D:618:PCW:H51	0.74	2.13	9	7
3:D:604:PCW:H452	3:D:606:PCW:H181	0.74	1.59	3	5
3:D:617:PCW:H431	3:C:204:PCW:C47	0.74	2.11	8	3
3:A:419:PCW:C44	4:B:210:17F:H76	0.74	2.12	20	2
3:C:205:PCW:H32	3:C:209:PCW:C13	0.74	2.12	12	3
3:A:420:PCW:H362	3:D:618:PCW:C41	0.74	2.09	20	1
3:A:420:PCW:H351	3:D:618:PCW:H431	0.74	1.58	5	3
3:A:403:PCW:H41	3:A:403:PCW:C3	0.74	2.12	5	9
3:C:207:PCW:H412	4:C:213:17F:H11A	0.74	1.59	18	3
3:A:406:PCW:H351	4:B:211:17F:H6	0.74	1.56	5	1
3:C:206:PCW:H372	3:C:208:PCW:C14	0.74	2.11	8	2
3:C:216:PCW:H241	3:C:216:PCW:C28	0.74	2.07	7	1
3:C:206:PCW:C5	4:C:214:17F:H37	0.74	2.10	8	1
3:A:408:PCW:O1P	3:A:411:PCW:H141	0.74	1.81	9	2

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
3:A:407:PCW:C5	3:A:410:PCW:H351	0.74	2.09	12	1
3:A:411:PCW:C26	3:B:205:PCW:H252	0.74	2.08	20	3
3:A:412:PCW:H483	3:C:204:PCW:C27	0.74	2.13	18	1
3:B:208:PCW:C40	3:C:216:PCW:H271	0.74	2.12	19	1
3:B:203:PCW:H332	4:B:210:17F:C2X	0.74	2.12	20	1
3:A:414:PCW:H141	4:A:415:17F:C32	0.74	2.12	2	5
3:A:418:PCW:H351	3:D:613:PCW:C13	0.74	2.12	11	6
3:D:613:PCW:H332	3:D:627:PCW:H132	0.74	1.56	5	6
3:B:208:PCW:H451	4:C:219:17F:H46	0.74	1.57	10	2
3:A:414:PCW:H162	4:A:415:17F:C20	0.74	2.11	11	1
3:D:616:PCW:H222	3:C:208:PCW:H272	0.74	1.57	12	1
3:A:411:PCW:H62	4:B:211:17F:O5	0.74	1.83	14	1
3:A:409:PCW:O1P	3:B:206:PCW:H62	0.74	1.82	15	1
4:D:632:17F:H5	4:D:632:17F:O8	0.74	1.81	17	17
3:C:204:PCW:H481	3:C:216:PCW:H40	0.74	1.57	5	2
4:A:422:17F:H54	3:D:606:PCW:C17	0.74	2.13	2	1
3:D:614:PCW:H261	4:B:209:17F:H69	0.74	1.56	3	2
3:C:203:PCW:H39	4:C:213:17F:H63	0.74	1.59	10	2
3:C:208:PCW:O31	3:C:208:PCW:H73	0.74	1.83	12	1
3:D:622:PCW:H32	3:D:622:PCW:O1P	0.74	1.82	16	1
3:A:419:PCW:H381	3:D:625:PCW:H251	0.74	1.56	6	14
3:A:417:PCW:H472	3:D:618:PCW:C25	0.74	2.12	8	5
3:D:606:PCW:C34	3:D:606:PCW:H132	0.74	2.12	3	8
3:A:403:PCW:C47	3:A:404:PCW:H283	0.74	2.12	12	3
3:D:625:PCW:H51	3:D:625:PCW:O11	0.74	1.81	5	2
3:C:205:PCW:C6	4:C:214:17F:H9	0.74	2.12	9	2
3:A:406:PCW:H332	4:B:211:17F:H4	0.74	1.58	11	1
3:A:406:PCW:H451	3:B:205:PCW:H262	0.74	1.60	11	1
3:A:417:PCW:H282	3:A:420:PCW:H251	0.74	1.59	13	2
3:C:207:PCW:C39	4:C:213:17F:H66	0.74	2.13	16	1
3:C:206:PCW:H19	3:C:207:PCW:H221	0.74	1.59	17	2
3:D:608:PCW:H19	4:D:629:17F:C26	0.74	2.06	15	10
3:D:610:PCW:H132	3:D:610:PCW:H342	0.74	1.59	4	7
3:D:614:PCW:C48	3:D:620:PCW:H411	0.74	2.12	1	2
3:D:617:PCW:H221	3:D:617:PCW:H172	0.74	1.58	2	10
3:B:203:PCW:C38	3:C:211:PCW:H182	0.74	2.12	3	1
3:A:403:PCW:H481	3:A:404:PCW:H281	0.74	1.58	8	1
3:C:207:PCW:C16	4:C:213:17F:H60	0.74	2.04	20	2
3:D:602:PCW:H272	4:D:629:17F:H76	0.74	1.59	11	2
3:C:203:PCW:C1	3:C:211:PCW:H73	0.74	2.12	13	2
3:A:408:PCW:O1P	3:A:408:PCW:H51	0.74	1.80	19	13

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
3:A:421:PCW:C6	4:D:630:17F:H4	0.74	2.11	20	6
4:A:422:17F:H19A	4:A:422:17F:H9	0.74	1.58	7	16
3:D:621:PCW:H132	4:D:632:17F:H18	0.74	1.60	13	3
3:C:203:PCW:O31	3:C:203:PCW:H11	0.74	1.82	17	17
3:D:606:PCW:C15	4:C:218:17F:H8	0.74	2.12	2	4
3:B:208:PCW:H161	3:C:203:PCW:H271	0.74	1.58	7	3
3:C:216:PCW:H152	3:C:217:PCW:C16	0.74	2.11	8	5
3:A:420:PCW:O1P	3:D:618:PCW:H372	0.74	1.82	13	11
3:C:206:PCW:C17	3:C:207:PCW:H222	0.74	2.13	13	3
3:C:205:PCW:H63	4:C:214:17F:H2	0.74	1.60	5	2
3:D:627:PCW:H281	4:D:631:17F:H51	0.74	1.59	14	4
3:A:401:PCW:H221	3:A:401:PCW:H182	0.74	1.56	20	5
3:A:418:PCW:C34	3:D:613:PCW:H132	0.74	2.09	13	5
3:B:208:PCW:O11	3:B:208:PCW:H82	0.74	1.82	8	3
3:C:205:PCW:H41	4:C:214:17F:H6A	0.74	1.60	8	1
3:B:206:PCW:H283	4:C:214:17F:H34	0.74	1.59	20	1
3:D:606:PCW:H132	3:D:606:PCW:C34	0.74	2.12	5	10
3:D:617:PCW:C40	3:D:619:PCW:H162	0.74	2.12	11	7
3:B:207:PCW:C38	3:B:207:PCW:H231	0.74	2.13	1	1
3:C:203:PCW:H171	3:C:203:PCW:C13	0.74	2.10	1	12
3:C:203:PCW:H132	3:C:203:PCW:C17	0.74	2.12	19	17
3:A:418:PCW:H411	3:A:418:PCW:C37	0.74	2.03	4	7
4:A:422:17F:H54	3:D:606:PCW:H172	0.74	1.57	2	1
3:B:203:PCW:H161	4:B:209:17F:H20A	0.74	1.59	5	3
3:D:613:PCW:H322	3:D:619:PCW:H132	0.74	1.59	7	6
3:B:205:PCW:H31	4:B:211:17F:O1	0.74	1.82	14	6
3:B:204:PCW:H12	3:B:207:PCW:C32	0.74	2.12	11	1
3:C:206:PCW:H141	3:C:208:PCW:C32	0.74	2.10	20	2
3:A:401:PCW:H442	3:D:615:PCW:C26	0.74	2.10	15	2
3:D:611:PCW:C48	3:B:208:PCW:H242	0.74	2.11	17	1
3:A:405:PCW:H283	3:A:418:PCW:H221	0.74	1.59	18	1
3:A:406:PCW:C40	3:B:205:PCW:H242	0.74	2.11	1	1
3:D:616:PCW:H82	4:D:632:17F:O4	0.74	1.83	15	11
3:B:206:PCW:H31	3:B:206:PCW:O4P	0.74	1.83	5	9
4:C:213:17F:H4	4:C:213:17F:O10	0.74	1.83	20	5
3:A:403:PCW:H322	3:A:404:PCW:C1	0.74	2.13	12	4
4:A:416:17F:H74	4:B:209:17F:H68	0.74	1.60	4	3
4:A:416:17F:C38	3:B:204:PCW:H272	0.74	2.13	5	2
3:B:208:PCW:H40	3:C:216:PCW:C26	0.74	2.13	6	1
3:B:207:PCW:H61	4:B:210:17F:H8	0.74	1.58	10	1
3:D:618:PCW:O31	3:D:618:PCW:H73	0.74	1.82	12	2

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
3:D:621:PCW:P	3:D:622:PCW:H41	0.74	2.23	14	1
3:C:203:PCW:H51	3:C:207:PCW:O31	0.74	1.83	14	1
1:A:244:SER:HA	1:A:248:GLU:HG3	0.73	1.59	18	2
3:A:408:PCW:C17	3:A:411:PCW:H232	0.73	2.13	3	4
3:D:627:PCW:O1P	3:D:627:PCW:H52	0.73	1.83	14	3
3:A:419:PCW:H322	3:D:625:PCW:H342	0.73	1.59	16	2
3:D:602:PCW:H341	4:C:214:17F:C33	0.73	2.13	3	1
3:C:205:PCW:H42	4:C:214:17F:H2	0.73	1.58	8	1
3:C:212:PCW:H40	4:C:215:17F:H67	0.73	1.57	12	1
3:A:419:PCW:H462	3:C:212:PCW:C28	0.73	2.11	13	1
3:D:607:PCW:H361	3:D:626:PCW:H422	0.73	1.59	13	2
4:B:210:17F:H30	4:C:215:17F:H29	0.73	1.57	19	3
3:D:618:PCW:O31	3:D:618:PCW:H12	0.73	1.83	14	5
3:D:621:PCW:O1P	3:D:622:PCW:H73	0.73	1.82	20	8
3:D:612:PCW:H161	3:D:620:PCW:H171	0.73	1.59	4	4
3:D:615:PCW:H452	3:D:620:PCW:C22	0.73	2.12	17	4
3:D:627:PCW:O1P	3:D:627:PCW:H51	0.73	1.82	17	14
3:D:610:PCW:H20	3:D:610:PCW:C24	0.73	2.13	3	2
3:A:409:PCW:H271	3:A:419:PCW:H271	0.73	1.59	11	8
3:C:207:PCW:H441	4:C:213:17F:C1Y	0.73	2.14	13	4
3:A:401:PCW:H421	3:D:612:PCW:H271	0.73	1.58	17	3
3:A:406:PCW:C20	4:B:211:17F:H31	0.73	2.14	1	5
3:B:207:PCW:H381	3:B:207:PCW:H231	0.73	1.59	1	1
1:A:231:ASN:HA	1:A:234:LYS:HD2	0.73	1.57	14	9
3:B:207:PCW:H31	3:B:207:PCW:O4P	0.73	1.83	2	3
3:C:217:PCW:H172	4:C:219:17F:H32	0.73	1.59	17	4
3:A:419:PCW:H82	3:D:626:PCW:O31	0.73	1.84	9	3
3:B:205:PCW:H182	3:C:203:PCW:H481	0.73	1.60	3	5
4:A:422:17F:H4A	3:D:622:PCW:C15	0.73	2.13	19	4
3:C:203:PCW:H40	4:C:213:17F:H66	0.73	1.60	19	4
3:C:216:PCW:C17	3:C:217:PCW:H162	0.73	2.13	18	7
3:C:208:PCW:H42	3:C:208:PCW:O31	0.73	1.83	12	1
3:D:606:PCW:C7	3:D:626:PCW:H19	0.73	2.12	17	4
3:C:206:PCW:H242	3:C:208:PCW:H381	0.73	1.59	3	3
3:D:614:PCW:H431	3:D:620:PCW:C39	0.73	2.13	12	5
3:D:614:PCW:H282	4:B:209:17F:H12	0.73	1.60	7	1
3:C:203:PCW:H441	3:C:217:PCW:C48	0.73	2.13	20	3
3:A:409:PCW:H272	3:A:419:PCW:H271	0.73	1.59	4	2
3:B:206:PCW:H31	3:B:206:PCW:O1P	0.73	1.84	17	14
3:C:206:PCW:H151	3:C:208:PCW:H171	0.73	1.59	1	4
3:A:403:PCW:H242	3:D:618:PCW:H282	0.73	1.59	7	5

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
3:D:605:PCW:H431	3:D:624:PCW:H421	0.73	1.61	12	5
1:A:214:PHE:HZ	3:A:405:PCW:H162	0.73	1.42	15	2
1:A:217:LEU:HD13	3:A:405:PCW:H222	0.73	1.58	13	1
3:A:411:PCW:H73	4:B:211:17F:O5	0.73	1.83	17	1
3:A:404:PCW:O31	3:A:404:PCW:C35	0.73	2.37	10	17
3:A:419:PCW:H431	3:D:625:PCW:H462	0.73	1.60	3	15
3:D:603:PCW:H331	3:D:624:PCW:H121	0.73	1.60	3	3
3:A:418:PCW:H442	3:D:613:PCW:H242	0.73	1.58	4	5
4:C:213:17F:H71	4:C:213:17F:H33	0.73	1.58	3	1
3:C:203:PCW:H51	4:C:213:17F:H6A	0.73	1.60	9	1
3:D:615:PCW:C43	3:D:620:PCW:H222	0.73	2.13	10	1
3:A:421:PCW:H122	4:D:630:17F:C10	0.73	2.12	11	2
3:A:406:PCW:H39	3:B:205:PCW:C12	0.73	2.12	17	2
3:D:612:PCW:C22	3:D:620:PCW:H461	0.73	2.14	20	2
3:D:618:PCW:H51	3:D:618:PCW:O31	0.73	1.83	19	1
3:C:212:PCW:H2	4:C:215:17F:O10	0.73	1.82	20	1
3:D:610:PCW:H12	4:D:631:17F:H4	0.73	1.59	4	4
3:A:408:PCW:C23	3:A:411:PCW:H222	0.73	2.12	20	4
3:A:413:PCW:H382	3:C:210:PCW:H161	0.73	1.61	15	8
4:A:422:17F:H35	4:C:218:17F:H77	0.73	1.59	4	1
3:D:605:PCW:H482	3:D:620:PCW:H441	0.73	1.61	16	2
3:C:207:PCW:C16	4:C:213:17F:H56	0.73	2.13	4	5
3:A:408:PCW:H51	3:A:408:PCW:O2P	0.73	1.83	20	5
3:D:604:PCW:H281	3:D:607:PCW:H462	0.73	1.59	5	1
3:D:621:PCW:H451	3:C:208:PCW:H481	0.73	1.58	8	2
3:D:604:PCW:H231	4:C:215:17F:C30	0.73	2.11	8	1
3:C:211:PCW:H132	4:C:215:17F:C31	0.73	2.14	13	2
3:B:203:PCW:C39	3:C:211:PCW:H441	0.73	2.13	12	1
3:A:411:PCW:H51	4:B:211:17F:C3	0.73	2.14	16	2
3:C:207:PCW:H121	4:C:213:17F:H18	0.73	1.61	19	2
3:B:205:PCW:H481	3:B:208:PCW:H232	0.73	1.60	18	1
3:D:603:PCW:H181	3:D:603:PCW:H441	0.73	1.58	19	1
3:A:403:PCW:H19	3:A:404:PCW:C14	0.73	2.03	20	1
4:A:416:17F:H54	3:D:605:PCW:H281	0.73	1.59	20	1
3:A:402:PCW:C38	3:C:208:PCW:H361	0.73	2.14	1	1
3:A:418:PCW:H422	3:D:613:PCW:C21	0.73	2.11	1	1
3:C:211:PCW:H151	4:C:215:17F:H61	0.73	1.60	2	2
3:D:622:PCW:H362	4:D:631:17F:C33	0.73	2.14	15	8
3:B:206:PCW:H142	3:C:209:PCW:H371	0.73	1.60	3	1
3:D:605:PCW:H451	3:D:624:PCW:C44	0.73	2.13	17	6
3:A:408:PCW:O1P	3:A:408:PCW:H31	0.73	1.82	5	7

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
3:D:602:PCW:H52	4:C:214:17F:H19	0.73	1.59	5	1
3:A:406:PCW:H371	4:B:211:17F:H10A	0.73	1.59	6	3
3:A:414:PCW:H232	4:A:415:17F:C1Z	0.73	2.13	14	1
3:A:412:PCW:H482	3:C:217:PCW:C47	0.73	2.13	18	1
3:D:615:PCW:H82	3:D:625:PCW:O1P	0.73	1.83	5	2
3:D:619:PCW:O1P	3:D:627:PCW:H63	0.73	1.84	18	5
3:C:210:PCW:H52	3:C:210:PCW:C32	0.73	2.13	19	7
3:C:207:PCW:H322	3:C:207:PCW:H63	0.73	1.59	3	1
4:A:422:17F:H4A	3:D:622:PCW:C14	0.73	2.12	13	6
3:B:203:PCW:H431	3:C:211:PCW:H221	0.73	1.60	4	3
3:A:414:PCW:H162	4:A:415:17F:H33	0.73	1.60	12	3
3:D:619:PCW:H131	3:D:627:PCW:C13	0.73	2.13	8	1
4:B:211:17F:C23	3:C:204:PCW:H422	0.73	2.13	11	2
3:C:204:PCW:C40	3:C:216:PCW:H251	0.73	2.13	14	3
3:A:403:PCW:H73	3:A:403:PCW:O11	0.73	1.83	16	5
3:C:207:PCW:H19	4:C:213:17F:C19	0.73	2.13	18	1
3:A:409:PCW:C37	4:B:210:17F:H65	0.73	2.13	1	1
3:A:407:PCW:C5	3:A:410:PCW:H321	0.73	2.14	2	2
3:D:602:PCW:H481	3:D:608:PCW:H232	0.73	1.60	11	4
3:D:602:PCW:H31	3:D:602:PCW:O31	0.73	1.83	5	13
3:D:607:PCW:H431	3:D:625:PCW:C47	0.73	2.08	6	5
3:B:208:PCW:H421	3:C:216:PCW:H262	0.73	1.61	15	5
3:C:203:PCW:H452	3:C:204:PCW:C23	0.73	2.13	11	5
3:C:205:PCW:H121	3:C:209:PCW:H342	0.73	1.59	13	2
3:B:206:PCW:H142	3:B:206:PCW:C40	0.73	2.14	8	1
3:C:211:PCW:H152	4:C:215:17F:C33	0.73	2.14	12	1
3:C:212:PCW:H371	4:C:215:17F:H59	0.73	1.61	12	1
3:C:205:PCW:H472	4:C:215:17F:C21	0.73	2.14	19	1
3:D:615:PCW:H41	3:D:625:PCW:O1P	0.72	1.84	16	3
3:D:616:PCW:H2	3:D:616:PCW:C4	0.72	2.14	9	10
3:D:617:PCW:H421	3:D:627:PCW:H232	0.72	1.58	14	5
3:C:211:PCW:H151	4:C:215:17F:C34	0.72	2.14	2	1
3:C:216:PCW:H172	3:C:217:PCW:C16	0.72	2.13	4	8
3:A:404:PCW:H132	3:B:205:PCW:C45	0.72	2.13	14	6
3:C:203:PCW:H41	3:C:211:PCW:O1P	0.72	1.84	10	2
3:A:408:PCW:H171	3:A:411:PCW:C22	0.72	2.14	18	7
3:B:206:PCW:H252	3:C:205:PCW:H19	0.72	1.59	8	2
3:B:205:PCW:H42	3:C:204:PCW:H62	0.72	1.59	11	2
3:D:602:PCW:H73	4:C:214:17F:C19	0.72	2.13	17	1
3:A:401:PCW:H472	3:D:612:PCW:C28	0.72	2.13	18	2
3:A:419:PCW:H242	4:B:210:17F:H73	0.72	1.61	18	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
3:C:211:PCW:H262	4:C:215:17F:H51	0.72	1.58	1	2
3:A:403:PCW:H281	3:A:414:PCW:C21	0.72	2.11	2	1
3:D:622:PCW:H262	3:C:217:PCW:C8	0.72	2.14	5	7
3:C:206:PCW:H63	3:C:212:PCW:C32	0.72	2.14	7	5
3:C:216:PCW:C44	3:C:217:PCW:H341	0.72	2.14	4	8
3:A:406:PCW:H341	3:B:205:PCW:H342	0.72	1.61	9	8
4:D:629:17F:H32	4:D:629:17F:H11A	0.72	1.61	3	1
1:A:301:LEU:HB3	1:D:473:LYS:HE3	0.72	1.60	20	5
3:A:409:PCW:O31	3:B:206:PCW:H62	0.72	1.84	4	1
3:A:420:PCW:H412	3:D:611:PCW:H181	0.72	1.59	4	2
3:B:205:PCW:H12	3:B:205:PCW:O31	0.72	1.81	4	12
3:C:209:PCW:H451	3:C:212:PCW:H432	0.72	1.59	6	1
3:D:602:PCW:C48	4:D:629:17F:H43	0.72	2.14	7	2
3:C:216:PCW:H462	4:C:218:17F:C42	0.72	2.03	15	2
3:B:204:PCW:C3	3:B:207:PCW:H372	0.72	2.14	13	1
3:C:212:PCW:H371	4:C:215:17F:H33	0.72	1.60	17	1
3:D:608:PCW:H171	4:D:629:17F:H18	0.72	1.59	10	2
3:C:209:PCW:H452	3:C:212:PCW:H212	0.72	1.61	1	1
3:D:607:PCW:H261	3:B:206:PCW:H481	0.72	1.60	5	2
3:A:406:PCW:H432	4:B:211:17F:C12	0.72	2.14	16	5
3:B:206:PCW:H272	3:C:205:PCW:C19	0.72	2.14	10	2
3:C:206:PCW:H12	4:C:214:17F:H29	0.72	1.60	20	2
3:A:404:PCW:H152	3:B:205:PCW:C47	0.72	2.13	16	2
3:A:413:PCW:H63	3:C:210:PCW:O2P	0.72	1.84	11	3
3:A:404:PCW:C43	3:A:414:PCW:H251	0.72	2.15	3	4
3:B:204:PCW:C31	3:B:204:PCW:H52	0.72	2.15	10	4
3:B:208:PCW:H161	3:C:203:PCW:C28	0.72	2.14	10	2
3:A:403:PCW:H341	3:A:404:PCW:H31	0.72	1.59	11	1
3:B:204:PCW:H412	3:B:207:PCW:H432	0.72	1.59	19	1
3:C:205:PCW:H122	3:C:212:PCW:H19	0.72	1.61	19	1
3:D:604:PCW:H31	3:D:604:PCW:P	0.72	2.24	11	13
3:D:616:PCW:H272	4:D:632:17F:C24	0.72	2.13	5	4
3:D:616:PCW:H483	3:C:207:PCW:H252	0.72	1.61	11	6
3:B:208:PCW:O3	3:C:211:PCW:H472	0.72	1.84	1	1
3:B:207:PCW:H31	3:B:207:PCW:P	0.72	2.23	3	9
3:C:209:PCW:H141	4:C:214:17F:H8A	0.72	1.61	2	1
3:C:209:PCW:H441	3:C:212:PCW:H271	0.72	1.61	11	2
3:A:403:PCW:H73	3:A:404:PCW:P	0.72	2.24	3	1
3:A:406:PCW:C24	3:A:411:PCW:H472	0.72	2.12	4	3
3:A:404:PCW:C15	3:B:205:PCW:H451	0.72	2.13	18	3
3:A:406:PCW:C39	3:B:205:PCW:H121	0.72	2.13	20	4

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
3:D:622:PCW:H222	4:D:631:17F:C19	0.72	2.11	6	2
3:D:606:PCW:H321	3:D:608:PCW:H73	0.72	1.60	9	2
3:D:616:PCW:H472	3:C:208:PCW:C22	0.72	2.01	17	4
3:C:203:PCW:H471	3:C:210:PCW:C20	0.72	2.14	20	3
3:A:409:PCW:O2P	3:B:206:PCW:H62	0.72	1.84	11	1
3:A:410:PCW:H221	3:D:622:PCW:C40	0.72	2.14	14	1
3:D:614:PCW:C47	3:D:620:PCW:H431	0.72	2.13	18	2
3:D:622:PCW:H371	4:D:631:17F:H63	0.72	1.62	14	2
3:C:212:PCW:H73	4:C:213:17F:C3	0.72	2.13	14	1
4:A:416:17F:H9A	4:A:416:17F:H18A	0.72	1.60	20	1
3:A:402:PCW:H39	3:A:407:PCW:H272	0.72	1.60	3	8
3:A:421:PCW:H372	3:D:618:PCW:C15	0.72	2.15	9	4
4:A:422:17F:H54	3:D:606:PCW:H211	0.72	1.60	1	3
3:B:204:PCW:C21	3:B:204:PCW:C17	0.72	2.67	12	11
3:A:407:PCW:H321	3:A:410:PCW:H352	0.72	1.59	11	3
3:C:217:PCW:H121	4:C:219:17F:C1Y	0.72	2.15	10	3
3:A:402:PCW:H442	3:C:208:PCW:H152	0.72	1.60	15	4
3:A:403:PCW:H141	3:A:403:PCW:H381	0.72	1.59	7	1
3:A:414:PCW:H332	4:B:209:17F:O8	0.72	1.84	18	2
3:D:604:PCW:C31	3:D:604:PCW:C11	0.72	2.68	7	7
3:D:619:PCW:H361	3:D:627:PCW:C17	0.72	2.14	16	7
3:D:618:PCW:H51	3:D:618:PCW:O3P	0.72	1.84	12	13
4:D:628:17F:C22	4:D:629:17F:H75	0.72	2.14	5	7
4:D:628:17F:C2X	4:D:629:17F:H75	0.72	2.14	17	7
3:A:413:PCW:C38	3:C:210:PCW:H441	0.72	2.15	5	1
3:C:206:PCW:O11	3:C:207:PCW:H261	0.72	1.85	6	1
3:C:205:PCW:C8	4:C:214:17F:H9	0.72	2.14	12	3
4:B:210:17F:H67	3:C:212:PCW:H271	0.72	1.58	8	1
3:D:602:PCW:H481	3:D:608:PCW:H231	0.72	1.61	14	4
3:D:627:PCW:H242	3:C:217:PCW:H372	0.72	1.61	14	2
3:C:211:PCW:H161	4:C:215:17F:C35	0.72	2.14	15	1
4:D:628:17F:H40	4:D:629:17F:H75	0.72	1.61	16	5
3:C:210:PCW:H352	3:C:210:PCW:C31	0.72	2.14	7	18
3:D:612:PCW:H221	3:D:612:PCW:H432	0.72	1.62	3	2
3:D:619:PCW:H63	3:C:217:PCW:P	0.72	2.25	17	6
4:A:416:17F:H77	3:D:612:PCW:H471	0.72	1.61	16	4
3:A:404:PCW:H132	3:B:205:PCW:H451	0.72	1.61	7	3
4:D:628:17F:C21	4:D:629:17F:H74	0.72	2.14	7	1
3:B:208:PCW:O2P	3:C:211:PCW:H342	0.72	1.85	20	2
4:B:211:17F:H69	4:B:211:17F:H10A	0.72	1.60	7	1
3:C:206:PCW:H162	3:C:208:PCW:C36	0.72	2.10	18	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
3:A:403:PCW:H82	3:A:404:PCW:O1P	0.72	1.84	19	1
3:A:417:PCW:C20	3:A:420:PCW:H431	0.72	2.13	1	2
3:D:612:PCW:H39	3:D:623:PCW:C46	0.72	2.14	10	8
3:D:612:PCW:H31	3:D:620:PCW:O11	0.72	1.84	2	7
3:D:615:PCW:H51	3:D:625:PCW:O1P	0.72	1.84	2	2
3:C:206:PCW:H352	3:C:208:PCW:H141	0.72	1.61	2	3
4:B:211:17F:C28	3:C:204:PCW:H422	0.72	2.14	18	2
3:D:605:PCW:H462	4:B:209:17F:H51	0.72	1.60	5	1
3:D:614:PCW:H472	3:D:620:PCW:H231	0.72	1.59	5	4
3:A:401:PCW:H471	3:D:615:PCW:H242	0.72	1.60	6	1
3:D:612:PCW:H222	3:D:620:PCW:C44	0.72	2.13	7	2
3:A:401:PCW:C47	3:D:612:PCW:H251	0.72	2.13	15	3
3:C:206:PCW:H62	4:C:213:17F:P1	0.72	2.25	8	1
3:A:409:PCW:H321	3:B:206:PCW:H341	0.72	1.60	14	5
3:C:206:PCW:H241	3:C:208:PCW:C41	0.72	2.13	20	4
3:A:420:PCW:H451	3:D:611:PCW:C21	0.72	2.15	7	10
2:B:47:ASP:HA	2:C:128:LYS:HB2	0.72	1.62	20	2
3:B:205:PCW:H12	3:B:205:PCW:C4	0.72	2.11	2	2
3:C:203:PCW:H341	3:C:204:PCW:C12	0.72	2.13	2	6
3:D:606:PCW:H132	3:D:606:PCW:H341	0.72	1.60	7	8
3:D:605:PCW:O3P	3:D:624:PCW:H82	0.72	1.85	16	7
3:D:605:PCW:H471	3:D:614:PCW:H162	0.72	1.62	20	4
3:A:410:PCW:C25	4:A:422:17F:H74	0.72	2.15	8	3
3:A:406:PCW:H462	3:D:619:PCW:H251	0.72	1.59	10	1
3:A:403:PCW:H151	3:A:403:PCW:H382	0.72	1.60	11	1
3:A:419:PCW:H471	3:D:607:PCW:H471	0.72	1.61	15	2
3:A:401:PCW:C34	3:B:207:PCW:H39	0.72	2.15	19	1
3:D:617:PCW:H372	3:D:619:PCW:H142	0.72	1.61	19	1
3:D:602:PCW:H172	3:D:602:PCW:C22	0.71	2.15	17	5
3:D:609:PCW:H452	3:C:208:PCW:H231	0.71	1.58	3	7
3:D:619:PCW:H422	3:D:627:PCW:H231	0.71	1.61	12	5
3:D:622:PCW:H371	4:D:631:17F:C34	0.71	2.15	2	7
3:A:406:PCW:H122	4:B:211:17F:C7	0.71	2.15	2	2
3:A:414:PCW:H252	4:A:415:17F:H60	0.71	1.62	4	5
3:D:601:PCW:H482	4:D:628:17F:H53	0.71	1.62	11	5
3:D:612:PCW:H452	3:D:612:PCW:H241	0.71	1.61	9	4
3:C:217:PCW:H172	4:C:219:17F:C1Z	0.71	2.15	16	6
3:C:212:PCW:H341	4:C:213:17F:O8	0.71	1.84	4	1
3:A:405:PCW:H252	3:A:418:PCW:H241	0.71	1.60	6	1
3:C:207:PCW:H172	4:C:213:17F:H18	0.71	1.62	7	1
3:C:208:PCW:H232	3:C:208:PCW:C27	0.71	2.12	8	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
3:A:414:PCW:H471	4:A:415:17F:C38	0.71	2.15	14	1
4:B:210:17F:H68	3:C:209:PCW:H421	0.71	1.61	3	1
3:D:613:PCW:H321	3:D:619:PCW:H152	0.71	1.62	4	4
3:A:420:PCW:H351	3:D:618:PCW:H412	0.71	1.60	6	2
3:A:406:PCW:H122	4:B:211:17F:O8	0.71	1.85	7	4
4:B:210:17F:C12	4:B:210:17F:H40	0.71	2.14	9	1
3:B:205:PCW:H232	3:C:210:PCW:H283	0.71	1.62	10	1
3:D:614:PCW:H20	4:B:209:17F:H48	0.71	1.61	16	3
3:D:601:PCW:H371	3:D:602:PCW:H151	0.71	1.63	9	2
3:D:619:PCW:C35	3:D:627:PCW:H341	0.71	2.16	16	4
3:D:624:PCW:H221	3:C:217:PCW:H231	0.71	1.61	15	8
3:A:404:PCW:H141	3:B:205:PCW:H451	0.71	1.61	2	2
3:D:610:PCW:H241	3:D:610:PCW:C20	0.71	2.15	3	1
3:B:207:PCW:H182	3:B:207:PCW:C34	0.71	2.15	3	6
3:A:401:PCW:H51	3:B:207:PCW:C31	0.71	2.15	17	4
4:A:422:17F:H8A	4:C:218:17F:C36	0.71	2.13	14	4
4:A:422:17F:C28	4:C:218:17F:H10	0.71	2.15	11	8
3:A:414:PCW:C31	3:A:414:PCW:H351	0.71	2.15	9	5
3:D:609:PCW:C27	4:D:628:17F:H73	0.71	2.05	17	2
3:D:614:PCW:H20	4:B:209:17F:C25	0.71	2.09	7	1
3:A:405:PCW:C28	3:A:418:PCW:H241	0.71	2.15	20	2
3:B:203:PCW:H222	4:B:209:17F:H19	0.71	1.59	16	2
4:A:422:17F:H6	3:D:622:PCW:C15	0.71	2.14	9	9
3:C:203:PCW:H73	4:C:213:17F:O2	0.71	1.86	1	1
3:A:405:PCW:H271	3:A:418:PCW:H241	0.71	1.62	3	10
3:D:608:PCW:C19	3:D:608:PCW:H151	0.71	2.15	2	1
3:C:211:PCW:C5	3:C:211:PCW:H12	0.71	2.15	2	1
1:A:275:LYS:HG2	1:D:499:LEU:HD21	0.71	1.60	18	5
3:A:413:PCW:C45	3:C:210:PCW:H232	0.71	2.14	8	3
3:A:408:PCW:H261	3:D:619:PCW:H462	0.71	1.61	5	4
3:A:419:PCW:H483	3:C:212:PCW:H381	0.71	1.61	5	1
3:D:604:PCW:H52	4:C:219:17F:H4A	0.71	1.62	19	3
3:B:206:PCW:H122	3:C:209:PCW:H352	0.71	1.61	5	2
3:D:609:PCW:H52	4:D:632:17F:HN1	0.71	1.43	11	5
3:C:212:PCW:H442	4:C:215:17F:H40	0.71	1.61	11	1
3:A:402:PCW:H442	3:C:206:PCW:H282	0.71	1.62	12	1
4:B:210:17F:C2X	4:C:215:17F:H29	0.71	2.16	15	1
3:A:401:PCW:H12	3:B:207:PCW:H152	0.71	1.60	16	1
3:A:403:PCW:H11	3:A:403:PCW:O31	0.71	1.85	16	20
4:B:210:17F:H41	4:B:210:17F:H12A	0.71	1.62	2	8
3:C:205:PCW:H11	4:C:214:17F:H10	0.71	1.62	2	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
3:B:206:PCW:H181	3:C:205:PCW:H152	0.71	1.60	3	1
3:D:614:PCW:H251	4:B:209:17F:H43	0.71	1.61	14	3
3:B:207:PCW:H361	3:B:207:PCW:H231	0.71	1.62	5	1
3:A:406:PCW:H221	3:A:411:PCW:H472	0.71	1.63	17	3
3:A:409:PCW:H2	4:B:210:17F:C1Z	0.71	2.15	10	3
3:D:627:PCW:H282	4:D:631:17F:H46	0.71	1.61	9	4
3:C:216:PCW:H442	3:C:217:PCW:H361	0.71	1.61	9	3
3:C:206:PCW:H211	3:C:208:PCW:H411	0.71	1.59	15	4
3:C:208:PCW:H42	3:C:208:PCW:C2	0.71	2.16	12	1
3:A:408:PCW:O11	3:A:411:PCW:H152	0.71	1.85	13	2
3:C:205:PCW:C20	3:C:209:PCW:H221	0.71	2.15	17	1
4:B:210:17F:H30	4:C:215:17F:C1X	0.71	2.14	19	1
3:A:411:PCW:C27	3:A:413:PCW:H39	0.71	2.14	2	4
3:D:606:PCW:O11	3:D:606:PCW:H2	0.71	1.83	11	20
3:D:609:PCW:H483	3:C:208:PCW:C47	0.71	2.15	19	5
3:D:613:PCW:H332	3:D:627:PCW:C13	0.71	2.15	5	9
3:D:605:PCW:H332	3:D:624:PCW:C8	0.71	2.15	13	10
3:C:206:PCW:H212	3:C:208:PCW:C17	0.71	2.16	2	2
4:B:211:17F:H43	3:C:204:PCW:H422	0.71	1.62	6	2
4:D:628:17F:H20A	4:D:628:17F:O9	0.71	1.86	7	1
3:C:205:PCW:H332	3:C:209:PCW:H332	0.71	1.62	7	1
3:D:617:PCW:C1	3:C:216:PCW:H342	0.71	2.16	10	2
3:D:614:PCW:C48	3:D:620:PCW:H211	0.71	2.15	5	11
3:A:417:PCW:H161	3:A:420:PCW:C33	0.71	2.15	20	5
3:A:405:PCW:H52	3:A:406:PCW:O11	0.71	1.85	18	3
3:B:206:PCW:C27	3:C:205:PCW:H19	0.71	2.13	18	4
3:A:402:PCW:C18	3:A:407:PCW:H211	0.71	2.16	19	4
3:A:402:PCW:O2P	3:A:410:PCW:H63	0.71	1.86	10	1
3:D:617:PCW:H381	3:D:619:PCW:H142	0.71	1.62	14	3
3:D:610:PCW:C6	4:D:631:17F:H6A	0.71	2.13	19	3
3:B:203:PCW:H482	4:C:215:17F:H47	0.71	1.62	13	2
3:A:412:PCW:H431	3:C:210:PCW:H182	0.71	1.61	17	1
3:D:619:PCW:H242	3:C:204:PCW:H442	0.71	1.61	19	2
3:D:614:PCW:O31	3:D:614:PCW:H12	0.71	1.85	4	20
3:B:207:PCW:H171	4:B:210:17F:O10	0.71	1.86	10	7
3:B:208:PCW:H321	3:C:211:PCW:C6	0.71	2.16	12	4
4:C:213:17F:H33	4:C:213:17F:C39	0.71	2.16	3	1
3:D:611:PCW:C48	3:B:208:PCW:H241	0.71	2.16	18	2
4:C:219:17F:H44	4:C:219:17F:H68	0.71	1.61	9	2
4:C:218:17F:H47	4:C:219:17F:C22	0.71	2.15	8	1
3:B:203:PCW:H222	4:B:209:17F:H20A	0.71	1.62	15	2

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
3:A:410:PCW:H262	3:D:621:PCW:H411	0.71	1.61	14	1
3:D:621:PCW:C28	4:D:632:17F:H37	0.71	2.15	14	2
3:C:205:PCW:H471	4:C:215:17F:C22	0.71	2.16	17	1
3:A:417:PCW:H172	3:A:420:PCW:H411	0.71	1.63	18	1
3:D:619:PCW:C24	3:C:204:PCW:H442	0.71	2.15	5	8
3:D:618:PCW:H51	3:D:618:PCW:H2	0.71	1.63	9	9
3:D:621:PCW:H412	3:D:621:PCW:C37	0.71	2.13	16	15
3:D:604:PCW:H372	3:D:604:PCW:H411	0.71	1.61	9	3
3:C:204:PCW:C22	3:C:210:PCW:H282	0.71	2.16	4	7
3:A:414:PCW:H141	4:A:415:17F:H63	0.71	1.62	5	1
3:A:406:PCW:H20	4:B:211:17F:H20	0.71	1.61	17	2
3:A:414:PCW:C32	4:A:415:17F:H32	0.71	2.14	15	2
3:C:211:PCW:H172	4:C:215:17F:H65	0.71	1.63	9	1
3:C:212:PCW:H222	4:C:215:17F:H12	0.71	1.61	12	1
4:A:422:17F:C36	4:D:632:17F:H67	0.71	2.16	13	1
3:A:401:PCW:H381	3:B:204:PCW:C17	0.71	2.13	16	1
3:C:205:PCW:H151	3:C:209:PCW:H321	0.71	1.61	17	1
3:D:605:PCW:O2P	3:D:614:PCW:H63	0.71	1.86	20	2
3:C:206:PCW:C24	3:C:208:PCW:H431	0.71	2.15	18	1
4:B:211:17F:H35	4:B:211:17F:H65	0.71	1.63	1	1
3:A:406:PCW:H321	3:B:205:PCW:C36	0.71	2.15	4	7
4:D:632:17F:H4	4:D:632:17F:O10	0.71	1.86	14	6
3:A:421:PCW:H381	3:D:618:PCW:C15	0.71	2.16	16	2
3:C:204:PCW:H272	3:C:217:PCW:C44	0.71	2.11	6	2
3:D:617:PCW:H431	3:C:204:PCW:H471	0.71	1.60	8	1
3:C:203:PCW:H152	4:C:213:17F:H38	0.71	1.62	13	3
3:B:206:PCW:C8	3:C:205:PCW:H341	0.71	2.16	18	2
3:C:204:PCW:H242	3:C:210:PCW:C20	0.70	2.16	2	3
3:C:207:PCW:O1P	3:C:207:PCW:C3	0.70	2.39	7	5
3:C:207:PCW:C3	3:C:207:PCW:O1P	0.70	2.39	4	3
3:A:409:PCW:H432	3:A:419:PCW:H241	0.70	1.62	10	8
3:A:409:PCW:H322	3:B:206:PCW:C34	0.70	2.15	8	1
3:A:405:PCW:C36	3:A:411:PCW:H421	0.70	2.15	15	2
3:A:414:PCW:C46	3:D:614:PCW:H231	0.70	2.16	19	1
3:D:627:PCW:H42	3:D:627:PCW:H2	0.70	1.61	1	1
3:B:208:PCW:C47	3:C:203:PCW:H152	0.70	2.16	5	1
3:D:608:PCW:H19	4:D:629:17F:C28	0.70	2.16	17	3
3:D:616:PCW:H483	3:C:207:PCW:H283	0.70	1.63	8	2
3:A:401:PCW:H62	3:B:207:PCW:C2	0.70	2.04	19	2
3:D:612:PCW:O11	3:D:620:PCW:H132	0.70	1.86	10	1
4:C:218:17F:H29	4:C:219:17F:H8	0.70	1.63	20	3

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
3:A:410:PCW:O3	3:C:208:PCW:H372	0.70	1.86	14	1
3:A:419:PCW:H441	4:B:210:17F:H76	0.70	1.62	20	1
3:A:402:PCW:H40	3:A:407:PCW:H282	0.70	1.63	19	2
3:A:404:PCW:O31	3:A:404:PCW:O3	0.70	2.09	11	13
3:A:414:PCW:H141	3:A:414:PCW:C18	0.70	2.12	9	3
4:D:630:17F:H5	4:D:630:17F:O8	0.70	1.86	19	8
3:C:207:PCW:O31	3:C:207:PCW:H11	0.70	1.86	1	18
3:B:204:PCW:H171	3:B:204:PCW:H211	0.70	1.63	14	7
3:C:207:PCW:H142	4:C:213:17F:H18	0.70	1.62	10	4
3:A:409:PCW:H82	3:B:206:PCW:H11	0.70	1.60	4	2
4:B:211:17F:H6A	4:B:211:17F:O10	0.70	1.85	8	8
3:C:212:PCW:H411	3:C:212:PCW:C18	0.70	2.16	17	4
3:C:212:PCW:H432	3:C:212:PCW:H211	0.70	1.61	14	3
4:D:632:17F:C37	4:D:632:17F:H58	0.70	2.16	8	1
3:B:203:PCW:H152	4:B:209:17F:O6	0.70	1.87	8	1
3:A:401:PCW:H62	3:B:207:PCW:C31	0.70	2.16	20	2
3:C:206:PCW:H182	3:C:208:PCW:C15	0.70	2.16	20	1
3:A:410:PCW:H283	4:A:422:17F:C41	0.70	2.17	3	1
4:A:422:17F:C35	3:D:622:PCW:H451	0.70	2.15	3	1
3:D:604:PCW:H31	3:D:604:PCW:C4	0.70	2.15	6	6
3:A:406:PCW:O3	4:B:211:17F:H75	0.70	1.84	7	2
4:D:628:17F:H58	4:D:629:17F:H47	0.70	1.63	7	1
3:D:625:PCW:H471	3:D:626:PCW:C48	0.70	2.16	16	2
3:A:403:PCW:C34	3:A:404:PCW:H31	0.70	2.16	11	1
3:A:414:PCW:H342	4:A:415:17F:H57	0.70	1.63	19	2
3:B:203:PCW:H271	4:B:210:17F:H53	0.70	1.62	20	1
3:A:421:PCW:H61	4:D:630:17F:C4	0.70	2.17	6	4
3:C:205:PCW:H341	3:C:209:PCW:H332	0.70	1.62	1	1
3:B:208:PCW:C40	3:C:216:PCW:H283	0.70	2.12	8	4
3:C:206:PCW:C18	3:C:208:PCW:H152	0.70	2.16	8	2
3:C:203:PCW:H441	3:C:217:PCW:H481	0.70	1.64	20	2
3:A:409:PCW:H39	4:B:210:17F:C36	0.70	2.16	13	1
3:D:608:PCW:H171	4:D:629:17F:H18A	0.70	1.63	16	3
3:B:206:PCW:H411	4:B:210:17F:H68	0.70	1.61	13	1
3:A:410:PCW:H31	3:A:410:PCW:P	0.70	2.26	14	1
3:D:605:PCW:O1P	3:D:614:PCW:H82	0.70	1.85	14	1
3:A:419:PCW:H441	4:B:210:17F:H72	0.70	1.63	16	1
3:D:617:PCW:H432	3:D:627:PCW:C23	0.70	2.16	19	2
4:B:210:17F:C27	3:C:205:PCW:H483	0.70	2.16	17	1
1:D:505:ASP:HA	1:D:508:ARG:HD2	0.70	1.62	8	6
3:D:602:PCW:H12	3:D:602:PCW:O31	0.70	1.85	1	7

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
3:D:606:PCW:C25	4:C:218:17F:H38	0.70	2.16	5	10
3:A:401:PCW:H462	3:D:615:PCW:H242	0.70	1.62	3	2
1:A:250:VAL:HG21	3:A:412:PCW:H271	0.70	1.64	4	5
3:C:212:PCW:H462	4:C:215:17F:H40	0.70	1.62	4	1
3:A:408:PCW:O4P	3:A:413:PCW:H32	0.70	1.87	20	4
3:D:617:PCW:H441	3:D:627:PCW:H261	0.70	1.63	5	3
3:D:608:PCW:H452	4:D:628:17F:H34	0.70	1.63	18	2
3:D:623:PCW:H281	3:D:624:PCW:H462	0.70	1.62	17	4
4:D:632:17F:H62	3:C:208:PCW:H482	0.70	1.61	13	3
3:D:605:PCW:C47	3:D:620:PCW:H432	0.70	2.15	12	3
3:D:616:PCW:C21	4:D:632:17F:H38	0.70	2.17	12	1
4:B:210:17F:C33	3:C:205:PCW:H441	0.70	2.15	12	1
3:D:621:PCW:O1P	3:D:622:PCW:H62	0.70	1.87	17	3
4:B:211:17F:H69	4:B:211:17F:H12A	0.70	1.61	19	1
3:A:417:PCW:H52	3:A:417:PCW:O1P	0.70	1.85	4	19
3:D:615:PCW:C5	3:D:625:PCW:O1P	0.70	2.40	20	19
3:C:204:PCW:H12	3:C:204:PCW:O31	0.70	1.84	16	13
3:C:204:PCW:C24	3:C:210:PCW:H282	0.70	2.15	9	6
4:C:214:17F:H5	4:C:214:17F:O8	0.70	1.86	10	9
3:A:411:PCW:O4P	4:B:211:17F:H1A	0.70	1.86	19	4
3:C:204:PCW:C40	3:C:216:PCW:H242	0.70	2.16	19	2
3:B:208:PCW:C16	3:C:203:PCW:H283	0.70	2.16	10	1
3:B:208:PCW:C44	3:C:204:PCW:H171	0.70	2.16	14	1
3:A:413:PCW:H422	3:C:210:PCW:C46	0.70	2.17	15	7
3:D:609:PCW:C18	3:D:616:PCW:H352	0.70	2.16	3	6
3:C:204:PCW:O1P	3:C:204:PCW:C3	0.70	2.40	9	20
3:D:603:PCW:H252	3:D:611:PCW:H171	0.70	1.63	3	3
3:D:608:PCW:H142	3:D:609:PCW:H171	0.70	1.63	18	2
3:D:608:PCW:H461	4:D:628:17F:C34	0.70	2.16	4	8
3:A:406:PCW:H122	4:B:211:17F:H6	0.70	1.61	4	3
3:B:205:PCW:C23	3:C:210:PCW:H262	0.70	2.16	5	3
2:B:84:ILE:HD12	2:B:123:ARG:HD3	0.70	1.63	8	1
3:B:206:PCW:H142	3:B:206:PCW:H40	0.70	1.61	8	1
3:A:401:PCW:H381	3:B:204:PCW:H262	0.70	1.63	17	1
3:D:627:PCW:C20	3:C:217:PCW:H331	0.70	2.17	18	1
3:D:621:PCW:C4	3:D:621:PCW:H2	0.70	2.16	19	1
3:C:209:PCW:O11	3:C:209:PCW:H2	0.70	1.86	20	19
3:A:407:PCW:O31	3:A:410:PCW:H352	0.70	1.87	6	5
3:D:608:PCW:H261	4:D:629:17F:H63	0.70	1.63	8	5
3:A:408:PCW:H242	3:A:411:PCW:C23	0.70	2.15	7	8
3:A:417:PCW:H283	3:A:420:PCW:H252	0.70	1.63	4	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
3:B:203:PCW:C45	3:C:211:PCW:H232	0.70	2.13	4	2
3:B:205:PCW:H482	3:B:208:PCW:C19	0.70	2.17	16	2
3:B:208:PCW:H362	3:C:203:PCW:H172	0.70	1.64	11	5
3:A:406:PCW:C45	4:B:211:17F:H58	0.70	2.16	13	2
3:D:609:PCW:H271	4:D:628:17F:C40	0.70	2.05	17	4
3:B:208:PCW:C40	3:C:204:PCW:H151	0.70	2.16	8	2
3:C:203:PCW:C47	3:C:204:PCW:H232	0.70	2.13	8	1
4:B:210:17F:H40	4:B:210:17F:H12	0.70	1.64	9	2
3:B:205:PCW:H11	4:B:211:17F:O1	0.70	1.87	11	2
3:B:203:PCW:H332	4:B:210:17F:C21	0.70	2.17	19	2
3:A:409:PCW:H141	3:A:419:PCW:H231	0.70	1.63	16	1
3:D:603:PCW:H181	3:D:624:PCW:H222	0.70	1.62	17	1
3:A:410:PCW:H221	4:A:422:17F:H76	0.70	1.64	20	1
3:A:408:PCW:H181	3:A:413:PCW:H262	0.70	1.63	16	3
3:D:605:PCW:H231	3:D:614:PCW:C38	0.70	2.17	7	13
3:D:616:PCW:O1P	3:D:616:PCW:H52	0.70	1.87	7	12
3:D:617:PCW:H31	3:D:617:PCW:O4P	0.70	1.87	13	8
4:B:211:17F:H2	4:B:211:17F:O2	0.70	1.87	2	18
3:C:205:PCW:C34	3:C:209:PCW:H332	0.70	2.17	1	1
3:A:401:PCW:C11	3:B:207:PCW:H39	0.70	2.16	3	1
3:B:206:PCW:H122	3:C:209:PCW:H371	0.70	1.63	3	1
3:D:604:PCW:H281	3:D:607:PCW:C46	0.70	2.17	5	1
3:D:603:PCW:H432	3:D:611:PCW:H351	0.70	1.63	11	2
2:C:36:ILE:HA	2:C:59:ALA:HB2	0.70	1.61	15	8
3:A:409:PCW:H321	3:B:206:PCW:H322	0.70	1.62	13	1
3:D:609:PCW:H451	3:C:206:PCW:H20	0.70	1.63	14	1
1:D:462:LYS:HB3	3:D:602:PCW:H281	0.70	1.64	17	2
3:A:401:PCW:H472	3:D:612:PCW:H283	0.70	1.63	18	2
3:A:403:PCW:C22	3:D:618:PCW:H282	0.70	2.17	20	1
3:A:409:PCW:H321	3:B:206:PCW:C33	0.70	2.17	20	1
3:A:406:PCW:H281	3:D:619:PCW:H231	0.69	1.64	1	1
3:A:419:PCW:H483	3:C:212:PCW:H471	0.69	1.64	17	4
3:D:614:PCW:C21	4:B:209:17F:H47	0.69	2.16	12	5
3:C:207:PCW:O3	4:C:213:17F:H4	0.69	1.87	11	3
3:C:211:PCW:H32	4:C:215:17F:H31	0.69	1.62	2	1
3:C:205:PCW:H121	3:C:209:PCW:C34	0.69	2.16	4	2
3:C:207:PCW:C14	4:C:213:17F:H20A	0.69	2.17	19	2
3:B:203:PCW:H461	4:C:215:17F:H42	0.69	1.63	5	1
3:B:205:PCW:H132	3:C:204:PCW:C4	0.69	2.17	5	1
3:A:402:PCW:H412	3:C:206:PCW:H251	0.69	1.64	12	1
3:D:619:PCW:H351	3:D:627:PCW:C34	0.69	2.15	16	2

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
2:C:32:TYR:HA	5:C:201:GSP:H3'	0.69	1.64	15	1
3:C:203:PCW:H82	3:C:211:PCW:O1P	0.69	1.86	3	5
3:A:411:PCW:H322	3:A:411:PCW:H41	0.69	1.64	12	4
3:D:615:PCW:O1P	3:D:615:PCW:H51	0.69	1.87	9	8
3:A:410:PCW:H40	3:A:412:PCW:H382	0.69	1.63	8	1
3:C:206:PCW:H142	3:C:208:PCW:C15	0.69	2.17	8	1
3:C:209:PCW:C44	3:C:212:PCW:H262	0.69	2.18	8	3
5:B:201:GSP:O2B	5:B:201:GSP:O3G	0.69	2.09	13	2
3:C:203:PCW:H12	3:C:211:PCW:C6	0.69	2.16	12	2
3:B:208:PCW:H142	3:C:203:PCW:H241	0.69	1.62	15	1
3:A:410:PCW:H12	3:C:207:PCW:C6	0.69	2.16	16	1
3:C:206:PCW:H82	4:C:214:17F:C10	0.69	2.17	18	1
3:A:406:PCW:H39	3:B:205:PCW:C16	0.69	2.16	1	2
3:D:619:PCW:H131	3:D:627:PCW:H142	0.69	1.61	13	4
3:C:203:PCW:H122	3:C:207:PCW:C40	0.69	2.18	1	1
3:C:216:PCW:O31	3:C:216:PCW:H11	0.69	1.86	18	20
4:B:209:17F:C19	4:B:209:17F:C31	0.69	2.70	9	14
4:D:628:17F:H36	4:D:629:17F:C39	0.69	2.18	10	3
3:A:406:PCW:C32	3:B:205:PCW:H362	0.69	2.18	4	3
3:A:408:PCW:H31	3:A:413:PCW:C11	0.69	2.17	17	5
3:C:204:PCW:H222	3:C:210:PCW:H282	0.69	1.63	17	4
4:A:422:17F:C27	4:C:218:17F:H10	0.69	2.16	5	3
3:C:207:PCW:C23	3:C:207:PCW:H483	0.69	2.17	5	1
3:D:614:PCW:C20	4:B:209:17F:H51	0.69	2.16	19	3
3:A:406:PCW:C27	4:B:211:17F:H60	0.69	2.16	14	5
3:A:417:PCW:H451	3:D:618:PCW:H252	0.69	1.63	18	4
3:D:627:PCW:H41	3:D:627:PCW:C2	0.69	2.16	18	2
4:B:210:17F:H72	3:C:209:PCW:H40	0.69	1.65	13	1
3:A:406:PCW:H262	3:A:411:PCW:H482	0.69	1.64	15	1
4:A:422:17F:H43	4:C:219:17F:C37	0.69	2.17	16	2
3:C:217:PCW:C12	4:C:218:17F:H67	0.69	2.14	16	1
3:A:414:PCW:C14	4:A:415:17F:H33	0.69	2.18	20	1
3:D:603:PCW:H462	3:D:611:PCW:H432	0.69	1.63	13	8
3:A:405:PCW:C34	3:A:406:PCW:H212	0.69	2.17	6	1
3:B:208:PCW:O3P	3:C:211:PCW:H342	0.69	1.86	10	2
3:D:619:PCW:H412	4:D:631:17F:C26	0.69	2.10	17	3
3:D:626:PCW:H372	3:D:626:PCW:H411	0.69	1.64	18	2
3:C:205:PCW:C21	3:C:209:PCW:H271	0.69	2.18	15	1
3:A:419:PCW:H431	3:D:625:PCW:H442	0.69	1.63	19	2
3:B:206:PCW:H142	3:C:209:PCW:H372	0.69	1.63	17	2
4:B:211:17F:H12	4:B:211:17F:C32	0.69	2.16	16	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
3:C:206:PCW:C5	4:C:214:17F:H10A	0.69	2.17	16	1
4:A:416:17F:H77	4:B:209:17F:H70	0.69	1.64	17	1
3:C:211:PCW:C23	4:C:215:17F:H48	0.69	2.18	18	1
3:A:408:PCW:H182	3:A:408:PCW:C23	0.69	2.17	7	9
3:C:205:PCW:H181	3:C:209:PCW:H261	0.69	1.63	14	4
3:A:403:PCW:C3	3:A:403:PCW:O1P	0.69	2.41	6	16
3:B:205:PCW:O31	3:B:208:PCW:H63	0.69	1.87	3	2
3:C:207:PCW:H322	3:C:207:PCW:H62	0.69	1.62	6	5
3:A:403:PCW:H321	3:A:406:PCW:C5	0.69	2.14	14	3
3:A:413:PCW:H322	3:C:210:PCW:H132	0.69	1.63	16	6
3:B:208:PCW:O2P	3:B:208:PCW:C3	0.69	2.40	8	2
3:B:203:PCW:O1P	4:B:210:17F:H37	0.69	1.87	9	1
3:A:420:PCW:O1P	3:A:420:PCW:H52	0.69	1.87	10	1
3:B:203:PCW:H461	4:C:215:17F:H47	0.69	1.64	10	3
3:B:203:PCW:C38	3:C:211:PCW:H421	0.69	2.18	13	1
3:C:203:PCW:H461	3:C:204:PCW:H152	0.69	1.65	13	2
3:A:408:PCW:H482	3:A:413:PCW:H231	0.69	1.65	15	1
3:C:216:PCW:H421	3:C:217:PCW:H151	0.69	1.64	15	1
3:C:211:PCW:H2	4:C:215:17F:C31	0.69	2.18	16	1
3:A:411:PCW:H73	4:B:211:17F:C3	0.69	2.18	17	1
3:D:625:PCW:O11	3:D:625:PCW:H2	0.69	1.88	11	15
3:D:616:PCW:H211	4:D:632:17F:H38	0.69	1.64	3	2
3:D:604:PCW:H372	3:D:604:PCW:C41	0.69	2.17	9	2
3:A:408:PCW:H212	3:A:413:PCW:H262	0.69	1.64	8	1
3:D:617:PCW:H39	3:D:619:PCW:H161	0.69	1.65	8	1
3:C:203:PCW:H472	3:C:204:PCW:C23	0.69	2.13	8	1
3:D:605:PCW:C37	3:D:612:PCW:H322	0.69	2.17	10	1
3:D:606:PCW:H52	3:D:626:PCW:H19	0.69	1.64	14	1
3:A:418:PCW:C43	3:D:613:PCW:H172	0.69	2.13	20	1
3:A:407:PCW:H122	3:A:410:PCW:C33	0.69	2.15	1	3
4:A:415:17F:H64	4:B:209:17F:H37	0.69	1.62	1	2
3:C:209:PCW:H162	4:C:214:17F:C8	0.69	2.18	3	4
3:D:621:PCW:C14	4:D:632:17F:H18	0.69	2.17	7	7
4:B:210:17F:H56	3:C:205:PCW:H442	0.69	1.64	3	1
3:A:406:PCW:H471	4:B:211:17F:C31	0.69	2.18	15	5
3:C:206:PCW:H361	3:C:208:PCW:H122	0.69	1.64	7	2
3:D:609:PCW:C48	3:C:208:PCW:H472	0.69	2.17	13	5
3:C:207:PCW:H172	4:C:213:17F:H20A	0.69	1.65	7	1
3:D:608:PCW:H261	4:D:629:17F:H58	0.69	1.63	8	2
3:D:624:PCW:O4P	3:D:624:PCW:C6	0.69	2.40	13	19
3:B:208:PCW:H342	3:C:203:PCW:H283	0.69	1.65	1	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
4:C:219:17F:H60	4:C:219:17F:H10A	0.69	1.65	13	6
3:A:401:PCW:H472	3:D:612:PCW:H241	0.69	1.64	2	1
3:B:203:PCW:C43	3:C:211:PCW:H232	0.69	2.16	2	1
3:C:212:PCW:C7	4:C:213:17F:H2	0.69	2.18	2	4
3:B:208:PCW:C35	3:C:203:PCW:H222	0.69	2.18	19	2
3:A:404:PCW:H372	4:A:415:17F:H11	0.69	1.63	4	1
3:B:207:PCW:H232	3:B:207:PCW:H381	0.69	1.65	12	3
3:C:206:PCW:H172	3:C:208:PCW:H342	0.69	1.63	4	4
3:B:205:PCW:H332	3:B:208:PCW:C7	0.69	2.18	10	4
3:A:401:PCW:C6	3:B:207:PCW:H11	0.69	2.07	7	1
3:A:409:PCW:H352	4:B:210:17F:C35	0.69	2.18	7	2
3:B:204:PCW:C42	3:B:207:PCW:H431	0.69	2.16	7	1
3:C:205:PCW:H141	3:C:209:PCW:H362	0.69	1.62	14	2
3:A:408:PCW:H272	3:D:619:PCW:H462	0.69	1.65	9	4
3:A:403:PCW:H472	3:A:404:PCW:C27	0.69	2.17	14	1
3:C:203:PCW:H471	3:C:210:PCW:H171	0.69	1.63	15	1
3:C:204:PCW:C39	3:C:216:PCW:H261	0.69	2.18	19	1
3:C:206:PCW:H52	4:C:214:17F:C10	0.69	2.18	16	3
3:A:404:PCW:H442	3:A:404:PCW:C17	0.69	2.18	2	2
3:D:612:PCW:H31	3:D:620:PCW:C11	0.69	2.18	2	5
3:C:211:PCW:H32	4:C:215:17F:H56	0.69	1.64	4	1
3:D:622:PCW:O1P	3:D:622:PCW:C3	0.69	2.41	5	1
3:A:406:PCW:C20	4:B:211:17F:H20	0.69	2.18	13	2
3:B:206:PCW:O3P	3:B:206:PCW:H63	0.69	1.88	6	2
4:D:632:17F:C29	3:C:208:PCW:H161	0.69	2.18	8	2
3:D:605:PCW:P	3:D:614:PCW:H52	0.69	2.28	9	7
3:C:209:PCW:H452	3:C:212:PCW:H241	0.69	1.64	12	1
3:C:209:PCW:H211	3:C:209:PCW:H172	0.69	1.63	15	1
4:A:416:17F:C36	3:B:204:PCW:H283	0.69	2.15	16	1
3:C:203:PCW:H432	3:C:210:PCW:C19	0.69	2.18	17	1
3:D:603:PCW:H261	3:D:611:PCW:C17	0.69	2.18	19	1
3:D:624:PCW:H62	3:D:624:PCW:O4P	0.69	1.87	12	6
3:C:210:PCW:H162	3:C:210:PCW:H422	0.69	1.63	9	3
1:D:512:ASP:HA	1:D:515:ARG:HD2	0.69	1.63	6	4
3:D:617:PCW:H461	3:D:627:PCW:H251	0.69	1.63	9	3
3:C:203:PCW:H182	3:C:211:PCW:H481	0.69	1.64	4	1
3:A:405:PCW:C26	3:A:418:PCW:H241	0.69	2.18	6	1
3:C:206:PCW:H171	3:C:208:PCW:H382	0.69	1.63	6	1
3:A:402:PCW:C42	3:C:208:PCW:H132	0.69	2.14	7	3
3:A:411:PCW:C5	4:B:211:17F:H1A	0.69	2.17	14	3
3:C:212:PCW:H441	4:C:215:17F:H30	0.69	1.65	9	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:388:SER:HB2	1:D:594:LYS:HG2	0.69	1.65	14	1
3:D:619:PCW:H322	3:D:627:PCW:C15	0.69	2.16	16	1
3:A:406:PCW:H252	4:B:211:17F:C33	0.69	2.18	18	1
3:A:408:PCW:H32	3:A:411:PCW:H142	0.68	1.63	6	6
3:D:609:PCW:C24	3:D:616:PCW:H381	0.68	2.14	3	7
3:A:406:PCW:H472	3:B:205:PCW:H222	0.68	1.64	2	1
3:A:408:PCW:H232	3:A:408:PCW:H171	0.68	1.65	8	4
4:A:415:17F:C12	4:B:209:17F:H5	0.68	2.18	2	1
3:A:403:PCW:H321	3:A:404:PCW:H12	0.68	1.65	3	2
3:A:420:PCW:H481	3:D:619:PCW:H281	0.68	1.65	3	2
4:B:211:17F:H65	4:B:211:17F:C12	0.68	2.15	9	3
4:C:218:17F:H47	4:C:219:17F:C23	0.68	2.10	11	5
3:B:207:PCW:H73	3:B:207:PCW:C11	0.68	2.18	6	1
3:D:614:PCW:H142	3:D:620:PCW:C39	0.68	2.18	15	3
3:D:627:PCW:C28	4:D:631:17F:H46	0.68	2.17	10	5
4:A:416:17F:H76	3:D:623:PCW:H242	0.68	1.64	10	1
3:A:401:PCW:H63	3:B:204:PCW:O2P	0.68	1.88	20	2
3:A:410:PCW:H221	4:A:422:17F:C42	0.68	2.17	20	1
3:C:211:PCW:H283	4:C:215:17F:H53	0.68	1.63	1	1
3:C:216:PCW:C15	3:C:217:PCW:H162	0.68	2.16	8	7
3:A:402:PCW:H431	3:C:206:PCW:H262	0.68	1.64	2	2
3:D:603:PCW:H261	3:D:611:PCW:H141	0.68	1.63	2	10
3:D:612:PCW:C2	3:D:620:PCW:H63	0.68	2.18	11	6
4:C:219:17F:O10	4:C:219:17F:H20A	0.68	1.88	5	1
3:A:406:PCW:H222	4:B:211:17F:H56	0.68	1.65	18	3
3:A:413:PCW:H421	3:C:210:PCW:H461	0.68	1.64	19	2
2:C:117:LYS:HE2	5:C:201:GSP:C5	0.68	2.23	12	2
3:A:412:PCW:C40	3:C:210:PCW:H362	0.68	2.19	20	3
3:A:411:PCW:C32	3:A:411:PCW:H42	0.68	2.18	14	1
3:B:206:PCW:H82	3:C:205:PCW:H341	0.68	1.64	18	1
3:D:615:PCW:H52	3:D:625:PCW:P	0.68	2.27	20	1
2:C:15:GLY:HA2	5:C:201:GSP:H8	0.68	1.48	3	9
3:D:604:PCW:H251	4:C:215:17F:C42	0.68	2.17	11	4
3:D:608:PCW:H221	4:D:628:17F:H19	0.68	1.65	2	1
3:A:402:PCW:C16	3:A:407:PCW:H211	0.68	2.17	9	7
3:D:625:PCW:C46	3:D:626:PCW:H482	0.68	2.17	4	10
4:A:416:17F:O5	3:B:204:PCW:H82	0.68	1.88	5	1
3:A:403:PCW:O1P	3:A:403:PCW:H31	0.68	1.89	6	2
3:D:610:PCW:H362	3:D:610:PCW:H132	0.68	1.64	6	1
4:D:632:17F:H58	4:D:632:17F:H66	0.68	1.66	8	1
3:B:206:PCW:O1P	3:B:206:PCW:H31	0.68	1.88	9	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
3:B:203:PCW:H152	4:B:209:17F:O1	0.68	1.88	14	1
3:A:406:PCW:H262	3:A:411:PCW:C48	0.68	2.18	15	1
3:C:207:PCW:H412	4:C:213:17F:C8	0.68	2.18	19	1
3:D:621:PCW:C15	4:D:632:17F:H18	0.68	2.19	2	7
3:D:601:PCW:H39	3:D:602:PCW:C15	0.68	2.15	5	1
3:D:603:PCW:C18	3:D:624:PCW:H222	0.68	2.14	19	6
3:D:605:PCW:H211	3:D:614:PCW:C38	0.68	2.16	17	4
3:B:203:PCW:C38	3:C:211:PCW:H442	0.68	2.18	7	1
3:B:206:PCW:C28	4:C:214:17F:H20	0.68	2.19	7	2
3:C:205:PCW:H332	3:C:209:PCW:C33	0.68	2.18	7	1
3:A:417:PCW:O31	3:D:618:PCW:H61	0.68	1.89	11	1
4:B:211:17F:H46	3:C:204:PCW:H381	0.68	1.65	12	1
3:C:203:PCW:H11	3:C:211:PCW:H73	0.68	1.65	13	2
3:B:208:PCW:H442	3:C:204:PCW:H171	0.68	1.66	14	1
3:C:203:PCW:H63	3:C:211:PCW:O1P	0.68	1.87	16	1
3:D:602:PCW:C21	3:D:602:PCW:H172	0.68	2.19	5	2
3:D:624:PCW:C19	3:B:208:PCW:H271	0.68	2.16	1	1
3:C:206:PCW:H222	3:C:208:PCW:C43	0.68	2.12	17	2
3:A:401:PCW:H12	3:B:207:PCW:H351	0.68	1.64	3	1
3:D:627:PCW:H262	3:C:210:PCW:C27	0.68	2.19	3	1
3:A:411:PCW:H241	3:A:413:PCW:H39	0.68	1.64	7	2
3:D:609:PCW:H281	4:C:214:17F:H54	0.68	1.64	18	3
4:B:210:17F:C42	3:C:209:PCW:H441	0.68	2.18	7	1
3:C:205:PCW:H421	3:C:212:PCW:H461	0.68	1.64	7	1
3:C:205:PCW:H32	3:C:209:PCW:H161	0.68	1.65	9	1
3:C:207:PCW:H281	4:C:214:17F:H46	0.68	1.62	10	1
3:A:401:PCW:H422	3:B:204:PCW:H283	0.68	1.66	12	2
3:D:609:PCW:H282	3:D:616:PCW:H411	0.68	1.64	12	1
4:A:422:17F:H29	4:C:219:17F:H62	0.68	1.66	20	3
3:A:410:PCW:H221	3:D:622:PCW:H40	0.68	1.65	14	1
3:A:414:PCW:H212	4:A:415:17F:H20A	0.68	1.63	14	1
1:A:214:PHE:CZ	3:A:405:PCW:H162	0.68	2.22	15	1
3:A:418:PCW:H422	3:D:613:PCW:C25	0.68	2.18	18	1
3:C:206:PCW:C26	3:C:208:PCW:H411	0.68	2.18	18	1
3:A:414:PCW:H351	3:A:414:PCW:C31	0.68	2.18	5	14
3:D:603:PCW:H221	3:D:611:PCW:H331	0.68	1.64	1	1
5:C:201:GSP:O3G	5:C:201:GSP:O2B	0.68	2.11	10	5
3:A:405:PCW:C27	3:A:418:PCW:H241	0.68	2.18	4	14
3:A:414:PCW:H341	4:A:415:17F:C1Z	0.68	2.18	3	3
3:D:622:PCW:H412	4:D:632:17F:C41	0.68	2.16	3	2
3:B:203:PCW:H222	4:B:209:17F:H18	0.68	1.63	4	3

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
3:A:414:PCW:H422	4:A:415:17F:C39	0.68	2.17	9	1
3:B:208:PCW:H221	3:C:211:PCW:H462	0.68	1.65	9	1
3:A:412:PCW:H462	3:C:210:PCW:H482	0.68	1.65	15	1
3:B:203:PCW:C22	4:B:209:17F:H19	0.68	2.18	16	1
3:C:212:PCW:H422	4:C:215:17F:H12	0.68	1.65	17	1
3:A:403:PCW:H221	3:D:618:PCW:H282	0.68	1.66	20	1
3:A:406:PCW:O1P	3:B:205:PCW:H362	0.68	1.87	1	1
3:A:408:PCW:H152	3:A:411:PCW:C24	0.68	2.18	1	1
3:A:403:PCW:H212	3:A:403:PCW:H422	0.68	1.63	5	2
3:D:614:PCW:H31	3:D:614:PCW:O31	0.68	1.87	8	9
3:D:622:PCW:H231	3:C:217:PCW:C8	0.68	2.15	13	7
3:D:623:PCW:C42	3:D:625:PCW:H261	0.68	2.16	2	3
3:C:203:PCW:C44	3:C:204:PCW:H212	0.68	2.19	4	2
3:D:623:PCW:H242	3:B:203:PCW:H472	0.68	1.65	6	1
3:A:401:PCW:H441	3:B:207:PCW:H481	0.68	1.63	8	2
3:B:205:PCW:H132	3:C:204:PCW:H51	0.68	1.65	10	2
4:A:422:17F:H40	4:C:219:17F:H67	0.68	1.63	19	4
3:A:411:PCW:H42	3:A:411:PCW:H322	0.68	1.65	14	1
3:D:606:PCW:C4	3:D:626:PCW:H19	0.68	2.19	14	1
3:C:203:PCW:H321	3:C:207:PCW:H332	0.68	1.65	14	1
3:A:404:PCW:H20	3:D:611:PCW:C28	0.68	2.19	16	1
3:A:401:PCW:H451	3:D:612:PCW:H283	0.68	1.64	17	1
3:C:207:PCW:H142	4:C:213:17F:C17	0.68	2.19	17	1
3:A:408:PCW:H272	3:D:619:PCW:H452	0.68	1.65	19	1
3:D:607:PCW:H12	3:D:626:PCW:C36	0.68	2.19	11	11
3:C:204:PCW:C27	3:C:217:PCW:H441	0.68	2.13	6	3
3:D:612:PCW:H162	3:D:620:PCW:H171	0.68	1.65	16	6
4:D:632:17F:H65	3:C:208:PCW:H482	0.68	1.65	11	3
3:A:406:PCW:H221	3:A:411:PCW:H452	0.68	1.66	12	4
3:D:605:PCW:C17	3:D:614:PCW:H132	0.68	2.17	3	4
3:D:624:PCW:H62	3:D:624:PCW:O31	0.68	1.89	12	3
3:D:625:PCW:H462	3:D:626:PCW:H482	0.68	1.64	11	6
3:A:401:PCW:C11	3:B:207:PCW:H231	0.68	2.18	6	1
3:D:622:PCW:C19	4:D:631:17F:H5	0.68	2.19	6	5
3:A:421:PCW:O1P	3:D:618:PCW:H82	0.68	1.89	19	3
4:C:213:17F:H43	4:C:215:17F:H74	0.68	1.64	8	1
3:D:609:PCW:C38	3:C:208:PCW:H283	0.68	2.19	9	3
3:C:207:PCW:H122	4:C:213:17F:H20A	0.68	1.66	14	1
3:D:619:PCW:H242	3:C:204:PCW:C44	0.68	2.18	19	1
4:B:211:17F:H65	4:B:211:17F:C1X	0.68	2.19	19	1
3:A:406:PCW:C41	3:C:204:PCW:H342	0.68	2.18	20	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
3:D:608:PCW:H20	4:D:628:17F:C18	0.68	2.18	2	2
3:A:401:PCW:H381	3:B:204:PCW:C23	0.68	2.18	3	2
3:C:205:PCW:C11	3:C:209:PCW:H151	0.68	2.18	4	1
3:A:420:PCW:H40	3:D:617:PCW:H221	0.68	1.66	5	1
3:D:601:PCW:H432	3:D:601:PCW:C47	0.68	2.11	14	2
3:B:203:PCW:H20	3:B:204:PCW:H142	0.68	1.66	8	1
4:D:631:17F:H8	3:C:217:PCW:H73	0.68	1.64	9	2
3:A:404:PCW:H382	3:A:404:PCW:H121	0.68	1.66	10	2
3:A:420:PCW:H471	3:D:611:PCW:H211	0.68	1.65	10	1
3:D:616:PCW:H172	3:D:616:PCW:H132	0.68	1.65	12	2
3:D:607:PCW:H361	3:D:626:PCW:C38	0.68	2.18	19	1
3:A:405:PCW:H82	4:B:211:17F:C3	0.68	2.18	1	1
3:A:417:PCW:H231	3:D:618:PCW:H481	0.68	1.66	1	2
3:A:407:PCW:H82	3:A:410:PCW:C35	0.68	2.07	3	6
3:D:603:PCW:H212	3:D:603:PCW:C44	0.68	2.18	4	4
3:C:207:PCW:O11	3:C:207:PCW:H82	0.68	1.87	4	2
3:C:208:PCW:H51	3:C:208:PCW:H322	0.68	1.66	4	1
3:D:602:PCW:C48	4:D:629:17F:H47	0.68	2.19	6	2
3:D:612:PCW:H172	3:D:612:PCW:C35	0.68	2.09	12	2
3:B:207:PCW:H362	3:B:207:PCW:H221	0.68	1.65	9	1
3:D:612:PCW:H61	3:D:625:PCW:C14	0.68	2.19	14	1
3:D:606:PCW:H252	4:C:218:17F:H41	0.68	1.63	17	2
3:D:607:PCW:H451	3:D:625:PCW:C47	0.67	2.19	1	1
3:B:205:PCW:P	3:B:205:PCW:C3	0.67	2.79	1	3
1:A:299:SER:HB2	1:A:300:PRO:HD3	0.67	1.65	9	5
3:A:414:PCW:H352	4:A:415:17F:H57	0.67	1.65	18	2
3:A:409:PCW:H482	3:A:419:PCW:H272	0.67	1.65	3	2
3:A:406:PCW:C39	3:B:205:PCW:H152	0.67	2.12	4	8
4:D:628:17F:H59	4:D:629:17F:H51	0.67	1.64	7	2
3:A:403:PCW:H481	3:A:404:PCW:C28	0.67	2.19	8	1
3:B:205:PCW:H212	3:C:203:PCW:C48	0.67	2.19	10	1
3:A:414:PCW:H232	4:A:415:17F:H20A	0.67	1.66	11	1
3:C:203:PCW:H152	4:C:213:17F:C22	0.67	2.18	11	2
3:C:205:PCW:O31	3:C:209:PCW:H32	0.67	1.88	12	2
3:C:203:PCW:C7	3:C:207:PCW:H11	0.67	2.13	14	1
3:A:403:PCW:H321	3:A:406:PCW:H62	0.67	1.66	15	1
3:C:203:PCW:H422	3:C:204:PCW:C16	0.67	2.09	19	2
3:A:410:PCW:H52	3:A:410:PCW:O1P	0.67	1.89	11	15
3:D:609:PCW:H261	3:D:616:PCW:H411	0.67	1.67	3	2
3:A:420:PCW:H451	3:D:611:PCW:C20	0.67	2.19	4	2
4:A:422:17F:H48	4:C:218:17F:C10	0.67	2.19	5	3

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
3:A:405:PCW:C25	3:A:418:PCW:H241	0.67	2.19	6	1
3:D:623:PCW:H2	3:D:624:PCW:H322	0.67	1.65	11	3
3:C:207:PCW:H19	4:C:213:17F:C20	0.67	2.19	17	3
4:A:415:17F:H61	4:B:209:17F:C21	0.67	2.18	20	3
3:C:212:PCW:H122	4:C:215:17F:C9	0.67	2.16	8	1
4:C:213:17F:H46	4:C:215:17F:H66	0.67	1.66	9	1
3:D:614:PCW:H141	3:D:620:PCW:C39	0.67	2.18	18	3
3:A:403:PCW:H161	3:A:404:PCW:C32	0.67	2.10	13	3
3:C:207:PCW:H361	4:C:213:17F:O10	0.67	1.90	13	1
3:B:206:PCW:H31	3:B:206:PCW:H42	0.67	1.64	17	1
3:D:614:PCW:O31	3:D:614:PCW:H31	0.67	1.88	6	11
4:D:632:17F:H52	3:C:208:PCW:C18	0.67	2.09	1	4
4:B:209:17F:C31	4:B:209:17F:C19	0.67	2.71	1	5
4:B:211:17F:C7	4:B:211:17F:C17	0.67	2.72	1	4
3:C:212:PCW:H412	4:C:215:17F:C32	0.67	2.18	2	1
3:C:210:PCW:C31	3:C:210:PCW:H352	0.67	2.20	5	1
3:A:421:PCW:O1P	3:D:618:PCW:H52	0.67	1.88	8	1
3:A:404:PCW:H351	3:A:404:PCW:H51	0.67	1.66	11	1
3:D:601:PCW:H482	4:D:628:17F:H51	0.67	1.65	13	2
3:A:408:PCW:O2P	3:A:408:PCW:H31	0.67	1.90	1	3
3:D:603:PCW:H281	3:D:611:PCW:H232	0.67	1.65	1	3
3:C:209:PCW:C22	3:C:209:PCW:C26	0.67	2.72	1	20
3:A:403:PCW:H452	3:A:404:PCW:C28	0.67	2.18	2	1
3:D:605:PCW:C42	3:D:620:PCW:H141	0.67	2.20	17	4
3:D:612:PCW:H432	3:D:620:PCW:H482	0.67	1.67	4	1
3:A:404:PCW:H51	3:B:205:PCW:H39	0.67	1.64	5	1
3:B:203:PCW:H381	3:C:211:PCW:H422	0.67	1.66	5	2
3:D:606:PCW:H331	3:D:608:PCW:H61	0.67	1.67	7	2
2:C:72:MET:HA	2:C:78:PHE:HZ	0.67	1.49	7	2
3:D:619:PCW:C13	3:D:627:PCW:H151	0.67	2.18	8	1
3:A:414:PCW:C23	4:A:415:17F:H34	0.67	2.12	14	1
3:C:211:PCW:C24	4:C:215:17F:H70	0.67	2.18	15	1
3:C:206:PCW:H152	3:C:207:PCW:C18	0.67	2.19	19	1
3:A:406:PCW:C40	3:B:205:PCW:H152	0.67	2.20	20	1
3:D:617:PCW:H421	3:D:627:PCW:H221	0.67	1.66	20	1
3:C:216:PCW:H372	3:C:216:PCW:C14	0.67	2.18	18	3
4:D:628:17F:H40	4:D:629:17F:H78	0.67	1.66	2	1
3:B:203:PCW:H451	3:C:211:PCW:H251	0.67	1.67	20	3
4:A:415:17F:C28	3:B:208:PCW:H231	0.67	2.19	18	3
3:D:603:PCW:H161	3:D:624:PCW:H211	0.67	1.64	12	6
3:A:418:PCW:H361	3:D:613:PCW:H151	0.67	1.65	15	4

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
3:A:421:PCW:H442	3:D:618:PCW:C20	0.67	2.20	14	6
3:B:207:PCW:O1P	3:B:207:PCW:C3	0.67	2.43	10	3
3:A:404:PCW:C18	3:A:404:PCW:H222	0.67	2.19	14	3
3:A:403:PCW:H412	3:A:403:PCW:H212	0.67	1.67	11	1
3:A:401:PCW:H341	3:B:207:PCW:C39	0.67	2.20	13	1
3:A:404:PCW:H421	3:A:404:PCW:H162	0.67	1.66	16	2
3:C:205:PCW:H412	3:C:212:PCW:C23	0.67	2.19	18	1
3:C:212:PCW:H371	4:C:215:17F:C10	0.67	2.20	18	1
3:D:623:PCW:H262	3:B:208:PCW:H281	0.67	1.66	19	1
3:D:602:PCW:H483	4:D:628:17F:H58	0.67	1.66	1	5
3:D:615:PCW:C46	3:D:615:PCW:C42	0.67	2.72	14	18
3:B:203:PCW:O11	3:C:211:PCW:H39	0.67	1.90	14	2
3:A:421:PCW:O31	3:D:618:PCW:H82	0.67	1.89	15	3
3:C:205:PCW:H411	3:C:212:PCW:H231	0.67	1.67	4	1
3:A:418:PCW:H441	3:D:613:PCW:C27	0.67	2.18	10	4
3:C:209:PCW:C47	3:C:209:PCW:H272	0.67	2.19	6	3
3:D:602:PCW:H42	4:C:214:17F:H32	0.67	1.64	8	1
3:D:614:PCW:H283	4:B:209:17F:H66	0.67	1.67	10	1
3:C:207:PCW:P	3:C:207:PCW:H31	0.67	2.30	14	5
3:D:627:PCW:H20	3:C:217:PCW:H321	0.67	1.64	1	3
2:C:64:TYR:HB3	2:C:67:MET:HB3	0.67	1.66	1	11
3:C:212:PCW:C20	3:C:212:PCW:C24	0.67	2.73	14	3
3:A:414:PCW:H341	4:A:415:17F:C1Y	0.67	2.17	2	3
3:D:618:PCW:C27	3:D:618:PCW:C23	0.67	2.70	2	16
3:C:206:PCW:H2	3:C:206:PCW:O1P	0.67	1.88	5	9
4:C:219:17F:H12A	4:C:219:17F:C33	0.67	2.20	7	10
3:A:403:PCW:H481	3:A:404:PCW:H283	0.67	1.66	3	2
4:A:422:17F:C11	4:C:218:17F:H69	0.67	2.17	14	5
4:B:210:17F:H68	3:C:209:PCW:C42	0.67	2.19	3	1
3:D:607:PCW:C3	3:D:626:PCW:H411	0.67	2.19	6	3
3:A:401:PCW:H39	3:B:204:PCW:H231	0.67	1.65	8	2
3:A:401:PCW:H252	3:D:615:PCW:C27	0.67	2.19	10	2
3:D:607:PCW:H241	3:B:206:PCW:H482	0.67	1.65	9	1
3:A:402:PCW:H51	3:A:402:PCW:O11	0.67	1.88	12	2
3:C:203:PCW:H51	3:C:207:PCW:C31	0.67	2.20	14	1
1:A:307:ASP:HA	1:A:310:ARG:HD2	0.67	1.66	5	9
3:C:217:PCW:H141	4:C:219:17F:H34	0.67	1.66	9	3
3:D:613:PCW:O11	3:D:613:PCW:H2	0.67	1.89	12	19
3:A:407:PCW:O31	3:A:410:PCW:H321	0.67	1.89	15	3
3:D:602:PCW:C36	4:C:214:17F:H67	0.67	2.08	17	4
3:A:413:PCW:H82	3:C:210:PCW:O31	0.67	1.89	11	2

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
4:C:215:17F:H63	4:C:215:17F:H12	0.67	1.66	18	1
3:B:205:PCW:O11	3:B:205:PCW:H2	0.67	1.88	6	11
3:D:605:PCW:C26	3:D:614:PCW:H181	0.67	2.20	17	4
3:A:402:PCW:H151	3:A:407:PCW:H211	0.67	1.67	4	2
3:B:208:PCW:H341	3:C:211:PCW:H63	0.67	1.65	5	2
4:B:211:17F:H50	3:C:204:PCW:H462	0.67	1.64	5	1
3:A:418:PCW:C41	3:D:613:PCW:H231	0.67	2.19	7	2
3:D:622:PCW:H212	4:D:631:17F:H31	0.67	1.66	7	8
3:D:614:PCW:C25	4:B:209:17F:H47	0.67	2.10	18	2
3:C:205:PCW:H152	3:C:209:PCW:H412	0.67	1.65	12	1
3:C:212:PCW:H222	3:C:212:PCW:H441	0.67	1.65	12	1
3:D:607:PCW:H361	3:D:626:PCW:C42	0.67	2.20	13	2
3:D:603:PCW:C23	3:D:611:PCW:H351	0.67	2.19	16	1
3:A:408:PCW:H32	3:A:411:PCW:C14	0.67	2.20	19	9
3:A:419:PCW:H452	3:D:625:PCW:H462	0.67	1.64	19	8
3:D:602:PCW:C36	4:C:214:17F:H61	0.67	2.19	1	5
4:D:631:17F:H11A	3:C:217:PCW:H73	0.67	1.65	3	3
3:C:206:PCW:H352	3:C:208:PCW:H121	0.67	1.67	18	4
3:A:401:PCW:C27	3:D:615:PCW:H281	0.67	2.13	6	1
3:D:609:PCW:H422	3:D:616:PCW:C45	0.67	2.20	6	2
3:C:203:PCW:H122	3:C:207:PCW:H382	0.67	1.66	7	1
3:A:406:PCW:H272	4:B:211:17F:C33	0.67	2.20	9	3
3:C:203:PCW:C40	4:C:213:17F:H70	0.67	2.19	11	3
3:C:211:PCW:C24	4:C:215:17F:H73	0.67	2.20	20	4
3:A:413:PCW:C39	3:C:210:PCW:H161	0.67	2.20	11	3
3:C:203:PCW:C32	3:C:207:PCW:H351	0.67	2.15	14	1
3:A:418:PCW:O3P	3:A:418:PCW:O31	0.66	2.13	16	10
3:D:612:PCW:H51	3:D:623:PCW:C34	0.66	2.17	6	6
3:D:621:PCW:H372	3:D:621:PCW:C41	0.66	2.16	15	5
4:B:211:17F:H12	4:B:211:17F:C37	0.66	2.20	2	1
3:B:204:PCW:H461	4:B:210:17F:H48	0.66	1.66	17	2
3:B:207:PCW:H382	3:B:207:PCW:C23	0.66	2.19	3	2
3:C:207:PCW:C15	4:C:213:17F:H56	0.66	2.18	3	4
2:B:161:ARG:HG2	2:C:135:ARG:HG3	0.66	1.67	6	2
3:C:205:PCW:C1	4:C:214:17F:H8A	0.66	2.20	6	1
3:D:619:PCW:O1P	3:D:627:PCW:H51	0.66	1.90	8	1
3:C:208:PCW:H2	3:C:208:PCW:C4	0.66	2.18	12	1
3:D:612:PCW:O2P	3:D:614:PCW:H62	0.66	1.90	14	1
3:C:209:PCW:H341	3:C:212:PCW:C27	0.66	2.20	19	1
3:C:209:PCW:P	3:C:209:PCW:C3	0.66	2.83	1	17
3:C:209:PCW:O31	3:C:209:PCW:H12	0.66	1.88	2	12

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
4:C:219:17F:H59	4:C:219:17F:C12	0.66	2.19	18	9
3:A:413:PCW:H422	3:C:210:PCW:H461	0.66	1.67	12	6
3:C:209:PCW:C44	3:C:212:PCW:H271	0.66	2.20	2	2
3:A:404:PCW:H471	4:A:415:17F:C30	0.66	2.20	9	3
3:B:208:PCW:H351	3:C:203:PCW:C22	0.66	2.20	9	5
3:D:609:PCW:H251	4:D:628:17F:C39	0.66	2.20	9	8
3:C:203:PCW:H451	3:C:210:PCW:C19	0.66	2.20	4	7
3:A:408:PCW:O1P	3:A:408:PCW:C3	0.66	2.42	5	2
3:B:205:PCW:H132	3:C:204:PCW:H41	0.66	1.67	14	5
3:B:206:PCW:H252	3:C:205:PCW:C19	0.66	2.20	5	3
3:D:603:PCW:H172	3:D:603:PCW:C21	0.66	2.19	13	5
3:D:615:PCW:H432	3:D:620:PCW:H20	0.66	1.66	16	2
3:C:207:PCW:H381	4:C:213:17F:O7	0.66	1.90	8	1
4:D:628:17F:C18	4:D:629:17F:H55	0.66	2.20	9	3
3:A:409:PCW:H2	4:B:210:17F:H31	0.66	1.67	11	2
3:B:208:PCW:H342	3:C:203:PCW:H172	0.66	1.67	11	2
3:A:406:PCW:H331	4:B:211:17F:O7	0.66	1.91	11	1
4:A:422:17F:H59	3:D:622:PCW:H421	0.66	1.65	11	2
3:A:411:PCW:C21	3:A:411:PCW:C17	0.66	2.72	14	1
3:C:207:PCW:H232	3:C:207:PCW:H483	0.66	1.66	19	1
3:A:410:PCW:O11	3:A:410:PCW:H2	0.66	1.90	4	19
3:D:616:PCW:H272	4:D:632:17F:H42	0.66	1.67	1	2
3:C:205:PCW:O1P	4:C:214:17F:N1	0.66	2.28	4	4
3:C:207:PCW:C41	4:C:213:17F:H8A	0.66	2.19	14	2
3:A:418:PCW:C41	3:A:418:PCW:C37	0.66	2.70	4	5
3:D:603:PCW:H351	3:D:624:PCW:H141	0.66	1.65	10	5
3:D:608:PCW:H221	4:D:628:17F:C19	0.66	2.21	2	1
2:C:68:ARG:HA	2:C:71:TYR:CE1	0.66	2.25	14	4
3:D:618:PCW:O31	3:D:618:PCW:C5	0.66	2.44	19	2
3:C:212:PCW:O3P	3:C:212:PCW:H82	0.66	1.91	12	1
3:D:605:PCW:C31	3:D:614:PCW:H82	0.66	2.20	15	3
3:A:418:PCW:H351	3:D:613:PCW:H151	0.66	1.67	18	1
3:D:604:PCW:H162	3:C:211:PCW:H283	0.66	1.66	19	1
3:B:205:PCW:H42	3:C:204:PCW:H61	0.66	1.66	20	1
3:D:609:PCW:H73	3:D:621:PCW:O11	0.66	1.89	17	11
3:C:203:PCW:C46	3:C:204:PCW:H161	0.66	2.21	5	2
3:C:204:PCW:C24	3:C:210:PCW:H20	0.66	2.21	2	4
3:D:613:PCW:H321	3:D:619:PCW:C13	0.66	2.20	2	11
3:C:204:PCW:C27	3:C:217:PCW:H421	0.66	2.20	7	3
3:A:417:PCW:C16	3:A:420:PCW:H341	0.66	2.20	5	1
3:C:209:PCW:H52	4:C:214:17F:H4	0.66	1.68	16	5

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
3:D:601:PCW:C43	3:D:601:PCW:C47	0.66	2.73	6	2
3:D:612:PCW:H63	3:D:623:PCW:H332	0.66	1.68	6	1
3:B:204:PCW:H52	3:B:204:PCW:H321	0.66	1.66	16	3
3:B:203:PCW:H472	3:C:211:PCW:H232	0.66	1.66	13	2
3:A:412:PCW:H482	3:C:217:PCW:H472	0.66	1.66	18	2
3:A:406:PCW:H31	4:B:211:17F:C42	0.66	2.19	19	1
4:A:415:17F:H65	4:B:209:17F:H41	0.66	1.66	20	1
3:A:409:PCW:H181	3:A:409:PCW:C22	0.66	2.16	15	2
3:A:403:PCW:H31	3:A:403:PCW:P	0.66	2.29	11	14
3:A:411:PCW:H62	4:B:211:17F:O4	0.66	1.91	13	6
3:A:419:PCW:H52	3:D:626:PCW:O31	0.66	1.90	2	2
3:C:217:PCW:H19	4:C:219:17F:H20	0.66	1.68	3	6
3:D:616:PCW:H242	4:D:632:17F:H41	0.66	1.67	3	1
3:A:419:PCW:C47	3:D:625:PCW:H483	0.66	2.20	19	5
3:A:401:PCW:C1	3:B:207:PCW:H342	0.66	2.17	6	1
3:C:203:PCW:C28	3:C:211:PCW:H471	0.66	2.21	7	1
3:C:206:PCW:C14	3:C:208:PCW:H342	0.66	2.18	18	4
3:A:404:PCW:H62	3:B:205:PCW:H40	0.66	1.66	12	1
3:D:616:PCW:C22	3:C:208:PCW:H272	0.66	2.20	12	1
3:D:604:PCW:C34	4:C:219:17F:H8	0.66	2.20	14	1
3:B:206:PCW:O11	3:C:209:PCW:H332	0.66	1.89	14	1
3:C:206:PCW:H262	3:C:208:PCW:C39	0.66	2.20	14	1
1:A:275:LYS:O	1:A:279:LEU:HG	0.66	1.91	10	19
2:C:84:ILE:HD12	2:C:123:ARG:HD3	0.66	1.67	1	1
3:A:406:PCW:C44	3:C:204:PCW:H442	0.66	2.13	2	1
3:D:617:PCW:C34	3:C:216:PCW:H362	0.66	2.20	10	6
3:B:206:PCW:O2P	3:B:206:PCW:H51	0.66	1.91	2	7
3:A:403:PCW:H231	3:A:403:PCW:C27	0.66	2.21	9	3
3:D:618:PCW:H51	3:D:618:PCW:C2	0.66	2.21	9	9
3:D:623:PCW:H211	3:B:203:PCW:C48	0.66	2.21	18	2
3:D:604:PCW:H482	3:D:626:PCW:H272	0.66	1.66	19	3
3:C:204:PCW:H261	3:C:217:PCW:H421	0.66	1.68	14	2
3:C:210:PCW:C22	3:C:210:PCW:C26	0.66	2.70	6	7
4:C:213:17F:H78	4:C:219:17F:H53	0.66	1.68	5	2
3:D:610:PCW:O1P	4:D:631:17F:N1	0.66	2.28	7	1
3:B:203:PCW:H361	3:C:211:PCW:H422	0.66	1.66	7	1
3:B:205:PCW:H63	3:B:205:PCW:C1	0.66	2.20	7	1
3:A:403:PCW:O11	3:A:403:PCW:H63	0.66	1.90	8	1
3:A:413:PCW:O31	3:A:413:PCW:H52	0.66	1.90	8	1
3:D:617:PCW:H482	3:C:210:PCW:C27	0.66	2.19	8	2
4:C:213:17F:C23	4:C:215:17F:H58	0.66	2.20	9	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
3:C:210:PCW:H372	3:C:210:PCW:H162	0.66	1.66	14	1
3:B:205:PCW:C23	3:C:210:PCW:H241	0.66	2.18	15	1
3:B:208:PCW:P	3:C:211:PCW:H342	0.66	2.30	20	2
4:B:211:17F:C28	3:C:216:PCW:H212	0.66	2.18	20	1
3:D:609:PCW:C12	3:D:616:PCW:C7	0.66	2.74	10	8
3:C:204:PCW:C46	3:C:204:PCW:C42	0.66	2.72	5	7
4:C:218:17F:C26	4:C:219:17F:H73	0.66	2.21	18	7
4:A:416:17F:H57	3:B:204:PCW:H171	0.66	1.66	18	3
3:A:418:PCW:C48	3:D:613:PCW:H281	0.66	2.20	2	1
4:C:214:17F:H30	4:C:214:17F:H39	0.66	1.67	6	2
3:A:414:PCW:H141	4:A:415:17F:H59	0.66	1.68	3	1
3:C:205:PCW:H63	4:C:214:17F:O5	0.66	1.91	3	1
3:A:408:PCW:H131	3:A:411:PCW:H211	0.66	1.68	4	1
3:D:614:PCW:C41	3:D:620:PCW:H39	0.66	2.21	12	2
3:C:203:PCW:H341	3:C:204:PCW:H32	0.66	1.67	5	1
3:A:403:PCW:H63	3:A:403:PCW:C11	0.66	2.21	8	2
3:B:208:PCW:H40	3:C:216:PCW:C28	0.66	2.13	8	2
3:B:203:PCW:C38	3:C:211:PCW:H441	0.66	2.21	12	2
3:A:404:PCW:H221	3:A:404:PCW:H181	0.66	1.67	12	1
3:D:623:PCW:C13	3:D:623:PCW:H39	0.66	2.21	14	1
3:B:207:PCW:H61	4:B:210:17F:H6	0.66	1.68	14	1
3:D:602:PCW:C42	4:D:628:17F:H41	0.66	2.19	15	1
3:D:621:PCW:H121	4:D:632:17F:C18	0.66	2.20	16	1
3:A:402:PCW:H411	3:C:208:PCW:H381	0.66	1.67	1	2
3:A:406:PCW:C3	4:B:211:17F:H75	0.66	2.21	1	2
3:A:417:PCW:H20	3:A:420:PCW:H431	0.66	1.67	1	2
3:A:417:PCW:H442	3:D:618:PCW:H212	0.66	1.67	1	3
3:D:619:PCW:H131	3:D:627:PCW:C14	0.66	2.20	13	7
3:C:206:PCW:H172	3:C:207:PCW:C19	0.66	2.20	1	1
3:C:217:PCW:H122	4:C:218:17F:H69	0.66	1.67	4	1
3:D:603:PCW:C45	3:D:611:PCW:H432	0.66	2.20	10	2
4:C:215:17F:N1	4:C:215:17F:O2	0.66	2.28	10	3
3:A:401:PCW:C43	3:D:615:PCW:H262	0.66	2.14	17	3
4:A:416:17F:H77	3:D:612:PCW:H472	0.66	1.66	14	1
3:B:204:PCW:H40	3:B:207:PCW:H63	0.66	1.67	17	2
3:C:209:PCW:H282	3:C:209:PCW:H40	0.66	1.67	15	1
3:D:625:PCW:C47	3:D:626:PCW:H482	0.66	2.21	16	1
3:A:403:PCW:O3	3:A:403:PCW:H382	0.66	1.90	8	4
4:A:416:17F:C36	3:B:204:PCW:H271	0.66	2.21	1	2
3:A:420:PCW:C2	3:D:618:PCW:H411	0.66	2.21	4	9
3:D:622:PCW:H181	3:D:622:PCW:C14	0.66	2.21	18	9

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
2:B:68:ARG:HA	2:B:71:TYR:CE1	0.66	2.25	13	4
5:B:201:GSP:O2A	5:B:201:GSP:S1G	0.66	2.54	17	4
3:B:205:PCW:C21	3:B:205:PCW:C25	0.66	2.73	1	10
4:B:211:17F:H12	4:B:211:17F:C35	0.66	2.20	1	2
3:C:203:PCW:O11	3:C:203:PCW:H2	0.66	1.89	20	13
3:D:621:PCW:C28	4:D:632:17F:H35	0.66	2.21	11	2
3:C:207:PCW:H442	4:C:213:17F:H32	0.66	1.66	4	2
3:A:408:PCW:C23	3:A:408:PCW:H182	0.66	2.21	5	3
3:D:613:PCW:H63	3:D:619:PCW:H12	0.66	1.66	5	6
3:A:414:PCW:H351	3:A:414:PCW:O3	0.66	1.91	13	5
3:A:405:PCW:H362	3:A:411:PCW:H461	0.66	1.66	13	5
3:A:418:PCW:H351	3:D:613:PCW:H132	0.66	1.65	11	4
3:D:603:PCW:H382	3:D:624:PCW:H141	0.66	1.66	12	5
3:D:623:PCW:H122	3:D:624:PCW:H331	0.66	1.68	8	1
3:A:401:PCW:H322	3:B:207:PCW:H242	0.66	1.66	10	1
3:C:211:PCW:H132	4:C:215:17F:H58	0.66	1.66	13	1
3:B:206:PCW:H231	3:C:205:PCW:H19	0.66	1.67	15	1
5:C:201:GSP:O3G	6:C:202:MG:MG	0.66	1.39	13	19
4:A:422:17F:C33	4:D:632:17F:H74	0.66	2.21	9	2
3:D:617:PCW:H19	3:D:618:PCW:H483	0.66	1.66	3	1
3:C:205:PCW:H122	3:C:209:PCW:H341	0.66	1.66	3	1
3:A:418:PCW:H341	3:D:613:PCW:H161	0.66	1.65	5	1
3:A:420:PCW:H372	3:D:618:PCW:H432	0.66	1.68	7	1
3:D:613:PCW:H63	3:D:619:PCW:H31	0.66	1.66	7	1
3:B:204:PCW:C3	3:B:207:PCW:H371	0.66	2.20	7	1
3:D:623:PCW:H39	3:D:623:PCW:C13	0.66	2.19	8	1
3:D:619:PCW:H422	3:D:627:PCW:C26	0.66	2.15	10	2
3:D:605:PCW:C21	3:D:614:PCW:H382	0.66	2.21	14	3
4:B:210:17F:H47	3:C:205:PCW:C48	0.66	2.21	17	1
3:B:206:PCW:C23	3:C:205:PCW:H132	0.66	2.21	18	1
4:A:416:17F:H57	3:B:204:PCW:H141	0.66	1.68	20	1
3:D:625:PCW:C15	3:D:625:PCW:C19	0.65	2.74	19	12
3:A:420:PCW:H121	3:D:618:PCW:C45	0.65	2.21	3	1
3:D:618:PCW:H51	3:D:618:PCW:C1	0.65	2.20	3	5
4:D:628:17F:C21	4:D:629:17F:H75	0.65	2.21	19	7
2:B:128:LYS:CB	2:C:47:ASP:HA	0.65	2.21	11	2
3:A:408:PCW:C26	3:D:619:PCW:H462	0.65	2.22	5	1
4:B:211:17F:H47	3:C:204:PCW:C42	0.65	2.19	5	2
3:A:407:PCW:C1	3:A:412:PCW:H11	0.65	2.20	16	4
3:C:206:PCW:C20	3:C:208:PCW:H411	0.65	2.22	6	1
3:B:206:PCW:H283	4:C:214:17F:H20	0.65	1.67	7	3

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
3:A:406:PCW:C39	3:C:204:PCW:H321	0.65	2.20	9	2
3:A:409:PCW:H472	3:A:409:PCW:C27	0.65	2.21	11	4
4:B:211:17F:H40	3:C:204:PCW:H422	0.65	1.67	11	2
3:A:409:PCW:H371	4:B:210:17F:H69	0.65	1.67	12	1
3:A:406:PCW:H40	3:B:205:PCW:H271	0.65	1.67	14	1
3:D:616:PCW:C45	4:C:214:17F:H54	0.65	2.18	16	1
3:A:405:PCW:C36	3:A:411:PCW:C44	0.65	2.74	1	3
3:D:624:PCW:C24	3:D:624:PCW:C20	0.65	2.73	7	20
3:C:209:PCW:C16	4:C:214:17F:H8	0.65	2.18	1	2
3:D:617:PCW:O1P	3:D:617:PCW:H52	0.65	1.92	2	3
3:D:621:PCW:H283	4:D:632:17F:C2X	0.65	2.21	15	4
4:B:210:17F:H2	4:B:210:17F:O2	0.65	1.91	7	13
3:C:205:PCW:H182	3:C:209:PCW:H19	0.65	1.65	4	1
3:D:609:PCW:H51	4:D:632:17F:O2	0.65	1.91	6	3
3:A:408:PCW:C3	3:A:408:PCW:O1P	0.65	2.44	13	5
3:D:621:PCW:H141	4:D:632:17F:H18	0.65	1.68	7	3
4:D:628:17F:H36	4:D:629:17F:H75	0.65	1.67	17	6
3:C:206:PCW:H131	3:C:207:PCW:C19	0.65	2.21	20	3
3:C:207:PCW:H422	4:C:213:17F:H10	0.65	1.69	9	3
3:A:403:PCW:H252	3:D:618:PCW:H222	0.65	1.68	10	1
3:A:406:PCW:C39	3:B:205:PCW:H172	0.65	2.20	11	2
3:A:407:PCW:P	3:A:412:PCW:O1P	0.65	2.54	11	2
3:C:205:PCW:P	3:C:205:PCW:C31	0.65	2.85	12	1
3:D:605:PCW:C38	3:D:612:PCW:H322	0.65	2.20	13	1
3:C:203:PCW:C32	3:C:207:PCW:H332	0.65	2.20	14	1
3:A:421:PCW:H351	3:D:618:PCW:H132	0.65	1.68	18	2
3:B:203:PCW:H161	4:B:209:17F:H18	0.65	1.68	1	1
3:B:207:PCW:H41	3:B:207:PCW:O11	0.65	1.91	5	15
3:C:210:PCW:C32	3:C:210:PCW:H52	0.65	2.22	1	4
3:A:421:PCW:H19	4:D:630:17F:H20	0.65	1.66	6	4
3:C:211:PCW:H262	4:C:215:17F:H52	0.65	1.68	15	3
4:C:218:17F:H51	4:C:219:17F:H78	0.65	1.68	20	5
4:A:415:17F:C34	4:B:209:17F:H37	0.65	2.20	18	5
3:D:603:PCW:O2	3:D:603:PCW:O1P	0.65	2.14	4	4
3:C:203:PCW:C44	3:C:204:PCW:H161	0.65	2.21	12	5
3:A:404:PCW:C31	3:A:404:PCW:C35	0.65	2.75	5	1
3:A:405:PCW:H63	3:A:406:PCW:O11	0.65	1.92	20	5
3:B:206:PCW:H212	3:C:209:PCW:C31	0.65	2.22	19	5
3:B:208:PCW:H482	3:C:216:PCW:C20	0.65	2.21	6	1
3:A:406:PCW:H471	4:B:211:17F:C32	0.65	2.20	8	2
3:A:406:PCW:H39	3:C:204:PCW:H321	0.65	1.68	9	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
3:A:403:PCW:H381	3:A:403:PCW:H151	0.65	1.67	13	1
3:A:419:PCW:C47	3:D:607:PCW:H471	0.65	2.21	15	1
3:A:401:PCW:C6	3:B:207:PCW:O31	0.65	2.44	8	12
3:A:406:PCW:C32	3:B:205:PCW:H321	0.65	2.21	1	1
3:D:616:PCW:H241	4:D:632:17F:H41	0.65	1.68	7	5
2:C:84:ILE:HD11	2:C:118:CYS:HA	0.65	1.68	1	3
4:C:218:17F:N1	4:C:218:17F:O10	0.65	2.30	2	2
1:A:330:ARG:HH21	1:D:447:GLU:HB3	0.65	1.49	7	8
3:D:618:PCW:H2	3:D:618:PCW:O11	0.65	1.92	9	6
3:C:207:PCW:C44	4:C:213:17F:H32	0.65	2.22	6	5
3:B:205:PCW:C17	3:C:204:PCW:H321	0.65	2.22	5	3
3:B:208:PCW:H41	3:C:211:PCW:H51	0.65	1.66	5	1
3:C:206:PCW:H352	3:C:208:PCW:H142	0.65	1.67	7	4
4:A:416:17F:C36	3:B:204:PCW:H222	0.65	2.22	6	1
3:C:206:PCW:C37	3:C:208:PCW:H142	0.65	2.21	8	1
3:D:614:PCW:C26	4:B:209:17F:H50	0.65	2.21	9	2
3:C:203:PCW:H152	4:C:213:17F:C21	0.65	2.22	11	1
3:D:627:PCW:C20	4:D:631:17F:H38	0.65	2.22	13	2
3:D:606:PCW:C5	3:D:626:PCW:H19	0.65	2.22	14	1
3:A:403:PCW:C31	3:A:403:PCW:C35	0.65	2.74	19	14
3:A:408:PCW:O2P	3:A:408:PCW:C3	0.65	2.45	1	4
3:A:408:PCW:H131	3:A:411:PCW:C23	0.65	2.21	2	1
3:D:616:PCW:H483	3:C:207:PCW:H271	0.65	1.68	2	1
3:A:409:PCW:C46	3:A:419:PCW:H241	0.65	2.22	3	1
3:A:414:PCW:H352	3:A:414:PCW:H121	0.65	1.69	17	5
3:A:409:PCW:H352	4:B:210:17F:H65	0.65	1.66	12	2
4:D:628:17F:H5	4:D:628:17F:O8	0.65	1.91	7	1
2:B:72:MET:HA	2:B:78:PHE:HZ	0.65	1.51	17	3
3:A:414:PCW:C21	4:A:415:17F:H20A	0.65	2.20	14	1
3:D:614:PCW:C25	4:B:209:17F:H43	0.65	2.20	14	1
4:C:218:17F:H9A	4:C:218:17F:H20A	0.65	1.68	14	1
3:D:605:PCW:H231	3:D:614:PCW:C39	0.65	2.20	17	11
3:A:406:PCW:H441	3:C:204:PCW:C44	0.65	2.16	2	1
3:D:604:PCW:O31	3:D:606:PCW:H82	0.65	1.91	15	9
4:C:218:17F:H5	4:C:218:17F:C19	0.65	2.14	5	6
3:B:205:PCW:C13	3:C:204:PCW:H42	0.65	2.22	5	1
3:C:205:PCW:C11	3:C:209:PCW:H152	0.65	2.22	11	3
3:C:206:PCW:C15	3:C:207:PCW:H221	0.65	2.20	5	1
3:D:605:PCW:C40	3:D:620:PCW:H141	0.65	2.21	20	5
3:D:608:PCW:H472	4:D:628:17F:H60	0.65	1.68	7	1
3:D:616:PCW:H231	3:C:208:PCW:H251	0.65	1.68	12	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
3:D:619:PCW:C42	3:D:627:PCW:H231	0.65	2.21	12	1
3:A:404:PCW:H52	3:A:406:PCW:P	0.65	2.32	17	1
3:A:406:PCW:H411	3:C:204:PCW:H342	0.65	1.69	20	2
4:D:631:17F:O7	4:D:631:17F:O10	0.65	2.15	15	18
3:C:203:PCW:H142	4:C:213:17F:H30	0.65	1.68	1	1
3:C:209:PCW:C45	3:C:212:PCW:H452	0.65	2.22	1	1
3:D:601:PCW:C42	3:D:601:PCW:C46	0.65	2.72	18	3
3:B:208:PCW:H12	3:C:211:PCW:H342	0.65	1.67	2	2
3:D:602:PCW:H341	4:C:214:17F:H60	0.65	1.68	3	1
3:D:602:PCW:H483	4:D:628:17F:H56	0.65	1.66	3	1
3:C:206:PCW:H352	3:C:208:PCW:C12	0.65	2.21	3	3
3:A:418:PCW:C47	3:D:613:PCW:H271	0.65	2.21	4	1
3:D:623:PCW:H122	3:D:624:PCW:C33	0.65	2.21	7	7
3:C:206:PCW:H61	4:C:213:17F:C9	0.65	2.20	5	1
3:C:206:PCW:H121	3:C:208:PCW:H162	0.65	1.67	6	1
3:A:421:PCW:C14	4:D:630:17F:H11	0.65	2.22	11	1
3:A:406:PCW:H141	4:B:211:17F:O8	0.65	1.92	12	1
3:B:208:PCW:H441	3:C:216:PCW:H271	0.65	1.69	12	2
3:C:205:PCW:H122	3:C:209:PCW:C48	0.65	2.20	12	1
3:B:203:PCW:H381	3:C:211:PCW:C42	0.65	2.22	13	1
3:D:614:PCW:H281	4:B:209:17F:H36	0.65	1.69	14	1
3:B:205:PCW:H131	3:C:204:PCW:C4	0.65	2.21	14	1
3:C:210:PCW:C35	3:C:210:PCW:H121	0.65	2.22	14	1
3:A:405:PCW:C37	3:A:411:PCW:H441	0.65	2.20	20	1
3:D:624:PCW:H221	3:C:217:PCW:C23	0.65	2.22	14	10
2:B:84:ILE:HD11	2:B:118:CYS:HA	0.65	1.67	8	5
3:B:207:PCW:C3	3:B:207:PCW:O1P	0.65	2.45	15	15
4:B:210:17F:H9	3:C:205:PCW:H451	0.65	1.69	15	2
3:A:405:PCW:C28	3:A:418:PCW:H221	0.65	2.21	16	5
3:C:204:PCW:C42	3:C:204:PCW:C46	0.65	2.73	2	13
3:C:209:PCW:H451	3:C:212:PCW:C26	0.65	2.22	3	2
3:A:418:PCW:H332	3:D:613:PCW:O3	0.65	1.92	7	3
3:D:610:PCW:H172	4:D:631:17F:C34	0.65	2.22	6	4
3:D:627:PCW:H42	3:D:627:PCW:C3	0.65	2.22	15	2
3:A:401:PCW:C47	3:D:615:PCW:H242	0.65	2.21	6	1
3:A:404:PCW:H20	3:D:611:PCW:H282	0.65	1.66	16	4
3:D:613:PCW:H212	3:D:613:PCW:H171	0.65	1.66	6	1
3:C:207:PCW:C17	4:C:213:17F:H18	0.65	2.21	7	1
3:A:405:PCW:H352	3:A:411:PCW:H421	0.65	1.66	10	1
3:D:616:PCW:H221	3:C:208:PCW:C23	0.65	2.06	14	1
3:B:205:PCW:H483	3:B:208:PCW:H232	0.65	1.67	15	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
3:B:208:PCW:H62	3:B:208:PCW:O11	0.65	1.92	15	1
3:A:401:PCW:H481	3:D:620:PCW:C27	0.65	2.22	18	1
3:B:208:PCW:H40	3:C:216:PCW:C27	0.65	2.17	19	1
3:D:617:PCW:H52	3:D:617:PCW:O2P	0.65	1.91	20	1
3:A:405:PCW:H361	3:A:411:PCW:H442	0.65	1.68	1	2
4:C:218:17F:H42	4:C:219:17F:C40	0.65	2.21	2	3
3:D:601:PCW:H142	3:B:206:PCW:H171	0.65	1.69	2	1
3:D:602:PCW:C48	3:D:608:PCW:H232	0.65	2.22	5	3
3:A:414:PCW:H483	4:B:209:17F:H65	0.65	1.69	19	3
3:B:208:PCW:H351	3:C:203:PCW:C20	0.65	2.18	17	5
3:C:203:PCW:H442	3:C:204:PCW:C16	0.65	2.22	12	3
3:B:206:PCW:H231	3:C:205:PCW:C17	0.65	2.21	5	2
3:C:203:PCW:C34	3:C:204:PCW:H32	0.65	2.21	5	1
3:A:421:PCW:H61	4:D:630:17F:H6A	0.65	1.67	6	1
3:A:405:PCW:H272	3:A:418:PCW:H241	0.65	1.69	7	3
3:D:610:PCW:H241	3:D:610:PCW:C19	0.65	2.21	8	1
3:B:203:PCW:H151	4:B:209:17F:H1	0.65	1.69	8	1
3:C:212:PCW:H73	4:C:213:17F:H2	0.65	1.67	11	2
3:B:208:PCW:O4P	3:B:208:PCW:O31	0.65	2.14	12	2
3:C:203:PCW:H11	3:C:211:PCW:H62	0.65	1.69	15	1
3:A:412:PCW:H483	3:C:204:PCW:H251	0.65	1.68	19	1
4:D:628:17F:C31	4:D:628:17F:C19	0.65	2.75	5	12
3:A:403:PCW:C32	3:A:404:PCW:H12	0.65	2.21	3	3
3:D:621:PCW:H132	4:D:632:17F:C18	0.65	2.21	13	5
3:B:206:PCW:H252	3:C:205:PCW:C17	0.65	2.18	10	5
4:C:213:17F:H78	4:C:219:17F:C30	0.65	2.22	5	1
3:D:607:PCW:C43	3:D:625:PCW:H471	0.65	2.10	6	1
3:A:418:PCW:O2	3:A:418:PCW:H342	0.65	1.91	15	3
3:D:616:PCW:H141	4:D:632:17F:C9	0.65	2.22	12	1
3:D:619:PCW:P	3:D:627:PCW:H52	0.65	2.32	12	1
3:C:206:PCW:H171	3:C:207:PCW:C18	0.65	2.21	12	1
3:D:618:PCW:O2	3:D:618:PCW:O1P	0.65	2.15	13	1
1:A:217:LEU:HD21	3:A:405:PCW:H252	0.65	1.69	17	3
3:C:203:PCW:H73	3:C:207:PCW:C1	0.65	2.15	14	1
3:A:401:PCW:H442	3:D:615:PCW:C27	0.65	2.22	18	1
3:A:414:PCW:C47	3:A:414:PCW:C43	0.64	2.74	11	15
4:A:415:17F:H4	4:A:415:17F:O10	0.64	1.92	13	9
3:D:610:PCW:H241	3:D:610:PCW:H20	0.64	1.69	17	12
3:D:612:PCW:H51	3:D:623:PCW:H321	0.64	1.69	1	1
3:B:208:PCW:H371	3:C:203:PCW:H221	0.64	1.68	2	2
4:A:416:17F:C1Y	3:B:204:PCW:H162	0.64	2.22	4	2

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
3:A:409:PCW:H483	3:A:419:PCW:H20	0.64	1.69	5	2
3:B:205:PCW:H483	3:B:208:PCW:H20	0.64	1.69	13	1
3:D:608:PCW:H251	4:D:629:17F:H63	0.64	1.68	17	1
3:A:421:PCW:H362	4:D:630:17F:C10	0.64	2.22	20	1
3:D:606:PCW:H161	4:C:218:17F:H12	0.64	1.67	20	1
3:D:608:PCW:C19	4:D:629:17F:H39	0.64	2.21	7	6
3:D:610:PCW:C24	3:D:610:PCW:H20	0.64	2.22	20	13
3:D:622:PCW:O3P	3:D:622:PCW:O31	0.64	2.16	13	18
5:B:201:GSP:O3G	6:B:202:MG:MG	0.64	1.41	10	19
4:C:215:17F:O2	4:C:215:17F:N1	0.64	2.29	5	16
4:C:218:17F:C25	4:C:219:17F:H73	0.64	2.23	13	5
3:A:407:PCW:H121	3:A:410:PCW:C33	0.64	2.22	3	5
3:A:418:PCW:H39	3:D:613:PCW:C43	0.64	2.21	9	3
3:D:616:PCW:H121	4:D:632:17F:C7	0.64	2.22	3	1
3:C:206:PCW:H161	3:C:207:PCW:H242	0.64	1.68	3	1
3:D:603:PCW:H222	3:D:611:PCW:H352	0.64	1.69	11	2
3:D:614:PCW:C21	4:B:209:17F:H51	0.64	2.23	6	3
4:A:415:17F:H37	3:C:211:PCW:H422	0.64	1.67	6	1
3:C:203:PCW:H152	4:C:218:17F:H54	0.64	1.69	6	1
3:A:417:PCW:H161	3:A:420:PCW:H352	0.64	1.70	16	4
3:D:603:PCW:H442	3:D:611:PCW:H362	0.64	1.68	1	1
3:D:610:PCW:C20	3:D:610:PCW:C24	0.64	2.75	6	19
3:B:204:PCW:H31	3:B:207:PCW:H352	0.64	1.67	19	2
3:C:204:PCW:H272	3:C:217:PCW:H472	0.64	1.69	1	2
3:C:204:PCW:C48	3:C:216:PCW:H40	0.64	2.22	1	2
3:D:602:PCW:O31	3:D:602:PCW:H12	0.64	1.93	3	13
3:D:614:PCW:H221	4:B:209:17F:H43	0.64	1.67	11	4
3:A:406:PCW:H483	3:A:406:PCW:C27	0.64	2.18	9	2
3:C:204:PCW:H231	3:C:210:PCW:C28	0.64	2.14	11	3
3:C:216:PCW:H442	3:C:217:PCW:C34	0.64	2.16	4	6
3:D:606:PCW:H41	3:D:606:PCW:O31	0.64	1.92	15	4
3:D:615:PCW:H442	3:D:620:PCW:H19	0.64	1.68	11	4
3:D:619:PCW:H341	4:D:631:17F:C21	0.64	2.22	5	3
3:C:205:PCW:C14	3:C:209:PCW:H321	0.64	2.23	17	2
3:C:207:PCW:H39	4:C:219:17F:C42	0.64	2.21	5	1
3:A:405:PCW:H252	3:A:418:PCW:C24	0.64	2.21	6	1
3:A:406:PCW:H20	4:B:211:17F:C20	0.64	2.21	17	2
3:C:207:PCW:H62	3:C:207:PCW:O11	0.64	1.91	7	1
2:B:15:GLY:HA3	5:B:201:GSP:C8	0.64	2.23	13	4
3:B:203:PCW:H411	3:C:211:PCW:H182	0.64	1.66	10	1
3:C:203:PCW:H281	3:C:211:PCW:C43	0.64	2.21	12	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
3:C:203:PCW:H122	3:C:207:PCW:C39	0.64	2.22	12	1
3:A:406:PCW:H371	4:B:211:17F:H8A	0.64	1.69	17	2
3:A:419:PCW:H82	3:D:626:PCW:H332	0.64	1.67	15	1
3:A:401:PCW:C48	3:D:612:PCW:H461	0.64	2.19	16	1
3:A:417:PCW:C45	3:A:421:PCW:H421	0.64	2.14	20	1
3:A:407:PCW:O3P	3:A:407:PCW:O31	0.64	2.15	20	5
3:D:609:PCW:H62	3:D:621:PCW:O11	0.64	1.91	12	5
3:C:210:PCW:C26	3:C:210:PCW:C22	0.64	2.72	2	13
3:D:609:PCW:C48	3:C:208:PCW:H451	0.64	2.21	3	2
3:B:208:PCW:H371	3:C:203:PCW:H222	0.64	1.67	5	3
3:C:210:PCW:H451	3:C:210:PCW:H181	0.64	1.69	5	1
3:C:210:PCW:O31	3:C:210:PCW:O4P	0.64	2.15	5	1
3:B:208:PCW:H2	3:B:208:PCW:C5	0.64	2.22	6	1
3:A:414:PCW:H252	4:A:415:17F:C34	0.64	2.22	9	2
3:B:208:PCW:H422	3:C:204:PCW:H171	0.64	1.70	8	1
3:A:404:PCW:H462	3:A:404:PCW:H171	0.64	1.68	10	1
3:D:604:PCW:C25	4:C:215:17F:H76	0.64	2.15	12	1
3:C:209:PCW:O3P	3:C:209:PCW:O31	0.64	2.16	14	2
3:B:203:PCW:H332	4:B:210:17F:C22	0.64	2.22	19	1
3:D:605:PCW:O1P	3:D:614:PCW:H62	0.64	1.93	5	3
3:C:211:PCW:O3	4:C:215:17F:H31	0.64	1.91	2	1
4:A:422:17F:H63	3:D:622:PCW:H471	0.64	1.69	16	2
4:A:422:17F:C4	3:D:622:PCW:H151	0.64	2.21	19	3
2:C:82:PHE:HB2	2:C:89:SER:HB2	0.64	1.69	5	3
3:A:419:PCW:H482	3:D:625:PCW:H483	0.64	1.70	6	1
4:B:210:17F:H11A	4:C:215:17F:H8A	0.64	1.68	6	1
3:B:208:PCW:H342	3:C:203:PCW:C19	0.64	2.22	18	3
3:D:606:PCW:C15	4:C:218:17F:H11A	0.64	2.22	14	2
3:A:406:PCW:H332	4:B:211:17F:O1	0.64	1.92	14	1
3:C:207:PCW:H11	3:C:207:PCW:O31	0.64	1.93	14	1
3:C:205:PCW:C2	3:C:209:PCW:H152	0.64	2.23	16	1
3:A:409:PCW:H142	3:A:409:PCW:C18	0.64	2.23	1	19
3:D:602:PCW:H341	4:C:214:17F:C34	0.64	2.23	3	3
3:D:602:PCW:C48	4:D:628:17F:H56	0.64	2.22	3	3
3:D:606:PCW:O11	3:D:606:PCW:H51	0.64	1.92	10	6
3:D:614:PCW:H261	4:B:209:17F:C38	0.64	2.22	3	2
3:C:212:PCW:H422	4:C:215:17F:H67	0.64	1.70	3	1
1:A:325:ASP:HA	1:A:328:ARG:HD2	0.64	1.69	4	5
3:C:205:PCW:C42	3:C:212:PCW:H252	0.64	2.21	4	1
3:A:406:PCW:H462	4:B:211:17F:H58	0.64	1.69	5	1
3:C:206:PCW:C28	3:C:206:PCW:C24	0.64	2.74	6	2

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
3:D:616:PCW:H481	3:C:207:PCW:H251	0.64	1.69	8	1
3:A:417:PCW:C19	3:A:420:PCW:H411	0.64	2.23	9	1
3:C:209:PCW:H42	4:C:214:17F:C4	0.64	2.20	17	1
3:A:404:PCW:H442	3:A:404:PCW:C16	0.64	2.21	10	2
3:A:409:PCW:H19	3:A:409:PCW:C15	0.64	2.23	19	6
3:D:608:PCW:O11	3:D:608:PCW:H2	0.64	1.93	18	20
4:D:632:17F:H65	3:C:208:PCW:C48	0.64	2.23	20	4
3:A:413:PCW:H362	3:C:210:PCW:H141	0.64	1.70	18	5
3:D:618:PCW:H62	3:D:618:PCW:C31	0.64	2.21	9	4
3:A:418:PCW:H352	3:D:613:PCW:H181	0.64	1.70	6	3
3:D:606:PCW:O4P	3:D:606:PCW:C6	0.64	2.46	6	2
4:D:632:17F:H59	4:D:632:17F:C37	0.64	2.23	6	1
3:C:206:PCW:C7	4:C:214:17F:H12A	0.64	2.23	6	1
4:C:219:17F:C33	4:C:219:17F:H10A	0.64	2.23	6	1
4:D:629:17F:H4	4:D:629:17F:C1	0.64	2.21	7	2
3:A:408:PCW:C48	3:A:413:PCW:H241	0.64	2.23	11	2
3:A:417:PCW:H382	3:A:421:PCW:H39	0.64	1.69	10	1
3:C:207:PCW:C41	4:C:213:17F:H11A	0.64	2.23	15	3
3:D:611:PCW:H483	3:B:208:PCW:C23	0.64	2.21	14	1
3:C:203:PCW:H11	3:C:211:PCW:C6	0.64	2.23	15	1
3:B:204:PCW:H432	3:B:207:PCW:C20	0.64	2.23	18	1
1:A:264:LYS:HE2	1:D:509:ALA:HB1	0.64	1.70	8	9
3:D:619:PCW:H381	3:D:627:PCW:C16	0.64	2.18	7	7
4:C:219:17F:H56	4:C:219:17F:H11	0.64	1.68	18	7
3:A:408:PCW:H372	3:A:413:PCW:H182	0.64	1.69	16	2
3:D:603:PCW:H242	3:D:611:PCW:C37	0.64	2.23	3	1
3:D:604:PCW:H452	3:D:606:PCW:C18	0.64	2.23	9	2
3:D:609:PCW:H422	3:D:616:PCW:C46	0.64	2.20	3	4
3:C:212:PCW:H352	4:C:213:17F:H11	0.64	1.70	3	1
3:D:622:PCW:C26	3:C:217:PCW:H61	0.64	2.23	16	3
3:A:408:PCW:H162	3:A:413:PCW:H412	0.64	1.69	5	1
3:A:414:PCW:H51	3:A:414:PCW:O2P	0.64	1.92	5	1
3:B:203:PCW:H361	3:C:211:PCW:C42	0.64	2.23	7	1
3:B:203:PCW:H2	3:C:211:PCW:C39	0.64	2.23	7	1
3:D:603:PCW:H451	3:D:611:PCW:H412	0.64	1.69	9	1
3:C:207:PCW:C41	4:C:213:17F:H12	0.64	2.19	11	2
3:B:205:PCW:H132	3:C:204:PCW:C5	0.64	2.23	20	2
3:A:412:PCW:C45	3:C:210:PCW:H472	0.64	2.23	20	3
4:A:416:17F:H77	4:B:209:17F:H78	0.64	1.70	13	1
3:C:208:PCW:C31	3:C:208:PCW:H51	0.64	2.23	14	1
3:C:206:PCW:H52	4:C:214:17F:H10A	0.64	1.68	16	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
3:C:205:PCW:C41	3:C:212:PCW:H231	0.64	2.20	18	1
3:B:207:PCW:H412	3:B:207:PCW:H232	0.64	1.69	1	1
3:D:615:PCW:H51	3:D:625:PCW:P	0.64	2.33	2	1
3:D:622:PCW:C28	4:D:631:17F:H30	0.64	2.22	10	7
3:A:401:PCW:C12	3:B:207:PCW:H39	0.64	2.23	3	1
3:A:406:PCW:H341	3:B:205:PCW:C34	0.64	2.23	3	4
3:A:414:PCW:H372	4:A:415:17F:C38	0.64	2.20	7	2
3:D:603:PCW:H442	3:D:611:PCW:H351	0.64	1.68	17	4
3:D:627:PCW:H52	3:D:627:PCW:C2	0.64	2.19	10	3
4:C:218:17F:H43	4:C:219:17F:H73	0.64	1.70	4	3
3:B:205:PCW:H12	3:B:208:PCW:H82	0.64	1.70	5	1
3:D:605:PCW:H39	3:D:612:PCW:C34	0.64	2.22	13	6
3:A:417:PCW:H382	3:D:618:PCW:H141	0.64	1.68	7	2
3:D:607:PCW:H12	3:D:626:PCW:C35	0.64	2.23	11	2
4:A:422:17F:O9	3:D:622:PCW:H121	0.64	1.93	15	3
3:A:404:PCW:H20	3:D:611:PCW:H261	0.64	1.70	10	1
3:B:208:PCW:C33	3:C:203:PCW:H20	0.64	2.19	14	1
3:D:602:PCW:H61	3:C:209:PCW:C7	0.64	2.23	16	1
3:C:205:PCW:H61	3:C:206:PCW:H63	0.64	1.70	16	1
3:C:211:PCW:H232	4:C:215:17F:H52	0.64	1.69	18	1
3:C:207:PCW:H172	4:C:213:17F:H19	0.64	1.69	19	1
3:A:408:PCW:H152	3:A:411:PCW:C23	0.64	2.23	18	6
3:D:601:PCW:C46	3:D:601:PCW:C42	0.64	2.75	20	15
3:C:210:PCW:H441	3:C:210:PCW:H161	0.64	1.70	1	3
3:C:212:PCW:H73	4:C:213:17F:O2	0.64	1.93	15	3
3:D:616:PCW:H261	4:D:632:17F:H46	0.64	1.70	3	1
3:B:205:PCW:C25	3:B:205:PCW:C21	0.64	2.72	18	6
3:D:616:PCW:H262	4:C:214:17F:H75	0.64	1.70	4	1
3:D:606:PCW:O11	3:D:606:PCW:C5	0.64	2.45	6	8
3:B:203:PCW:C46	4:C:215:17F:H42	0.64	2.21	5	1
3:A:403:PCW:H131	3:A:403:PCW:H381	0.64	1.70	6	1
3:D:608:PCW:H20	4:D:629:17F:C26	0.64	2.21	11	2
3:D:621:PCW:C13	4:D:632:17F:H18	0.64	2.22	13	2
3:C:205:PCW:C3	3:C:209:PCW:H132	0.64	2.23	14	1
3:D:616:PCW:H122	4:D:632:17F:H8	0.64	1.70	16	1
3:C:206:PCW:H161	3:C:207:PCW:H182	0.64	1.68	16	1
3:A:414:PCW:C14	3:A:414:PCW:C18	0.63	2.76	1	2
3:A:417:PCW:O3P	3:A:417:PCW:O31	0.63	2.17	4	7
3:D:609:PCW:H431	3:C:208:PCW:H242	0.63	1.69	20	3
3:D:624:PCW:C27	3:B:208:PCW:H272	0.63	2.23	1	1
4:D:632:17F:H65	3:C:208:PCW:H483	0.63	1.68	10	2

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
4:B:210:17F:C12	4:B:210:17F:C24	0.63	2.71	16	5
3:D:602:PCW:H341	4:C:214:17F:H61	0.63	1.68	16	4
3:C:212:PCW:H51	4:C:213:17F:O8	0.63	1.93	5	1
3:A:406:PCW:H281	3:D:619:PCW:C26	0.63	2.23	14	4
4:D:632:17F:C30	3:C:206:PCW:H39	0.63	2.20	8	1
3:A:401:PCW:O2	3:B:207:PCW:H231	0.63	1.93	9	1
3:A:408:PCW:C3	3:A:411:PCW:H152	0.63	2.23	9	2
3:C:212:PCW:H441	4:C:215:17F:C1X	0.63	2.23	9	1
3:A:414:PCW:C16	4:A:415:17F:H33	0.63	2.23	16	2
3:A:414:PCW:C31	4:A:415:17F:H10A	0.63	2.23	20	1
3:D:623:PCW:C36	3:D:623:PCW:C32	0.63	2.69	10	17
2:C:37:GLU:HG2	2:C:56:LEU:HD11	0.63	1.71	14	3
3:C:203:PCW:C21	3:C:203:PCW:C25	0.63	2.74	16	15
3:C:204:PCW:O1P	3:C:204:PCW:H32	0.63	1.93	8	12
3:C:209:PCW:H32	3:C:209:PCW:O2P	0.63	1.93	3	5
3:A:402:PCW:H483	3:C:206:PCW:H39	0.63	1.70	2	1
3:A:406:PCW:H141	4:B:211:17F:H8	0.63	1.69	18	2
3:D:624:PCW:H451	4:B:209:17F:H75	0.63	1.69	14	2
3:A:414:PCW:C16	4:A:415:17F:C1Z	0.63	2.75	18	3
3:A:418:PCW:C35	3:D:613:PCW:H132	0.63	2.24	11	5
3:C:216:PCW:H372	3:C:216:PCW:H141	0.63	1.71	4	3
3:A:401:PCW:H73	3:B:207:PCW:O31	0.63	1.94	9	10
3:A:401:PCW:H39	3:B:204:PCW:C23	0.63	2.23	8	2
3:B:208:PCW:O3P	3:C:211:PCW:H321	0.63	1.94	7	5
3:D:603:PCW:H52	4:C:219:17F:O1	0.63	1.93	17	1
3:C:209:PCW:C11	4:C:214:17F:H6	0.63	2.23	18	1
3:A:403:PCW:C45	3:D:618:PCW:H281	0.63	2.23	20	1
3:D:604:PCW:H361	4:C:218:17F:H36	0.63	1.69	18	7
3:C:210:PCW:H52	3:C:210:PCW:H322	0.63	1.69	2	1
3:D:608:PCW:C44	3:C:205:PCW:H271	0.63	2.23	5	1
3:D:612:PCW:H41	3:D:623:PCW:H342	0.63	1.71	9	3
3:A:409:PCW:H272	3:A:409:PCW:H482	0.63	1.71	7	1
3:D:604:PCW:H252	4:C:215:17F:C42	0.63	2.23	10	1
3:C:210:PCW:H321	3:C:210:PCW:H73	0.63	1.68	11	1
3:D:617:PCW:O1P	3:C:216:PCW:H42	0.63	1.92	12	1
3:D:619:PCW:O2P	3:D:627:PCW:H52	0.63	1.94	12	3
3:A:413:PCW:C37	3:C:210:PCW:H141	0.63	2.24	16	2
3:C:203:PCW:C36	3:C:204:PCW:H142	0.63	2.23	17	2
3:A:414:PCW:H63	4:A:415:17F:C7	0.63	2.23	20	1
3:A:418:PCW:O4P	3:A:418:PCW:C6	0.63	2.46	3	15
3:D:608:PCW:H212	4:D:629:17F:H30	0.63	1.69	9	3

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
3:D:626:PCW:C27	3:D:626:PCW:C23	0.63	2.71	11	19
3:A:418:PCW:C35	3:D:613:PCW:C13	0.63	2.76	7	5
1:D:523:ASP:HA	1:D:526:ARG:HD2	0.63	1.70	2	5
3:D:610:PCW:H62	4:D:631:17F:O6	0.63	1.94	20	2
3:D:624:PCW:O4P	3:D:624:PCW:H62	0.63	1.93	13	14
3:C:212:PCW:C24	3:C:212:PCW:C20	0.63	2.73	4	14
3:A:401:PCW:H2	3:A:401:PCW:O2P	0.63	1.93	14	7
3:D:624:PCW:H282	3:C:217:PCW:C27	0.63	2.22	10	2
3:C:206:PCW:H152	3:C:207:PCW:H222	0.63	1.70	8	2
3:A:404:PCW:H39	3:B:205:PCW:C44	0.63	2.23	12	3
3:D:623:PCW:H142	3:D:624:PCW:C35	0.63	2.23	7	3
3:C:207:PCW:H422	4:C:213:17F:C1Z	0.63	2.24	7	1
3:D:617:PCW:H271	3:D:619:PCW:C28	0.63	2.22	16	2
3:B:204:PCW:H52	3:B:204:PCW:C32	0.63	2.24	10	3
3:A:404:PCW:C39	3:B:205:PCW:H451	0.63	2.23	13	3
3:A:414:PCW:C16	4:A:415:17F:H20	0.63	2.20	11	1
3:A:421:PCW:C12	4:D:630:17F:H11	0.63	2.14	17	4
3:D:606:PCW:H252	4:C:218:17F:C24	0.63	2.23	20	4
3:C:207:PCW:H171	3:C:208:PCW:H331	0.63	1.71	12	3
3:A:401:PCW:H472	3:D:612:PCW:C27	0.63	2.23	19	2
1:A:246:ASP:HA	1:D:528:ARG:NH1	0.63	2.08	16	18
3:D:607:PCW:C1	3:D:626:PCW:C37	0.63	2.75	10	5
3:D:610:PCW:O1P	3:D:610:PCW:H52	0.63	1.94	6	9
3:D:614:PCW:C14	3:D:620:PCW:H382	0.63	2.24	11	4
3:B:204:PCW:C11	3:B:204:PCW:O31	0.63	2.46	7	8
3:C:205:PCW:H432	4:C:215:17F:H29	0.63	1.71	2	1
3:A:421:PCW:H19	4:D:630:17F:C31	0.63	2.24	7	4
3:A:402:PCW:H441	3:C:208:PCW:H132	0.63	1.70	5	2
3:D:616:PCW:H221	3:C:208:PCW:C25	0.63	2.19	16	3
3:C:206:PCW:H121	3:C:208:PCW:C16	0.63	2.23	6	1
3:B:204:PCW:C23	3:B:204:PCW:C27	0.63	2.74	13	3
3:A:409:PCW:H2	4:B:210:17F:C20	0.63	2.22	8	1
3:D:612:PCW:H39	3:D:623:PCW:H461	0.63	1.70	10	1
1:A:388:SER:HB2	1:D:594:LYS:HE3	0.63	1.69	11	1
3:C:207:PCW:H351	4:C:213:17F:H66	0.63	1.71	12	1
3:C:212:PCW:H73	4:C:213:17F:O1	0.63	1.92	13	2
3:C:207:PCW:H421	4:C:213:17F:H33	0.63	1.69	14	1
4:C:215:17F:P1	4:C:215:17F:H18A	0.63	2.34	14	1
3:D:622:PCW:H362	4:D:631:17F:C34	0.63	2.23	15	1
3:A:404:PCW:C34	4:A:415:17F:H6	0.63	2.24	17	1
3:D:604:PCW:H283	4:C:213:17F:H51	0.63	1.69	1	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
3:D:621:PCW:O4P	3:D:621:PCW:H2	0.63	1.93	18	4
3:A:417:PCW:C8	4:D:630:17F:H1	0.63	2.23	15	3
3:B:207:PCW:H221	3:B:207:PCW:C36	0.63	2.22	6	4
2:C:117:LYS:HE2	5:C:201:GSP:C4	0.63	2.29	4	9
3:D:602:PCW:C32	4:C:214:17F:H60	0.63	2.24	16	3
3:D:612:PCW:C3	3:D:620:PCW:H63	0.63	2.24	3	4
3:D:619:PCW:H63	3:C:217:PCW:O2P	0.63	1.93	3	5
3:D:603:PCW:H162	3:D:624:PCW:C21	0.63	2.23	16	6
3:B:208:PCW:H73	3:B:208:PCW:O11	0.63	1.94	4	3
4:C:218:17F:H46	4:C:219:17F:H78	0.63	1.71	4	3
3:A:419:PCW:H471	3:C:209:PCW:H462	0.63	1.69	5	1
3:C:205:PCW:H412	3:C:212:PCW:H232	0.63	1.69	7	1
3:B:203:PCW:H242	4:B:209:17F:C19	0.63	2.18	11	1
3:C:211:PCW:H282	4:C:215:17F:C42	0.63	2.21	17	1
3:C:212:PCW:H332	4:C:215:17F:C20	0.63	2.22	17	1
3:D:627:PCW:H222	3:C:216:PCW:H431	0.63	1.68	19	1
4:B:211:17F:H11	4:B:211:17F:H65	0.63	1.70	20	1
3:A:404:PCW:H132	3:B:205:PCW:H442	0.63	1.71	9	3
4:A:416:17F:O9	4:A:416:17F:H20	0.63	1.94	5	6
2:B:32:TYR:CE1	5:B:201:GSP:H5'2	0.63	2.29	10	7
3:B:204:PCW:C17	3:B:204:PCW:C21	0.63	2.68	2	2
3:B:205:PCW:H11	3:B:205:PCW:O31	0.63	1.93	8	4
3:A:407:PCW:H241	3:C:206:PCW:H272	0.63	1.70	3	1
3:A:421:PCW:H162	4:D:630:17F:H20	0.63	1.70	4	4
4:A:422:17F:H43	4:C:219:17F:H67	0.63	1.70	3	4
2:B:36:ILE:HA	2:B:59:ALA:HB2	0.63	1.69	16	7
3:B:203:PCW:O11	3:B:203:PCW:H2	0.63	1.94	12	5
4:C:215:17F:O6	4:C:215:17F:C18	0.63	2.47	3	11
3:A:410:PCW:H281	4:D:631:17F:C42	0.63	2.23	4	1
3:C:205:PCW:H131	3:C:209:PCW:H181	0.63	1.68	4	1
3:B:208:PCW:C22	3:C:211:PCW:H483	0.63	2.23	8	1
4:C:213:17F:H43	4:C:215:17F:C41	0.63	2.23	8	1
4:D:628:17F:H19A	4:D:629:17F:H51	0.63	1.69	9	5
3:D:616:PCW:C14	4:D:632:17F:H9A	0.63	2.23	12	2
3:A:403:PCW:C20	3:A:404:PCW:H251	0.63	2.24	19	1
3:A:414:PCW:H462	3:D:614:PCW:C23	0.63	2.24	19	1
3:C:203:PCW:H381	3:C:204:PCW:C14	0.63	2.24	19	1
4:D:629:17F:O7	4:D:629:17F:C17	0.63	2.47	11	20
3:A:412:PCW:C39	3:C:210:PCW:H362	0.63	2.24	4	1
3:D:604:PCW:H411	4:C:218:17F:C2X	0.63	2.14	6	1
3:C:210:PCW:C18	3:C:210:PCW:H461	0.63	2.24	15	2

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
3:C:209:PCW:C16	4:C:214:17F:H11A	0.63	2.24	7	3
3:A:411:PCW:H283	3:C:210:PCW:C22	0.63	2.18	8	1
4:A:422:17F:C27	4:C:218:17F:H12	0.63	2.23	13	3
3:C:211:PCW:H172	4:C:215:17F:C36	0.63	2.24	9	1
3:C:211:PCW:H132	4:C:215:17F:C32	0.63	2.23	13	1
3:C:211:PCW:H242	4:C:215:17F:H70	0.63	1.71	15	1
3:A:405:PCW:C34	3:A:411:PCW:H441	0.63	2.24	16	1
3:A:418:PCW:C38	3:D:613:PCW:H151	0.63	2.20	17	1
3:D:624:PCW:C45	4:B:209:17F:H74	0.63	2.24	18	1
3:C:203:PCW:C8	4:C:215:17F:H20	0.63	2.24	18	1
1:A:243:MET:HG3	1:A:247:LEU:HD12	0.63	1.71	13	12
3:D:621:PCW:O1P	3:D:622:PCW:H42	0.63	1.94	9	5
3:B:206:PCW:O1P	3:B:206:PCW:C3	0.63	2.47	17	8
1:A:388:SER:HB2	1:D:594:LYS:HE2	0.63	1.68	2	4
3:D:619:PCW:H341	4:D:631:17F:C2X	0.63	2.22	3	4
3:D:627:PCW:C20	3:C:217:PCW:C35	0.63	2.76	13	9
4:D:628:17F:C19	4:D:628:17F:C31	0.63	2.76	2	8
3:B:208:PCW:C47	3:B:208:PCW:C43	0.63	2.76	8	18
3:A:404:PCW:C7	3:B:205:PCW:H40	0.63	2.23	14	3
3:B:203:PCW:H222	4:B:209:17F:C19	0.63	2.24	12	2
3:C:203:PCW:H351	3:C:207:PCW:H371	0.63	1.71	3	1
3:A:407:PCW:H51	3:A:407:PCW:O31	0.63	1.93	7	4
3:A:402:PCW:H452	3:C:206:PCW:H231	0.63	1.70	8	2
3:D:612:PCW:H211	3:D:620:PCW:H442	0.63	1.68	10	1
3:A:414:PCW:H212	4:A:415:17F:C20	0.63	2.24	14	1
3:C:212:PCW:C16	3:C:212:PCW:H221	0.63	2.24	14	1
3:A:406:PCW:H371	4:B:211:17F:C10	0.63	2.24	17	2
3:B:207:PCW:C20	4:B:210:17F:H31	0.63	2.19	15	1
3:D:604:PCW:H231	4:C:215:17F:C41	0.63	2.24	17	1
3:C:211:PCW:H261	4:C:215:17F:H73	0.63	1.70	17	1
3:C:207:PCW:H231	3:C:207:PCW:C27	0.63	2.24	18	1
3:A:418:PCW:H451	3:D:613:PCW:C17	0.63	2.24	20	1
3:A:401:PCW:H73	3:B:207:PCW:H131	0.62	1.70	1	2
3:D:606:PCW:H422	3:D:609:PCW:C3	0.62	2.19	18	3
3:D:606:PCW:O11	3:D:606:PCW:H63	0.62	1.94	15	6
4:C:219:17F:C7	4:C:219:17F:C17	0.62	2.77	5	1
3:D:610:PCW:H31	4:D:631:17F:O9	0.62	1.94	8	4
4:B:210:17F:H36	4:C:215:17F:H30	0.62	1.71	6	1
3:C:207:PCW:H62	3:C:207:PCW:C32	0.62	2.24	20	3
3:A:406:PCW:C25	4:B:211:17F:H60	0.62	2.24	7	1
3:C:206:PCW:H131	3:C:207:PCW:H171	0.62	1.70	7	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
4:C:219:17F:H12A	4:C:219:17F:H59	0.62	1.69	7	1
3:C:206:PCW:H62	4:C:213:17F:O1	0.62	1.94	18	3
3:C:217:PCW:C14	4:C:219:17F:H32	0.62	2.20	8	1
3:A:414:PCW:H452	4:B:209:17F:H40	0.62	1.69	9	2
3:C:210:PCW:O31	3:C:210:PCW:H73	0.62	1.94	13	3
1:A:213:THR:HA	1:D:561:LYS:HE2	0.62	1.70	10	1
3:B:208:PCW:C4	3:B:208:PCW:H2	0.62	2.24	10	2
3:D:614:PCW:H63	3:D:624:PCW:C8	0.62	2.24	11	1
3:A:405:PCW:H82	4:B:211:17F:H4A	0.62	1.70	16	2
4:A:422:17F:H66	3:D:622:PCW:C42	0.62	2.23	15	2
3:A:401:PCW:C46	3:D:612:PCW:H251	0.62	2.24	14	2
3:A:413:PCW:H412	3:C:210:PCW:H442	0.62	1.71	15	1
3:B:206:PCW:H31	3:B:206:PCW:C5	0.62	2.24	17	1
4:A:416:17F:H57	3:B:204:PCW:C14	0.62	2.24	20	1
3:D:601:PCW:C38	4:D:628:17F:H52	0.62	2.23	13	2
2:C:22:GLN:O	2:C:26:ASN:HA	0.62	1.94	1	17
4:C:215:17F:O10	4:C:215:17F:H20A	0.62	1.93	2	16
3:D:608:PCW:C18	4:D:629:17F:H46	0.62	2.24	2	1
3:B:207:PCW:O11	3:B:207:PCW:H41	0.62	1.95	2	2
3:A:403:PCW:C48	3:A:404:PCW:H283	0.62	2.24	19	3
3:A:406:PCW:H161	4:B:211:17F:H19A	0.62	1.71	6	3
3:A:419:PCW:C38	3:D:625:PCW:H251	0.62	2.24	8	2
3:D:603:PCW:H271	3:D:611:PCW:C21	0.62	2.20	7	2
3:D:604:PCW:H52	4:C:219:17F:O2	0.62	1.93	7	1
3:B:203:PCW:H19	3:B:204:PCW:H39	0.62	1.71	7	1
3:C:212:PCW:H211	3:C:212:PCW:H162	0.62	1.68	7	2
4:C:213:17F:H29	4:C:215:17F:H56	0.62	1.71	9	1
3:A:403:PCW:O11	3:A:403:PCW:C4	0.62	2.46	15	5
3:C:210:PCW:H121	3:C:210:PCW:H352	0.62	1.71	14	1
3:C:203:PCW:H222	3:C:203:PCW:H181	0.62	1.70	2	4
3:C:209:PCW:C47	3:C:209:PCW:C43	0.62	2.77	7	18
3:D:604:PCW:O31	3:D:604:PCW:O3	0.62	2.16	9	14
3:D:606:PCW:H161	4:C:218:17F:C12	0.62	2.24	20	4
3:D:616:PCW:H211	4:D:632:17F:C22	0.62	2.23	3	1
3:A:409:PCW:H332	3:B:206:PCW:H361	0.62	1.69	4	1
3:A:413:PCW:H382	3:C:210:PCW:H441	0.62	1.71	5	1
3:B:208:PCW:H321	3:C:211:PCW:O4P	0.62	1.94	5	1
4:A:415:17F:C21	3:C:211:PCW:H422	0.62	2.23	6	1
3:D:612:PCW:O31	3:D:620:PCW:H61	0.62	1.93	6	1
3:D:621:PCW:H141	4:D:632:17F:C18	0.62	2.25	7	3
2:B:68:ARG:HA	2:B:71:TYR:CE2	0.62	2.29	7	2

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
3:C:205:PCW:H41	4:C:214:17F:O8	0.62	1.94	7	2
3:D:619:PCW:P	3:D:627:PCW:H51	0.62	2.34	8	1
3:C:216:PCW:H422	3:C:217:PCW:H341	0.62	1.71	8	3
3:D:614:PCW:C20	4:B:209:17F:H48	0.62	2.24	11	5
3:A:408:PCW:C15	3:A:411:PCW:H211	0.62	2.21	20	3
3:D:625:PCW:H371	3:D:626:PCW:H121	0.62	1.69	11	1
4:C:213:17F:H50	4:C:215:17F:C39	0.62	2.24	11	1
4:A:422:17F:H58	4:D:632:17F:H77	0.62	1.69	12	1
3:D:610:PCW:H82	4:D:631:17F:O8	0.62	1.95	12	2
3:C:208:PCW:H42	3:C:208:PCW:C31	0.62	2.23	12	1
3:D:616:PCW:H362	3:C:208:PCW:H283	0.62	1.71	14	1
3:C:207:PCW:H281	4:C:214:17F:H42	0.62	1.71	20	1
3:A:406:PCW:O31	3:A:406:PCW:O3P	0.62	2.16	2	18
3:D:605:PCW:H261	3:D:614:PCW:H181	0.62	1.71	2	3
3:B:208:PCW:H483	4:C:218:17F:H54	0.62	1.70	7	3
3:A:406:PCW:H271	3:A:406:PCW:C48	0.62	2.19	9	2
3:D:605:PCW:O1P	3:D:614:PCW:C5	0.62	2.47	19	4
3:C:206:PCW:C24	3:C:206:PCW:C28	0.62	2.73	8	3
3:D:623:PCW:C38	3:D:625:PCW:H171	0.62	2.25	11	2
3:C:206:PCW:C15	3:C:207:PCW:H242	0.62	2.24	8	1
3:C:211:PCW:H212	4:C:215:17F:H69	0.62	1.70	9	2
4:A:416:17F:C42	3:D:623:PCW:H242	0.62	2.25	10	1
3:A:418:PCW:H42	3:A:418:PCW:C2	0.62	2.23	10	1
3:D:607:PCW:H262	3:B:206:PCW:H481	0.62	1.69	20	2
3:D:612:PCW:C13	3:D:620:PCW:H171	0.62	2.24	10	1
3:B:205:PCW:O11	3:C:204:PCW:C5	0.62	2.47	10	3
3:A:402:PCW:H451	4:D:632:17F:H47	0.62	1.69	14	1
3:A:404:PCW:H39	3:B:205:PCW:H421	0.62	1.71	1	1
3:A:406:PCW:C20	3:A:411:PCW:H472	0.62	2.25	1	1
3:A:406:PCW:H272	3:D:617:PCW:H281	0.62	1.71	1	1
3:B:207:PCW:C34	3:B:207:PCW:H182	0.62	2.25	2	2
3:C:203:PCW:H39	4:C:213:17F:C35	0.62	2.23	1	3
3:C:206:PCW:C15	3:C:208:PCW:H171	0.62	2.24	13	4
3:C:207:PCW:H172	3:C:208:PCW:H331	0.62	1.72	1	1
3:A:403:PCW:O11	3:A:403:PCW:O2	0.62	2.17	11	15
3:A:413:PCW:C11	3:A:413:PCW:O31	0.62	2.48	15	11
3:A:419:PCW:H381	3:D:625:PCW:C25	0.62	2.23	8	5
3:A:417:PCW:H121	3:D:618:PCW:C33	0.62	2.24	16	4
3:A:408:PCW:H261	3:C:210:PCW:H242	0.62	1.70	4	2
3:D:615:PCW:C6	3:D:625:PCW:O1P	0.62	2.46	8	10
3:D:602:PCW:H142	3:D:602:PCW:C38	0.62	2.10	5	3

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
3:A:413:PCW:H451	3:C:210:PCW:H242	0.62	1.70	7	1
3:D:612:PCW:H211	3:D:620:PCW:C44	0.62	2.24	10	1
4:B:211:17F:H11	4:B:211:17F:C38	0.62	2.23	14	3
3:D:620:PCW:C45	4:B:209:17F:H74	0.62	2.24	19	2
3:C:212:PCW:C22	4:C:215:17F:H10A	0.62	2.24	13	1
3:D:604:PCW:H82	4:C:219:17F:H6	0.62	1.72	14	1
3:C:210:PCW:H181	3:C:210:PCW:H441	0.62	1.72	14	1
3:D:619:PCW:C46	3:B:205:PCW:H232	0.62	2.22	16	1
4:B:210:17F:H1A	3:C:205:PCW:C37	0.62	2.24	18	1
3:A:405:PCW:H362	3:A:411:PCW:H441	0.62	1.68	3	2
3:B:208:PCW:H412	3:C:216:PCW:H283	0.62	1.69	1	1
3:D:620:PCW:H11	3:D:620:PCW:O31	0.62	1.95	6	17
3:C:204:PCW:C20	3:C:216:PCW:H281	0.62	2.25	3	1
3:A:421:PCW:O31	3:D:618:PCW:H52	0.62	1.94	12	7
3:D:612:PCW:H20	3:D:620:PCW:H482	0.62	1.70	4	1
2:B:47:ASP:HB2	2:B:164:ARG:HH12	0.62	1.54	4	1
3:B:204:PCW:C1	3:B:204:PCW:H73	0.62	2.24	12	5
3:A:410:PCW:C22	4:A:422:17F:H74	0.62	2.24	11	2
4:D:632:17F:C37	4:D:632:17F:C32	0.62	2.77	8	2
3:C:206:PCW:H171	3:C:208:PCW:C38	0.62	2.24	6	1
3:A:411:PCW:H11	3:B:205:PCW:H131	0.62	1.71	13	3
1:A:288:ARG:O	1:A:292:HIS:HB2	0.62	1.94	8	2
3:A:409:PCW:H272	3:A:409:PCW:C47	0.62	2.24	9	4
3:A:410:PCW:H122	3:C:207:PCW:H171	0.62	1.71	13	1
3:C:208:PCW:H252	4:C:214:17F:H53	0.62	1.72	13	1
3:A:406:PCW:C22	3:A:411:PCW:H472	0.62	2.24	16	1
3:A:418:PCW:O4P	3:A:418:PCW:O31	0.62	2.16	2	4
3:D:603:PCW:C22	3:D:611:PCW:H331	0.62	2.24	1	4
3:D:606:PCW:C18	3:D:606:PCW:C14	0.62	2.77	3	13
3:D:618:PCW:C23	3:D:618:PCW:C27	0.62	2.75	4	4
3:D:622:PCW:H19	4:D:631:17F:O10	0.62	1.94	9	7
3:A:411:PCW:H271	3:C:210:PCW:C23	0.62	2.23	6	2
4:A:416:17F:C41	4:B:209:17F:H74	0.62	2.22	9	1
3:A:421:PCW:H381	3:D:618:PCW:H141	0.62	1.72	10	1
3:C:216:PCW:H142	3:C:216:PCW:C37	0.62	2.21	18	2
4:A:422:17F:O10	4:A:422:17F:P1	0.62	2.58	18	3
3:C:207:PCW:H411	4:C:213:17F:H8A	0.62	1.69	14	2
3:C:206:PCW:C4	4:C:214:17F:H10A	0.62	2.25	16	1
3:A:409:PCW:H182	3:A:419:PCW:H261	0.62	1.72	17	1
4:C:213:17F:H47	4:C:215:17F:H67	0.62	1.72	17	1
3:B:208:PCW:H342	3:C:203:PCW:H19	0.62	1.71	18	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
3:C:209:PCW:H341	3:C:212:PCW:H271	0.62	1.71	19	1
4:D:628:17F:O10	4:D:628:17F:C7	0.62	2.48	17	17
3:C:203:PCW:H461	3:C:204:PCW:C16	0.62	2.23	5	3
1:D:465:GLU:O	1:D:469:LEU:HG	0.62	1.93	14	12
2:B:32:TYR:HE1	5:B:201:GSP:H5'2	0.62	1.55	2	1
4:C:213:17F:O10	4:C:213:17F:H20	0.62	1.94	13	4
3:C:205:PCW:H421	3:C:212:PCW:H242	0.62	1.70	3	2
3:C:211:PCW:H181	3:C:211:PCW:C22	0.62	2.14	11	8
4:D:632:17F:C30	3:C:208:PCW:H161	0.62	2.24	19	7
4:A:416:17F:H69	3:B:204:PCW:H272	0.62	1.70	5	1
3:D:607:PCW:H472	3:C:209:PCW:H251	0.62	1.72	5	1
5:B:201:GSP:H5'1	5:B:201:GSP:O1B	0.62	1.95	5	1
3:D:619:PCW:C43	3:D:627:PCW:H282	0.62	2.25	11	4
3:A:401:PCW:H322	3:B:207:PCW:H232	0.62	1.71	7	1
3:D:615:PCW:C42	3:D:615:PCW:C46	0.62	2.72	17	2
3:D:616:PCW:H161	4:D:632:17F:H11A	0.62	1.70	12	2
3:A:414:PCW:H122	4:A:415:17F:H33	0.62	1.72	14	1
3:C:206:PCW:H19	3:C:207:PCW:H182	0.62	1.70	16	1
3:A:404:PCW:H342	4:A:415:17F:O8	0.62	1.94	17	1
3:C:203:PCW:H82	4:C:215:17F:H20	0.62	1.71	18	1
3:A:401:PCW:H341	3:B:207:PCW:H39	0.62	1.71	19	1
3:D:602:PCW:O31	3:D:602:PCW:H31	0.62	1.94	20	7
3:D:605:PCW:O31	3:D:605:PCW:O3P	0.62	2.18	7	18
3:C:207:PCW:H31	3:C:207:PCW:P	0.62	2.35	20	8
3:A:417:PCW:C41	3:A:417:PCW:H371	0.62	2.24	2	8
3:D:604:PCW:C3	3:D:604:PCW:O1P	0.62	2.48	16	10
3:A:403:PCW:H282	3:A:403:PCW:C24	0.62	2.24	3	3
3:C:203:PCW:H282	3:C:211:PCW:H471	0.62	1.69	7	2
3:D:604:PCW:H82	4:C:219:17F:H4A	0.62	1.68	4	1
3:D:606:PCW:H73	3:D:626:PCW:C19	0.62	2.25	20	4
3:C:205:PCW:H2	4:C:214:17F:O7	0.62	1.94	4	1
3:C:207:PCW:H372	3:C:207:PCW:C42	0.62	2.22	4	1
3:A:421:PCW:H162	4:D:630:17F:C31	0.62	2.24	10	5
3:D:617:PCW:H451	3:C:204:PCW:C45	0.62	2.23	11	3
3:D:617:PCW:H40	3:D:619:PCW:H162	0.62	1.71	11	2
3:C:207:PCW:C19	4:C:213:17F:H57	0.62	2.25	8	1
3:A:411:PCW:P	4:B:211:17F:H1A	0.62	2.35	10	2
3:C:203:PCW:H40	4:C:213:17F:H70	0.62	1.72	11	3
4:D:632:17F:H62	3:C:208:PCW:C48	0.62	2.24	13	1
3:A:406:PCW:H271	4:B:211:17F:H60	0.62	1.71	15	1
4:A:415:17F:C30	3:B:208:PCW:H232	0.62	2.24	19	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
3:A:408:PCW:H31	3:A:408:PCW:P	0.62	2.35	1	3
3:A:406:PCW:H372	3:B:205:PCW:O3	0.62	1.95	5	2
3:A:421:PCW:C11	4:D:630:17F:H9	0.62	2.25	12	3
3:A:420:PCW:C44	3:D:611:PCW:H211	0.62	2.24	6	1
3:D:606:PCW:C14	3:D:606:PCW:C18	0.62	2.78	8	7
3:C:212:PCW:H411	3:C:212:PCW:C17	0.62	2.24	19	3
3:D:603:PCW:H141	3:D:624:PCW:H181	0.62	1.70	17	4
3:B:203:PCW:C15	4:B:209:17F:H1	0.62	2.25	8	1
3:C:216:PCW:H121	3:C:217:PCW:H171	0.62	1.72	8	2
3:C:217:PCW:H362	4:C:218:17F:H77	0.62	1.70	10	3
3:A:418:PCW:H332	3:D:613:PCW:H152	0.62	1.70	12	1
3:A:408:PCW:H32	3:A:411:PCW:H141	0.62	1.69	14	1
3:A:411:PCW:H472	4:B:211:17F:H32	0.62	1.71	19	1
3:D:607:PCW:H31	3:D:626:PCW:H39	0.62	1.70	19	1
4:D:631:17F:H30	3:C:217:PCW:H61	0.62	1.70	20	1
3:D:615:PCW:H452	3:D:620:PCW:H20	0.61	1.70	2	5
3:D:617:PCW:H341	3:C:216:PCW:C34	0.61	2.19	4	7
3:D:624:PCW:C6	3:D:624:PCW:C31	0.61	2.78	17	12
2:B:22:GLN:O	2:B:26:ASN:HA	0.61	1.95	14	16
3:A:402:PCW:H441	3:C:208:PCW:H152	0.61	1.70	2	2
3:D:617:PCW:H341	3:C:216:PCW:H362	0.61	1.72	15	4
3:A:420:PCW:H11	3:D:618:PCW:H381	0.61	1.72	3	1
3:B:203:PCW:O31	3:C:211:PCW:H39	0.61	1.94	5	2
3:A:401:PCW:H51	3:B:207:PCW:O31	0.61	1.95	13	2
3:A:402:PCW:C45	4:D:632:17F:H51	0.61	2.23	8	4
3:C:207:PCW:H441	4:C:213:17F:C1Z	0.61	2.25	18	6
3:A:414:PCW:H141	4:A:415:17F:C35	0.61	2.21	8	2
3:B:206:PCW:H141	3:B:206:PCW:H39	0.61	1.71	8	1
3:D:604:PCW:H271	3:C:212:PCW:H451	0.61	1.72	13	1
3:B:206:PCW:H231	3:C:205:PCW:C19	0.61	2.24	16	2
3:B:203:PCW:H371	4:B:210:17F:H37	0.61	1.72	18	1
3:D:607:PCW:C31	3:D:626:PCW:H371	0.61	2.25	19	1
4:A:415:17F:O1	4:A:415:17F:C2	0.61	2.48	8	11
3:B:204:PCW:C6	3:B:204:PCW:O4P	0.61	2.47	2	1
3:C:203:PCW:C25	3:C:203:PCW:C21	0.61	2.73	4	5
3:A:412:PCW:H381	3:C:210:PCW:C36	0.61	2.25	4	1
3:D:604:PCW:H482	3:D:626:PCW:C27	0.61	2.25	19	3
3:D:605:PCW:H232	3:D:614:PCW:H161	0.61	1.72	15	2
3:D:614:PCW:H482	3:D:620:PCW:H181	0.61	1.69	7	4
2:B:78:PHE:HB2	2:B:111:MET:HG2	0.61	1.71	19	7
4:C:213:17F:H20	4:C:213:17F:O10	0.61	1.94	9	8

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
4:D:629:17F:H1	4:D:629:17F:C4	0.61	2.22	7	1
3:D:616:PCW:H63	4:D:632:17F:C2	0.61	2.24	17	2
3:A:414:PCW:H452	4:B:209:17F:H29	0.61	1.69	11	1
3:D:619:PCW:H442	3:D:627:PCW:H282	0.61	1.72	11	1
3:D:616:PCW:H222	3:C:208:PCW:C27	0.61	2.25	12	1
3:D:619:PCW:C35	3:D:627:PCW:C34	0.61	2.78	16	2
4:C:219:17F:H10A	4:C:219:17F:C33	0.61	2.25	13	1
3:A:418:PCW:O31	3:A:418:PCW:H41	0.61	1.95	16	1
3:A:413:PCW:H283	3:A:413:PCW:C41	0.61	2.24	18	1
3:D:608:PCW:H19	3:D:608:PCW:C15	0.61	2.18	18	1
3:D:624:PCW:C26	3:C:217:PCW:H242	0.61	2.24	18	1
3:D:607:PCW:H471	3:C:209:PCW:C48	0.61	2.22	20	1
3:D:603:PCW:H141	3:D:624:PCW:H182	0.61	1.73	1	2
3:A:401:PCW:H342	3:B:207:PCW:C39	0.61	2.25	2	4
3:D:620:PCW:H481	3:D:624:PCW:C44	0.61	2.25	2	1
3:A:407:PCW:C12	3:A:410:PCW:C33	0.61	2.78	3	2
3:A:409:PCW:H461	3:A:419:PCW:H241	0.61	1.71	3	1
3:A:413:PCW:H40	3:C:210:PCW:C23	0.61	2.26	15	2
3:A:414:PCW:C43	3:A:414:PCW:C47	0.61	2.74	5	5
3:A:406:PCW:H321	3:B:205:PCW:H342	0.61	1.72	14	3
3:D:613:PCW:H321	3:D:619:PCW:C15	0.61	2.25	4	2
3:A:408:PCW:H162	3:A:413:PCW:H411	0.61	1.70	5	1
3:D:604:PCW:H41	3:D:604:PCW:O11	0.61	1.94	8	3
3:C:211:PCW:O4P	3:C:211:PCW:C6	0.61	2.47	5	1
3:A:401:PCW:H481	3:D:615:PCW:H471	0.61	1.71	9	1
3:A:404:PCW:H141	3:A:404:PCW:C38	0.61	2.23	9	4
3:D:614:PCW:C3	3:D:620:PCW:H2	0.61	2.25	19	2
3:D:616:PCW:C23	3:C:208:PCW:H272	0.61	2.26	12	1
3:A:401:PCW:H39	3:B:204:PCW:H281	0.61	1.72	13	1
3:B:208:PCW:C8	3:C:204:PCW:H12	0.61	2.25	15	1
3:C:203:PCW:H381	3:C:204:PCW:H141	0.61	1.70	19	1
3:A:401:PCW:H272	3:D:615:PCW:H283	0.61	1.72	1	1
3:A:401:PCW:H41	3:B:207:PCW:H321	0.61	1.73	1	2
3:A:401:PCW:C31	3:A:401:PCW:O3	0.61	2.49	18	14
4:A:416:17F:H9A	4:A:416:17F:C18	0.61	2.24	20	3
3:D:615:PCW:C4	3:D:625:PCW:O1P	0.61	2.49	1	3
3:D:625:PCW:C19	3:D:625:PCW:C15	0.61	2.75	1	3
3:C:211:PCW:H262	4:C:215:17F:C29	0.61	2.25	1	3
3:A:406:PCW:H472	3:B:205:PCW:C26	0.61	2.25	13	3
1:D:444:ASP:O	1:D:448:VAL:HB	0.61	1.96	6	7
3:D:609:PCW:C45	3:C:208:PCW:H20	0.61	2.25	3	2

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
3:C:206:PCW:C16	3:C:207:PCW:H242	0.61	2.25	3	2
1:A:396:LYS:HE2	1:D:587:ALA:HA	0.61	1.72	12	8
3:C:205:PCW:H141	3:C:209:PCW:H321	0.61	1.72	5	4
3:A:414:PCW:H452	4:B:209:17F:H36	0.61	1.70	17	3
3:A:419:PCW:H481	3:D:607:PCW:H471	0.61	1.71	6	1
1:D:463:TRP:CD1	4:D:629:17F:H71	0.61	2.30	17	4
3:D:604:PCW:H482	3:D:626:PCW:H281	0.61	1.68	13	2
4:B:209:17F:H10	4:B:209:17F:H62	0.61	1.72	10	1
3:C:216:PCW:H161	3:C:217:PCW:H162	0.61	1.73	18	2
3:C:212:PCW:H441	3:C:212:PCW:C22	0.61	2.24	12	1
3:C:206:PCW:C17	3:C:208:PCW:H342	0.61	2.25	16	2
1:A:245:LYS:HA	1:A:249:GLU:HG3	0.61	1.73	1	3
3:A:402:PCW:H412	3:C:208:PCW:H381	0.61	1.73	1	4
3:A:408:PCW:H182	3:A:408:PCW:H231	0.61	1.73	16	11
3:A:414:PCW:C35	4:A:415:17F:H57	0.61	2.24	18	3
3:B:205:PCW:O4P	3:B:205:PCW:C6	0.61	2.49	6	6
3:D:609:PCW:H483	3:C:208:PCW:C45	0.61	2.25	3	1
3:D:616:PCW:C47	3:C:208:PCW:H20	0.61	2.25	4	1
2:B:117:LYS:HE2	5:B:201:GSP:C4	0.61	2.29	12	7
3:D:616:PCW:C48	3:C:206:PCW:H122	0.61	2.25	5	1
3:B:205:PCW:H172	3:C:204:PCW:H321	0.61	1.71	19	2
3:C:203:PCW:H182	3:C:211:PCW:H131	0.61	1.71	5	1
3:C:212:PCW:H211	3:C:212:PCW:C16	0.61	2.26	7	2
4:A:415:17F:O1	4:A:415:17F:H2	0.61	1.96	8	2
3:A:418:PCW:C42	3:D:613:PCW:H251	0.61	2.26	12	5
3:D:614:PCW:C43	3:D:620:PCW:H39	0.61	2.26	17	2
3:C:203:PCW:H351	3:C:207:PCW:H332	0.61	1.72	12	1
4:A:416:17F:H72	4:B:209:17F:H73	0.61	1.73	13	1
3:D:619:PCW:H342	3:D:627:PCW:H341	0.61	1.72	14	1
1:D:563:LYS:HB2	1:D:564:PRO:HD3	0.61	1.70	18	3
3:C:207:PCW:H452	4:C:213:17F:H74	0.61	1.72	16	1
3:C:206:PCW:H12	4:C:214:17F:C1X	0.61	2.25	20	1
3:A:406:PCW:H371	3:A:406:PCW:H412	0.61	1.70	1	5
3:D:623:PCW:C38	3:D:625:PCW:H182	0.61	2.26	4	6
3:B:204:PCW:C27	3:B:204:PCW:C23	0.61	2.77	15	10
3:A:417:PCW:H371	3:A:417:PCW:H411	0.61	1.71	2	3
3:A:418:PCW:H371	3:D:613:PCW:H151	0.61	1.71	11	2
3:B:208:PCW:O4P	3:B:208:PCW:H2	0.61	1.96	3	3
3:C:211:PCW:H242	4:C:215:17F:H72	0.61	1.73	3	1
4:A:416:17F:H74	4:B:209:17F:C38	0.61	2.26	4	1
3:C:210:PCW:H432	3:C:210:PCW:H162	0.61	1.71	5	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
3:C:216:PCW:H172	3:C:217:PCW:H182	0.61	1.73	5	2
3:A:420:PCW:H52	3:A:420:PCW:O2P	0.61	1.95	17	5
3:D:607:PCW:H361	3:D:626:PCW:C44	0.61	2.26	18	3
3:A:409:PCW:H352	4:B:210:17F:C36	0.61	2.25	12	2
3:C:216:PCW:H52	3:C:216:PCW:H322	0.61	1.70	17	2
3:A:406:PCW:C43	4:B:211:17F:H12	0.61	2.26	8	1
3:A:410:PCW:H431	3:A:412:PCW:C38	0.61	2.26	8	1
3:B:206:PCW:C24	3:B:206:PCW:C28	0.61	2.74	8	1
3:B:207:PCW:C23	3:B:207:PCW:H362	0.61	2.26	10	1
3:D:605:PCW:C45	3:D:624:PCW:H441	0.61	2.14	20	3
1:A:301:LEU:HD13	1:D:473:LYS:HG3	0.61	1.73	1	1
4:B:210:17F:H10	3:C:205:PCW:H471	0.61	1.71	1	1
3:A:412:PCW:C45	3:C:210:PCW:H182	0.61	2.21	15	3
3:B:205:PCW:H462	3:B:208:PCW:H19	0.61	1.71	2	1
3:C:207:PCW:C20	4:C:213:17F:H57	0.61	2.26	2	1
3:A:410:PCW:H283	4:A:422:17F:H75	0.61	1.72	3	2
4:D:628:17F:C23	4:D:629:17F:H75	0.61	2.24	16	5
3:A:408:PCW:H351	3:A:413:PCW:H151	0.61	1.70	6	3
3:D:611:PCW:H82	3:C:216:PCW:H73	0.61	1.71	11	5
3:D:616:PCW:H221	3:C:208:PCW:H261	0.61	1.71	8	1
3:C:207:PCW:H2	4:C:213:17F:H4A	0.61	1.72	11	2
3:C:212:PCW:C37	4:C:215:17F:H20A	0.61	2.23	9	1
3:D:605:PCW:H262	3:D:614:PCW:H181	0.61	1.72	17	2
3:D:617:PCW:H63	3:D:617:PCW:O11	0.61	1.95	12	1
3:D:606:PCW:H41	3:D:606:PCW:H2	0.61	1.71	15	2
3:D:617:PCW:H412	3:D:617:PCW:C37	0.61	2.26	14	1
3:A:402:PCW:H332	3:A:407:PCW:H121	0.61	1.73	1	2
3:A:419:PCW:H82	3:D:626:PCW:H362	0.61	1.71	4	5
3:A:420:PCW:O2	3:D:618:PCW:C41	0.61	2.49	4	9
3:A:419:PCW:H63	3:D:626:PCW:O31	0.61	1.95	20	4
3:D:606:PCW:H162	4:C:218:17F:H30	0.61	1.71	18	6
3:C:217:PCW:O3	4:C:218:17F:H68	0.61	1.96	4	1
3:A:402:PCW:H82	3:A:407:PCW:C3	0.61	2.26	5	1
3:A:408:PCW:H151	3:A:413:PCW:H372	0.61	1.72	7	4
3:B:206:PCW:C23	3:C:205:PCW:H171	0.61	2.25	5	3
3:D:607:PCW:C48	3:C:209:PCW:H483	0.61	2.26	6	1
3:D:623:PCW:H142	3:D:624:PCW:H351	0.61	1.72	14	3
3:C:205:PCW:H182	3:C:209:PCW:H221	0.61	1.72	19	5
3:D:617:PCW:C19	3:D:618:PCW:H482	0.61	2.26	10	1
3:D:622:PCW:C23	3:C:217:PCW:H82	0.61	2.21	13	4
3:C:212:PCW:C42	4:C:215:17F:H36	0.61	2.23	10	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
3:A:410:PCW:H42	3:A:410:PCW:H12	0.61	1.73	12	1
3:D:627:PCW:C24	3:C:217:PCW:H372	0.61	2.26	14	1
3:C:209:PCW:H40	3:C:209:PCW:C28	0.61	2.25	15	1
3:B:208:PCW:C35	3:C:203:PCW:H20	0.61	2.20	17	1
3:B:203:PCW:C27	4:B:210:17F:H53	0.61	2.25	20	1
3:B:204:PCW:H39	3:B:207:PCW:H63	0.61	1.71	20	1
4:A:416:17F:H65	3:B:204:PCW:C26	0.61	2.24	2	2
3:D:602:PCW:C6	3:D:602:PCW:O4P	0.61	2.49	12	19
3:D:611:PCW:O11	3:D:617:PCW:H41	0.61	1.95	3	3
3:B:206:PCW:C6	3:B:206:PCW:O4P	0.61	2.49	4	9
3:B:207:PCW:H162	3:B:207:PCW:H342	0.61	1.72	1	2
4:B:210:17F:H64	3:C:212:PCW:H282	0.61	1.72	2	1
3:C:210:PCW:H321	3:C:210:PCW:C7	0.61	2.25	11	4
3:A:406:PCW:H361	3:B:205:PCW:C32	0.61	2.24	9	3
3:D:604:PCW:C41	3:D:604:PCW:H372	0.61	2.25	11	2
3:C:206:PCW:C18	3:C:208:PCW:H362	0.61	2.26	3	2
3:D:612:PCW:H241	3:D:612:PCW:C46	0.61	2.26	4	2
4:C:219:17F:H10A	4:C:219:17F:H60	0.61	1.71	6	1
4:C:213:17F:O10	4:C:213:17F:C4	0.61	2.48	20	3
4:C:218:17F:H43	4:C:219:17F:H35	0.61	1.72	8	1
3:D:627:PCW:H283	4:D:631:17F:H51	0.61	1.70	20	2
3:D:617:PCW:H442	3:D:627:PCW:H261	0.61	1.73	14	1
3:A:401:PCW:H362	3:B:207:PCW:H39	0.61	1.70	16	1
3:D:616:PCW:H272	4:D:632:17F:C26	0.61	2.26	16	1
3:C:206:PCW:H241	3:C:208:PCW:H382	0.61	1.72	16	1
4:C:218:17F:H64	4:C:219:17F:C34	0.61	2.25	16	1
3:A:420:PCW:H31	3:D:618:PCW:C42	0.61	2.25	19	4
3:D:616:PCW:C20	4:D:632:17F:H38	0.61	2.26	6	9
2:C:78:PHE:HB2	2:C:111:MET:HG2	0.61	1.71	17	10
3:D:610:PCW:C28	4:D:631:17F:H72	0.61	2.26	3	2
3:C:203:PCW:H461	3:C:204:PCW:C15	0.61	2.25	13	3
4:A:416:17F:H65	3:B:204:PCW:H222	0.61	1.71	6	1
3:C:206:PCW:H182	3:C:208:PCW:H151	0.61	1.71	11	2
3:C:210:PCW:H121	3:C:210:PCW:C34	0.61	2.25	14	1
3:B:205:PCW:H32	3:C:204:PCW:H52	0.61	1.73	19	1
3:A:414:PCW:H121	4:A:415:17F:C1Z	0.61	2.26	20	1
2:B:79:LEU:HD13	2:B:159:LEU:HD22	0.60	1.73	2	2
3:C:203:PCW:H141	4:C:213:17F:H37	0.60	1.72	2	3
4:B:211:17F:H10	4:B:211:17F:C37	0.60	2.25	3	1
3:A:407:PCW:H321	3:A:410:PCW:C35	0.60	2.26	5	4
3:A:419:PCW:C8	3:D:626:PCW:H331	0.60	2.25	11	3

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
3:A:411:PCW:C25	3:B:205:PCW:H231	0.60	2.26	6	1
3:A:401:PCW:H482	3:D:612:PCW:H441	0.60	1.72	7	1
3:A:417:PCW:H61	4:D:630:17F:O4	0.60	1.96	15	2
3:D:612:PCW:C28	3:D:620:PCW:H272	0.60	2.25	7	1
4:A:416:17F:H77	3:D:605:PCW:H482	0.60	1.72	9	1
3:A:403:PCW:H441	3:D:618:PCW:H281	0.60	1.72	11	1
3:C:212:PCW:H162	4:C:215:17F:H10	0.60	1.71	11	1
3:A:402:PCW:H331	3:A:410:PCW:H332	0.60	1.73	12	1
3:A:414:PCW:O31	4:A:415:17F:H19A	0.60	1.95	14	1
4:C:218:17F:H9A	4:C:218:17F:C20	0.60	2.26	14	1
3:C:205:PCW:H332	3:C:209:PCW:H11	0.60	1.73	15	1
3:C:203:PCW:H361	3:C:204:PCW:C14	0.60	2.25	17	1
3:C:212:PCW:C3	4:C:215:17F:H32	0.60	2.25	19	1
4:A:416:17F:H71	3:B:203:PCW:C27	0.60	2.26	1	1
3:A:417:PCW:O31	3:A:417:PCW:P	0.60	2.59	19	12
3:C:205:PCW:O31	3:C:205:PCW:O3	0.60	2.19	11	15
3:A:402:PCW:C31	3:A:402:PCW:C35	0.60	2.79	11	14
5:B:201:GSP:S1G	5:B:201:GSP:O3A	0.60	2.59	2	1
3:C:212:PCW:H431	4:C:213:17F:H55	0.60	1.73	2	1
3:A:419:PCW:C8	3:D:626:PCW:O31	0.60	2.49	3	2
3:C:205:PCW:H421	3:C:212:PCW:C24	0.60	2.27	3	1
3:A:408:PCW:H241	3:A:413:PCW:H432	0.60	1.73	4	1
3:A:421:PCW:O31	3:A:421:PCW:O3P	0.60	2.19	12	2
4:B:211:17F:H54	3:C:204:PCW:C48	0.60	2.25	4	1
3:C:207:PCW:C16	4:C:213:17F:H20A	0.60	2.25	4	3
3:A:418:PCW:C7	3:D:618:PCW:H40	0.60	2.26	8	3
2:B:64:TYR:HB3	2:B:67:MET:HB3	0.60	1.72	17	4
3:B:208:PCW:H472	3:C:203:PCW:H232	0.60	1.72	6	1
3:A:411:PCW:H241	3:A:413:PCW:C39	0.60	2.26	7	3
3:D:617:PCW:H371	3:D:619:PCW:C14	0.60	2.15	7	2
3:D:624:PCW:C28	3:C:211:PCW:H282	0.60	2.25	7	1
3:C:206:PCW:H131	3:C:207:PCW:C17	0.60	2.26	7	1
3:C:205:PCW:H11	4:C:214:17F:O7	0.60	1.96	17	4
3:D:609:PCW:C25	3:D:616:PCW:H381	0.60	2.25	16	2
3:C:209:PCW:H171	4:C:214:17F:C1X	0.60	2.19	16	1
3:A:414:PCW:H362	4:B:209:17F:O8	0.60	1.96	17	1
3:D:614:PCW:C28	4:B:209:17F:H46	0.60	2.26	20	1
3:D:606:PCW:H471	4:D:632:17F:C1Y	0.60	2.26	1	2
4:D:629:17F:O7	4:D:629:17F:O10	0.60	2.19	11	19
4:D:632:17F:O10	4:D:632:17F:H4	0.60	1.96	1	12
3:C:209:PCW:C3	3:C:209:PCW:O2P	0.60	2.48	7	10

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
3:D:613:PCW:O3P	3:D:613:PCW:O31	0.60	2.19	16	16
3:B:203:PCW:H2	3:C:211:PCW:H39	0.60	1.73	7	2
3:B:204:PCW:H441	4:B:210:17F:H48	0.60	1.72	2	1
1:D:466:GLU:OE2	3:D:602:PCW:H261	0.60	1.96	4	1
3:B:204:PCW:C45	3:B:207:PCW:H20	0.60	2.25	4	2
3:B:206:PCW:H241	3:C:205:PCW:C17	0.60	2.20	4	1
3:A:401:PCW:H182	3:A:401:PCW:C22	0.60	2.24	5	4
3:D:624:PCW:C31	3:D:624:PCW:H62	0.60	2.27	17	3
3:D:605:PCW:O3P	3:D:624:PCW:C8	0.60	2.50	6	1
3:A:421:PCW:H19	4:D:630:17F:H57	0.60	1.74	7	5
3:D:617:PCW:C34	3:C:216:PCW:C34	0.60	2.78	9	1
3:D:605:PCW:O3P	3:D:605:PCW:O31	0.60	2.19	10	2
4:D:632:17F:H64	3:C:208:PCW:H461	0.60	1.73	20	2
3:B:206:PCW:O1P	3:B:206:PCW:H51	0.60	1.97	16	4
3:C:206:PCW:H12	4:C:214:17F:C12	0.60	2.25	12	1
3:A:401:PCW:H482	3:D:612:PCW:H232	0.60	1.72	14	2
3:B:207:PCW:H20	4:B:210:17F:C1Y	0.60	2.21	15	1
4:D:632:17F:O10	4:D:632:17F:C6	0.60	2.49	2	11
3:C:211:PCW:O31	3:C:211:PCW:O3P	0.60	2.19	16	11
3:D:605:PCW:C31	3:D:614:PCW:H42	0.60	2.26	3	1
3:D:604:PCW:H252	4:C:215:17F:H76	0.60	1.74	10	1
3:C:206:PCW:C8	4:C:214:17F:H10A	0.60	2.26	20	2
4:A:416:17F:O1	4:A:416:17F:H2	0.60	1.96	15	5
3:C:207:PCW:H121	4:C:213:17F:O10	0.60	1.96	12	1
3:A:404:PCW:H19	3:A:417:PCW:H481	0.60	1.74	14	1
3:A:410:PCW:H262	3:D:621:PCW:C41	0.60	2.26	14	1
3:D:619:PCW:H361	3:D:627:PCW:C16	0.60	2.26	16	1
3:D:622:PCW:H283	3:C:217:PCW:C6	0.60	2.27	16	1
3:A:420:PCW:C11	3:D:618:PCW:H421	0.60	2.26	18	1
3:A:406:PCW:H211	3:A:406:PCW:H162	0.60	1.71	9	6
3:D:617:PCW:O2P	3:D:617:PCW:C3	0.60	2.48	5	8
3:C:206:PCW:H151	3:C:208:PCW:C15	0.60	2.23	13	6
3:A:406:PCW:H321	3:B:205:PCW:H361	0.60	1.71	3	3
3:A:421:PCW:C19	4:D:630:17F:H20	0.60	2.26	3	4
3:A:412:PCW:H381	3:C:210:PCW:H362	0.60	1.73	4	1
3:A:413:PCW:C42	3:C:210:PCW:H461	0.60	2.27	8	3
4:A:422:17F:H39	4:C:219:17F:C37	0.60	2.20	4	3
3:C:207:PCW:O1P	3:C:207:PCW:H32	0.60	1.96	4	2
3:C:209:PCW:C43	3:C:209:PCW:C47	0.60	2.78	4	2
4:B:210:17F:H47	3:C:205:PCW:H481	0.60	1.73	5	1
4:A:415:17F:H37	3:C:211:PCW:C42	0.60	2.26	6	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
3:D:605:PCW:C41	3:D:620:PCW:H121	0.60	2.25	6	2
3:A:401:PCW:C39	3:B:204:PCW:H231	0.60	2.27	7	2
4:A:422:17F:H36	4:C:219:17F:H67	0.60	1.74	20	5
3:D:614:PCW:H221	4:B:209:17F:C25	0.60	2.27	14	2
3:D:616:PCW:H212	4:D:632:17F:H38	0.60	1.74	12	1
5:B:201:GSP:O2B	6:B:202:MG:MG	0.60	1.43	13	1
3:C:210:PCW:H161	3:C:210:PCW:H441	0.60	1.73	15	1
3:D:602:PCW:C8	4:C:214:17F:H4A	0.60	2.27	17	1
3:B:205:PCW:C33	3:B:208:PCW:H73	0.60	2.21	20	1
3:B:206:PCW:H283	4:C:214:17F:C1Z	0.60	2.26	20	1
3:A:407:PCW:O4P	3:A:407:PCW:H2	0.60	1.97	7	15
3:A:408:PCW:C6	3:A:408:PCW:O4P	0.60	2.49	7	19
3:A:418:PCW:C14	3:D:618:PCW:H483	0.60	2.24	1	1
3:C:206:PCW:H171	3:C:207:PCW:C22	0.60	2.26	1	2
3:A:402:PCW:H342	3:A:407:PCW:H141	0.60	1.73	5	2
3:A:403:PCW:O11	3:A:403:PCW:C5	0.60	2.48	11	11
3:A:404:PCW:H442	3:A:404:PCW:C18	0.60	2.27	8	2
3:D:612:PCW:C11	3:D:612:PCW:O31	0.60	2.48	18	8
3:D:627:PCW:H262	3:C:210:PCW:H281	0.60	1.73	2	2
3:D:606:PCW:H2	3:D:606:PCW:H41	0.60	1.73	5	11
3:D:610:PCW:C24	3:D:610:PCW:C20	0.60	2.78	3	1
3:D:611:PCW:O11	3:D:617:PCW:H63	0.60	1.96	3	1
3:D:625:PCW:H411	3:D:626:PCW:H412	0.60	1.74	10	5
3:A:412:PCW:H381	3:C:210:PCW:H382	0.60	1.74	4	1
3:A:404:PCW:C41	4:A:415:17F:H40	0.60	2.21	5	1
3:A:409:PCW:H271	3:A:419:PCW:C27	0.60	2.26	10	5
3:B:208:PCW:H471	3:C:203:PCW:H181	0.60	1.72	6	1
3:D:608:PCW:H172	4:D:629:17F:H18	0.60	1.72	10	1
3:D:604:PCW:H482	3:D:606:PCW:H61	0.60	1.74	11	1
3:A:405:PCW:H352	3:A:411:PCW:H441	0.60	1.72	16	2
3:D:613:PCW:H471	3:D:613:PCW:H252	0.60	1.73	12	2
3:B:204:PCW:H472	3:B:207:PCW:H262	0.60	1.72	14	1
3:C:206:PCW:H73	4:C:213:17F:H18A	0.60	1.73	14	1
3:A:412:PCW:C48	3:C:204:PCW:H271	0.60	2.27	17	1
3:A:403:PCW:O31	3:A:403:PCW:C1	0.60	2.48	16	15
3:D:611:PCW:H122	3:D:611:PCW:H332	0.60	1.73	1	1
3:D:603:PCW:H461	3:D:611:PCW:H412	0.60	1.74	7	4
3:C:206:PCW:H212	3:C:208:PCW:H19	0.60	1.74	16	3
3:D:616:PCW:H261	4:D:632:17F:C26	0.60	2.26	3	1
3:D:624:PCW:H481	4:B:209:17F:C30	0.60	2.26	3	3
3:C:205:PCW:C12	3:C:209:PCW:C34	0.60	2.79	3	2

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
3:B:205:PCW:H231	3:C:210:PCW:H262	0.60	1.74	4	1
3:D:605:PCW:P	3:D:624:PCW:H82	0.60	2.36	16	3
3:D:605:PCW:H40	3:D:620:PCW:H141	0.60	1.72	20	4
3:D:603:PCW:H141	3:D:624:PCW:C18	0.60	2.26	17	4
3:B:208:PCW:H442	4:C:213:17F:H77	0.60	1.74	12	1
3:C:212:PCW:H142	4:C:215:17F:O8	0.60	1.97	13	2
3:A:409:PCW:H432	3:A:419:PCW:H221	0.60	1.74	16	1
3:A:418:PCW:H451	3:D:613:PCW:H171	0.60	1.71	20	1
3:D:602:PCW:O1P	3:D:602:PCW:H51	0.60	1.97	5	5
3:C:207:PCW:O31	3:C:207:PCW:C1	0.60	2.48	1	15
4:C:215:17F:O9	4:C:215:17F:O8	0.60	2.20	15	10
3:A:419:PCW:O31	3:A:419:PCW:O3	0.60	2.18	11	15
3:D:603:PCW:C26	3:D:611:PCW:H171	0.60	2.27	10	6
3:A:409:PCW:C27	3:A:419:PCW:H271	0.60	2.26	4	3
3:A:409:PCW:H332	3:B:206:PCW:H341	0.60	1.73	13	2
3:C:207:PCW:H412	4:C:213:17F:H8	0.60	1.73	4	1
3:D:612:PCW:H32	3:D:620:PCW:O11	0.60	1.96	5	1
3:D:617:PCW:H421	3:D:627:PCW:C23	0.60	2.26	14	5
3:C:205:PCW:C48	4:C:215:17F:H37	0.60	2.26	6	1
3:D:617:PCW:C43	3:C:204:PCW:H472	0.60	2.26	19	2
3:C:203:PCW:H281	3:C:211:PCW:H451	0.60	1.73	18	2
3:C:208:PCW:H73	3:C:208:PCW:C32	0.60	2.27	12	1
3:B:203:PCW:H431	3:C:211:PCW:C16	0.60	2.26	13	1
3:B:203:PCW:H452	4:C:215:17F:H43	0.60	1.73	15	1
3:C:211:PCW:H212	4:C:215:17F:H65	0.60	1.71	17	1
3:D:619:PCW:O2P	3:D:627:PCW:H41	0.60	1.97	19	1
4:D:630:17F:O10	4:D:630:17F:H20A	0.60	1.94	19	12
3:B:208:PCW:O31	3:B:208:PCW:O3P	0.60	2.19	12	12
3:A:408:PCW:C11	3:A:413:PCW:H121	0.60	2.27	15	5
1:D:475:GLU:HB2	1:D:476:PRO:HD3	0.60	1.74	9	5
3:D:608:PCW:H262	4:D:629:17F:C1X	0.60	2.27	18	3
3:D:611:PCW:H341	3:D:611:PCW:O31	0.60	1.96	5	11
3:D:608:PCW:C6	3:D:626:PCW:H222	0.60	2.26	12	6
3:D:612:PCW:C20	3:D:620:PCW:H482	0.60	2.27	4	2
4:B:210:17F:H41	4:B:210:17F:H36	0.60	1.72	4	1
4:B:211:17F:H55	3:C:216:PCW:H39	0.60	1.74	5	1
3:C:206:PCW:C22	3:C:208:PCW:H411	0.60	2.26	5	1
3:D:609:PCW:O11	3:D:616:PCW:H61	0.60	1.97	6	6
3:B:205:PCW:H483	3:B:208:PCW:C20	0.60	2.26	13	1
3:C:203:PCW:H471	3:C:210:PCW:C17	0.60	2.27	15	1
3:C:206:PCW:H82	4:C:214:17F:H10A	0.60	1.71	18	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
3:A:408:PCW:H181	3:A:413:PCW:H261	0.60	1.72	1	7
3:A:413:PCW:C5	3:C:210:PCW:O2P	0.60	2.50	4	6
3:D:619:PCW:C13	3:D:627:PCW:H142	0.60	2.25	13	3
3:B:206:PCW:H212	3:C:209:PCW:H322	0.60	1.74	1	2
1:A:396:LYS:HG2	1:D:587:ALA:HB2	0.60	1.74	12	3
2:C:84:ILE:HD12	2:C:123:ARG:HB3	0.60	1.74	8	8
3:C:207:PCW:H161	4:C:213:17F:C31	0.60	2.26	8	3
3:D:606:PCW:O11	3:D:606:PCW:C2	0.60	2.47	11	9
3:C:203:PCW:H12	3:C:211:PCW:C7	0.60	2.27	3	1
3:A:402:PCW:H162	3:A:407:PCW:H231	0.60	1.74	7	5
3:A:408:PCW:H242	3:A:411:PCW:H252	0.60	1.73	5	4
3:A:420:PCW:O2	3:D:618:PCW:H422	0.60	1.97	5	1
4:A:416:17F:H69	3:B:204:PCW:C26	0.60	2.25	6	1
3:C:209:PCW:H452	3:C:212:PCW:H182	0.60	1.72	6	1
3:A:419:PCW:O1P	3:D:615:PCW:C4	0.60	2.50	15	3
3:A:408:PCW:C24	3:A:411:PCW:C22	0.60	2.79	11	4
1:D:503:MET:HA	1:D:506:ARG:HD2	0.60	1.74	17	3
3:C:205:PCW:H452	4:C:215:17F:H38	0.60	1.73	10	1
3:C:212:PCW:H421	4:C:215:17F:C10	0.60	2.24	14	1
3:B:208:PCW:H121	3:B:208:PCW:H73	0.60	1.74	15	1
3:C:203:PCW:H141	4:C:213:17F:C22	0.60	2.25	15	1
3:C:205:PCW:H181	3:C:209:PCW:H262	0.60	1.74	15	1
3:C:205:PCW:H122	3:C:212:PCW:C19	0.60	2.27	19	2
3:B:203:PCW:H472	3:C:211:PCW:C25	0.60	2.27	16	1
3:D:605:PCW:C32	3:D:612:PCW:H12	0.60	2.27	18	1
3:C:203:PCW:C32	3:C:204:PCW:H122	0.60	2.26	20	1
3:A:402:PCW:H382	3:C:208:PCW:H361	0.59	1.73	1	1
3:A:405:PCW:O11	3:A:405:PCW:H2	0.59	1.97	1	16
3:D:624:PCW:C20	3:C:217:PCW:H232	0.59	2.27	1	4
3:A:402:PCW:H431	3:C:206:PCW:C26	0.59	2.26	2	1
3:A:418:PCW:H422	3:D:613:PCW:C24	0.59	2.26	18	9
3:C:205:PCW:C12	3:C:209:PCW:H341	0.59	2.27	3	2
4:A:416:17F:C31	3:B:204:PCW:H151	0.59	2.21	6	4
3:D:617:PCW:H461	3:D:627:PCW:C26	0.59	2.27	5	3
4:D:632:17F:H65	3:C:208:PCW:C46	0.59	2.27	5	1
3:B:206:PCW:H322	3:B:206:PCW:H61	0.59	1.74	6	1
3:D:603:PCW:C14	3:D:624:PCW:H181	0.59	2.27	8	1
3:D:605:PCW:C40	3:D:620:PCW:H121	0.59	2.27	11	4
3:A:412:PCW:H452	3:C:210:PCW:H472	0.59	1.72	20	2
3:A:402:PCW:H462	4:D:632:17F:H51	0.59	1.73	12	1
3:A:407:PCW:H332	3:A:410:PCW:C35	0.59	2.26	14	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
2:B:47:ASP:HA	2:C:128:LYS:HG3	0.59	1.73	14	1
3:A:408:PCW:H482	3:A:413:PCW:C23	0.59	2.27	15	1
3:A:419:PCW:H441	4:B:210:17F:C40	0.59	2.26	16	1
3:C:208:PCW:H63	4:C:213:17F:H1A	0.59	1.74	17	1
3:B:207:PCW:C11	3:B:207:PCW:C31	0.59	2.80	19	6
3:B:208:PCW:C43	3:B:208:PCW:C47	0.59	2.74	1	2
3:D:605:PCW:H462	4:B:209:17F:C30	0.59	2.27	10	3
3:B:203:PCW:H42	3:C:211:PCW:H352	0.59	1.73	14	2
3:A:421:PCW:C31	3:D:618:PCW:H52	0.59	2.27	4	2
3:D:604:PCW:H372	3:D:604:PCW:C42	0.59	2.27	11	7
3:B:208:PCW:H462	4:C:218:17F:H49	0.59	1.72	4	1
4:D:628:17F:H36	4:D:629:17F:H71	0.59	1.72	8	1
3:B:206:PCW:C3	3:B:206:PCW:P	0.59	2.91	8	1
3:A:406:PCW:C13	4:B:211:17F:H71	0.59	2.25	9	1
3:B:206:PCW:H242	3:C:209:PCW:C12	0.59	2.26	9	2
2:C:23:LEU:HD21	2:C:153:ASP:HA	0.59	1.75	10	1
4:A:422:17F:C23	4:C:219:17F:H71	0.59	2.23	15	1
3:D:601:PCW:C39	4:D:628:17F:H54	0.59	2.26	16	1
1:A:356:HIS:CB	3:A:401:PCW:H20	0.59	2.27	18	1
3:A:406:PCW:H411	3:C:204:PCW:C34	0.59	2.26	19	1
3:B:203:PCW:C33	4:B:210:17F:H35	0.59	2.24	20	1
4:A:416:17F:C7	4:A:416:17F:C17	0.59	2.79	5	3
3:D:607:PCW:C11	3:D:607:PCW:O31	0.59	2.50	15	20
3:D:609:PCW:O31	3:D:609:PCW:O3	0.59	2.20	8	19
3:C:209:PCW:H442	3:C:212:PCW:C26	0.59	2.15	14	3
3:A:409:PCW:H412	3:A:419:PCW:H282	0.59	1.74	9	4
4:A:416:17F:O10	4:A:416:17F:O6	0.59	2.19	10	7
3:D:606:PCW:C42	3:D:609:PCW:H31	0.59	2.20	18	3
1:D:462:LYS:HB3	3:D:602:PCW:H283	0.59	1.74	5	3
3:D:627:PCW:H283	3:C:210:PCW:H272	0.59	1.74	3	3
3:C:206:PCW:O31	3:C:206:PCW:P	0.59	2.60	8	2
2:B:34:PRO:HA	5:B:201:GSP:S1G	0.59	2.38	19	4
3:D:602:PCW:H471	4:D:629:17F:H43	0.59	1.74	6	2
3:C:209:PCW:H452	3:C:212:PCW:C18	0.59	2.27	6	1
3:C:207:PCW:H461	4:C:213:17F:H73	0.59	1.73	8	1
3:C:208:PCW:C23	3:C:208:PCW:C27	0.59	2.79	8	1
3:D:605:PCW:H322	3:D:612:PCW:O3P	0.59	1.96	20	5
3:D:619:PCW:C44	3:D:627:PCW:H282	0.59	2.28	11	1
3:A:414:PCW:H252	4:A:415:17F:C32	0.59	2.27	19	2
4:A:416:17F:O5	3:B:204:PCW:H63	0.59	1.97	12	2
3:A:414:PCW:C12	4:A:415:17F:H33	0.59	2.27	14	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
3:C:209:PCW:H422	3:C:212:PCW:H262	0.59	1.73	15	1
3:A:402:PCW:H141	3:A:407:PCW:H171	0.59	1.72	1	1
3:A:405:PCW:H52	4:B:211:17F:O5	0.59	1.97	1	1
3:A:406:PCW:C38	3:B:205:PCW:H161	0.59	2.28	1	1
3:D:602:PCW:H172	3:D:602:PCW:H221	0.59	1.72	5	2
3:D:604:PCW:H451	3:D:606:PCW:C18	0.59	2.16	5	8
3:C:207:PCW:H151	4:C:213:17F:C20	0.59	2.18	1	1
3:A:401:PCW:C18	3:A:401:PCW:C22	0.59	2.76	20	8
3:A:401:PCW:H181	3:A:401:PCW:C22	0.59	2.18	12	3
3:D:603:PCW:C16	3:D:624:PCW:H211	0.59	2.28	5	6
3:D:605:PCW:O1P	3:D:605:PCW:H52	0.59	1.96	16	11
3:D:612:PCW:C3	3:D:620:PCW:O11	0.59	2.50	5	4
3:D:617:PCW:H452	3:D:627:PCW:H251	0.59	1.74	8	3
3:C:204:PCW:H252	3:C:217:PCW:H441	0.59	1.73	14	4
3:C:206:PCW:H352	3:C:208:PCW:C14	0.59	2.27	6	5
3:B:203:PCW:H332	4:B:210:17F:H37	0.59	1.74	17	5
3:D:602:PCW:H261	4:D:629:17F:C42	0.59	2.27	17	5
4:B:211:17F:H49	3:C:204:PCW:H462	0.59	1.74	5	1
3:B:208:PCW:O3P	3:C:211:PCW:H52	0.59	1.98	19	2
4:C:213:17F:O1	4:C:213:17F:H2	0.59	1.96	6	1
3:A:414:PCW:H352	4:A:415:17F:H65	0.59	1.75	7	1
3:B:203:PCW:H451	3:C:211:PCW:H222	0.59	1.74	11	2
3:A:409:PCW:C47	3:A:409:PCW:H272	0.59	2.28	8	1
3:D:605:PCW:H82	4:D:630:17F:O4	0.59	1.97	9	1
2:C:23:LEU:HG	2:C:42:LYS:HE2	0.59	1.73	9	1
3:C:205:PCW:H52	4:C:214:17F:O5	0.59	1.96	10	1
3:B:208:PCW:H40	3:C:216:PCW:H281	0.59	1.74	11	1
3:C:205:PCW:C15	3:C:209:PCW:H412	0.59	2.27	12	1
3:C:205:PCW:H421	3:C:212:PCW:C26	0.59	2.20	18	1
4:B:211:17F:H54	3:C:216:PCW:H232	0.59	1.74	19	1
3:B:203:PCW:C28	4:B:210:17F:H53	0.59	2.27	20	1
3:A:406:PCW:C14	4:B:211:17F:H63	0.59	2.27	1	1
3:A:410:PCW:C24	4:A:422:17F:H74	0.59	2.25	17	2
4:A:415:17F:H64	4:B:209:17F:C21	0.59	2.27	1	1
3:A:414:PCW:C34	4:A:415:17F:H32	0.59	2.25	6	2
3:D:619:PCW:O2P	3:D:627:PCW:H82	0.59	1.97	18	3
3:B:205:PCW:H483	3:B:208:PCW:H19	0.59	1.75	2	4
3:C:212:PCW:O31	3:C:212:PCW:O3	0.59	2.20	2	7
3:A:420:PCW:C48	3:D:619:PCW:H281	0.59	2.27	16	4
3:A:404:PCW:H152	3:B:205:PCW:H452	0.59	1.75	4	1
3:A:401:PCW:C7	3:B:207:PCW:O31	0.59	2.50	9	9

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
3:D:603:PCW:C8	3:D:603:PCW:H131	0.59	2.28	6	2
3:D:602:PCW:C46	4:D:628:17F:H65	0.59	2.23	7	2
3:C:216:PCW:C24	3:C:216:PCW:C28	0.59	2.77	7	1
3:A:406:PCW:H20	4:B:211:17F:H19A	0.59	1.75	8	3
3:D:604:PCW:H411	3:D:604:PCW:C37	0.59	2.26	9	2
3:D:623:PCW:H40	3:D:625:PCW:H261	0.59	1.73	9	1
2:B:6:LEU:HD12	2:B:55:ILE:HG12	0.59	1.74	10	1
3:D:605:PCW:H461	4:B:209:17F:H74	0.59	1.73	14	1
3:A:414:PCW:C47	4:B:209:17F:H12A	0.59	2.17	15	1
3:A:409:PCW:H162	3:A:419:PCW:H211	0.59	1.73	16	1
3:A:403:PCW:H271	3:A:414:PCW:C20	0.59	2.27	17	1
3:D:619:PCW:P	3:D:627:PCW:H63	0.59	2.36	18	2
3:D:614:PCW:H272	4:B:209:17F:H46	0.59	1.74	2	4
3:D:602:PCW:H483	4:D:628:17F:C31	0.59	2.28	3	2
3:A:405:PCW:C5	3:A:406:PCW:O11	0.59	2.51	18	3
2:C:13:GLY:HA2	5:C:201:GSP:C5'	0.59	2.26	13	2
3:C:207:PCW:H441	4:C:213:17F:H31	0.59	1.73	13	2
3:A:418:PCW:H332	3:D:613:PCW:C11	0.59	2.27	7	1
3:A:418:PCW:H371	3:A:418:PCW:H411	0.59	1.73	11	2
3:D:617:PCW:C2	3:C:216:PCW:H342	0.59	2.28	16	2
4:C:215:17F:N1	4:C:215:17F:H4	0.59	2.13	13	2
3:B:203:PCW:H431	3:C:211:PCW:H162	0.59	1.75	13	1
3:C:203:PCW:H361	3:C:204:PCW:H122	0.59	1.74	19	2
3:C:207:PCW:H283	3:C:207:PCW:C24	0.59	2.27	18	1
3:A:404:PCW:C6	3:A:404:PCW:H372	0.59	2.28	1	1
3:A:407:PCW:O2	3:A:407:PCW:H342	0.59	1.96	8	5
3:D:605:PCW:O31	3:D:614:PCW:C6	0.59	2.48	2	8
3:B:205:PCW:O1P	3:B:205:PCW:C5	0.59	2.50	1	2
3:C:211:PCW:O11	3:C:211:PCW:O2	0.59	2.20	5	12
3:A:418:PCW:H39	3:D:613:PCW:H451	0.59	1.73	18	4
3:A:421:PCW:O3P	3:A:421:PCW:O31	0.59	2.21	19	16
3:C:205:PCW:H382	3:C:212:PCW:C22	0.59	2.27	2	1
3:D:603:PCW:H441	3:D:603:PCW:H212	0.59	1.73	19	2
3:D:618:PCW:C47	3:D:618:PCW:C43	0.59	2.74	3	1
3:D:626:PCW:H51	3:D:626:PCW:O11	0.59	1.97	15	2
3:C:207:PCW:H162	4:C:213:17F:C31	0.59	2.26	4	3
3:B:203:PCW:H461	4:C:215:17F:C24	0.59	2.28	5	1
3:A:413:PCW:C32	3:C:210:PCW:H132	0.59	2.27	7	5
1:D:497:SER:HB2	1:D:498:PRO:HD3	0.59	1.74	13	3
3:D:612:PCW:C31	3:D:623:PCW:H352	0.59	2.26	20	2
3:D:608:PCW:H452	4:D:628:17F:C33	0.59	2.23	11	2

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
3:B:207:PCW:C19	4:B:210:17F:O10	0.59	2.51	11	2
3:A:414:PCW:C42	4:A:415:17F:H69	0.59	2.18	12	1
3:C:207:PCW:H142	4:C:213:17F:H57	0.59	1.74	14	1
3:A:418:PCW:H381	3:D:613:PCW:H432	0.59	1.71	16	1
3:A:406:PCW:H241	3:A:411:PCW:H472	0.59	1.75	20	1
3:A:405:PCW:H82	4:B:211:17F:O5	0.59	1.97	1	1
3:D:614:PCW:O31	3:D:614:PCW:C1	0.59	2.50	4	12
3:C:203:PCW:C13	3:C:203:PCW:C17	0.59	2.79	1	3
3:A:408:PCW:C13	3:A:411:PCW:H231	0.59	2.26	2	1
3:D:603:PCW:H371	3:D:603:PCW:C41	0.59	2.12	6	7
3:B:208:PCW:H421	3:C:216:PCW:C26	0.59	2.27	9	5
3:A:420:PCW:H382	3:D:611:PCW:C16	0.59	2.28	15	7
3:D:603:PCW:H242	3:D:611:PCW:H371	0.59	1.74	3	1
3:A:414:PCW:C25	4:A:415:17F:H60	0.59	2.26	4	3
3:C:210:PCW:H351	3:C:210:PCW:C11	0.59	2.27	5	1
3:D:617:PCW:C33	3:C:216:PCW:H341	0.59	2.28	7	2
3:A:409:PCW:C2	4:B:210:17F:H20A	0.59	2.21	8	1
3:D:619:PCW:C13	3:D:627:PCW:H132	0.59	2.26	8	1
2:B:16:LYS:HG2	5:B:201:GSP:O2B	0.59	1.98	19	3
3:D:624:PCW:H321	3:D:624:PCW:H41	0.59	1.74	11	1
3:D:601:PCW:H482	4:D:628:17F:C29	0.59	2.27	13	1
3:A:405:PCW:H221	3:A:418:PCW:H262	0.59	1.73	18	1
3:C:206:PCW:C22	3:C:208:PCW:H19	0.59	2.28	18	1
3:B:203:PCW:H39	3:C:211:PCW:H421	0.59	1.75	19	1
3:D:615:PCW:C45	3:D:620:PCW:H20	0.59	2.28	3	3
3:D:623:PCW:O1P	3:D:623:PCW:H52	0.59	1.97	7	9
3:C:203:PCW:H452	3:C:204:PCW:C21	0.59	2.23	20	3
4:A:416:17F:H69	3:B:204:PCW:C27	0.59	2.28	5	1
3:A:420:PCW:H351	3:D:618:PCW:C43	0.59	2.26	5	1
3:B:203:PCW:C36	3:C:211:PCW:H40	0.59	2.10	5	1
4:C:219:17F:O10	4:C:219:17F:C20	0.59	2.51	5	1
3:B:208:PCW:H452	3:C:203:PCW:C15	0.59	2.27	6	2
3:D:617:PCW:H271	3:D:619:PCW:H283	0.59	1.74	9	5
3:A:412:PCW:C46	3:C:210:PCW:H472	0.59	2.28	11	4
3:C:211:PCW:H242	4:C:215:17F:H73	0.59	1.74	10	2
3:D:623:PCW:H382	3:D:625:PCW:C17	0.59	2.27	13	3
2:C:32:TYR:HD1	5:C:201:GSP:H4'	0.59	1.57	15	1
3:C:205:PCW:H211	3:C:209:PCW:H271	0.59	1.73	15	1
4:B:211:17F:H65	4:B:211:17F:H37	0.59	1.74	16	1
3:A:405:PCW:H321	3:A:406:PCW:H182	0.59	1.75	17	1
3:D:602:PCW:O4P	3:D:602:PCW:H62	0.59	1.98	15	18

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
2:C:15:GLY:HA2	5:C:201:GSP:C8	0.59	2.33	15	5
3:D:608:PCW:C46	4:D:628:17F:H61	0.59	2.27	4	7
3:C:211:PCW:H412	3:C:211:PCW:C37	0.59	2.15	15	8
3:A:401:PCW:C41	3:B:204:PCW:H262	0.59	2.25	12	3
3:D:604:PCW:H412	3:D:606:PCW:C24	0.59	2.28	19	4
3:D:603:PCW:H41	3:D:603:PCW:C3	0.59	2.28	6	1
3:C:206:PCW:C21	3:C:206:PCW:C25	0.59	2.76	6	4
3:A:406:PCW:C44	3:C:204:PCW:H431	0.59	2.28	17	2
3:B:204:PCW:O3P	3:B:207:PCW:H11	0.59	1.97	9	1
4:C:218:17F:H42	4:C:219:17F:H74	0.59	1.74	10	1
3:A:413:PCW:H341	3:A:413:PCW:C13	0.59	2.18	11	2
4:A:422:17F:H6	3:D:622:PCW:H132	0.59	1.75	11	1
3:D:603:PCW:H382	3:D:624:PCW:C14	0.59	2.28	12	1
3:A:403:PCW:H362	3:A:403:PCW:O31	0.59	1.97	16	2
3:C:212:PCW:H73	4:C:213:17F:O5	0.59	1.97	14	1
3:D:617:PCW:C19	3:D:618:PCW:H461	0.59	2.28	18	1
3:D:607:PCW:H452	3:D:626:PCW:H481	0.58	1.73	15	2
3:D:627:PCW:C21	3:C:217:PCW:H352	0.58	2.28	11	10
3:B:208:PCW:O31	3:B:208:PCW:C4	0.58	2.51	5	5
1:A:301:LEU:HD13	1:D:473:LYS:HG2	0.58	1.75	14	7
3:A:411:PCW:H51	4:B:211:17F:C1	0.58	2.23	14	4
3:B:206:PCW:O4P	3:B:206:PCW:C6	0.58	2.50	13	10
3:C:203:PCW:C17	3:C:203:PCW:C13	0.58	2.81	7	12
4:C:219:17F:H56	4:C:219:17F:C11	0.58	2.28	18	3
3:A:408:PCW:C26	4:D:631:17F:H55	0.58	2.28	3	1
3:D:602:PCW:H483	4:D:628:17F:C32	0.58	2.28	20	4
2:B:117:LYS:HB3	2:B:120:LEU:HD12	0.58	1.74	3	3
3:D:623:PCW:H231	3:B:203:PCW:H481	0.58	1.73	4	2
3:B:206:PCW:H121	3:B:206:PCW:H362	0.58	1.75	4	1
3:A:409:PCW:O2P	3:B:206:PCW:H63	0.58	1.98	5	1
3:B:203:PCW:C21	4:B:209:17F:H19	0.58	2.25	18	2
3:A:402:PCW:H412	3:C:206:PCW:H252	0.58	1.75	6	1
3:B:206:PCW:C7	4:B:210:17F:H33	0.58	2.28	6	1
3:B:207:PCW:H462	4:B:210:17F:H50	0.58	1.75	8	2
3:C:209:PCW:H141	4:C:214:17F:C6	0.58	2.27	9	1
3:A:408:PCW:H482	3:A:413:PCW:H241	0.58	1.74	11	1
3:C:203:PCW:H432	3:C:210:PCW:H171	0.58	1.75	14	1
3:D:615:PCW:H51	3:D:625:PCW:H42	0.58	1.75	15	2
3:B:204:PCW:O4P	3:B:204:PCW:O31	0.58	2.21	19	1
3:A:404:PCW:H40	4:A:415:17F:H44	0.58	1.75	20	1
3:A:406:PCW:H281	3:D:619:PCW:H262	0.58	1.75	1	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
3:A:417:PCW:H141	3:A:420:PCW:C34	0.58	2.27	1	5
3:A:404:PCW:H341	3:A:404:PCW:O31	0.58	1.96	2	1
3:A:418:PCW:H431	3:D:613:PCW:C16	0.58	2.26	19	4
3:D:603:PCW:O4P	4:C:219:17F:H1A	0.58	1.98	2	1
3:D:613:PCW:H342	3:D:613:PCW:O2	0.58	1.98	4	18
3:D:607:PCW:C2	3:D:626:PCW:H372	0.58	2.28	3	5
3:D:616:PCW:H272	4:D:632:17F:H46	0.58	1.75	4	3
3:C:205:PCW:H132	3:C:209:PCW:C14	0.58	2.28	4	1
3:B:205:PCW:H171	3:C:204:PCW:H321	0.58	1.75	5	2
3:A:406:PCW:C47	3:B:205:PCW:H262	0.58	2.27	9	2
3:A:401:PCW:H342	3:B:207:PCW:H382	0.58	1.73	8	1
3:D:605:PCW:H431	3:D:624:PCW:C42	0.58	2.28	11	3
3:D:609:PCW:C44	3:D:616:PCW:H472	0.58	2.23	8	1
3:D:621:PCW:O1P	3:D:622:PCW:C6	0.58	2.50	17	2
2:B:92:ASP:HA	2:B:95:HIS:HD2	0.58	1.57	11	1
3:C:209:PCW:O31	3:C:209:PCW:C4	0.58	2.48	12	2
3:A:408:PCW:O11	3:A:408:PCW:H2	0.58	1.98	13	1
3:D:616:PCW:H211	4:D:632:17F:C24	0.58	2.23	13	2
3:B:204:PCW:H32	3:B:207:PCW:H372	0.58	1.74	13	1
3:A:414:PCW:C47	4:A:415:17F:H68	0.58	2.25	14	1
3:D:612:PCW:H11	3:D:620:PCW:H63	0.58	1.75	14	1
3:B:207:PCW:C31	3:B:207:PCW:C11	0.58	2.82	17	2
3:C:206:PCW:H171	3:C:208:PCW:C36	0.58	2.18	17	1
3:D:604:PCW:P	3:D:604:PCW:C3	0.58	2.91	11	10
4:D:632:17F:H53	3:C:208:PCW:C16	0.58	2.27	9	3
3:A:402:PCW:H162	3:A:407:PCW:C21	0.58	2.28	17	3
3:A:414:PCW:H351	3:A:414:PCW:O31	0.58	1.98	13	4
3:A:420:PCW:C35	3:D:618:PCW:H422	0.58	2.27	3	2
3:D:604:PCW:H412	3:D:606:PCW:H252	0.58	1.75	10	4
3:D:625:PCW:C41	3:D:626:PCW:C41	0.58	2.78	3	2
4:A:416:17F:H72	3:D:612:PCW:H481	0.58	1.75	18	4
3:A:401:PCW:O2	3:B:207:PCW:H362	0.58	1.98	6	1
3:A:401:PCW:N	3:B:207:PCW:O31	0.58	2.36	9	7
3:A:419:PCW:H39	3:D:625:PCW:H422	0.58	1.75	6	1
3:D:606:PCW:O4P	3:D:606:PCW:H62	0.58	1.98	6	2
3:A:407:PCW:H321	3:A:410:PCW:H371	0.58	1.75	7	1
3:C:205:PCW:H121	3:C:212:PCW:H251	0.58	1.74	7	1
3:C:206:PCW:C7	4:C:213:17F:O1	0.58	2.51	11	5
3:C:205:PCW:H63	4:C:214:17F:H9	0.58	1.75	9	1
3:A:410:PCW:H39	3:A:412:PCW:H351	0.58	1.75	18	1
3:C:206:PCW:H82	4:C:214:17F:C9	0.58	2.28	18	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
3:A:411:PCW:H472	4:B:211:17F:C1Y	0.58	2.29	19	1
3:C:207:PCW:H471	3:C:207:PCW:C28	0.58	2.23	19	1
3:A:408:PCW:H171	3:A:411:PCW:C23	0.58	2.28	3	5
3:C:209:PCW:O11	3:C:209:PCW:C2	0.58	2.48	20	11
3:A:419:PCW:H39	3:D:625:PCW:H441	0.58	1.75	5	2
3:D:615:PCW:C45	3:D:620:PCW:H222	0.58	2.27	17	2
3:D:620:PCW:H481	4:B:209:17F:C41	0.58	2.28	15	2
3:D:603:PCW:H361	3:D:611:PCW:H321	0.58	1.76	4	1
3:D:605:PCW:C48	3:D:620:PCW:H421	0.58	2.29	4	1
3:C:212:PCW:H412	4:C:215:17F:H75	0.58	1.73	5	1
3:A:402:PCW:O31	3:A:402:PCW:O3	0.58	2.20	6	4
2:B:82:PHE:HB2	2:B:89:SER:HB2	0.58	1.74	14	4
3:A:408:PCW:C23	3:A:411:PCW:C22	0.58	2.80	20	4
4:A:416:17F:H2	4:A:416:17F:O2	0.58	1.98	10	1
3:C:206:PCW:C19	3:C:208:PCW:H171	0.58	2.29	11	2
3:D:610:PCW:H171	4:D:631:17F:H61	0.58	1.75	16	3
3:A:407:PCW:H61	3:A:410:PCW:H371	0.58	1.73	15	1
3:C:210:PCW:H441	3:C:210:PCW:C16	0.58	2.28	15	1
3:D:615:PCW:O4P	3:D:615:PCW:H31	0.58	1.98	17	1
4:B:210:17F:C1	3:C:205:PCW:H371	0.58	2.23	18	1
3:D:616:PCW:O3	3:D:616:PCW:O31	0.58	2.21	20	15
3:B:205:PCW:H82	3:B:205:PCW:O4P	0.58	1.99	11	14
3:C:217:PCW:O4P	3:C:217:PCW:C6	0.58	2.51	1	2
3:A:417:PCW:H2	3:A:417:PCW:O2P	0.58	1.98	2	1
3:C:216:PCW:O31	3:C:216:PCW:C1	0.58	2.51	11	17
3:D:609:PCW:H462	3:C:208:PCW:C45	0.58	2.27	13	3
3:D:622:PCW:H262	3:C:217:PCW:C6	0.58	2.28	16	2
4:B:211:17F:H29	4:B:211:17F:H41	0.58	1.74	3	1
3:A:408:PCW:C26	3:C:210:PCW:H242	0.58	2.28	13	2
3:B:204:PCW:H40	4:B:210:17F:C12	0.58	2.28	4	1
3:B:208:PCW:C45	4:C:218:17F:H54	0.58	2.28	4	2
3:D:605:PCW:C38	3:D:612:PCW:H31	0.58	2.28	5	1
3:D:610:PCW:H42	4:D:631:17F:H6	0.58	1.74	18	2
3:B:207:PCW:H232	3:B:207:PCW:C45	0.58	2.27	13	1
3:C:207:PCW:H381	4:C:213:17F:C8	0.58	2.28	14	1
3:A:403:PCW:H19	3:A:404:PCW:H122	0.58	1.74	16	1
3:A:408:PCW:H272	3:D:619:PCW:C45	0.58	2.28	16	1
3:B:206:PCW:H431	3:C:205:PCW:H252	0.58	1.74	16	1
4:A:422:17F:H69	4:D:632:17F:H67	0.58	1.75	17	1
3:D:616:PCW:H283	3:C:206:PCW:H482	0.58	1.75	1	1
3:A:403:PCW:H51	3:A:404:PCW:P	0.58	2.38	2	3

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
3:A:411:PCW:H62	4:B:211:17F:H1A	0.58	1.76	2	1
3:D:617:PCW:C45	3:D:627:PCW:H251	0.58	2.28	2	2
3:C:204:PCW:H181	3:C:217:PCW:H482	0.58	1.76	2	1
3:C:207:PCW:H483	3:C:207:PCW:H283	0.58	1.76	2	1
4:A:422:17F:H63	3:D:622:PCW:H451	0.58	1.73	3	2
3:A:406:PCW:H381	3:C:204:PCW:C34	0.58	2.29	4	3
3:C:205:PCW:H162	3:C:209:PCW:C19	0.58	2.29	4	1
3:A:420:PCW:C20	3:A:420:PCW:C24	0.58	2.73	5	1
1:D:561:LYS:HE3	1:D:561:LYS:HA	0.58	1.73	13	2
3:D:613:PCW:H62	3:D:627:PCW:O11	0.58	1.98	6	3
3:A:410:PCW:C23	4:A:422:17F:H74	0.58	2.29	7	2
3:D:622:PCW:C21	4:D:631:17F:H31	0.58	2.28	7	9
3:C:212:PCW:H181	3:C:212:PCW:C43	0.58	2.25	7	1
3:A:402:PCW:H483	3:C:206:PCW:H40	0.58	1.75	8	1
3:C:206:PCW:H472	4:C:214:17F:H74	0.58	1.74	9	1
3:C:211:PCW:C21	4:C:215:17F:H69	0.58	2.26	17	2
3:C:206:PCW:H19	3:C:207:PCW:C19	0.58	2.28	16	1
3:C:212:PCW:H122	4:C:215:17F:C20	0.58	2.22	1	1
3:A:406:PCW:H482	3:D:619:PCW:H483	0.58	1.76	2	2
4:A:415:17F:H12A	4:B:209:17F:H5	0.58	1.76	2	1
3:C:206:PCW:H19	3:C:207:PCW:C24	0.58	2.15	2	1
3:A:420:PCW:H40	3:D:617:PCW:H231	0.58	1.74	6	1
3:D:607:PCW:H481	3:C:209:PCW:H483	0.58	1.75	6	1
3:B:208:PCW:O31	3:C:211:PCW:H82	0.58	1.98	19	4
3:A:408:PCW:H42	3:A:413:PCW:C1	0.58	2.27	20	3
3:D:605:PCW:O31	3:D:614:PCW:C5	0.58	2.50	7	4
3:D:604:PCW:H381	4:C:218:17F:H40	0.58	1.75	16	4
4:D:628:17F:H18A	4:D:629:17F:H55	0.58	1.76	9	3
3:B:208:PCW:C1	3:C:211:PCW:H321	0.58	2.29	15	3
3:D:602:PCW:H481	3:D:608:PCW:C23	0.58	2.28	20	3
4:A:415:17F:H61	4:B:209:17F:H29	0.58	1.75	12	1
3:A:418:PCW:H332	3:D:613:PCW:C15	0.58	2.29	12	1
3:B:206:PCW:C21	3:C:205:PCW:H171	0.58	2.28	12	2
3:C:206:PCW:H141	3:C:208:PCW:H331	0.58	1.75	14	1
3:A:418:PCW:H382	3:D:613:PCW:H231	0.58	1.74	18	1
3:A:410:PCW:H232	4:A:422:17F:H71	0.58	1.76	1	1
3:D:609:PCW:C11	3:D:609:PCW:O31	0.58	2.52	15	11
3:B:204:PCW:H422	4:B:210:17F:C24	0.58	2.29	1	1
3:A:403:PCW:C4	3:A:403:PCW:O11	0.58	2.52	2	5
3:D:627:PCW:H421	3:D:627:PCW:H372	0.58	1.76	5	4
3:C:206:PCW:H20	3:C:208:PCW:H19	0.58	1.74	9	2

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
3:A:420:PCW:H351	3:D:618:PCW:C41	0.58	2.29	6	2
3:B:204:PCW:H31	3:B:207:PCW:C35	0.58	2.27	4	4
3:D:619:PCW:H422	3:D:627:PCW:H282	0.58	1.74	5	2
3:A:405:PCW:H252	3:A:418:PCW:C25	0.58	2.28	6	1
3:B:203:PCW:H41	3:B:203:PCW:H12	0.58	1.76	6	4
3:B:203:PCW:H451	3:C:211:PCW:C22	0.58	2.28	7	1
3:A:409:PCW:H483	3:A:419:PCW:H212	0.58	1.76	14	1
3:C:209:PCW:C42	3:C:212:PCW:H271	0.58	2.25	17	1
1:D:462:LYS:HD2	3:D:602:PCW:C28	0.58	2.28	20	2
3:A:417:PCW:C16	3:A:420:PCW:H331	0.58	2.21	20	1
3:D:616:PCW:H121	4:D:632:17F:H8	0.58	1.73	20	1
3:D:607:PCW:H32	3:D:626:PCW:H372	0.58	1.74	1	2
2:C:68:ARG:HA	2:C:71:TYR:CZ	0.58	2.34	4	9
3:C:210:PCW:C31	3:C:210:PCW:C35	0.58	2.82	5	17
3:C:206:PCW:H212	3:C:208:PCW:H171	0.58	1.73	18	2
3:A:406:PCW:C20	4:B:211:17F:H19A	0.58	2.29	8	5
3:D:606:PCW:C21	3:D:606:PCW:C17	0.58	2.77	3	6
3:C:204:PCW:C28	3:C:217:PCW:H421	0.58	2.28	15	2
3:A:401:PCW:H483	3:D:615:PCW:H471	0.58	1.75	20	2
3:D:609:PCW:O1P	4:D:632:17F:H20A	0.58	1.98	4	2
3:D:625:PCW:H432	3:D:626:PCW:H461	0.58	1.75	5	3
4:B:210:17F:H67	3:C:212:PCW:H281	0.58	1.75	4	2
3:D:603:PCW:C7	3:C:216:PCW:H31	0.58	2.29	5	2
3:C:210:PCW:H351	3:C:210:PCW:H121	0.58	1.76	5	1
3:D:614:PCW:H241	4:B:209:17F:H71	0.58	1.76	6	2
3:A:404:PCW:H241	3:D:618:PCW:C28	0.58	2.29	7	1
3:C:206:PCW:H73	4:C:213:17F:O6	0.58	1.99	15	2
3:A:421:PCW:O2P	3:D:618:PCW:H82	0.58	1.99	10	2
3:D:609:PCW:H431	3:C:208:PCW:C24	0.58	2.28	10	3
3:B:203:PCW:C47	3:C:211:PCW:H271	0.58	2.27	20	2
3:B:206:PCW:H63	4:B:210:17F:P1	0.58	2.39	10	1
3:A:401:PCW:H51	3:B:204:PCW:C1	0.58	2.29	11	1
3:A:403:PCW:H482	3:A:404:PCW:H211	0.58	1.76	11	1
3:D:614:PCW:H141	3:D:620:PCW:H382	0.58	1.75	12	1
3:B:208:PCW:C1	3:C:211:PCW:H362	0.58	2.29	17	2
3:B:208:PCW:H361	3:C:211:PCW:H63	0.58	1.75	18	1
3:C:207:PCW:C21	4:C:213:17F:H57	0.58	2.28	20	1
3:A:408:PCW:O31	3:A:408:PCW:H11	0.58	1.99	11	9
3:A:414:PCW:O3	3:A:414:PCW:O31	0.58	2.21	1	12
3:A:417:PCW:C28	3:A:420:PCW:H251	0.58	2.29	13	4
3:A:414:PCW:H121	4:A:415:17F:H58	0.58	1.73	2	2

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
2:B:68:ARG:HA	2:B:71:TYR:CZ	0.58	2.34	15	9
3:A:403:PCW:P	3:A:403:PCW:C3	0.58	2.91	19	5
3:D:612:PCW:H20	3:D:612:PCW:H412	0.58	1.75	3	3
3:A:420:PCW:H362	3:D:618:PCW:H382	0.58	1.75	6	4
3:D:605:PCW:H212	3:D:614:PCW:C15	0.58	2.29	4	2
3:A:411:PCW:H11	3:B:205:PCW:C11	0.58	2.29	6	4
3:C:210:PCW:H351	3:C:210:PCW:C12	0.58	2.29	5	1
3:A:419:PCW:O1P	3:D:625:PCW:H321	0.58	1.99	6	1
3:D:610:PCW:O31	3:D:610:PCW:O3P	0.58	2.22	6	1
3:D:612:PCW:O11	3:D:620:PCW:C6	0.58	2.51	7	6
3:D:604:PCW:H251	4:C:215:17F:H52	0.58	1.74	8	1
3:D:623:PCW:C12	3:D:624:PCW:H331	0.58	2.28	8	1
3:C:207:PCW:H412	4:C:213:17F:H30	0.58	1.75	10	2
3:D:625:PCW:C39	3:D:626:PCW:H141	0.58	2.27	11	1
3:C:204:PCW:C39	3:C:216:PCW:H251	0.58	2.29	14	3
3:D:614:PCW:C48	3:D:620:PCW:H431	0.58	2.28	18	3
3:B:205:PCW:H132	3:C:204:PCW:C1	0.58	2.20	14	1
3:C:205:PCW:C22	3:C:209:PCW:H242	0.58	2.28	17	1
3:C:203:PCW:H222	3:C:203:PCW:C18	0.58	2.29	20	1
3:D:621:PCW:O1P	3:D:622:PCW:C5	0.57	2.51	13	11
3:C:212:PCW:H441	4:C:215:17F:H10	0.57	1.75	1	1
3:B:207:PCW:O11	3:B:207:PCW:C5	0.57	2.52	17	10
3:B:205:PCW:O31	3:B:205:PCW:H12	0.57	1.99	3	1
4:C:213:17F:H71	4:C:213:17F:H58	0.57	1.75	3	1
3:D:602:PCW:H141	4:D:628:17F:H54	0.57	1.74	4	2
3:D:615:PCW:H442	3:D:620:PCW:C19	0.57	2.28	11	6
3:B:205:PCW:C13	3:C:204:PCW:C4	0.57	2.82	5	1
3:C:204:PCW:H232	3:C:210:PCW:C20	0.57	2.12	5	1
3:A:417:PCW:H61	4:D:630:17F:O5	0.57	1.99	14	3
3:D:606:PCW:H61	3:D:626:PCW:C28	0.57	2.29	13	4
3:D:616:PCW:H12	3:D:616:PCW:O31	0.57	1.99	12	2
4:A:416:17F:H78	3:B:203:PCW:H272	0.57	1.75	7	1
3:D:609:PCW:H281	4:C:214:17F:C30	0.57	2.29	7	1
4:B:210:17F:H4	4:B:210:17F:H2	0.57	1.76	8	1
3:B:208:PCW:C40	3:C:216:PCW:H262	0.57	2.25	9	1
3:A:420:PCW:C31	3:A:420:PCW:C11	0.57	2.82	10	1
1:D:466:GLU:OE2	3:D:602:PCW:H262	0.57	1.99	15	2
3:D:607:PCW:C36	3:D:626:PCW:H442	0.57	2.29	18	2
2:B:15:GLY:HA2	5:B:201:GSP:C8	0.57	2.33	12	3
5:B:201:GSP:H3'	5:B:201:GSP:PA	0.57	2.38	13	1
3:A:414:PCW:C7	4:B:209:17F:O5	0.57	2.52	14	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
3:D:605:PCW:O31	3:D:614:PCW:C8	0.57	2.52	14	4
3:D:607:PCW:H442	3:D:625:PCW:H471	0.57	1.76	20	2
3:D:617:PCW:H452	3:C:204:PCW:C47	0.57	2.24	14	1
3:A:401:PCW:C39	3:B:204:PCW:H281	0.57	2.29	15	1
3:A:406:PCW:H371	4:B:211:17F:C8	0.57	2.29	17	1
3:D:624:PCW:C6	3:D:624:PCW:O4P	0.57	2.52	17	1
3:A:420:PCW:O31	3:A:420:PCW:O3	0.57	2.22	18	1
3:C:203:PCW:O3	4:C:213:17F:H37	0.57	1.99	19	1
3:D:615:PCW:O4P	3:D:615:PCW:H73	0.57	1.99	2	19
3:C:206:PCW:H151	3:C:208:PCW:C17	0.57	2.28	1	1
3:D:603:PCW:C22	3:D:603:PCW:H441	0.57	2.30	3	2
1:A:388:SER:HB2	1:D:594:LYS:HD3	0.57	1.76	5	1
3:D:608:PCW:H221	4:D:628:17F:H18	0.57	1.75	7	1
3:A:402:PCW:C45	3:C:206:PCW:H231	0.57	2.29	8	1
3:A:405:PCW:H82	4:B:211:17F:C5	0.57	2.26	9	1
3:D:608:PCW:H241	4:D:629:17F:H40	0.57	1.75	11	1
3:C:208:PCW:C8	4:C:213:17F:O4	0.57	2.53	11	1
3:D:616:PCW:H122	4:D:632:17F:C8	0.57	2.29	16	1
3:B:206:PCW:H382	3:C:205:PCW:H283	0.57	1.74	16	1
3:B:203:PCW:H42	3:C:211:PCW:O2P	0.57	1.98	19	1
3:D:607:PCW:H432	3:D:626:PCW:C48	0.57	2.29	15	2
3:D:613:PCW:H372	3:D:627:PCW:H31	0.57	1.76	1	1
3:A:403:PCW:H472	3:A:404:PCW:H272	0.57	1.75	2	1
3:D:614:PCW:H212	4:B:209:17F:H47	0.57	1.75	2	4
3:D:625:PCW:O31	3:D:625:PCW:O3P	0.57	2.22	17	9
3:A:404:PCW:H431	3:A:414:PCW:H251	0.57	1.75	8	2
3:A:420:PCW:H11	3:D:618:PCW:H39	0.57	1.76	3	1
3:D:608:PCW:H63	3:D:626:PCW:C24	0.57	2.26	6	5
3:B:206:PCW:H62	3:B:206:PCW:O4P	0.57	2.00	11	3
3:C:205:PCW:H182	3:C:209:PCW:C19	0.57	2.29	4	1
3:D:608:PCW:O1P	3:D:626:PCW:H212	0.57	1.99	5	1
3:D:612:PCW:C22	3:D:620:PCW:H482	0.57	2.29	20	3
3:D:617:PCW:H481	3:B:205:PCW:H222	0.57	1.73	14	2
3:B:203:PCW:H461	4:C:215:17F:H46	0.57	1.74	5	1
3:A:406:PCW:H381	3:C:204:PCW:H362	0.57	1.76	6	1
2:C:72:MET:HA	2:C:78:PHE:CZ	0.57	2.34	7	3
3:A:406:PCW:H462	4:B:211:17F:H32	0.57	1.76	11	1
4:A:416:17F:H68	4:B:209:17F:H68	0.57	1.75	13	1
3:C:207:PCW:C6	3:C:207:PCW:H341	0.57	2.28	13	1
3:B:208:PCW:H421	3:C:216:PCW:C28	0.57	2.29	18	2
3:A:414:PCW:H121	4:A:415:17F:H62	0.57	1.75	15	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
3:C:212:PCW:H2	4:C:215:17F:O1	0.57	1.99	17	2
4:B:211:17F:H59	4:B:211:17F:C12	0.57	2.26	16	1
3:D:621:PCW:H122	4:D:632:17F:H4A	0.57	1.75	17	1
3:A:406:PCW:H39	3:B:205:PCW:H122	0.57	1.75	19	1
3:A:409:PCW:H11	3:A:409:PCW:O31	0.57	1.99	17	8
3:D:602:PCW:O31	3:D:602:PCW:C3	0.57	2.51	16	11
3:D:603:PCW:H441	3:D:603:PCW:C21	0.57	2.24	2	4
2:B:117:LYS:HG2	5:B:201:GSP:C6	0.57	2.34	4	3
3:B:204:PCW:H483	3:C:205:PCW:H481	0.57	1.75	4	1
3:D:604:PCW:H272	3:D:625:PCW:H481	0.57	1.76	5	1
3:C:206:PCW:C18	3:C:208:PCW:C17	0.57	2.79	11	6
1:A:301:LEU:HD22	1:D:473:LYS:HG2	0.57	1.74	6	2
5:C:201:GSP:H2'	5:C:201:GSP:O5'	0.57	2.00	15	2
3:D:611:PCW:H51	3:D:617:PCW:O1P	0.57	1.98	11	1
3:A:405:PCW:P	3:A:406:PCW:H151	0.57	2.39	12	1
3:A:418:PCW:C32	3:D:613:PCW:H132	0.57	2.29	12	1
3:D:607:PCW:H361	3:D:626:PCW:H442	0.57	1.76	18	2
3:B:208:PCW:H341	3:C:211:PCW:C8	0.57	2.30	17	1
3:D:610:PCW:H52	4:D:631:17F:O1	0.57	2.00	18	1
4:C:215:17F:H4	4:C:215:17F:N1	0.57	2.13	18	1
3:C:204:PCW:H39	3:C:216:PCW:H261	0.57	1.75	19	1
3:B:204:PCW:H411	3:B:207:PCW:H341	0.57	1.77	20	1
4:A:422:17F:C30	3:D:606:PCW:H211	0.57	2.29	1	1
3:D:606:PCW:O3P	3:D:606:PCW:O31	0.57	2.23	11	13
3:B:204:PCW:H431	4:B:210:17F:C10	0.57	2.25	1	3
3:B:205:PCW:H172	3:C:204:PCW:O2	0.57	2.00	1	1
3:A:411:PCW:H281	3:C:203:PCW:H471	0.57	1.77	13	2
3:C:206:PCW:C19	3:C:207:PCW:H242	0.57	2.15	2	1
3:D:612:PCW:O4P	3:D:620:PCW:H62	0.57	2.00	7	7
3:B:204:PCW:H441	3:C:205:PCW:C48	0.57	2.30	6	1
4:B:210:17F:H72	3:C:209:PCW:C42	0.57	2.30	7	1
3:B:206:PCW:H32	3:B:206:PCW:O1P	0.57	1.98	8	1
3:D:609:PCW:H431	3:C:208:PCW:H231	0.57	1.77	19	2
3:C:207:PCW:H182	3:C:208:PCW:H331	0.57	1.77	20	2
3:D:614:PCW:H251	4:B:209:17F:C26	0.57	2.29	12	1
3:D:618:PCW:O31	3:D:618:PCW:C7	0.57	2.52	12	1
3:A:419:PCW:C6	3:D:626:PCW:H2	0.57	2.22	13	1
3:D:617:PCW:H481	3:B:205:PCW:H221	0.57	1.77	14	1
3:A:403:PCW:C32	3:A:404:PCW:O2P	0.57	2.53	15	1
3:D:619:PCW:C32	3:D:627:PCW:H121	0.57	2.29	15	1
3:A:404:PCW:H51	3:B:205:PCW:H40	0.57	1.77	16	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
3:B:205:PCW:O1P	3:C:204:PCW:H62	0.57	2.00	17	2
2:C:117:LYS:HG2	5:C:201:GSP:C6	0.57	2.33	19	3
3:A:410:PCW:H39	3:A:412:PCW:C37	0.57	2.29	18	1
3:A:418:PCW:H382	3:D:613:PCW:C23	0.57	2.29	18	1
3:D:615:PCW:O4P	3:D:615:PCW:C7	0.57	2.53	2	18
3:D:621:PCW:O1P	3:D:622:PCW:C4	0.57	2.52	9	5
3:A:402:PCW:H483	3:C:206:PCW:C39	0.57	2.30	2	1
3:A:411:PCW:O1P	3:A:411:PCW:O2	0.57	2.22	2	2
3:B:208:PCW:C32	3:C:211:PCW:H82	0.57	2.20	2	1
3:C:209:PCW:H121	4:C:214:17F:C7	0.57	2.28	2	1
3:C:211:PCW:H172	4:C:215:17F:C34	0.57	2.29	2	1
3:A:413:PCW:H452	4:D:631:17F:H52	0.57	1.75	3	2
4:A:422:17F:O7	4:A:422:17F:O10	0.57	2.22	7	11
3:A:408:PCW:H31	3:A:413:PCW:C12	0.57	2.29	4	1
3:B:205:PCW:P	4:B:211:17F:O1	0.57	2.63	4	1
4:D:631:17F:O10	4:D:631:17F:O7	0.57	2.23	9	2
3:D:603:PCW:H421	3:D:611:PCW:H382	0.57	1.76	9	1
3:C:209:PCW:C12	4:C:214:17F:H6	0.57	2.28	9	2
3:C:211:PCW:H32	4:C:215:17F:H19A	0.57	1.76	9	1
5:B:201:GSP:S1G	5:B:201:GSP:O1B	0.57	2.63	16	2
4:A:415:17F:C34	4:B:209:17F:H30	0.57	2.25	14	1
3:B:204:PCW:H442	3:C:205:PCW:C46	0.57	2.23	17	1
3:A:420:PCW:O3	3:A:420:PCW:C31	0.57	2.52	18	1
3:A:408:PCW:P	3:A:408:PCW:H63	0.57	2.40	7	5
3:B:204:PCW:O4P	3:B:204:PCW:H2	0.57	1.99	8	3
3:C:203:PCW:H122	3:C:207:PCW:H40	0.57	1.76	1	1
3:B:205:PCW:O4P	3:B:205:PCW:H62	0.57	1.99	6	6
3:B:206:PCW:C12	3:C:209:PCW:H371	0.57	2.30	3	1
3:B:208:PCW:H2	3:B:208:PCW:O11	0.57	1.99	15	5
3:C:206:PCW:H181	3:C:208:PCW:H362	0.57	1.77	3	1
3:D:605:PCW:C17	3:D:614:PCW:H131	0.57	2.30	15	2
3:B:205:PCW:C48	3:B:208:PCW:H20	0.57	2.30	4	1
3:C:209:PCW:H271	3:C:209:PCW:C47	0.57	2.27	4	1
3:C:211:PCW:H242	4:C:215:17F:H47	0.57	1.77	4	1
3:D:601:PCW:C7	3:D:602:PCW:H32	0.57	2.29	5	1
3:A:401:PCW:O3P	3:B:207:PCW:H321	0.57	1.98	6	1
3:D:616:PCW:C4	3:D:616:PCW:H2	0.57	2.29	18	5
3:C:205:PCW:H482	4:C:215:17F:H37	0.57	1.77	6	1
3:D:622:PCW:H283	3:C:217:PCW:H73	0.57	1.77	7	1
3:A:401:PCW:H342	3:B:207:PCW:C38	0.57	2.29	8	1
4:D:632:17F:H53	3:C:208:PCW:H141	0.57	1.74	8	2

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
3:A:409:PCW:H2	4:B:210:17F:C1Y	0.57	2.29	11	2
2:B:46:ILE:HD13	2:B:160:VAL:HG21	0.57	1.74	18	2
3:C:206:PCW:C3	4:C:214:17F:H35	0.57	2.29	12	1
3:A:414:PCW:C18	3:A:414:PCW:C14	0.57	2.82	14	1
3:D:619:PCW:C34	3:D:627:PCW:H341	0.57	2.29	14	1
3:D:608:PCW:H41	3:D:626:PCW:H221	0.57	1.76	15	1
3:B:208:PCW:H2	3:B:208:PCW:C4	0.57	2.16	15	1
3:A:405:PCW:C8	4:B:211:17F:H4A	0.57	2.30	16	1
2:C:19:LEU:HD23	2:C:146:ALA:HB2	0.57	1.75	19	1
3:A:406:PCW:H2	3:A:406:PCW:O11	0.57	1.98	1	6
3:D:617:PCW:P	3:D:617:PCW:C3	0.57	2.90	18	9
3:D:625:PCW:H19	3:D:625:PCW:C14	0.57	2.30	19	11
3:D:626:PCW:O31	3:D:626:PCW:O3	0.57	2.23	8	13
4:D:630:17F:H1	4:D:630:17F:H4A	0.57	1.76	1	2
4:A:416:17F:H59	3:B:204:PCW:H222	0.57	1.75	2	1
3:D:604:PCW:H2	3:D:606:PCW:H63	0.57	1.75	2	1
3:D:617:PCW:O2	3:D:617:PCW:P	0.57	2.62	11	4
3:D:605:PCW:O31	3:D:614:PCW:H42	0.57	1.99	3	1
3:D:610:PCW:C6	4:D:631:17F:O1	0.57	2.53	5	3
3:D:614:PCW:H52	3:D:614:PCW:O2P	0.57	2.00	3	1
3:D:616:PCW:C24	4:D:632:17F:H41	0.57	2.29	3	1
3:C:207:PCW:C40	4:C:213:17F:H77	0.57	2.30	3	1
3:D:605:PCW:H481	3:D:620:PCW:H421	0.57	1.76	6	4
3:D:627:PCW:C31	3:D:627:PCW:O3	0.57	2.53	12	5
3:B:208:PCW:H451	4:C:213:17F:H37	0.57	1.76	5	1
4:D:628:17F:C32	4:D:629:17F:H47	0.57	2.30	7	1
3:D:623:PCW:H131	3:D:623:PCW:C39	0.57	2.22	8	1
3:C:203:PCW:H441	3:C:217:PCW:H482	0.57	1.76	8	3
3:C:206:PCW:H132	3:C:208:PCW:H321	0.57	1.77	10	1
3:B:205:PCW:C1	4:B:211:17F:O1	0.57	2.53	11	1
3:B:206:PCW:C16	3:C:209:PCW:H372	0.57	2.29	12	1
3:C:208:PCW:H73	3:C:208:PCW:C31	0.57	2.30	12	1
4:A:416:17F:C1Y	3:B:204:PCW:H151	0.57	2.29	15	1
3:D:614:PCW:H462	3:D:620:PCW:C39	0.57	2.30	17	1
3:A:412:PCW:H462	3:C:204:PCW:H251	0.57	1.74	18	1
3:A:414:PCW:O2	3:A:414:PCW:C35	0.57	2.44	18	1
3:D:607:PCW:H341	3:D:626:PCW:H422	0.57	1.77	18	1
3:A:401:PCW:O3	3:A:401:PCW:O31	0.57	2.23	17	17
3:A:420:PCW:H421	3:D:617:PCW:H232	0.57	1.76	6	2
4:B:209:17F:O10	4:B:209:17F:H20	0.57	2.00	13	11
3:C:209:PCW:H31	4:C:214:17F:N1	0.57	2.15	2	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
3:A:412:PCW:O31	3:A:412:PCW:O3	0.57	2.22	10	15
3:B:207:PCW:H232	3:B:207:PCW:C38	0.57	2.30	12	4
3:A:408:PCW:C23	3:A:408:PCW:H171	0.57	2.29	4	1
3:C:204:PCW:H231	3:C:210:PCW:H261	0.57	1.76	4	1
3:A:417:PCW:H161	3:A:420:PCW:C35	0.57	2.30	5	2
3:D:618:PCW:O31	3:D:618:PCW:H62	0.57	2.00	17	6
3:D:607:PCW:H361	3:D:626:PCW:H432	0.57	1.74	6	1
3:C:212:PCW:H371	4:C:215:17F:C20	0.57	2.27	9	1
4:A:415:17F:H60	4:B:209:17F:H41	0.57	1.77	10	1
3:A:401:PCW:H51	3:B:204:PCW:H11	0.57	1.75	11	1
3:C:206:PCW:H12	4:C:214:17F:H12A	0.57	1.72	12	1
3:A:406:PCW:C35	4:B:211:17F:H8	0.57	2.28	14	2
3:B:206:PCW:C16	3:C:209:PCW:H352	0.57	2.30	15	1
4:A:415:17F:O10	4:A:415:17F:O6	0.57	2.22	17	1
3:D:624:PCW:H19	3:B:208:PCW:C27	0.57	2.23	1	1
3:A:403:PCW:H132	3:A:404:PCW:C1	0.57	2.28	2	1
3:D:612:PCW:O2P	3:D:620:PCW:C6	0.57	2.52	6	5
3:D:604:PCW:C40	3:D:606:PCW:H252	0.57	2.30	3	1
3:A:414:PCW:H122	4:A:415:17F:H72	0.57	1.76	17	2
3:B:208:PCW:C46	3:C:203:PCW:H161	0.57	2.29	6	1
3:D:608:PCW:C45	4:D:628:17F:H34	0.57	2.28	18	2
4:D:630:17F:O8	4:D:630:17F:C5	0.57	2.51	7	6
3:C:204:PCW:H272	3:C:217:PCW:C42	0.57	2.30	7	1
3:A:421:PCW:C13	4:D:630:17F:H11A	0.57	2.29	10	1
3:D:607:PCW:O2	3:D:626:PCW:H372	0.57	1.99	10	1
3:A:402:PCW:C46	3:A:407:PCW:H261	0.57	2.29	14	1
3:C:212:PCW:H61	4:C:213:17F:O5	0.57	1.99	18	1
3:A:409:PCW:C32	3:B:206:PCW:H332	0.57	2.28	20	1
3:D:617:PCW:H483	3:D:619:PCW:H482	0.57	1.76	20	1
3:A:402:PCW:H412	3:C:206:PCW:H262	0.56	1.76	5	5
3:D:614:PCW:O11	3:D:614:PCW:H2	0.56	1.99	2	13
3:D:615:PCW:H452	3:D:620:PCW:C20	0.56	2.30	14	5
3:C:212:PCW:O2	3:C:212:PCW:O1P	0.56	2.23	2	5
3:A:420:PCW:H422	3:D:617:PCW:H231	0.56	1.76	2	2
4:C:213:17F:O7	4:C:213:17F:O10	0.56	2.23	7	3
3:A:420:PCW:C35	3:D:618:PCW:C42	0.56	2.82	3	1
3:B:205:PCW:H331	3:B:208:PCW:C12	0.56	2.20	3	1
3:D:603:PCW:H42	3:D:603:PCW:C31	0.56	2.30	8	2
3:A:404:PCW:H51	3:B:205:PCW:C39	0.56	2.29	5	1
3:A:420:PCW:C35	3:D:618:PCW:H431	0.56	2.28	5	1
3:D:605:PCW:H382	3:D:612:PCW:H31	0.56	1.77	5	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
3:D:607:PCW:H472	3:C:209:PCW:H483	0.56	1.77	7	2
3:A:414:PCW:H351	3:A:414:PCW:C3	0.56	2.30	9	1
3:A:417:PCW:H172	3:A:420:PCW:H361	0.56	1.75	10	1
3:A:406:PCW:H31	4:B:211:17F:C41	0.56	2.30	12	1
3:A:412:PCW:H411	3:C:210:PCW:H371	0.56	1.74	14	1
3:A:413:PCW:H422	3:C:210:PCW:C44	0.56	2.12	14	1
3:D:617:PCW:O2	3:D:617:PCW:O2P	0.56	2.23	14	1
4:C:213:17F:H77	4:C:219:17F:C28	0.56	2.17	16	1
3:D:608:PCW:H221	4:D:628:17F:H8A	0.56	1.77	17	1
3:D:617:PCW:C46	3:C:204:PCW:H472	0.56	2.30	17	1
3:C:211:PCW:H231	4:C:215:17F:H48	0.56	1.77	18	1
4:A:422:17F:H49	3:D:606:PCW:H161	0.56	1.74	14	2
3:B:203:PCW:H332	4:B:210:17F:C1X	0.56	2.30	2	2
3:A:408:PCW:P	3:A:408:PCW:H31	0.56	2.40	3	3
4:A:415:17F:H49	3:B:205:PCW:H483	0.56	1.76	3	1
1:D:514:LEU:HA	1:D:517:HIS:HB2	0.56	1.77	3	5
3:D:611:PCW:H41	3:D:617:PCW:H42	0.56	1.77	3	1
3:B:207:PCW:P	3:B:207:PCW:C3	0.56	2.93	3	1
3:C:211:PCW:H371	3:C:211:PCW:C41	0.56	2.26	15	7
3:D:603:PCW:H222	3:D:611:PCW:H332	0.56	1.75	4	2
1:D:591:TYR:HB3	4:D:630:17F:H48	0.56	1.75	5	1
3:D:602:PCW:C46	3:D:608:PCW:H482	0.56	2.28	5	1
3:D:608:PCW:H172	4:D:629:17F:O10	0.56	1.99	11	6
3:D:616:PCW:H181	4:D:632:17F:C21	0.56	2.30	19	3
3:D:623:PCW:H242	3:B:203:PCW:C47	0.56	2.29	6	1
3:A:401:PCW:C32	3:B:207:PCW:H232	0.56	2.30	7	1
3:C:205:PCW:H2	3:C:209:PCW:C15	0.56	2.27	9	1
3:B:208:PCW:H341	3:C:203:PCW:O11	0.56	2.00	11	2
3:C:212:PCW:C40	4:C:215:17F:H67	0.56	2.30	12	1
2:B:15:GLY:HA2	5:B:201:GSP:H8	0.56	1.60	16	3
3:D:608:PCW:O1P	3:D:626:PCW:H232	0.56	2.00	15	1
3:C:212:PCW:H471	4:C:215:17F:H45	0.56	1.75	15	1
3:C:205:PCW:C23	3:C:209:PCW:H283	0.56	2.30	19	2
3:A:402:PCW:H381	3:C:208:PCW:H361	0.56	1.77	1	2
1:D:573:LEU:HA	1:D:576:VAL:HG12	0.56	1.77	4	7
3:D:609:PCW:C6	3:D:621:PCW:O11	0.56	2.53	12	4
3:D:615:PCW:O31	3:D:615:PCW:H11	0.56	2.00	17	18
3:D:620:PCW:H82	3:D:620:PCW:O4P	0.56	2.01	6	20
3:C:205:PCW:H42	4:C:214:17F:HN1A	0.56	1.59	16	3
3:A:412:PCW:H411	3:C:210:PCW:C36	0.56	2.29	2	1
3:D:617:PCW:H39	3:D:619:PCW:C15	0.56	2.31	9	5

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
3:D:621:PCW:O4P	3:D:621:PCW:C7	0.56	2.54	7	8
3:D:623:PCW:H122	3:D:624:PCW:H352	0.56	1.76	2	4
3:C:207:PCW:C3	4:C:213:17F:H4	0.56	2.29	2	1
3:C:211:PCW:H32	4:C:215:17F:C1Y	0.56	2.29	2	1
3:A:401:PCW:H31	3:B:207:PCW:H371	0.56	1.76	3	1
3:A:409:PCW:C37	4:B:210:17F:H66	0.56	2.31	3	1
3:D:601:PCW:H482	4:D:628:17F:C30	0.56	2.29	10	4
3:D:608:PCW:H62	3:D:626:PCW:H222	0.56	1.77	15	3
3:A:402:PCW:C15	3:A:407:PCW:H211	0.56	2.29	4	2
4:A:415:17F:H44	3:B:205:PCW:H462	0.56	1.76	4	1
3:C:203:PCW:C43	3:C:204:PCW:H161	0.56	2.30	4	1
3:C:205:PCW:H321	4:C:214:17F:N1	0.56	2.15	4	1
3:A:408:PCW:H251	3:A:411:PCW:H221	0.56	1.78	10	2
3:A:407:PCW:H181	3:A:407:PCW:C40	0.56	2.31	6	1
3:A:421:PCW:H442	3:D:618:PCW:H20	0.56	1.75	7	6
3:A:401:PCW:C48	3:D:615:PCW:H471	0.56	2.30	9	1
3:D:609:PCW:H251	4:D:628:17F:C40	0.56	2.31	9	1
3:B:204:PCW:C44	3:C:205:PCW:H462	0.56	2.27	9	1
3:C:204:PCW:H39	3:C:216:PCW:C25	0.56	2.30	19	2
3:C:205:PCW:C43	3:C:212:PCW:H231	0.56	2.27	10	1
3:A:403:PCW:H332	3:A:406:PCW:H12	0.56	1.76	12	1
3:A:404:PCW:H39	3:B:205:PCW:C45	0.56	2.30	16	2
5:B:201:GSP:O2A	5:B:201:GSP:C3'	0.56	2.49	13	1
3:D:611:PCW:O11	3:D:617:PCW:C6	0.56	2.51	19	2
3:D:615:PCW:O1P	3:D:625:PCW:H73	0.56	2.01	15	1
3:D:606:PCW:H442	3:D:609:PCW:H12	0.56	1.76	18	1
3:A:403:PCW:C8	3:A:404:PCW:O1P	0.56	2.53	19	1
3:D:607:PCW:O2	3:D:626:PCW:H371	0.56	2.00	19	1
3:A:407:PCW:H221	3:C:206:PCW:C27	0.56	2.28	20	1
2:B:5:LYS:HA	2:B:54:ASP:HB3	0.56	1.75	9	8
3:B:208:PCW:C34	3:C:203:PCW:H283	0.56	2.30	1	1
4:B:210:17F:H10	3:C:205:PCW:C47	0.56	2.30	1	1
3:C:206:PCW:O31	3:C:206:PCW:O3	0.56	2.21	5	8
3:A:420:PCW:H351	3:D:618:PCW:H421	0.56	1.77	3	1
3:C:207:PCW:H39	4:C:219:17F:H77	0.56	1.76	5	1
3:B:208:PCW:H412	3:C:203:PCW:H231	0.56	1.76	6	1
3:B:208:PCW:O3P	3:B:208:PCW:O31	0.56	2.24	19	2
3:A:414:PCW:H262	4:B:209:17F:C21	0.56	2.30	8	1
3:B:208:PCW:H32	3:B:208:PCW:P	0.56	2.40	8	2
3:C:211:PCW:H221	3:C:211:PCW:C18	0.56	2.27	13	4
3:A:407:PCW:C8	3:A:410:PCW:H351	0.56	2.27	11	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
3:D:605:PCW:O2P	3:D:624:PCW:C8	0.56	2.53	11	2
4:D:632:17F:C36	3:C:208:PCW:H461	0.56	2.31	11	2
3:C:206:PCW:C18	3:C:208:PCW:C15	0.56	2.84	20	3
3:C:206:PCW:H61	3:C:212:PCW:H322	0.56	1.75	12	1
3:A:402:PCW:H442	3:C:206:PCW:H251	0.56	1.76	14	1
2:B:37:GLU:HG2	2:B:56:LEU:HD11	0.56	1.78	17	3
3:D:609:PCW:H252	3:D:616:PCW:H381	0.56	1.76	16	1
4:B:210:17F:C33	3:C:205:PCW:H462	0.56	2.29	16	1
3:A:406:PCW:O2P	3:B:205:PCW:H422	0.56	2.01	17	1
3:B:203:PCW:C38	3:C:211:PCW:H162	0.56	2.30	17	1
3:A:401:PCW:C42	3:D:612:PCW:H271	0.56	2.31	20	1
3:A:408:PCW:O4P	3:A:408:PCW:C6	0.56	2.54	20	1
3:A:404:PCW:O31	3:A:404:PCW:C36	0.56	2.53	11	5
1:A:356:HIS:NE2	3:A:401:PCW:H222	0.56	2.14	2	1
3:A:412:PCW:H12	3:A:412:PCW:H41	0.56	1.76	9	4
3:A:414:PCW:H371	3:A:414:PCW:C11	0.56	2.31	19	7
3:A:420:PCW:H382	3:D:611:PCW:H162	0.56	1.77	11	5
3:D:622:PCW:C14	3:D:622:PCW:H181	0.56	2.31	5	10
3:B:203:PCW:C4	3:C:211:PCW:H352	0.56	2.31	2	1
3:A:406:PCW:H471	4:B:211:17F:H32	0.56	1.75	3	2
3:A:420:PCW:C1	3:D:618:PCW:H381	0.56	2.29	3	1
3:A:408:PCW:H182	3:A:413:PCW:H262	0.56	1.76	4	1
3:C:207:PCW:C4	3:C:207:PCW:O11	0.56	2.54	4	1
3:C:210:PCW:O31	3:C:210:PCW:C35	0.56	2.45	11	5
3:A:420:PCW:O2	3:D:618:PCW:C42	0.56	2.53	6	3
3:D:617:PCW:C39	3:D:619:PCW:C16	0.56	2.83	8	4
3:D:618:PCW:H2	3:D:618:PCW:H62	0.56	1.76	5	3
3:D:610:PCW:O11	3:D:610:PCW:H2	0.56	1.99	6	1
3:D:616:PCW:C48	3:C:207:PCW:H241	0.56	2.31	6	1
3:D:604:PCW:O11	3:D:604:PCW:H41	0.56	1.99	10	3
3:C:206:PCW:H472	4:C:214:17F:C41	0.56	2.31	9	1
3:B:205:PCW:H31	4:B:211:17F:P1	0.56	2.40	10	1
3:C:209:PCW:H52	4:C:214:17F:O2	0.56	2.00	19	4
3:A:420:PCW:H40	3:D:617:PCW:H232	0.56	1.78	11	1
3:A:414:PCW:H252	4:A:415:17F:C33	0.56	2.31	19	3
4:B:210:17F:H52	4:C:215:17F:H42	0.56	1.77	13	1
3:D:609:PCW:H342	4:D:632:17F:H20A	0.56	1.74	14	1
3:C:206:PCW:H132	3:C:208:PCW:H62	0.56	1.77	14	1
3:C:212:PCW:C40	4:C:215:17F:H59	0.56	2.30	14	1
3:A:402:PCW:H322	3:A:410:PCW:C4	0.56	2.30	15	1
3:D:601:PCW:H132	3:D:601:PCW:H471	0.56	1.78	18	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
4:D:628:17F:H78	4:C:214:17F:C30	0.56	2.28	18	1
3:B:203:PCW:H73	3:C:211:PCW:O2P	0.56	2.00	19	1
3:D:607:PCW:H411	3:D:626:PCW:H472	0.56	1.76	20	1
1:A:356:HIS:CD2	3:A:401:PCW:H222	0.56	2.36	2	1
1:A:365:LYS:HB2	1:A:366:PRO:CD	0.56	2.27	11	10
3:A:407:PCW:O31	3:A:407:PCW:O3	0.56	2.23	13	7
3:A:411:PCW:H42	3:A:411:PCW:C31	0.56	2.30	17	3
3:A:418:PCW:O31	3:A:418:PCW:O3P	0.56	2.24	3	2
3:D:614:PCW:O31	3:D:614:PCW:C3	0.56	2.52	6	10
3:D:620:PCW:H481	3:D:624:PCW:H442	0.56	1.78	2	1
3:B:203:PCW:H321	4:B:210:17F:H29	0.56	1.78	2	1
3:A:412:PCW:H451	3:C:210:PCW:C19	0.56	2.31	4	2
3:D:618:PCW:H2	3:D:618:PCW:C6	0.56	2.28	12	2
3:C:206:PCW:C8	3:C:212:PCW:H73	0.56	2.29	5	1
3:A:410:PCW:H232	4:A:422:17F:H74	0.56	1.78	13	2
3:A:418:PCW:C35	3:D:613:PCW:H131	0.56	2.31	16	2
3:D:622:PCW:H19	4:D:631:17F:C17	0.56	2.31	9	1
3:A:414:PCW:H471	4:B:209:17F:C12	0.56	2.16	15	2
3:B:204:PCW:H32	3:B:207:PCW:H352	0.56	1.76	13	1
4:C:218:17F:C24	4:C:219:17F:H73	0.56	2.31	13	2
1:A:321:ALA:HB3	1:A:322:PRO:HD3	0.56	1.78	14	1
3:A:412:PCW:H381	3:C:210:PCW:H381	0.56	1.76	14	2
3:D:614:PCW:C28	4:B:209:17F:H36	0.56	2.31	14	1
3:D:614:PCW:H282	4:B:209:17F:H40	0.56	1.77	14	1
3:C:203:PCW:H182	3:C:211:PCW:H122	0.56	1.78	14	1
3:B:206:PCW:H232	3:C:205:PCW:H19	0.56	1.75	15	1
3:B:208:PCW:H42	3:B:208:PCW:O11	0.56	2.00	15	1
3:A:406:PCW:C23	3:A:411:PCW:H472	0.56	2.31	16	2
3:D:608:PCW:H221	4:D:628:17F:O10	0.56	2.00	18	1
3:D:614:PCW:H221	4:B:209:17F:C27	0.56	2.31	18	1
3:D:617:PCW:H471	3:C:204:PCW:H412	0.56	1.76	19	1
3:D:603:PCW:H461	3:D:611:PCW:H432	0.56	1.74	20	1
3:A:402:PCW:H442	3:C:206:PCW:H212	0.56	1.76	1	1
3:A:413:PCW:O1P	3:C:210:PCW:P	0.56	2.64	1	1
3:D:602:PCW:C21	3:D:602:PCW:C17	0.56	2.76	12	4
3:C:208:PCW:O31	3:C:208:PCW:O3	0.56	2.24	9	18
3:A:417:PCW:O31	3:A:417:PCW:O3P	0.56	2.24	19	5
3:D:617:PCW:C36	3:C:216:PCW:H362	0.56	2.31	3	3
3:D:626:PCW:O11	3:D:626:PCW:O2	0.56	2.23	9	2
3:A:421:PCW:C12	4:D:630:17F:C9	0.56	2.83	14	5
3:D:606:PCW:H62	3:D:626:PCW:H281	0.56	1.74	4	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:246:ASP:HA	1:D:528:ARG:CZ	0.56	2.31	18	8
3:B:207:PCW:O1P	3:B:207:PCW:H32	0.56	2.01	9	7
3:A:402:PCW:O2P	3:A:410:PCW:C7	0.56	2.54	8	3
3:A:421:PCW:O2P	3:D:618:PCW:C4	0.56	2.46	7	1
3:C:212:PCW:H432	3:C:212:PCW:C18	0.56	2.26	7	1
3:A:410:PCW:C46	3:A:412:PCW:H432	0.56	2.24	8	1
3:A:402:PCW:H331	3:A:410:PCW:O2	0.56	2.01	10	1
3:D:609:PCW:H271	4:D:628:17F:C39	0.56	2.30	14	2
3:C:209:PCW:O31	3:C:209:PCW:O3P	0.56	2.24	12	1
3:C:203:PCW:H11	3:C:211:PCW:C7	0.56	2.31	13	1
3:C:207:PCW:H342	4:C:213:17F:H5	0.56	1.77	15	2
1:A:320:LEU:HD21	3:D:601:PCW:H20	0.56	1.76	14	1
3:A:406:PCW:H412	4:B:211:17F:H10	0.56	1.78	15	1
3:B:203:PCW:H331	4:B:210:17F:H37	0.56	1.78	15	1
3:C:209:PCW:H121	4:C:214:17F:C18	0.56	2.31	16	2
3:A:406:PCW:H471	4:B:211:17F:C1Z	0.56	2.31	17	1
3:A:406:PCW:C3	4:B:211:17F:H77	0.56	2.26	19	1
3:C:207:PCW:H231	3:C:207:PCW:H462	0.56	1.77	19	1
3:B:208:PCW:H39	3:C:204:PCW:C35	0.56	2.30	1	1
4:B:211:17F:H19	4:B:211:17F:C8	0.56	2.30	1	2
3:B:208:PCW:H372	3:C:204:PCW:H331	0.56	1.77	2	1
3:B:204:PCW:H40	4:B:210:17F:C10	0.56	2.30	4	4
3:C:207:PCW:H40	4:C:213:17F:H77	0.56	1.77	3	1
3:C:216:PCW:H422	3:C:217:PCW:C33	0.56	2.31	16	9
3:B:204:PCW:O31	3:B:204:PCW:O3P	0.56	2.23	19	3
3:A:419:PCW:H31	3:D:615:PCW:C12	0.56	2.31	5	2
3:B:205:PCW:H171	3:C:204:PCW:C32	0.56	2.31	5	1
1:A:260:ASP:HA	1:A:263:LYS:HE2	0.56	1.76	6	1
3:D:623:PCW:H242	3:B:203:PCW:C48	0.56	2.30	6	1
3:B:203:PCW:O11	3:C:211:PCW:H372	0.56	2.00	6	1
3:D:604:PCW:C31	3:D:606:PCW:H82	0.56	2.31	19	3
3:B:208:PCW:H12	3:C:211:PCW:C32	0.56	2.31	12	2
3:A:403:PCW:H211	3:A:403:PCW:H422	0.56	1.77	13	1
3:A:404:PCW:C13	3:B:205:PCW:H452	0.56	2.30	13	1
3:D:602:PCW:H471	4:D:629:17F:C25	0.56	2.31	13	1
3:B:203:PCW:H42	3:C:211:PCW:C35	0.56	2.31	14	1
1:A:237:GLU:HA	1:A:240:ARG:HD2	0.56	1.77	15	1
4:A:422:17F:H49	4:C:218:17F:C12	0.56	2.29	16	1
3:D:608:PCW:C44	4:D:628:17F:H34	0.56	2.30	18	1
3:A:408:PCW:H482	3:A:413:PCW:C22	0.56	2.31	19	1
3:B:204:PCW:C48	3:C:205:PCW:H471	0.56	2.30	20	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
3:A:406:PCW:H272	3:D:617:PCW:C28	0.56	2.31	1	1
3:A:417:PCW:O11	3:A:417:PCW:H2	0.56	2.00	10	7
3:D:616:PCW:C28	3:C:206:PCW:H482	0.56	2.31	9	2
3:B:204:PCW:H40	4:B:210:17F:H12A	0.56	1.78	4	2
3:B:204:PCW:C3	3:B:207:PCW:H352	0.56	2.31	13	3
3:C:205:PCW:O4P	3:C:205:PCW:H82	0.56	2.01	1	20
3:A:409:PCW:C41	3:A:419:PCW:H251	0.56	2.26	2	1
3:C:211:PCW:H151	4:C:215:17F:C33	0.56	2.30	2	1
4:B:210:17F:H68	3:C:209:PCW:H441	0.56	1.78	3	2
3:D:621:PCW:H271	4:D:632:17F:H37	0.56	1.75	5	1
3:B:205:PCW:O31	3:B:208:PCW:C8	0.56	2.54	12	5
4:B:210:17F:H71	3:C:212:PCW:H262	0.56	1.76	6	1
1:D:451:LYS:HB3	3:D:601:PCW:H283	0.56	1.77	7	1
3:B:204:PCW:H40	4:B:210:17F:H10	0.56	1.76	8	1
3:B:203:PCW:H442	4:C:215:17F:H46	0.56	1.76	9	1
3:D:624:PCW:H41	3:D:624:PCW:C32	0.56	2.31	11	1
3:D:616:PCW:H212	4:D:632:17F:C22	0.56	2.31	12	1
3:A:407:PCW:H142	3:A:410:PCW:H322	0.56	1.78	14	1
4:B:210:17F:C36	3:C:212:PCW:H281	0.56	2.27	14	1
3:D:622:PCW:H431	4:D:631:17F:H67	0.56	1.76	16	1
3:C:206:PCW:C19	3:C:207:PCW:H182	0.56	2.30	16	1
3:C:209:PCW:C17	4:C:214:17F:H30	0.56	2.22	16	1
3:C:211:PCW:H152	4:C:215:17F:C36	0.56	2.29	18	1
1:D:519:ALA:HB3	1:D:520:PRO:HD3	0.56	1.78	8	19
3:D:608:PCW:H181	4:D:629:17F:C11	0.56	2.21	1	4
3:B:203:PCW:C11	3:B:203:PCW:O31	0.56	2.54	9	11
3:C:216:PCW:O11	3:C:216:PCW:O2	0.56	2.24	3	19
4:A:416:17F:H72	3:B:203:PCW:H272	0.56	1.76	2	2
3:D:608:PCW:C19	3:D:608:PCW:C15	0.56	2.82	2	2
3:B:204:PCW:H39	4:B:210:17F:C10	0.56	2.30	2	1
3:B:208:PCW:H371	3:C:204:PCW:H352	0.56	1.78	2	1
3:A:403:PCW:H212	3:A:404:PCW:C25	0.56	2.31	3	1
2:C:126:ASP:OD1	2:C:128:LYS:HG2	0.56	2.01	3	2
3:D:603:PCW:O31	3:D:603:PCW:O3	0.56	2.23	9	4
3:A:405:PCW:H362	3:A:406:PCW:H232	0.56	1.77	6	1
3:D:604:PCW:H381	4:C:218:17F:C21	0.56	2.31	7	2
3:C:211:PCW:H231	4:C:213:17F:H43	0.56	1.78	7	1
3:A:421:PCW:C36	3:D:618:PCW:H141	0.56	2.31	11	2
3:B:205:PCW:H63	3:B:208:PCW:H62	0.56	1.78	8	1
3:C:205:PCW:H231	3:C:209:PCW:H283	0.56	1.77	8	1
3:D:603:PCW:C45	3:D:611:PCW:H412	0.56	2.30	9	2

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
3:A:402:PCW:C7	3:A:407:PCW:H32	0.56	2.31	10	1
3:A:404:PCW:H252	4:B:211:17F:H73	0.56	1.77	10	1
3:A:409:PCW:O2P	3:B:206:PCW:H73	0.56	2.01	10	1
3:D:604:PCW:H31	3:D:604:PCW:H41	0.56	1.78	10	1
3:D:605:PCW:C8	4:D:630:17F:O5	0.56	2.54	10	1
3:D:605:PCW:H422	3:D:620:PCW:H483	0.56	1.77	10	1
3:D:611:PCW:C46	3:B:208:PCW:H261	0.56	2.30	13	3
3:D:614:PCW:H20	4:B:209:17F:C27	0.56	2.31	16	1
3:B:206:PCW:H431	3:C:205:PCW:C26	0.56	2.31	16	1
3:A:402:PCW:H442	3:C:208:PCW:H172	0.56	1.78	18	1
4:B:211:17F:C30	3:C:216:PCW:H182	0.56	2.29	20	1
4:C:214:17F:O8	4:C:214:17F:C5	0.55	2.50	14	9
3:D:608:PCW:H182	4:D:629:17F:C26	0.55	2.28	2	1
3:D:612:PCW:C4	3:D:623:PCW:H342	0.55	2.31	18	7
4:B:211:17F:H50	3:C:204:PCW:H422	0.55	1.78	3	2
1:D:532:ARG:O	1:D:536:LEU:HG	0.55	2.02	20	4
3:B:204:PCW:H2	3:B:204:PCW:O11	0.55	2.00	18	3
3:A:404:PCW:H32	3:B:205:PCW:H431	0.55	1.75	5	1
3:A:419:PCW:H31	3:D:615:PCW:H121	0.55	1.78	5	1
3:C:207:PCW:H483	3:C:207:PCW:H231	0.55	1.77	5	1
3:D:616:PCW:H2	3:D:616:PCW:O4P	0.55	2.01	12	4
4:C:213:17F:O10	4:C:213:17F:O7	0.55	2.23	11	8
1:A:330:ARG:HH22	1:D:448:VAL:HG23	0.55	1.60	12	1
3:B:208:PCW:C1	3:C:211:PCW:C34	0.55	2.82	12	2
3:A:409:PCW:H371	4:B:210:17F:H62	0.55	1.78	13	1
3:C:212:PCW:H221	3:C:212:PCW:H162	0.55	1.75	14	1
3:D:613:PCW:H51	3:D:619:PCW:O11	0.55	2.01	17	2
3:B:208:PCW:O31	3:B:208:PCW:H41	0.55	2.00	17	1
3:A:409:PCW:O1P	4:B:210:17F:N1	0.55	2.35	19	1
3:B:203:PCW:H461	4:C:215:17F:C29	0.55	2.28	19	1
3:A:414:PCW:H121	4:A:415:17F:H57	0.55	1.77	20	1
3:D:616:PCW:C5	4:D:632:17F:O4	0.55	2.53	13	5
3:A:411:PCW:H322	3:A:411:PCW:C8	0.55	2.31	14	3
3:A:411:PCW:H283	3:C:210:PCW:H231	0.55	1.78	2	1
3:B:205:PCW:H231	3:C:210:PCW:H251	0.55	1.78	2	1
3:D:603:PCW:H241	3:D:611:PCW:H142	0.55	1.78	6	2
3:C:216:PCW:H422	3:C:217:PCW:H331	0.55	1.78	6	3
3:D:605:PCW:H2	3:D:614:PCW:C6	0.55	2.31	5	2
3:D:603:PCW:H41	3:D:603:PCW:H32	0.55	1.76	6	1
3:C:209:PCW:H442	3:C:212:PCW:C25	0.55	2.31	8	1
3:A:419:PCW:H82	3:D:626:PCW:C32	0.55	2.30	9	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
3:D:622:PCW:H222	4:D:631:17F:C1Y	0.55	2.30	17	4
3:A:412:PCW:H451	3:C:210:PCW:C18	0.55	2.23	15	3
3:B:203:PCW:H261	4:B:209:17F:C34	0.55	2.31	14	1
3:C:203:PCW:C7	3:C:212:PCW:H11	0.55	2.32	17	1
1:A:356:HIS:HB3	3:A:401:PCW:H20	0.55	1.78	18	1
3:A:410:PCW:H221	4:A:422:17F:C41	0.55	2.31	20	1
3:A:414:PCW:H121	4:A:415:17F:C31	0.55	2.31	20	1
3:A:406:PCW:H283	3:D:619:PCW:H211	0.55	1.79	1	1
3:D:616:PCW:C48	3:C:207:PCW:H252	0.55	2.32	13	5
4:D:629:17F:H9A	4:D:629:17F:C19	0.55	2.31	3	3
3:D:605:PCW:H421	3:D:620:PCW:C14	0.55	2.31	3	5
3:C:206:PCW:C21	3:C:208:PCW:H19	0.55	2.32	2	2
4:B:210:17F:H78	3:C:209:PCW:H461	0.55	1.78	10	2
4:A:415:17F:H44	3:B:205:PCW:H483	0.55	1.77	4	1
3:B:208:PCW:H41	3:C:211:PCW:H82	0.55	1.78	4	1
3:A:419:PCW:H482	3:D:604:PCW:H271	0.55	1.77	5	1
3:D:624:PCW:H261	3:C:217:PCW:H262	0.55	1.78	9	3
3:C:205:PCW:O1P	3:C:205:PCW:O2	0.55	2.24	6	1
1:D:570:ARG:O	1:D:574:LEU:HG	0.55	2.01	10	1
3:C:209:PCW:H471	3:C:209:PCW:C27	0.55	2.30	11	2
3:C:211:PCW:C22	3:C:211:PCW:H181	0.55	2.23	10	1
3:A:403:PCW:H422	3:A:403:PCW:C21	0.55	2.30	13	1
3:B:207:PCW:C23	3:B:207:PCW:C36	0.55	2.82	14	1
4:A:416:17F:H62	3:B:204:PCW:C25	0.55	2.30	15	1
3:A:410:PCW:C18	3:A:410:PCW:C23	0.55	2.83	18	1
3:A:401:PCW:H452	3:D:612:PCW:C28	0.55	2.32	20	1
3:D:605:PCW:H182	3:D:614:PCW:C36	0.55	2.29	15	9
3:D:623:PCW:O3	3:D:624:PCW:H332	0.55	2.00	2	6
2:B:125:VAL:HG13	2:B:129:GLN:HG3	0.55	1.78	2	1
3:C:205:PCW:H382	3:C:212:PCW:H222	0.55	1.77	2	1
3:A:407:PCW:H63	3:A:410:PCW:C37	0.55	2.31	3	2
3:D:612:PCW:H432	3:D:612:PCW:H20	0.55	1.76	3	2
3:D:615:PCW:C5	3:D:625:PCW:H42	0.55	2.31	20	2
3:B:207:PCW:H41	3:B:207:PCW:H31	0.55	1.79	4	1
4:A:416:17F:O5	3:B:204:PCW:C5	0.55	2.53	5	2
3:A:405:PCW:H342	3:A:406:PCW:H182	0.55	1.76	19	2
2:C:162:GLU:HA	2:C:165:LYS:HE2	0.55	1.79	9	1
3:D:605:PCW:O1P	3:D:614:PCW:H51	0.55	2.01	10	1
3:B:208:PCW:H342	3:C:203:PCW:H171	0.55	1.75	11	1
3:C:205:PCW:H11	4:C:214:17F:C7	0.55	2.32	18	4
3:C:206:PCW:C7	3:C:212:PCW:O1P	0.55	2.54	13	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
4:B:211:17F:C22	3:C:204:PCW:H431	0.55	2.31	15	1
3:A:403:PCW:H181	3:A:403:PCW:H232	0.55	1.77	16	1
3:A:418:PCW:H331	3:D:613:PCW:C13	0.55	2.29	18	1
3:C:205:PCW:C41	3:C:212:PCW:C23	0.55	2.83	18	1
3:C:205:PCW:H121	3:C:209:PCW:H321	0.55	1.77	18	1
3:C:203:PCW:H471	3:C:210:PCW:H20	0.55	1.79	20	1
4:C:213:17F:H50	4:C:215:17F:H71	0.55	1.79	20	1
3:D:605:PCW:C31	3:D:614:PCW:H61	0.55	2.30	5	4
3:C:206:PCW:C15	3:C:208:PCW:C15	0.55	2.84	13	5
3:C:212:PCW:H432	3:C:212:PCW:C21	0.55	2.32	9	5
4:A:415:17F:H10	4:B:209:17F:H4	0.55	1.77	2	1
3:C:206:PCW:C22	3:C:208:PCW:H431	0.55	2.15	17	2
3:A:404:PCW:H121	3:A:404:PCW:C37	0.55	2.31	17	2
3:A:404:PCW:H341	4:A:415:17F:H6	0.55	1.77	17	2
3:A:408:PCW:H171	3:A:408:PCW:H232	0.55	1.78	4	1
3:A:408:PCW:H162	3:A:413:PCW:H261	0.55	1.77	4	1
3:A:412:PCW:H381	3:C:210:PCW:C38	0.55	2.30	4	2
3:D:603:PCW:H421	3:D:611:PCW:C36	0.55	2.31	4	1
3:C:203:PCW:H442	3:C:204:PCW:C17	0.55	2.31	4	1
3:C:205:PCW:H172	3:C:205:PCW:C21	0.55	2.30	16	2
3:D:602:PCW:H221	3:D:602:PCW:C17	0.55	2.26	15	2
3:D:610:PCW:H63	4:D:631:17F:O8	0.55	2.02	19	4
3:B:208:PCW:H451	4:C:219:17F:H42	0.55	1.78	6	1
3:D:607:PCW:H451	3:D:626:PCW:H481	0.55	1.79	7	2
3:B:204:PCW:H11	3:B:207:PCW:H351	0.55	1.78	7	1
3:A:413:PCW:O11	3:A:413:PCW:H2	0.55	2.00	8	1
3:B:208:PCW:H421	3:C:204:PCW:H171	0.55	1.75	8	1
3:C:205:PCW:O11	3:C:212:PCW:H152	0.55	2.00	15	2
4:A:415:17F:C28	3:B:208:PCW:H232	0.55	2.25	9	1
3:D:605:PCW:O2P	3:D:614:PCW:H51	0.55	2.02	11	1
3:B:208:PCW:C1	3:C:211:PCW:H322	0.55	2.31	11	1
3:C:206:PCW:C13	3:C:208:PCW:H321	0.55	2.24	18	2
3:B:208:PCW:C32	3:C:211:PCW:H63	0.55	2.25	15	2
3:D:624:PCW:H442	4:B:209:17F:C42	0.55	2.30	14	1
3:D:621:PCW:H41	3:D:621:PCW:C2	0.55	2.26	15	1
4:B:210:17F:C1X	4:C:215:17F:H29	0.55	2.31	15	2
3:C:205:PCW:H122	3:C:212:PCW:C20	0.55	2.32	15	1
3:A:405:PCW:C35	3:A:411:PCW:H441	0.55	2.31	16	1
3:D:622:PCW:C19	4:D:631:17F:O10	0.55	2.55	8	12
3:C:203:PCW:O31	3:C:203:PCW:C1	0.55	2.46	17	6
1:A:313:VAL:HG12	1:A:317:ARG:HE	0.55	1.60	2	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:D:418:GLN:O	1:D:422:VAL:HB	0.55	2.01	5	2
3:B:208:PCW:O31	3:B:208:PCW:H12	0.55	2.02	3	3
3:C:206:PCW:H242	3:C:208:PCW:C38	0.55	2.31	13	3
3:A:402:PCW:H431	3:C:206:PCW:H272	0.55	1.76	18	2
3:B:204:PCW:C47	3:B:207:PCW:H271	0.55	2.32	4	2
3:A:408:PCW:H331	3:A:413:PCW:H122	0.55	1.79	6	1
3:D:614:PCW:H261	4:B:209:17F:H66	0.55	1.78	6	1
3:C:206:PCW:H32	3:C:207:PCW:C26	0.55	2.31	6	1
3:D:617:PCW:C37	3:D:619:PCW:C14	0.55	2.80	7	2
3:C:205:PCW:H381	3:C:212:PCW:H261	0.55	1.77	7	1
3:A:403:PCW:H242	3:A:403:PCW:H422	0.55	1.77	9	1
3:D:604:PCW:H181	3:C:211:PCW:C28	0.55	2.31	9	1
3:A:409:PCW:O2P	3:B:206:PCW:C7	0.55	2.54	10	1
3:D:610:PCW:C4	4:D:631:17F:O8	0.55	2.55	12	5
3:B:203:PCW:H411	3:C:211:PCW:C18	0.55	2.31	10	1
3:C:206:PCW:H62	4:C:213:17F:H6	0.55	1.78	12	2
3:A:404:PCW:H352	3:A:404:PCW:H51	0.55	1.77	11	1
3:A:411:PCW:C1	3:B:205:PCW:H131	0.55	2.31	13	2
3:B:205:PCW:H151	3:C:204:PCW:C31	0.55	2.31	14	1
3:D:614:PCW:C12	3:D:620:PCW:H382	0.55	2.31	1	4
3:D:617:PCW:O31	3:D:617:PCW:O3	0.55	2.25	14	11
3:A:408:PCW:O31	3:A:408:PCW:O3P	0.55	2.25	4	5
3:D:601:PCW:H341	3:D:601:PCW:O31	0.55	2.00	14	12
3:B:205:PCW:H42	3:B:205:PCW:C1	0.55	2.21	2	1
3:A:411:PCW:O3	3:A:411:PCW:C31	0.55	2.55	20	14
3:C:203:PCW:H451	3:C:210:PCW:H19	0.55	1.78	18	5
3:C:217:PCW:O3P	3:C:217:PCW:O31	0.55	2.25	6	8
3:A:409:PCW:O2P	3:B:206:PCW:H61	0.55	2.01	7	1
3:A:402:PCW:H51	3:A:402:PCW:C32	0.55	2.29	9	1
3:D:621:PCW:O1P	3:D:622:PCW:H63	0.55	2.01	9	1
3:B:206:PCW:H63	4:B:210:17F:O1	0.55	2.02	10	1
3:D:602:PCW:O4P	3:D:602:PCW:C6	0.55	2.55	15	1
3:A:408:PCW:O1P	3:A:408:PCW:C5	0.55	2.54	19	5
3:D:624:PCW:H62	3:D:624:PCW:C31	0.55	2.32	1	8
3:C:207:PCW:O11	3:C:207:PCW:O2	0.55	2.25	10	12
4:A:416:17F:H71	3:B:203:PCW:H252	0.55	1.78	2	2
3:C:207:PCW:H31	3:C:207:PCW:O1P	0.55	2.02	14	3
3:C:207:PCW:O11	3:C:207:PCW:C8	0.55	2.55	4	2
3:D:624:PCW:O31	3:D:624:PCW:C6	0.55	2.55	6	2
3:D:610:PCW:H162	4:D:631:17F:C34	0.55	2.31	8	1
4:C:215:17F:N1	4:C:215:17F:H4A	0.55	2.16	8	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
3:A:406:PCW:H441	3:C:204:PCW:H431	0.55	1.78	9	2
3:D:608:PCW:C17	4:D:629:17F:C18	0.55	2.85	16	4
3:A:410:PCW:H40	3:A:412:PCW:H362	0.55	1.79	13	1
3:A:407:PCW:H332	3:A:410:PCW:H371	0.55	1.78	14	1
3:C:207:PCW:C12	4:C:213:17F:H20A	0.55	2.32	14	1
3:D:612:PCW:H51	3:D:623:PCW:C32	0.55	2.32	1	1
3:D:612:PCW:O3	3:D:612:PCW:O31	0.55	2.25	17	7
3:C:210:PCW:O2P	3:C:210:PCW:H2	0.55	2.00	11	3
3:D:612:PCW:H412	3:D:612:PCW:C20	0.55	2.32	3	1
3:B:206:PCW:H142	3:C:209:PCW:C37	0.55	2.30	3	3
3:A:404:PCW:C40	4:A:415:17F:H29	0.55	2.32	5	1
3:D:605:PCW:H481	3:D:614:PCW:H162	0.55	1.78	5	1
4:B:210:17F:H30	4:C:215:17F:C11	0.55	2.29	15	2
3:C:209:PCW:O11	3:C:209:PCW:C5	0.55	2.50	6	6
3:A:413:PCW:H451	3:C:210:PCW:C23	0.55	2.25	8	1
3:C:209:PCW:O31	3:C:209:PCW:O4P	0.55	2.25	15	1
3:A:418:PCW:C37	3:A:418:PCW:C41	0.55	2.77	20	2
3:B:208:PCW:H372	3:C:204:PCW:O31	0.55	2.01	17	1
3:C:206:PCW:H82	4:C:214:17F:H9	0.55	1.78	18	1
3:A:421:PCW:H11	3:A:421:PCW:C4	0.55	2.32	1	1
3:D:612:PCW:C5	3:D:623:PCW:H321	0.55	2.32	1	1
3:D:627:PCW:O2	3:D:627:PCW:C11	0.55	2.54	17	3
3:B:206:PCW:H441	3:C:209:PCW:C39	0.55	2.32	1	1
3:B:206:PCW:H63	3:B:206:PCW:O2P	0.55	2.02	11	6
3:D:624:PCW:H481	4:B:209:17F:H50	0.55	1.79	5	3
2:C:80:CYS:HB3	2:C:93:ILE:HD12	0.55	1.78	10	6
3:C:206:PCW:H212	3:C:208:PCW:H172	0.55	1.79	16	2
4:C:214:17F:C7	4:C:214:17F:O10	0.55	2.54	2	7
3:A:417:PCW:C44	3:D:618:PCW:H242	0.55	2.32	10	3
3:B:204:PCW:H411	3:B:207:PCW:H61	0.55	1.79	3	1
3:B:206:PCW:H431	3:B:206:PCW:H141	0.55	1.79	3	1
3:C:206:PCW:C16	3:C:207:PCW:H222	0.55	2.32	13	2
3:C:207:PCW:H432	4:C:213:17F:H77	0.55	1.79	3	1
3:C:217:PCW:C14	4:C:219:17F:C1Z	0.55	2.85	4	2
4:B:211:17F:H10	4:B:211:17F:H69	0.55	1.77	5	1
3:D:617:PCW:H331	3:C:216:PCW:H341	0.55	1.78	7	2
3:D:621:PCW:C7	3:D:621:PCW:O4P	0.55	2.55	6	5
2:B:22:GLN:HB3	2:B:149:ARG:HG3	0.55	1.79	6	1
3:B:205:PCW:C3	4:B:211:17F:O8	0.55	2.54	6	1
3:B:206:PCW:H271	3:C:205:PCW:H171	0.55	1.77	6	1
4:B:210:17F:H76	3:C:212:PCW:H472	0.55	1.77	6	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
3:D:602:PCW:C34	4:C:214:17F:H61	0.55	2.32	7	2
3:A:410:PCW:O1P	3:A:410:PCW:H51	0.55	2.02	12	1
3:C:205:PCW:O31	4:C:214:17F:N1	0.55	2.40	12	1
3:B:208:PCW:H11	3:C:211:PCW:H362	0.55	1.77	13	1
3:B:203:PCW:C44	3:C:211:PCW:H232	0.55	2.32	14	1
3:C:206:PCW:C17	3:C:208:PCW:H151	0.55	2.20	18	3
3:A:414:PCW:C34	4:A:415:17F:H59	0.55	2.32	17	1
3:A:406:PCW:H40	3:B:205:PCW:C15	0.55	2.32	20	1
2:B:135:ARG:HB2	2:C:165:LYS:HD3	0.55	1.78	20	1
3:A:413:PCW:C43	3:C:210:PCW:H232	0.54	2.31	8	6
3:D:602:PCW:O31	3:D:602:PCW:C1	0.54	2.54	10	7
3:A:408:PCW:C35	3:A:413:PCW:C16	0.54	2.83	18	7
3:D:609:PCW:C45	3:C:208:PCW:H231	0.54	2.33	2	1
3:D:610:PCW:C17	4:D:631:17F:H61	0.54	2.32	11	7
3:B:205:PCW:H483	3:B:208:PCW:C19	0.54	2.32	2	3
4:B:210:17F:H1A	4:C:215:17F:O8	0.54	2.00	2	1
4:A:416:17F:H64	3:B:204:PCW:C27	0.54	2.32	3	1
3:D:609:PCW:C40	3:D:616:PCW:H441	0.54	2.32	16	3
3:B:206:PCW:C14	3:C:209:PCW:H371	0.54	2.31	3	1
3:D:612:PCW:C20	3:D:620:PCW:C48	0.54	2.85	4	1
3:A:406:PCW:C46	4:B:211:17F:H58	0.54	2.32	5	1
3:D:608:PCW:H441	3:C:205:PCW:H271	0.54	1.79	5	1
3:A:406:PCW:H242	3:A:411:PCW:C48	0.54	2.30	8	3
4:A:415:17F:H37	3:C:211:PCW:H40	0.54	1.79	8	1
3:D:624:PCW:H461	4:B:209:17F:H75	0.54	1.77	8	1
3:C:212:PCW:C14	4:C:215:17F:H9A	0.54	2.18	10	1
3:B:204:PCW:H461	3:C:205:PCW:H462	0.54	1.76	11	1
3:B:204:PCW:H52	3:B:204:PCW:C31	0.54	2.32	13	2
4:C:218:17F:H68	4:C:219:17F:H63	0.54	1.80	16	1
3:A:417:PCW:H262	3:A:420:PCW:H242	0.54	1.77	17	1
3:B:204:PCW:H212	3:B:204:PCW:H171	0.54	1.79	17	1
3:B:205:PCW:H20	3:C:204:PCW:H432	0.54	1.79	17	1
3:D:606:PCW:H442	3:D:609:PCW:C1	0.54	2.31	18	1
3:C:204:PCW:H39	3:C:216:PCW:C26	0.54	2.31	19	1
3:C:205:PCW:H232	3:C:209:PCW:H283	0.54	1.79	19	1
3:A:405:PCW:H371	3:A:411:PCW:H441	0.54	1.80	20	1
3:B:204:PCW:O31	3:B:204:PCW:C11	0.54	2.55	8	6
3:B:205:PCW:H11	3:B:208:PCW:C8	0.54	2.33	2	1
3:B:205:PCW:O31	3:B:205:PCW:C1	0.54	2.49	12	5
4:A:416:17F:H31	3:B:204:PCW:H162	0.54	1.78	4	2
3:D:606:PCW:H2	3:D:606:PCW:C4	0.54	2.32	15	10

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
3:D:612:PCW:H483	3:B:207:PCW:H482	0.54	1.78	4	1
3:A:413:PCW:C42	3:C:210:PCW:H452	0.54	2.15	5	1
3:A:402:PCW:H451	4:D:632:17F:C29	0.54	2.29	8	3
3:A:420:PCW:H40	3:D:617:PCW:C23	0.54	2.32	11	3
3:D:604:PCW:H451	3:D:606:PCW:H141	0.54	1.79	11	5
3:D:618:PCW:O31	3:D:618:PCW:O3P	0.54	2.25	7	2
3:D:618:PCW:H182	3:D:618:PCW:H221	0.54	1.78	7	1
3:D:621:PCW:C45	3:C:208:PCW:H481	0.54	2.31	8	2
3:B:208:PCW:H221	3:C:211:PCW:H483	0.54	1.78	8	1
3:A:406:PCW:C36	3:B:205:PCW:H321	0.54	2.30	9	1
3:A:419:PCW:H82	3:D:626:PCW:C31	0.54	2.31	9	1
2:B:47:ASP:HB3	2:C:132:ASP:HB2	0.54	1.79	9	1
3:B:205:PCW:H212	3:C:203:PCW:H482	0.54	1.77	10	1
3:D:612:PCW:H461	3:D:612:PCW:H241	0.54	1.79	11	2
3:A:418:PCW:H331	3:D:613:PCW:H152	0.54	1.79	12	1
3:D:621:PCW:H2	3:D:621:PCW:C7	0.54	2.33	12	1
3:C:217:PCW:C36	4:C:218:17F:H76	0.54	2.29	13	1
3:D:608:PCW:C26	4:D:629:17F:H62	0.54	2.20	14	2
3:D:624:PCW:C45	4:B:209:17F:H75	0.54	2.32	14	1
4:A:416:17F:H59	3:B:204:PCW:H252	0.54	1.79	15	1
3:A:401:PCW:H411	3:B:204:PCW:H281	0.54	1.79	16	1
3:A:409:PCW:H242	3:A:419:PCW:H271	0.54	1.79	17	1
3:C:203:PCW:C42	3:C:204:PCW:H161	0.54	2.14	17	1
3:A:410:PCW:H181	3:A:410:PCW:H231	0.54	1.80	18	1
3:A:410:PCW:O1P	3:C:207:PCW:H41	0.54	2.03	19	1
3:A:408:PCW:O4P	3:A:408:PCW:H62	0.54	2.02	10	18
3:A:411:PCW:C28	3:C:203:PCW:H471	0.54	2.32	2	2
3:A:417:PCW:C47	3:D:618:PCW:H252	0.54	2.32	2	2
3:D:615:PCW:H51	3:D:625:PCW:O3P	0.54	2.02	2	1
3:D:604:PCW:H412	3:D:606:PCW:C23	0.54	2.26	3	1
3:B:206:PCW:C3	3:B:206:PCW:O1P	0.54	2.55	4	5
3:C:206:PCW:C25	3:C:206:PCW:C21	0.54	2.82	4	1
3:A:404:PCW:C5	3:B:205:PCW:H39	0.54	2.31	5	1
3:A:401:PCW:C5	3:B:207:PCW:O31	0.54	2.55	6	6
3:A:418:PCW:C37	3:D:613:PCW:H151	0.54	2.33	6	1
3:B:207:PCW:H31	3:B:207:PCW:O1P	0.54	2.02	10	7
4:A:415:17F:H40	4:B:209:17F:C33	0.54	2.32	10	1
3:B:208:PCW:H452	4:C:218:17F:C30	0.54	2.27	10	1
3:D:601:PCW:C48	4:D:628:17F:H51	0.54	2.31	13	2
4:D:628:17F:C8	4:D:629:17F:H33	0.54	2.32	13	3
3:C:206:PCW:H41	4:C:214:17F:H35	0.54	1.79	14	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
3:A:403:PCW:O31	3:A:403:PCW:C36	0.54	2.54	16	1
3:A:414:PCW:H262	4:A:415:17F:C34	0.54	2.31	17	1
3:A:421:PCW:H441	3:D:618:PCW:H211	0.54	1.78	19	1
4:B:210:17F:H36	4:C:215:17F:C22	0.54	2.31	19	1
3:A:402:PCW:C33	3:A:407:PCW:H121	0.54	2.32	1	2
3:B:208:PCW:O11	3:B:208:PCW:H2	0.54	2.02	8	10
3:C:203:PCW:H39	4:C:213:17F:C34	0.54	2.33	1	1
4:A:416:17F:H77	3:D:612:PCW:C47	0.54	2.31	14	4
3:C:209:PCW:O2P	3:C:209:PCW:C3	0.54	2.55	3	1
3:A:402:PCW:O4P	3:A:402:PCW:O2	0.54	2.25	4	8
3:B:203:PCW:C7	3:C:211:PCW:O31	0.54	2.55	4	5
3:A:405:PCW:H82	4:B:211:17F:O2	0.54	2.02	6	1
1:D:451:LYS:O	1:D:455:TYR:HB2	0.54	2.02	6	8
3:D:607:PCW:C47	3:C:209:PCW:H483	0.54	2.32	6	1
4:A:422:17F:H9	4:A:422:17F:C19	0.54	2.32	20	5
3:D:614:PCW:C28	4:B:209:17F:H12	0.54	2.31	7	1
3:D:618:PCW:O31	3:D:618:PCW:H51	0.54	2.02	7	1
4:D:628:17F:H59	4:D:629:17F:C29	0.54	2.33	7	1
3:C:207:PCW:H131	3:C:207:PCW:H61	0.54	1.76	8	1
3:C:212:PCW:H351	4:C:215:17F:C20	0.54	2.33	9	1
3:C:209:PCW:C44	3:C:212:PCW:H283	0.54	2.31	10	2
3:D:608:PCW:O1P	3:D:626:PCW:C22	0.54	2.55	19	4
3:B:207:PCW:C6	4:B:210:17F:H6	0.54	2.32	14	1
3:A:413:PCW:H482	3:C:204:PCW:H261	0.54	1.79	16	1
4:A:415:17F:H50	3:B:208:PCW:H231	0.54	1.79	18	1
3:D:602:PCW:C25	4:D:629:17F:H76	0.54	2.29	18	1
3:C:211:PCW:H232	4:C:215:17F:H48	0.54	1.79	18	1
4:D:630:17F:O10	4:D:630:17F:O6	0.54	2.25	12	11
3:C:211:PCW:H283	4:C:215:17F:C30	0.54	2.32	1	2
3:A:406:PCW:H371	3:A:406:PCW:C41	0.54	2.33	5	2
3:A:409:PCW:H261	3:A:409:PCW:H482	0.54	1.79	2	3
3:D:615:PCW:O1P	3:D:625:PCW:C6	0.54	2.55	2	1
3:D:621:PCW:O31	3:D:621:PCW:O3P	0.54	2.26	5	7
3:A:406:PCW:H381	3:C:204:PCW:C33	0.54	2.32	4	2
2:C:84:ILE:CD1	2:C:118:CYS:HA	0.54	2.33	17	9
3:B:204:PCW:O11	3:B:204:PCW:C7	0.54	2.55	8	1
3:A:414:PCW:H321	4:A:415:17F:C1Y	0.54	2.33	9	2
3:D:612:PCW:C23	3:D:620:PCW:H442	0.54	2.33	9	1
3:A:409:PCW:O31	4:B:210:17F:H33	0.54	2.03	10	1
3:A:406:PCW:C12	4:B:211:17F:C6	0.54	2.83	11	1
3:A:408:PCW:C24	3:A:411:PCW:H221	0.54	2.16	11	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
3:A:403:PCW:C14	3:A:404:PCW:H322	0.54	2.33	17	4
3:A:408:PCW:O3	3:A:413:PCW:H121	0.54	2.03	12	2
3:A:409:PCW:H352	4:B:210:17F:H59	0.54	1.80	13	1
3:D:610:PCW:H151	4:D:631:17F:C34	0.54	2.32	19	1
3:A:406:PCW:H211	3:A:406:PCW:C16	0.54	2.31	13	5
3:D:618:PCW:O31	3:D:618:PCW:C1	0.54	2.53	15	7
4:B:209:17F:O7	4:B:209:17F:O10	0.54	2.26	16	7
2:C:15:GLY:CA	5:C:201:GSP:C8	0.54	2.91	19	4
3:A:401:PCW:C3	3:B:207:PCW:H371	0.54	2.33	3	1
3:D:610:PCW:H283	4:D:631:17F:H72	0.54	1.78	11	3
3:B:203:PCW:H62	3:C:211:PCW:H331	0.54	1.80	3	1
3:B:206:PCW:C14	3:C:209:PCW:H39	0.54	2.32	3	1
3:A:410:PCW:H142	3:C:207:PCW:H171	0.54	1.80	4	1
3:A:411:PCW:O2P	4:B:211:17F:O3	0.54	2.26	11	3
3:D:623:PCW:O31	3:D:623:PCW:O3P	0.54	2.26	6	3
3:B:207:PCW:H162	3:B:207:PCW:H332	0.54	1.78	4	1
3:D:623:PCW:O31	3:D:624:PCW:C32	0.54	2.56	8	2
3:B:206:PCW:H52	3:C:205:PCW:H341	0.54	1.78	8	1
3:B:208:PCW:H442	4:C:213:17F:C42	0.54	2.32	12	1
3:C:205:PCW:C14	3:C:209:PCW:H412	0.54	2.33	12	1
4:B:209:17F:H10	4:B:209:17F:H59	0.54	1.79	13	1
3:B:206:PCW:C39	3:C:205:PCW:H283	0.54	2.33	16	1
3:C:211:PCW:H2	4:C:215:17F:H57	0.54	1.79	16	1
3:A:406:PCW:H472	3:B:205:PCW:H283	0.54	1.78	17	1
3:A:420:PCW:H31	3:D:618:PCW:C41	0.54	2.32	18	1
3:D:623:PCW:H211	3:B:203:PCW:H483	0.54	1.79	18	1
3:A:403:PCW:C46	3:D:618:PCW:H281	0.54	2.33	20	1
3:D:616:PCW:C8	4:D:632:17F:O4	0.54	2.55	10	7
2:B:80:CYS:HB3	2:B:93:ILE:HD12	0.54	1.79	4	4
4:B:211:17F:C17	4:B:211:17F:O7	0.54	2.56	2	4
3:A:419:PCW:C6	3:D:626:PCW:O31	0.54	2.56	3	2
2:B:12:ASP:HA	5:B:201:GSP:O1B	0.54	2.03	14	2
3:C:206:PCW:H62	3:C:212:PCW:O2P	0.54	2.03	3	1
3:A:406:PCW:H321	3:B:205:PCW:C34	0.54	2.33	14	2
3:A:420:PCW:H362	3:D:618:PCW:C38	0.54	2.32	18	5
3:D:603:PCW:C37	3:D:611:PCW:H342	0.54	2.31	4	1
3:D:612:PCW:H20	3:D:620:PCW:C48	0.54	2.33	4	1
3:C:212:PCW:H461	4:C:215:17F:H36	0.54	1.80	9	1
3:C:207:PCW:C28	4:C:214:17F:H46	0.54	2.32	10	1
3:A:406:PCW:H341	3:B:205:PCW:O2	0.54	2.03	11	2
3:A:421:PCW:H161	4:D:630:17F:H60	0.54	1.78	11	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
3:C:206:PCW:H141	3:C:208:PCW:C34	0.54	2.33	11	1
3:D:621:PCW:O31	3:D:621:PCW:O3	0.54	2.26	18	4
3:A:413:PCW:H461	3:C:210:PCW:H483	0.54	1.79	14	1
3:A:421:PCW:C34	3:D:618:PCW:H132	0.54	2.32	17	3
3:A:403:PCW:H321	3:A:404:PCW:O2P	0.54	2.03	15	1
2:B:15:GLY:O	2:B:19:LEU:HG	0.54	2.03	15	1
3:C:205:PCW:H432	4:C:215:17F:H67	0.54	1.80	19	1
3:A:408:PCW:C23	3:A:408:PCW:C18	0.54	2.85	2	8
4:A:422:17F:O10	4:A:422:17F:O6	0.54	2.26	18	5
3:D:608:PCW:O11	3:D:608:PCW:C2	0.54	2.54	18	12
3:D:608:PCW:H211	4:D:629:17F:H20	0.54	1.80	10	2
3:C:206:PCW:C17	3:C:207:PCW:C19	0.54	2.86	1	1
3:A:407:PCW:O31	3:A:410:PCW:C35	0.54	2.56	6	6
3:A:419:PCW:H431	3:D:625:PCW:H461	0.54	1.78	15	9
3:D:612:PCW:O2P	3:D:620:PCW:C4	0.54	2.55	2	6
3:D:627:PCW:O4P	3:D:627:PCW:H82	0.54	2.03	9	7
3:B:208:PCW:H482	3:C:216:PCW:H221	0.54	1.80	2	1
2:C:146:ALA:HB3	5:C:201:GSP:N7	0.54	2.18	8	2
3:C:217:PCW:H172	4:C:219:17F:C1Y	0.54	2.32	20	5
3:D:620:PCW:H481	4:B:209:17F:H74	0.54	1.78	3	2
3:A:421:PCW:H141	4:D:630:17F:H11A	0.54	1.80	4	2
3:B:205:PCW:O1P	4:B:211:17F:N1	0.54	2.41	14	2
3:D:606:PCW:P	3:D:606:PCW:O31	0.54	2.65	6	1
3:D:604:PCW:H181	3:C:211:PCW:H283	0.54	1.79	9	1
3:D:614:PCW:H261	4:B:209:17F:C39	0.54	2.32	9	1
3:A:404:PCW:H382	3:A:404:PCW:C12	0.54	2.31	10	1
3:A:405:PCW:C7	3:A:406:PCW:O11	0.54	2.54	11	1
2:B:16:LYS:HB2	5:B:201:GSP:O3B	0.54	2.02	11	2
3:B:208:PCW:H12	3:C:211:PCW:H322	0.54	1.80	11	1
3:C:207:PCW:C16	4:C:213:17F:C31	0.54	2.85	20	2
3:A:401:PCW:C47	3:D:612:PCW:H271	0.54	2.32	12	1
3:D:609:PCW:H232	3:D:616:PCW:H361	0.54	1.80	13	2
3:B:204:PCW:C7	3:B:204:PCW:C13	0.54	2.85	13	1
3:C:207:PCW:H63	3:C:207:PCW:C32	0.54	2.24	13	2
4:D:632:17F:H52	3:C:208:PCW:C15	0.54	2.32	14	1
3:A:409:PCW:H432	3:A:419:PCW:H282	0.54	1.80	15	1
3:D:605:PCW:H172	3:D:614:PCW:H131	0.54	1.78	15	1
3:C:212:PCW:H451	4:C:215:17F:C38	0.54	2.32	15	1
3:A:410:PCW:O1P	3:A:410:PCW:H52	0.54	2.03	19	1
1:A:349:TYR:HE1	3:A:401:PCW:H19	0.54	1.62	1	1
4:A:422:17F:O8	4:A:422:17F:O9	0.54	2.26	19	2

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
3:D:614:PCW:H261	4:B:209:17F:H71	0.54	1.80	1	2
3:D:627:PCW:H211	3:C:217:PCW:H352	0.54	1.80	1	4
3:C:204:PCW:O1P	3:C:204:PCW:H31	0.54	2.03	13	6
3:A:408:PCW:H232	3:A:408:PCW:C17	0.54	2.32	8	2
4:A:415:17F:O2	4:A:415:17F:O9	0.54	2.26	8	2
3:D:614:PCW:H482	3:D:620:PCW:C21	0.54	2.26	11	4
3:D:622:PCW:C28	3:C:217:PCW:H61	0.54	2.33	16	4
3:C:205:PCW:H212	3:C:205:PCW:C17	0.54	2.24	16	3
3:C:203:PCW:H451	3:C:210:PCW:H20	0.54	1.77	4	3
3:A:412:PCW:C42	3:C:210:PCW:H182	0.54	2.33	7	1
1:A:386:PHE:HZ	4:A:415:17F:H76	0.54	1.62	15	4
3:A:421:PCW:H362	3:D:618:PCW:H141	0.54	1.79	8	1
3:C:205:PCW:C3	3:C:209:PCW:H161	0.54	2.33	9	1
4:D:630:17F:P1	4:D:630:17F:O10	0.54	2.66	11	1
3:B:206:PCW:H271	3:C:205:PCW:C19	0.54	2.27	11	1
3:C:209:PCW:C45	3:C:212:PCW:H262	0.54	2.33	12	1
3:A:417:PCW:H282	3:A:420:PCW:C25	0.54	2.32	13	1
3:D:601:PCW:H382	4:D:628:17F:C29	0.54	2.33	13	1
3:B:204:PCW:H73	3:B:204:PCW:O11	0.54	2.02	13	1
3:C:207:PCW:O3	4:C:213:17F:H1	0.54	2.02	13	1
3:D:607:PCW:H442	3:D:625:PCW:C48	0.54	2.32	14	1
3:B:203:PCW:C33	4:B:210:17F:C21	0.54	2.84	15	2
3:A:401:PCW:C39	3:B:204:PCW:H172	0.54	2.33	16	1
3:D:623:PCW:C12	3:D:624:PCW:H332	0.54	2.33	16	1
3:C:206:PCW:H52	4:C:214:17F:C9	0.54	2.33	16	1
3:D:608:PCW:H211	4:D:629:17F:H20A	0.54	1.78	18	1
3:B:206:PCW:P	3:B:206:PCW:C3	0.54	2.96	3	12
1:D:534:GLU:HA	1:D:537:LYS:HE3	0.54	1.78	2	2
3:D:605:PCW:H132	3:D:614:PCW:H2	0.54	1.79	18	6
3:A:408:PCW:C37	3:A:413:PCW:H162	0.54	2.33	20	2
3:D:607:PCW:C3	3:D:626:PCW:C39	0.54	2.83	3	5
4:A:422:17F:H49	4:C:218:17F:C10	0.54	2.28	18	2
2:B:73:ARG:HG3	2:B:103:VAL:HG12	0.54	1.79	18	3
3:B:204:PCW:H462	3:C:205:PCW:C47	0.54	2.32	4	1
3:C:203:PCW:H341	3:C:204:PCW:C3	0.54	2.33	5	1
3:A:418:PCW:C36	3:D:613:PCW:H151	0.54	2.33	6	2
3:D:615:PCW:N	3:D:625:PCW:O1P	0.54	2.41	9	4
3:A:421:PCW:H52	3:A:421:PCW:H11	0.54	1.80	9	1
3:B:204:PCW:H452	3:B:207:PCW:H20	0.54	1.78	9	1
3:D:604:PCW:H412	3:D:606:PCW:C25	0.54	2.33	10	2
3:C:206:PCW:H62	4:C:213:17F:C7	0.54	2.33	12	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
3:C:209:PCW:H451	3:C:212:PCW:H251	0.54	1.80	13	1
3:B:203:PCW:C48	4:C:215:17F:H55	0.54	2.27	17	1
3:C:205:PCW:O11	3:C:209:PCW:H151	0.54	2.03	18	1
3:A:404:PCW:H441	3:A:414:PCW:C25	0.54	2.31	19	1
3:A:414:PCW:H342	4:B:209:17F:H29	0.54	1.79	20	1
3:A:417:PCW:C14	3:A:420:PCW:H341	0.53	2.24	17	5
3:A:420:PCW:C48	3:D:617:PCW:H271	0.53	2.32	15	2
3:B:208:PCW:H322	3:C:211:PCW:O11	0.53	2.03	7	3
3:D:622:PCW:C27	3:C:217:PCW:H61	0.53	2.33	11	2
4:B:210:17F:H1	4:B:210:17F:H4	0.53	1.78	7	2
1:A:217:LEU:HD11	3:A:405:PCW:H251	0.53	1.79	20	3
3:A:419:PCW:H31	3:D:615:PCW:C11	0.53	2.33	3	3
4:B:210:17F:C12	4:B:210:17F:C23	0.53	2.86	12	3
3:A:409:PCW:H52	3:B:206:PCW:C32	0.53	2.33	4	1
3:D:619:PCW:O2P	3:D:627:PCW:H42	0.53	2.04	4	2
3:D:627:PCW:H20	3:C:217:PCW:C32	0.53	2.32	18	2
3:A:404:PCW:H421	3:A:404:PCW:C17	0.53	2.33	9	3
3:D:606:PCW:H352	4:C:218:17F:H6	0.53	1.80	6	1
3:B:208:PCW:H482	3:C:216:PCW:C19	0.53	2.32	6	1
4:C:218:17F:C27	4:C:219:17F:H39	0.53	2.33	7	2
3:C:205:PCW:C36	3:C:212:PCW:H252	0.53	2.20	7	1
3:A:420:PCW:C44	3:D:617:PCW:H232	0.53	2.30	10	1
2:C:68:ARG:O	2:C:72:MET:HG2	0.53	2.03	10	1
3:A:410:PCW:H232	4:A:422:17F:H76	0.53	1.79	17	1
3:D:617:PCW:H432	3:D:627:PCW:C22	0.53	2.33	17	1
3:D:617:PCW:H462	3:C:204:PCW:H472	0.53	1.79	17	1
3:A:406:PCW:H262	3:A:411:PCW:H481	0.53	1.79	19	1
3:D:624:PCW:C28	3:C:217:PCW:H262	0.53	2.26	19	2
4:B:210:17F:H72	3:C:209:PCW:H461	0.53	1.79	20	1
3:A:405:PCW:H341	3:A:411:PCW:H421	0.53	1.80	12	2
3:D:603:PCW:H121	3:D:624:PCW:H161	0.53	1.80	9	2
3:D:613:PCW:C11	3:D:613:PCW:O31	0.53	2.56	1	2
3:D:616:PCW:H432	3:C:208:PCW:H283	0.53	1.79	1	1
3:D:619:PCW:C42	3:D:627:PCW:H261	0.53	2.22	10	3
3:D:602:PCW:C26	4:D:629:17F:H78	0.53	2.30	3	1
3:D:606:PCW:H132	3:D:606:PCW:H342	0.53	1.80	15	6
3:C:206:PCW:H211	3:C:208:PCW:H382	0.53	1.78	15	3
3:C:212:PCW:H422	4:C:215:17F:C37	0.53	2.33	3	1
3:A:414:PCW:O31	4:A:415:17F:H20	0.53	2.03	13	2
3:D:614:PCW:O31	3:D:620:PCW:H2	0.53	2.03	6	6
3:D:623:PCW:H371	3:D:623:PCW:H131	0.53	1.78	15	2

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
3:D:616:PCW:H181	4:D:632:17F:H12	0.53	1.80	5	1
3:B:205:PCW:H171	3:C:204:PCW:O2	0.53	2.03	5	1
3:B:206:PCW:H212	3:C:209:PCW:O31	0.53	2.03	13	3
3:B:208:PCW:H342	3:C:211:PCW:H31	0.53	1.80	5	1
3:C:207:PCW:H483	3:C:207:PCW:H232	0.53	1.78	5	1
3:A:405:PCW:H63	4:B:211:17F:O2	0.53	2.02	6	1
3:A:413:PCW:H421	3:C:210:PCW:C46	0.53	2.33	8	1
3:B:208:PCW:O11	3:B:208:PCW:C8	0.53	2.55	11	3
4:C:215:17F:H77	4:C:215:17F:C27	0.53	2.26	8	1
3:C:216:PCW:H422	3:C:217:PCW:C34	0.53	2.33	8	1
4:A:416:17F:H32	3:B:204:PCW:H182	0.53	1.79	18	2
3:B:206:PCW:H182	3:C:205:PCW:H171	0.53	1.80	12	1
3:C:208:PCW:O31	3:C:208:PCW:C7	0.53	2.54	12	1
3:D:605:PCW:C39	3:D:612:PCW:H341	0.53	2.27	13	3
4:C:215:17F:H48	4:C:215:17F:H78	0.53	1.79	13	1
4:B:210:17F:H36	4:C:215:17F:H29	0.53	1.79	15	1
3:B:208:PCW:H181	3:C:203:PCW:H271	0.53	1.80	16	1
4:A:415:17F:C36	4:B:209:17F:H37	0.53	2.33	1	1
3:D:605:PCW:C39	3:D:612:PCW:H322	0.53	2.32	13	2
2:B:146:ALA:HB3	5:B:201:GSP:N7	0.53	2.18	4	3
3:A:405:PCW:H412	3:A:411:PCW:H442	0.53	1.79	20	2
3:D:608:PCW:H451	3:C:205:PCW:H281	0.53	1.81	5	1
3:D:603:PCW:H82	3:D:603:PCW:C11	0.53	2.33	6	1
3:B:208:PCW:C47	3:C:203:PCW:H181	0.53	2.33	6	1
4:B:210:17F:H30	4:C:215:17F:H11A	0.53	1.79	6	1
3:C:206:PCW:C12	3:C:208:PCW:H171	0.53	2.33	6	1
3:B:207:PCW:O11	3:B:207:PCW:O2	0.53	2.26	15	9
3:D:616:PCW:C48	3:C:207:PCW:H251	0.53	2.33	8	2
3:C:212:PCW:C42	4:C:215:17F:H40	0.53	2.22	8	1
3:D:607:PCW:H432	3:D:626:PCW:H481	0.53	1.79	10	2
3:A:405:PCW:H281	3:A:418:PCW:C24	0.53	2.33	10	2
3:A:421:PCW:H131	4:D:630:17F:C11	0.53	2.33	10	1
3:D:619:PCW:C42	3:D:627:PCW:H282	0.53	2.33	10	2
3:A:406:PCW:H331	4:B:211:17F:C7	0.53	2.33	11	1
3:D:604:PCW:H432	3:D:606:PCW:H181	0.53	1.80	11	1
3:C:206:PCW:C23	3:C:208:PCW:H431	0.53	2.28	16	1
3:A:402:PCW:H412	3:C:206:PCW:C26	0.53	2.33	17	1
3:D:604:PCW:H251	4:C:215:17F:H75	0.53	1.80	17	1
3:C:206:PCW:H351	3:C:208:PCW:C12	0.53	2.33	17	1
3:A:417:PCW:H481	3:D:611:PCW:H282	0.53	1.80	18	1
4:A:416:17F:H62	3:B:204:PCW:H222	0.53	1.80	1	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
3:D:604:PCW:H282	3:D:607:PCW:H483	0.53	1.79	1	1
3:D:609:PCW:H73	3:D:621:PCW:H31	0.53	1.80	1	3
3:C:212:PCW:C42	3:C:212:PCW:H222	0.53	2.34	1	1
3:B:203:PCW:H11	3:B:203:PCW:O31	0.53	2.02	10	3
3:A:417:PCW:C3	3:D:611:PCW:O3	0.53	2.56	3	1
4:D:628:17F:H40	4:D:629:17F:C41	0.53	2.33	16	3
4:C:218:17F:H46	4:C:219:17F:C40	0.53	2.32	3	2
3:A:420:PCW:C41	3:D:611:PCW:H181	0.53	2.34	4	1
3:D:623:PCW:H381	3:D:625:PCW:H182	0.53	1.80	15	4
3:A:414:PCW:C14	4:A:415:17F:H63	0.53	2.31	5	1
3:D:606:PCW:H161	4:C:218:17F:H8	0.53	1.80	6	1
3:D:607:PCW:C3	3:D:626:PCW:C37	0.53	2.84	7	1
3:A:404:PCW:H161	3:B:205:PCW:H451	0.53	1.80	8	1
4:A:415:17F:H54	3:D:624:PCW:H451	0.53	1.79	10	1
1:D:462:LYS:HB3	3:D:602:PCW:C28	0.53	2.34	10	2
3:C:205:PCW:H472	4:C:215:17F:H42	0.53	1.80	10	1
3:A:413:PCW:C8	3:C:210:PCW:H372	0.53	2.33	11	1
3:D:609:PCW:H412	4:D:632:17F:H60	0.53	1.80	11	1
3:A:407:PCW:C46	3:A:410:PCW:H262	0.53	2.31	12	1
3:C:212:PCW:H351	4:C:215:17F:H57	0.53	1.79	12	1
3:D:619:PCW:H342	3:D:627:PCW:C34	0.53	2.32	14	1
3:B:206:PCW:C21	3:C:209:PCW:C32	0.53	2.77	14	1
3:A:406:PCW:H371	4:B:211:17F:H10	0.53	1.79	15	1
3:D:602:PCW:C7	4:C:214:17F:H19A	0.53	2.26	17	1
3:C:205:PCW:C47	4:C:215:17F:H38	0.53	2.23	17	1
3:D:608:PCW:C26	4:D:629:17F:H35	0.53	2.28	18	1
3:D:607:PCW:C3	3:D:626:PCW:H371	0.53	2.32	19	1
3:D:610:PCW:H322	4:D:631:17F:H9	0.53	1.80	20	1
3:A:420:PCW:C39	3:D:611:PCW:H161	0.53	2.34	2	1
3:D:608:PCW:O3P	3:D:608:PCW:O31	0.53	2.25	2	5
3:B:207:PCW:O11	3:B:207:PCW:C7	0.53	2.57	2	1
3:A:410:PCW:C28	4:A:422:17F:H75	0.53	2.33	10	3
3:A:418:PCW:O4P	3:A:418:PCW:H62	0.53	2.04	3	11
3:A:412:PCW:C38	3:C:210:PCW:H362	0.53	2.34	4	1
2:B:83:ALA:HB3	2:B:86:ASN:HB3	0.53	1.80	16	4
3:C:212:PCW:C40	4:C:215:17F:H63	0.53	2.34	4	1
3:B:206:PCW:C24	3:C:205:PCW:H171	0.53	2.34	20	2
3:A:405:PCW:H232	3:A:418:PCW:H262	0.53	1.80	6	1
3:D:608:PCW:H171	4:D:629:17F:C18	0.53	2.34	13	7
3:D:602:PCW:O2	4:C:214:17F:H60	0.53	2.02	8	2
4:C:215:17F:H64	4:C:215:17F:H35	0.53	1.81	8	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
3:A:401:PCW:C25	3:D:615:PCW:H271	0.53	2.31	10	1
3:B:208:PCW:C39	3:C:204:PCW:H151	0.53	2.33	10	1
3:B:205:PCW:H332	3:B:208:PCW:C6	0.53	2.33	11	1
3:C:206:PCW:C15	3:C:207:PCW:C19	0.53	2.85	11	2
3:A:406:PCW:H222	4:B:211:17F:H32	0.53	1.81	13	1
3:A:414:PCW:C48	4:B:209:17F:H65	0.53	2.33	19	2
2:B:110:PRO:HB3	2:B:162:GLU:HB3	0.53	1.81	13	1
3:A:406:PCW:H131	4:B:211:17F:C39	0.53	2.33	15	1
4:A:416:17F:H62	3:B:204:PCW:H252	0.53	1.79	15	1
3:B:208:PCW:C14	3:C:203:PCW:H241	0.53	2.34	15	1
3:C:205:PCW:H251	3:C:209:PCW:C40	0.53	2.34	16	1
4:C:218:17F:H68	4:C:219:17F:C35	0.53	2.33	16	1
3:A:414:PCW:C18	3:A:414:PCW:C22	0.53	2.70	17	1
3:A:403:PCW:H62	3:A:404:PCW:O2	0.53	2.04	20	1
3:D:603:PCW:H212	3:D:603:PCW:C47	0.53	2.33	20	1
3:A:409:PCW:H321	3:B:206:PCW:C34	0.53	2.32	1	3
3:C:210:PCW:H121	3:C:210:PCW:H351	0.53	1.81	1	4
3:A:404:PCW:O4P	3:A:404:PCW:H2	0.53	2.03	2	3
3:D:605:PCW:C32	3:D:614:PCW:H62	0.53	2.34	4	3
3:A:419:PCW:H483	3:C:212:PCW:C38	0.53	2.32	5	1
1:A:360:LEU:HD12	1:A:363:LYS:HD2	0.53	1.79	8	1
3:A:411:PCW:H262	3:C:210:PCW:C23	0.53	2.34	8	1
3:D:616:PCW:C48	3:C:207:PCW:H283	0.53	2.34	8	2
3:B:204:PCW:H12	3:B:207:PCW:C31	0.53	2.33	11	2
3:B:203:PCW:H482	4:C:215:17F:C29	0.53	2.31	10	1
3:D:604:PCW:C3	3:D:606:PCW:H82	0.53	2.33	11	1
3:A:404:PCW:H371	3:A:404:PCW:C12	0.53	2.30	13	1
3:D:605:PCW:H382	3:D:612:PCW:H322	0.53	1.79	13	1
3:C:212:PCW:H131	4:C:215:17F:O10	0.53	2.04	14	1
3:A:409:PCW:H182	3:A:419:PCW:C26	0.53	2.34	17	1
3:C:205:PCW:H221	3:C:209:PCW:H261	0.53	1.79	19	1
3:B:205:PCW:O11	3:C:204:PCW:C6	0.53	2.55	20	1
3:A:406:PCW:H232	3:A:411:PCW:H472	0.53	1.80	2	2
3:A:421:PCW:C7	4:D:630:17F:O2	0.53	2.57	14	3
3:D:625:PCW:H39	3:D:626:PCW:C14	0.53	2.34	4	2
3:B:207:PCW:O31	3:B:207:PCW:O3	0.53	2.27	4	1
3:A:406:PCW:H452	3:B:205:PCW:H283	0.53	1.81	5	2
3:D:605:PCW:C47	3:D:614:PCW:H162	0.53	2.33	20	3
3:B:206:PCW:C8	3:C:205:PCW:H362	0.53	2.34	5	1
3:C:212:PCW:H421	4:C:215:17F:C2X	0.53	2.30	10	1
3:A:419:PCW:H381	3:D:625:PCW:C26	0.53	2.34	11	2

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
3:C:205:PCW:H161	3:C:209:PCW:C22	0.53	2.34	12	1
3:A:403:PCW:C36	3:A:403:PCW:O31	0.53	2.56	13	1
3:C:209:PCW:H2	3:C:209:PCW:O11	0.53	2.02	15	1
3:A:401:PCW:H481	3:D:612:PCW:H241	0.53	1.81	16	1
3:D:608:PCW:H421	3:B:206:PCW:H452	0.53	1.81	16	1
3:D:612:PCW:H221	3:D:620:PCW:H461	0.53	1.79	17	1
3:D:602:PCW:H381	3:D:602:PCW:C14	0.53	2.34	18	1
3:C:211:PCW:C15	4:C:215:17F:H64	0.53	2.29	18	1
3:A:411:PCW:H452	4:B:211:17F:H20	0.53	1.80	19	1
4:B:210:17F:H30	4:C:215:17F:C21	0.53	2.34	19	1
3:A:403:PCW:H461	3:D:618:PCW:H281	0.53	1.80	20	1
3:A:420:PCW:C31	3:A:420:PCW:O3	0.53	2.57	17	17
3:D:602:PCW:H52	4:C:214:17F:C17	0.53	2.31	1	1
3:D:614:PCW:O4P	3:D:614:PCW:H63	0.53	2.03	16	8
1:A:316:LEU:HD11	3:D:602:PCW:H283	0.53	1.80	2	1
3:D:610:PCW:C17	4:D:631:17F:H65	0.53	2.34	3	1
3:C:206:PCW:C6	4:C:213:17F:O1	0.53	2.56	4	3
3:C:207:PCW:C41	4:C:213:17F:H8	0.53	2.33	4	1
1:D:435:GLU:O	1:D:439:GLN:HG3	0.53	2.03	12	5
3:C:205:PCW:O11	3:C:209:PCW:C15	0.53	2.57	10	3
3:A:403:PCW:H152	3:A:404:PCW:H322	0.53	1.80	11	1
3:D:616:PCW:H161	4:D:632:17F:C11	0.53	2.34	12	1
3:A:403:PCW:H132	3:A:404:PCW:H322	0.53	1.80	13	1
3:B:208:PCW:H73	3:B:208:PCW:C12	0.53	2.34	15	1
3:C:216:PCW:C42	3:C:217:PCW:H151	0.53	2.33	15	1
3:C:211:PCW:H2	4:C:215:17F:H56	0.53	1.81	16	1
3:A:406:PCW:H271	3:A:406:PCW:H481	0.53	1.80	19	1
3:D:607:PCW:H471	3:D:625:PCW:H481	0.53	1.80	19	1
3:A:404:PCW:H132	3:B:205:PCW:C44	0.53	2.33	1	2
3:A:406:PCW:H131	4:B:211:17F:C37	0.53	2.34	1	1
3:D:607:PCW:H451	3:D:625:PCW:C48	0.53	2.34	1	1
3:D:608:PCW:C43	4:D:628:17F:H34	0.53	2.31	7	6
4:B:211:17F:O2	4:B:211:17F:C2	0.53	2.57	14	7
3:B:207:PCW:O3	3:B:207:PCW:O31	0.53	2.25	3	2
3:A:419:PCW:O11	3:A:419:PCW:H2	0.53	2.04	5	3
3:B:205:PCW:O31	3:B:208:PCW:C6	0.53	2.57	3	1
3:C:205:PCW:H182	3:C:209:PCW:C20	0.53	2.33	3	1
3:A:408:PCW:C37	3:A:413:PCW:H182	0.53	2.29	4	3
3:A:408:PCW:C41	3:A:408:PCW:H372	0.53	2.33	4	1
3:D:609:PCW:O11	3:D:616:PCW:C7	0.53	2.57	13	5
3:A:409:PCW:H351	4:B:210:17F:H62	0.53	1.80	5	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
3:D:603:PCW:C44	3:D:603:PCW:H231	0.53	2.33	5	1
2:C:79:LEU:HD13	2:C:159:LEU:HD22	0.53	1.81	5	3
3:B:203:PCW:H381	3:C:211:PCW:H461	0.53	1.80	6	1
3:B:203:PCW:C5	3:C:211:PCW:O31	0.53	2.57	6	2
4:D:632:17F:H53	3:C:208:PCW:C14	0.53	2.33	8	1
3:B:206:PCW:H39	3:B:206:PCW:C14	0.53	2.33	8	1
3:A:414:PCW:C42	4:A:415:17F:H70	0.53	2.29	9	1
3:A:420:PCW:H32	3:A:420:PCW:P	0.53	2.43	10	1
4:B:211:17F:H39	3:C:204:PCW:H422	0.53	1.81	11	2
3:C:205:PCW:H231	3:C:209:PCW:C24	0.53	2.33	12	1
3:D:604:PCW:C27	3:C:212:PCW:H451	0.53	2.34	13	1
4:B:210:17F:H40	4:C:215:17F:H35	0.53	1.81	13	1
3:A:407:PCW:H331	3:A:410:PCW:H321	0.53	1.79	14	1
3:D:612:PCW:H222	3:D:620:PCW:C46	0.53	2.29	18	1
2:C:32:TYR:HE1	5:C:201:GSP:C5'	0.53	2.16	18	1
3:A:408:PCW:O2P	3:A:411:PCW:H142	0.53	2.04	1	1
3:D:604:PCW:C28	3:D:607:PCW:H483	0.53	2.34	1	1
3:D:607:PCW:C45	3:D:625:PCW:H471	0.53	2.31	1	1
3:D:622:PCW:H262	3:C:217:PCW:C7	0.53	2.34	1	1
3:A:406:PCW:H352	3:B:205:PCW:H321	0.53	1.80	2	1
3:D:609:PCW:O31	3:D:609:PCW:C11	0.53	2.57	13	7
3:A:401:PCW:H331	3:B:207:PCW:H40	0.53	1.80	3	1
3:A:408:PCW:H252	4:D:631:17F:C30	0.53	2.34	3	1
3:D:603:PCW:C16	3:D:624:PCW:H222	0.53	2.34	5	2
4:A:416:17F:C41	4:B:209:17F:H68	0.53	2.34	4	3
3:A:406:PCW:C33	4:B:211:17F:H8	0.53	2.30	7	1
4:D:629:17F:O10	4:D:629:17F:O7	0.53	2.27	8	1
3:A:421:PCW:H141	4:D:630:17F:H29	0.53	1.81	11	1
3:D:617:PCW:P	3:C:216:PCW:H51	0.53	2.44	11	1
2:B:19:LEU:HD23	2:B:146:ALA:HB2	0.53	1.80	15	3
3:D:614:PCW:H142	3:D:620:PCW:H412	0.53	1.81	12	1
3:A:401:PCW:H122	3:B:207:PCW:H281	0.53	1.80	13	1
3:C:203:PCW:H321	3:C:207:PCW:C33	0.53	2.34	14	1
3:C:204:PCW:C25	3:C:217:PCW:H472	0.53	2.34	14	2
3:B:203:PCW:H222	4:B:209:17F:C20	0.53	2.34	15	1
3:D:616:PCW:H142	4:D:632:17F:C9	0.53	2.33	16	1
3:C:206:PCW:H19	3:C:207:PCW:C18	0.53	2.34	16	1
3:B:208:PCW:O3P	3:C:211:PCW:H362	0.53	2.04	18	2
3:D:616:PCW:O3	3:D:616:PCW:C31	0.52	2.57	17	15
3:A:404:PCW:H32	3:A:406:PCW:O2P	0.52	2.04	2	1
3:A:418:PCW:H471	3:D:613:PCW:H272	0.52	1.80	2	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
3:C:207:PCW:H412	4:C:213:17F:C12	0.52	2.23	11	3
3:A:401:PCW:H331	3:B:207:PCW:C40	0.52	2.34	3	1
3:A:408:PCW:O2P	3:A:411:PCW:H141	0.52	2.04	3	1
3:B:203:PCW:H472	4:C:215:17F:H47	0.52	1.82	3	1
1:A:247:LEU:O	1:A:250:VAL:HG12	0.52	2.04	9	7
3:D:613:PCW:H321	3:D:619:PCW:C14	0.52	2.33	4	4
3:D:614:PCW:H20	4:B:209:17F:H44	0.52	1.79	5	1
3:A:411:PCW:H262	3:B:205:PCW:H212	0.52	1.78	6	1
3:A:418:PCW:C41	3:A:418:PCW:H371	0.52	2.34	7	1
3:D:612:PCW:H162	3:D:620:PCW:C19	0.52	2.29	7	1
3:B:203:PCW:H381	3:C:211:PCW:C44	0.52	2.33	7	1
3:B:208:PCW:H371	3:C:203:PCW:H231	0.52	1.81	9	1
3:A:401:PCW:H342	3:B:207:PCW:H242	0.52	1.80	13	1
3:D:617:PCW:C42	3:D:627:PCW:C23	0.52	2.86	14	1
3:B:206:PCW:H431	3:C:205:PCW:C25	0.52	2.33	16	1
3:A:403:PCW:H461	3:D:618:PCW:C27	0.52	2.34	20	1
4:A:422:17F:C37	3:D:622:PCW:H451	0.52	2.34	3	6
3:D:619:PCW:H451	4:D:631:17F:C30	0.52	2.34	7	2
3:A:413:PCW:H51	3:A:413:PCW:O1P	0.52	2.05	12	2
3:B:204:PCW:O31	3:B:204:PCW:C7	0.52	2.57	2	1
4:B:211:17F:H12	4:B:211:17F:H62	0.52	1.79	2	1
3:A:403:PCW:C23	3:A:403:PCW:C28	0.52	2.61	9	3
3:A:417:PCW:H121	3:D:618:PCW:H332	0.52	1.81	3	1
3:B:207:PCW:O3	3:B:207:PCW:C31	0.52	2.58	3	2
3:A:408:PCW:C27	3:C:210:PCW:H242	0.52	2.34	4	1
2:B:13:GLY:HA2	5:B:201:GSP:H4'	0.52	1.81	5	1
3:A:414:PCW:H431	4:B:209:17F:C12	0.52	2.34	6	1
3:C:204:PCW:H241	3:C:210:PCW:C28	0.52	2.26	6	2
3:A:403:PCW:H381	3:A:403:PCW:C14	0.52	2.34	7	1
3:D:613:PCW:C6	3:D:619:PCW:H31	0.52	2.34	7	1
3:C:207:PCW:H121	4:C:213:17F:H5	0.52	1.80	7	1
3:C:203:PCW:H231	3:C:216:PCW:H251	0.52	1.79	8	1
3:A:421:PCW:H131	4:D:630:17F:H11A	0.52	1.80	10	1
3:D:609:PCW:H281	4:C:214:17F:H50	0.52	1.80	12	1
3:D:614:PCW:C13	3:D:620:PCW:H382	0.52	2.34	13	2
3:D:616:PCW:H342	3:C:208:PCW:H281	0.52	1.79	14	1
3:A:401:PCW:C45	3:D:612:PCW:H283	0.52	2.32	17	1
3:B:205:PCW:H132	3:C:204:PCW:O2	0.52	2.03	17	1
3:B:203:PCW:H332	4:B:210:17F:H38	0.52	1.81	19	1
3:A:402:PCW:O2P	3:A:410:PCW:C4	0.52	2.54	1	3
3:A:410:PCW:O11	3:A:410:PCW:C2	0.52	2.55	20	10

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
3:D:622:PCW:C18	3:D:622:PCW:C14	0.52	2.82	11	6
3:C:203:PCW:C7	4:C:213:17F:H4A	0.52	2.35	1	1
1:A:279:LEU:O	1:A:283:LEU:HG	0.52	2.03	2	3
3:A:414:PCW:C14	4:A:415:17F:H58	0.52	2.31	6	3
3:D:620:PCW:C48	3:D:624:PCW:H442	0.52	2.34	2	1
3:B:207:PCW:H82	3:B:207:PCW:H331	0.52	1.80	3	1
3:A:410:PCW:H431	3:A:412:PCW:H382	0.52	1.80	8	1
4:C:215:17F:H47	4:C:215:17F:C42	0.52	2.26	8	1
3:A:413:PCW:C8	3:C:210:PCW:O31	0.52	2.57	9	1
3:C:212:PCW:H332	4:C:215:17F:H32	0.52	1.80	12	1
3:D:614:PCW:H221	4:B:209:17F:H44	0.52	1.81	14	1
3:D:608:PCW:O1P	3:D:626:PCW:C23	0.52	2.57	15	1
3:A:403:PCW:H181	3:A:403:PCW:C23	0.52	2.33	16	1
3:A:414:PCW:C40	4:A:415:17F:H69	0.52	2.34	18	1
3:C:206:PCW:C15	3:C:208:PCW:H342	0.52	2.35	18	1
4:A:422:17F:C1X	4:C:219:17F:H62	0.52	2.34	20	2
1:D:478:ARG:O	1:D:482:GLN:HB2	0.52	2.03	13	4
2:B:8:VAL:HG12	2:B:16:LYS:HD2	0.52	1.81	6	7
3:B:205:PCW:O11	3:B:205:PCW:C2	0.52	2.53	6	5
3:C:205:PCW:H411	4:C:215:17F:C12	0.52	2.33	2	1
3:C:205:PCW:C43	4:C:215:17F:H37	0.52	2.34	2	1
3:C:207:PCW:H2	4:C:213:17F:C4	0.52	2.34	2	3
3:D:605:PCW:H461	3:D:620:PCW:H483	0.52	1.81	3	1
3:C:203:PCW:C45	3:C:210:PCW:C20	0.52	2.82	4	1
3:A:413:PCW:H422	3:C:210:PCW:C45	0.52	2.16	5	1
3:D:605:PCW:O31	3:D:614:PCW:C7	0.52	2.57	6	2
3:D:612:PCW:H41	3:D:623:PCW:C34	0.52	2.34	5	2
3:A:411:PCW:H262	3:B:205:PCW:H231	0.52	1.81	6	1
3:C:206:PCW:H121	3:C:208:PCW:C17	0.52	2.34	6	1
3:D:604:PCW:H51	4:C:219:17F:H4A	0.52	1.81	7	1
3:D:607:PCW:C45	3:D:626:PCW:H481	0.52	2.34	7	1
3:D:601:PCW:C40	4:D:628:17F:H52	0.52	2.35	8	2
3:D:617:PCW:C48	3:B:205:PCW:H222	0.52	2.35	11	1
3:A:404:PCW:H222	3:A:404:PCW:H181	0.52	1.82	13	2
3:C:207:PCW:H411	4:C:213:17F:H11A	0.52	1.80	13	1
3:A:406:PCW:H351	4:B:211:17F:O7	0.52	2.04	20	2
3:A:413:PCW:C42	3:C:210:PCW:H442	0.52	2.12	14	1
3:D:614:PCW:C8	3:D:614:PCW:O4P	0.52	2.58	14	4
3:D:620:PCW:H481	4:B:209:17F:H78	0.52	1.81	14	1
2:B:132:ASP:HB2	2:C:47:ASP:HB3	0.52	1.79	14	1
3:D:622:PCW:H11	3:D:622:PCW:O31	0.52	2.04	16	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
3:B:207:PCW:H441	4:B:210:17F:H55	0.52	1.81	16	1
3:B:204:PCW:H73	3:B:204:PCW:H2	0.52	1.82	18	1
3:C:205:PCW:C12	3:C:212:PCW:H19	0.52	2.32	19	1
3:A:401:PCW:H12	3:B:207:PCW:H362	0.52	1.80	1	1
3:A:418:PCW:H372	3:D:613:PCW:H182	0.52	1.81	1	1
3:D:606:PCW:H321	3:D:608:PCW:H82	0.52	1.82	1	1
3:D:624:PCW:O3	3:D:624:PCW:O31	0.52	2.28	5	11
2:B:33:ASP:O	5:B:201:GSP:S1G	0.52	2.67	17	4
3:C:207:PCW:P	3:C:207:PCW:C3	0.52	2.98	14	10
3:A:418:PCW:C39	3:D:613:PCW:H451	0.52	2.35	18	2
3:C:211:PCW:H262	4:C:215:17F:C27	0.52	2.35	2	1
3:A:408:PCW:H261	4:D:631:17F:H55	0.52	1.82	3	1
3:B:203:PCW:H51	3:C:211:PCW:H352	0.52	1.80	18	2
4:B:210:17F:H68	3:C:209:PCW:C44	0.52	2.34	3	1
1:A:273:ARG:HA	1:A:276:VAL:HG12	0.52	1.80	14	5
3:A:404:PCW:H352	4:A:415:17F:H9A	0.52	1.81	4	1
4:A:416:17F:H68	3:B:204:PCW:H281	0.52	1.82	4	2
3:D:602:PCW:C14	4:D:628:17F:H54	0.52	2.35	4	1
3:C:204:PCW:C20	3:C:217:PCW:H482	0.52	2.35	4	2
3:D:602:PCW:H362	4:C:214:17F:C37	0.52	2.09	17	2
3:D:621:PCW:O1P	3:D:622:PCW:C7	0.52	2.57	7	5
3:A:404:PCW:O3P	3:A:404:PCW:O31	0.52	2.28	8	1
3:A:412:PCW:H452	3:C:210:PCW:H452	0.52	1.81	10	1
3:D:627:PCW:H52	3:D:627:PCW:C31	0.52	2.34	10	1
3:B:203:PCW:C48	4:C:215:17F:H51	0.52	2.31	10	1
4:C:215:17F:H77	4:C:215:17F:C29	0.52	2.35	12	1
3:A:419:PCW:C46	3:C:212:PCW:H283	0.52	2.18	13	1
3:D:604:PCW:H52	3:D:604:PCW:O11	0.52	2.04	13	1
3:C:205:PCW:H242	3:C:209:PCW:H283	0.52	1.80	15	1
3:C:206:PCW:C31	3:C:206:PCW:O3	0.52	2.57	1	6
3:D:612:PCW:O11	3:D:620:PCW:C8	0.52	2.57	19	7
3:D:616:PCW:C19	4:D:632:17F:H38	0.52	2.35	4	3
3:C:210:PCW:H211	3:C:210:PCW:C17	0.52	2.28	2	1
3:D:619:PCW:C38	3:D:627:PCW:H181	0.52	2.34	12	3
3:A:404:PCW:C44	3:A:414:PCW:H251	0.52	2.35	4	3
3:C:205:PCW:H121	3:C:209:PCW:H341	0.52	1.82	4	1
3:D:616:PCW:H212	3:C:208:PCW:H272	0.52	1.81	5	1
3:D:614:PCW:H283	4:B:209:17F:H63	0.52	1.82	6	1
3:B:208:PCW:H182	3:C:211:PCW:H471	0.52	1.81	8	1
3:A:402:PCW:H341	3:A:410:PCW:O3	0.52	2.04	10	1
3:D:608:PCW:C48	4:D:628:17F:H61	0.52	2.30	10	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
3:D:617:PCW:O2	3:D:617:PCW:O4P	0.52	2.28	11	1
3:B:205:PCW:C4	3:C:204:PCW:H62	0.52	2.34	11	1
3:B:206:PCW:H161	3:C:209:PCW:H372	0.52	1.80	12	1
3:A:401:PCW:H39	3:B:204:PCW:C28	0.52	2.34	13	1
3:D:607:PCW:H442	3:D:625:PCW:C47	0.52	2.34	14	1
2:B:72:MET:HA	2:B:78:PHE:CZ	0.52	2.38	14	2
4:C:213:17F:C42	4:C:219:17F:H49	0.52	2.18	16	1
3:A:407:PCW:H61	3:A:412:PCW:C37	0.52	2.34	18	1
3:A:419:PCW:C45	3:D:625:PCW:H462	0.52	2.34	19	1
3:A:414:PCW:C13	4:A:415:17F:H33	0.52	2.31	1	1
3:A:418:PCW:O31	3:A:418:PCW:P	0.52	2.67	2	4
3:D:607:PCW:O31	3:D:607:PCW:O3	0.52	2.28	15	9
3:D:616:PCW:C27	4:D:632:17F:H46	0.52	2.34	1	3
3:C:212:PCW:C44	4:C:215:17F:H10	0.52	2.34	1	1
3:A:411:PCW:H271	3:A:413:PCW:C39	0.52	2.25	2	1
4:A:416:17F:H57	3:B:204:PCW:C21	0.52	2.30	2	1
4:A:422:17F:O7	4:A:422:17F:C17	0.52	2.58	10	13
2:B:62:GLU:HG3	2:B:63:GLU:H	0.52	1.65	5	2
3:B:203:PCW:C46	4:C:215:17F:H73	0.52	2.28	7	1
3:D:604:PCW:O11	3:D:604:PCW:H73	0.52	2.04	8	1
4:A:416:17F:H74	4:B:209:17F:C41	0.52	2.31	9	1
3:C:209:PCW:H382	3:C:209:PCW:C42	0.52	2.17	11	2
3:C:203:PCW:C1	3:C:211:PCW:C7	0.52	2.88	13	1
3:C:212:PCW:H222	4:C:215:17F:H10A	0.52	1.80	13	2
3:D:602:PCW:C35	4:C:214:17F:H77	0.52	2.35	14	1
3:D:608:PCW:H283	4:D:629:17F:H35	0.52	1.81	18	1
3:B:208:PCW:H342	3:C:203:PCW:C20	0.52	2.35	18	1
3:C:203:PCW:H422	3:C:204:PCW:C18	0.52	2.35	18	1
3:C:211:PCW:C23	4:C:215:17F:H52	0.52	2.35	18	1
3:A:403:PCW:C21	3:D:618:PCW:H282	0.52	2.35	20	1
3:A:406:PCW:H381	3:B:205:PCW:H161	0.52	1.82	1	1
3:C:204:PCW:H39	3:C:216:PCW:H251	0.52	1.82	10	7
3:C:210:PCW:H371	3:C:210:PCW:C13	0.52	2.35	15	2
3:D:604:PCW:H432	3:D:606:PCW:H221	0.52	1.80	4	3
3:A:411:PCW:C34	3:A:411:PCW:H121	0.52	2.35	19	3
3:A:420:PCW:C36	3:D:618:PCW:H422	0.52	2.34	3	1
4:A:422:17F:H19A	4:A:422:17F:C9	0.52	2.35	3	3
3:C:211:PCW:H461	3:C:211:PCW:C14	0.52	2.34	15	2
4:C:218:17F:H42	4:C:219:17F:H70	0.52	1.80	3	1
3:C:209:PCW:H432	3:C:209:PCW:H271	0.52	1.81	4	1
3:A:401:PCW:H472	3:D:612:PCW:C26	0.52	2.29	5	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
3:A:408:PCW:O2P	3:A:408:PCW:C5	0.52	2.57	5	5
3:B:203:PCW:H461	4:C:215:17F:C26	0.52	2.34	5	1
3:A:405:PCW:C6	4:B:211:17F:O2	0.52	2.58	6	1
3:A:421:PCW:H342	3:D:618:PCW:H132	0.52	1.81	6	1
3:D:604:PCW:H31	3:D:604:PCW:O1P	0.52	2.05	6	2
1:D:549:ALA:O	1:D:553:GLU:HG3	0.52	2.04	15	2
3:D:616:PCW:H483	3:C:207:PCW:H221	0.52	1.80	7	1
3:D:616:PCW:C43	3:C:208:PCW:H262	0.52	2.29	13	3
4:A:415:17F:C33	4:B:209:17F:H41	0.52	2.35	10	1
3:D:607:PCW:C38	3:D:626:PCW:H452	0.52	2.35	20	2
3:D:608:PCW:C45	4:D:628:17F:H60	0.52	2.25	11	1
3:B:204:PCW:C1	3:B:207:PCW:H322	0.52	2.28	11	1
3:A:420:PCW:H451	3:D:611:PCW:H231	0.52	1.81	14	1
3:C:207:PCW:H412	4:C:213:17F:H10	0.52	1.82	14	1
4:A:416:17F:H74	4:B:209:17F:C39	0.52	2.34	15	1
4:A:422:17F:C25	4:C:219:17F:H67	0.52	2.35	16	1
3:D:601:PCW:O31	3:D:601:PCW:H472	0.52	2.05	18	2
3:A:406:PCW:C24	3:A:411:PCW:H452	0.52	2.35	20	1
3:D:605:PCW:H2	3:D:605:PCW:O1P	0.52	2.05	11	4
4:C:213:17F:H51	4:C:215:17F:H71	0.52	1.79	2	1
3:C:207:PCW:C20	4:C:213:17F:H19	0.52	2.34	3	1
3:A:406:PCW:H352	3:B:205:PCW:O2	0.52	2.05	4	1
3:D:623:PCW:H281	3:D:624:PCW:H451	0.52	1.81	4	1
3:A:410:PCW:H221	4:A:422:17F:H74	0.52	1.81	19	3
3:A:421:PCW:H341	3:D:618:PCW:H132	0.52	1.81	17	6
2:C:8:VAL:HG12	2:C:16:LYS:HD2	0.52	1.81	10	3
3:D:617:PCW:C31	3:D:617:PCW:O3	0.52	2.58	8	4
3:C:206:PCW:H182	3:C:208:PCW:H152	0.52	1.80	8	1
3:A:401:PCW:H421	3:D:612:PCW:C27	0.52	2.35	20	2
3:D:609:PCW:H251	4:D:628:17F:H73	0.52	1.80	9	1
1:A:308:ARG:HG3	1:D:469:LEU:HD11	0.52	1.82	13	1
3:A:402:PCW:H322	3:A:410:PCW:O4P	0.52	2.05	15	1
3:C:211:PCW:H242	4:C:215:17F:H48	0.52	1.81	15	1
3:A:404:PCW:H51	3:B:205:PCW:C40	0.52	2.35	16	1
4:A:422:17F:C25	4:C:219:17F:C37	0.52	2.87	16	1
3:B:204:PCW:H212	3:B:204:PCW:C17	0.52	2.32	16	1
4:A:416:17F:H74	3:D:614:PCW:H241	0.52	1.81	17	1
3:A:417:PCW:H362	3:A:421:PCW:C37	0.52	2.33	17	1
3:C:212:PCW:H411	3:C:212:PCW:H182	0.52	1.81	17	1
3:D:627:PCW:H122	3:D:627:PCW:H332	0.52	1.81	18	1
3:C:203:PCW:C14	4:C:213:17F:H30	0.52	2.33	1	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
3:A:411:PCW:H132	3:B:205:PCW:H281	0.52	1.81	2	1
3:D:617:PCW:H221	3:D:617:PCW:C17	0.52	2.33	2	1
4:B:211:17F:H66	4:B:211:17F:C12	0.52	2.31	2	1
3:A:408:PCW:H231	3:A:411:PCW:C22	0.52	2.35	3	1
3:A:410:PCW:H222	4:A:422:17F:C42	0.52	2.36	7	4
3:B:204:PCW:C40	4:B:210:17F:H10A	0.52	2.32	11	2
3:A:419:PCW:C3	3:D:615:PCW:H121	0.52	2.35	5	1
3:D:615:PCW:O11	3:D:615:PCW:O2	0.52	2.28	17	4
3:C:205:PCW:H2	3:C:209:PCW:H132	0.52	1.81	8	1
4:D:628:17F:H8	4:D:629:17F:H33	0.52	1.81	17	4
3:A:420:PCW:H11	3:D:618:PCW:C40	0.52	2.34	10	1
3:A:421:PCW:O1P	3:D:618:PCW:C8	0.52	2.58	11	3
3:C:210:PCW:H182	3:C:210:PCW:H461	0.52	1.80	15	1
3:A:417:PCW:C16	3:A:420:PCW:H352	0.52	2.34	16	1
3:A:408:PCW:H52	3:A:413:PCW:O2P	0.52	2.05	17	1
3:C:203:PCW:H422	3:C:204:PCW:H181	0.52	1.80	18	1
3:D:610:PCW:H73	4:D:631:17F:O1	0.52	2.05	20	1
3:C:205:PCW:H432	4:C:215:17F:C1X	0.51	2.36	2	1
3:A:401:PCW:H411	3:B:204:PCW:H241	0.51	1.82	3	1
3:A:402:PCW:C42	3:C:208:PCW:H152	0.51	2.31	17	5
3:B:205:PCW:H283	4:B:211:17F:H20A	0.51	1.80	12	2
3:A:409:PCW:H39	4:B:210:17F:C35	0.51	2.34	4	2
3:B:204:PCW:C7	3:B:204:PCW:C2	0.51	2.86	4	3
3:C:205:PCW:O31	4:C:214:17F:H6	0.51	2.05	4	1
3:A:420:PCW:H40	3:D:617:PCW:C22	0.51	2.34	5	1
3:A:405:PCW:C8	4:B:211:17F:O2	0.51	2.58	6	2
4:D:628:17F:H69	4:D:629:17F:H44	0.51	1.81	7	1
3:D:601:PCW:H371	3:D:602:PCW:C12	0.51	2.31	8	1
3:C:207:PCW:H461	4:C:213:17F:H78	0.51	1.82	8	1
3:C:211:PCW:C28	4:C:215:17F:H55	0.51	2.15	8	1
3:A:408:PCW:C4	3:A:413:PCW:C3	0.51	2.83	9	1
3:A:421:PCW:H11	3:A:421:PCW:C5	0.51	2.36	9	1
3:D:602:PCW:H272	4:D:629:17F:C42	0.51	2.35	11	3
1:D:463:TRP:CD1	4:D:629:17F:H77	0.51	2.40	12	2
1:A:217:LEU:CD1	3:A:405:PCW:H222	0.51	2.35	13	1
3:D:616:PCW:H222	3:C:208:PCW:H251	0.51	1.82	14	1
3:D:625:PCW:H382	3:D:626:PCW:C39	0.51	2.35	18	1
3:B:208:PCW:O3	3:C:203:PCW:H283	0.51	2.05	18	1
3:C:209:PCW:H451	3:C:212:PCW:H283	0.51	1.82	20	1
1:D:540:GLY:O	1:D:544:LEU:HG	0.51	2.05	4	2
4:C:219:17F:O7	4:C:219:17F:O10	0.51	2.28	8	12

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
4:D:631:17F:C11	3:C:217:PCW:H73	0.51	2.33	3	2
3:B:208:PCW:O31	3:B:208:PCW:O4P	0.51	2.27	15	2
3:C:209:PCW:H431	3:C:212:PCW:C26	0.51	2.20	4	1
3:A:413:PCW:H381	3:C:210:PCW:H441	0.51	1.82	5	1
3:D:623:PCW:C2	3:D:624:PCW:H322	0.51	2.35	6	3
4:C:218:17F:H51	4:C:219:17F:C42	0.51	2.36	18	3
1:D:437:LEU:O	1:D:441:MET:HB2	0.51	2.04	7	1
4:B:211:17F:C28	3:C:203:PCW:H242	0.51	2.31	7	1
3:B:203:PCW:H62	3:C:211:PCW:O31	0.51	2.05	8	3
3:C:210:PCW:H142	3:C:210:PCW:C39	0.51	2.34	16	4
3:A:402:PCW:O31	3:A:402:PCW:H11	0.51	2.04	19	6
3:D:607:PCW:C48	3:C:209:PCW:H251	0.51	2.35	10	1
3:A:418:PCW:O4P	3:A:418:PCW:H82	0.51	2.04	14	2
3:A:410:PCW:H121	3:C:208:PCW:C39	0.51	2.35	14	1
3:C:207:PCW:H352	4:C:213:17F:C31	0.51	2.35	14	1
3:A:406:PCW:H482	3:D:619:PCW:C48	0.51	2.35	16	1
3:C:203:PCW:H442	3:C:204:PCW:C21	0.51	2.15	18	1
3:A:404:PCW:H472	4:A:415:17F:H53	0.51	1.82	13	3
4:A:415:17F:H39	4:A:415:17F:H29	0.51	1.82	2	1
3:A:417:PCW:H411	3:A:417:PCW:C37	0.51	2.33	2	3
3:D:608:PCW:H231	4:D:629:17F:H47	0.51	1.82	2	1
3:B:203:PCW:H332	4:B:210:17F:H30	0.51	1.81	2	1
3:B:204:PCW:H382	4:B:210:17F:H42	0.51	1.81	2	1
3:B:208:PCW:H342	3:C:203:PCW:H20	0.51	1.82	2	1
3:D:607:PCW:C24	3:B:206:PCW:C48	0.51	2.88	3	1
3:B:203:PCW:H412	3:B:203:PCW:H371	0.51	1.81	3	1
3:B:206:PCW:H141	3:C:209:PCW:H39	0.51	1.83	3	1
3:C:207:PCW:H142	4:C:213:17F:C20	0.51	2.35	3	1
3:D:609:PCW:H42	4:D:632:17F:H18A	0.51	1.83	4	1
3:D:614:PCW:C48	3:D:620:PCW:H181	0.51	2.35	7	3
3:D:608:PCW:O1P	3:D:626:PCW:C21	0.51	2.58	5	1
3:A:401:PCW:H361	3:B:204:PCW:H182	0.51	1.83	7	1
3:A:412:PCW:H462	3:C:210:PCW:H472	0.51	1.81	11	4
4:A:416:17F:H57	3:B:204:PCW:H182	0.51	1.81	11	1
3:A:421:PCW:H141	4:D:630:17F:C11	0.51	2.29	11	1
3:C:212:PCW:H222	4:C:215:17F:H12A	0.51	1.82	11	2
3:C:205:PCW:C39	3:C:212:PCW:H242	0.51	2.36	12	1
3:A:412:PCW:C41	3:C:210:PCW:H362	0.51	2.36	15	2
3:A:410:PCW:P	3:A:410:PCW:C3	0.51	2.97	14	1
3:D:612:PCW:O11	3:D:620:PCW:H61	0.51	2.05	14	1
3:A:409:PCW:O2P	3:A:409:PCW:H52	0.51	2.04	15	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
3:D:611:PCW:H482	3:B:208:PCW:H241	0.51	1.81	15	1
3:D:609:PCW:H483	3:C:208:PCW:H482	0.51	1.83	18	1
3:D:624:PCW:H452	4:B:209:17F:H74	0.51	1.82	18	1
3:D:608:PCW:C21	4:D:629:17F:H20	0.51	2.36	1	1
2:B:35:THR:OG1	5:B:201:GSP:O3G	0.51	2.29	8	15
3:A:407:PCW:O3	3:A:410:PCW:H331	0.51	2.05	2	2
3:D:604:PCW:C45	3:D:606:PCW:C18	0.51	2.89	14	4
2:B:128:LYS:HG2	2:C:47:ASP:H	0.51	1.65	3	3
4:B:210:17F:O6	4:B:210:17F:C18	0.51	2.57	12	4
4:C:213:17F:H71	4:C:213:17F:C1Z	0.51	2.34	3	1
1:A:213:THR:O	1:A:217:LEU:HG	0.51	2.05	9	3
3:D:617:PCW:H281	3:D:619:PCW:C28	0.51	2.34	5	2
3:B:208:PCW:H371	3:C:203:PCW:C22	0.51	2.36	5	2
3:C:206:PCW:H82	3:C:212:PCW:H73	0.51	1.82	5	1
3:D:623:PCW:O3	3:D:624:PCW:C33	0.51	2.58	11	2
3:B:208:PCW:H472	3:C:203:PCW:C23	0.51	2.35	6	1
3:C:216:PCW:H483	3:C:217:PCW:H411	0.51	1.81	18	2
2:C:57:ASP:OD2	5:C:201:GSP:O3G	0.51	2.28	17	3
3:C:205:PCW:H332	3:C:209:PCW:C34	0.51	2.34	7	1
3:D:606:PCW:C26	4:C:218:17F:H42	0.51	2.36	8	1
3:C:206:PCW:C17	3:C:208:PCW:H152	0.51	2.34	8	1
3:A:414:PCW:H321	4:A:415:17F:C20	0.51	2.35	9	1
3:D:609:PCW:H272	4:C:214:17F:C30	0.51	2.35	12	1
3:A:417:PCW:H39	3:A:417:PCW:H142	0.51	1.81	15	1
3:D:610:PCW:C12	4:D:631:17F:H18	0.51	2.35	16	1
3:C:206:PCW:H162	3:C:208:PCW:C34	0.51	2.30	17	1
3:C:207:PCW:C19	4:C:213:17F:H19	0.51	2.33	18	1
3:C:212:PCW:H171	3:C:212:PCW:C38	0.51	2.34	19	1
3:A:402:PCW:C7	3:A:410:PCW:O2P	0.51	2.58	20	1
3:A:411:PCW:C4	3:A:411:PCW:C32	0.51	2.85	5	7
3:A:420:PCW:H321	3:D:618:PCW:H441	0.51	1.81	3	1
3:D:623:PCW:H331	3:D:624:PCW:C32	0.51	2.35	3	1
3:B:206:PCW:O31	3:B:206:PCW:H11	0.51	2.03	3	3
3:C:203:PCW:H32	3:C:211:PCW:H62	0.51	1.82	3	1
3:C:211:PCW:H142	3:C:211:PCW:C48	0.51	2.33	3	1
3:C:211:PCW:H472	3:C:211:PCW:H122	0.51	1.81	3	1
3:A:410:PCW:H40	3:A:412:PCW:H371	0.51	1.81	4	1
3:D:606:PCW:O11	3:D:606:PCW:C6	0.51	2.55	8	5
2:B:120:LEU:HD11	5:B:201:GSP:N2	0.51	2.20	10	2
2:C:99:GLN:O	2:C:103:VAL:HG23	0.51	2.05	10	3
3:C:212:PCW:H12	4:C:215:17F:H57	0.51	1.83	5	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
3:B:208:PCW:H161	3:C:203:PCW:C27	0.51	2.36	13	2
3:D:613:PCW:C33	3:D:619:PCW:H132	0.51	2.36	8	2
3:D:602:PCW:H272	4:D:629:17F:H78	0.51	1.81	10	1
1:A:246:ASP:O	1:A:250:VAL:HB	0.51	2.05	12	2
3:B:203:PCW:H73	3:C:211:PCW:H2	0.51	1.82	12	1
3:D:617:PCW:H442	3:D:619:PCW:H422	0.51	1.83	14	1
3:D:611:PCW:H483	3:B:208:PCW:H251	0.51	1.83	15	1
3:C:211:PCW:H231	4:C:215:17F:H66	0.51	1.82	15	1
3:D:619:PCW:H481	3:C:204:PCW:H442	0.51	1.80	16	1
4:B:211:17F:H62	4:B:211:17F:H30	0.51	1.81	16	1
3:A:401:PCW:C38	3:B:204:PCW:H262	0.51	2.34	17	1
3:D:601:PCW:C15	3:D:601:PCW:H451	0.51	2.35	17	1
4:C:218:17F:C7	4:C:218:17F:C18	0.51	2.88	17	1
3:D:619:PCW:H372	3:D:627:PCW:H141	0.51	1.82	19	1
3:C:203:PCW:H242	3:C:204:PCW:H372	0.51	1.81	20	1
1:A:330:ARG:HH21	1:D:447:GLU:HB2	0.51	1.63	1	1
3:A:403:PCW:H382	3:A:403:PCW:C11	0.51	2.36	1	1
1:A:247:LEU:HD23	3:A:412:PCW:H283	0.51	1.81	4	4
3:D:617:PCW:O2P	3:D:617:PCW:O2	0.51	2.29	7	4
3:D:622:PCW:O11	3:D:622:PCW:O2	0.51	2.28	2	13
3:D:623:PCW:C31	3:D:624:PCW:H322	0.51	2.35	3	7
3:A:403:PCW:C11	3:A:403:PCW:H382	0.51	2.35	8	2
3:D:602:PCW:H362	4:C:214:17F:C33	0.51	2.36	6	1
4:D:632:17F:H59	4:D:632:17F:H67	0.51	1.81	6	1
3:B:207:PCW:H61	4:B:210:17F:C6	0.51	2.35	7	1
2:C:2:THR:HB	2:C:4:TYR:CE2	0.51	2.41	7	2
4:C:213:17F:H72	4:C:219:17F:H49	0.51	1.83	7	1
3:D:607:PCW:C43	3:D:626:PCW:H481	0.51	2.35	10	2
3:A:403:PCW:C25	3:D:618:PCW:H222	0.51	2.35	10	1
4:A:415:17F:H41	4:A:415:17F:H36	0.51	1.82	10	1
3:D:612:PCW:H39	3:D:623:PCW:C45	0.51	2.34	10	1
3:D:603:PCW:H12	3:D:603:PCW:O31	0.51	2.05	12	2
3:A:403:PCW:H142	3:A:403:PCW:H382	0.51	1.82	13	1
3:A:419:PCW:H452	3:D:625:PCW:H483	0.51	1.81	15	1
3:C:209:PCW:C42	3:C:212:PCW:H262	0.51	2.35	15	1
3:B:204:PCW:H432	3:B:207:PCW:C19	0.51	2.35	18	1
3:A:408:PCW:C27	3:D:619:PCW:H452	0.51	2.35	19	1
3:A:417:PCW:O31	3:A:417:PCW:O3	0.51	2.29	15	5
3:D:618:PCW:O11	3:D:618:PCW:H2	0.51	2.06	17	4
3:A:410:PCW:H283	4:A:422:17F:H74	0.51	1.83	3	1
1:D:421:PRO:O	1:D:425:GLU:HG2	0.51	2.06	16	8

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
3:A:408:PCW:H261	3:D:619:PCW:C46	0.51	2.36	20	2
3:D:604:PCW:H342	4:C:219:17F:O8	0.51	2.05	5	2
3:A:418:PCW:H431	3:D:613:PCW:H171	0.51	1.82	6	1
3:A:406:PCW:H39	3:B:205:PCW:C14	0.51	2.36	7	1
3:C:206:PCW:C8	3:C:212:PCW:O1P	0.51	2.59	8	2
3:D:612:PCW:H471	3:B:203:PCW:C28	0.51	2.31	9	1
3:D:612:PCW:C47	3:B:203:PCW:H281	0.51	2.31	9	1
3:C:204:PCW:C48	3:C:216:PCW:H231	0.51	2.32	12	1
3:C:212:PCW:H42	4:C:213:17F:O5	0.51	2.05	14	1
4:D:632:17F:H52	3:C:208:PCW:H172	0.51	1.83	15	1
3:C:209:PCW:C39	3:C:209:PCW:H272	0.51	2.35	15	1
3:C:209:PCW:C17	4:C:214:17F:H11A	0.51	2.36	16	1
3:C:204:PCW:H11	3:C:204:PCW:C4	0.51	2.29	17	1
3:C:205:PCW:C19	3:C:209:PCW:H221	0.51	2.35	17	1
3:D:608:PCW:H211	4:D:629:17F:C20	0.51	2.35	18	1
3:A:402:PCW:H121	3:A:407:PCW:H151	0.51	1.81	1	2
4:D:631:17F:H53	3:C:210:PCW:C25	0.51	2.36	18	3
3:B:206:PCW:O4P	3:B:206:PCW:H62	0.51	2.06	20	13
3:B:204:PCW:O31	3:B:204:PCW:O3	0.51	2.28	15	3
3:A:409:PCW:H372	4:B:210:17F:H66	0.51	1.82	3	1
3:A:414:PCW:H341	4:A:415:17F:H33	0.51	1.82	3	2
4:A:422:17F:H5	4:A:422:17F:O1	0.51	2.05	9	10
3:A:418:PCW:H483	3:D:613:PCW:C28	0.51	2.36	4	1
1:D:487:GLN:O	1:D:491:GLU:HG3	0.51	2.06	4	2
3:A:402:PCW:C8	3:A:407:PCW:C3	0.51	2.88	6	4
2:B:17:SER:HB2	5:B:201:GSP:O1A	0.51	2.06	19	3
3:D:616:PCW:C26	4:C:214:17F:H72	0.51	2.26	6	1
3:C:206:PCW:C16	3:C:208:PCW:H362	0.51	2.36	6	2
3:D:604:PCW:C41	3:D:604:PCW:C37	0.51	2.84	9	1
2:B:149:ARG:HH21	2:B:152:VAL:HB	0.51	1.65	9	2
3:B:206:PCW:H82	4:B:210:17F:O1	0.51	2.05	11	1
3:A:401:PCW:H122	3:B:207:PCW:C28	0.51	2.36	13	1
3:A:404:PCW:H161	3:A:404:PCW:C40	0.51	2.36	13	1
3:A:411:PCW:C6	4:B:211:17F:O4	0.51	2.57	13	1
3:A:402:PCW:C48	3:A:407:PCW:H261	0.51	2.35	14	1
3:A:407:PCW:H331	3:A:410:PCW:H351	0.51	1.83	14	1
3:B:203:PCW:H431	3:C:211:PCW:C23	0.51	2.34	17	2
3:C:203:PCW:H441	3:C:210:PCW:C19	0.51	2.36	14	1
3:B:203:PCW:H451	3:C:211:PCW:C23	0.51	2.35	16	1
3:A:402:PCW:H422	3:C:208:PCW:H361	0.51	1.83	19	1
3:A:421:PCW:H321	3:D:618:PCW:H63	0.51	1.81	19	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
4:B:211:17F:H40	3:C:204:PCW:H411	0.51	1.82	20	1
3:A:404:PCW:H62	3:A:404:PCW:H372	0.51	1.83	1	1
3:A:417:PCW:H151	3:D:603:PCW:H272	0.51	1.82	11	5
3:A:409:PCW:H321	3:B:206:PCW:C7	0.51	2.36	2	1
3:A:421:PCW:H332	4:D:630:17F:H8A	0.51	1.81	15	3
3:D:621:PCW:O4P	3:D:621:PCW:H73	0.51	2.05	2	13
3:D:627:PCW:O1P	3:D:627:PCW:C5	0.51	2.58	17	6
2:B:13:GLY:CA	5:B:201:GSP:H5'1	0.51	2.32	13	2
3:A:408:PCW:H331	3:A:413:PCW:H151	0.51	1.83	17	2
3:A:401:PCW:C5	3:B:204:PCW:O2P	0.51	2.59	5	1
3:A:403:PCW:H131	3:A:403:PCW:C38	0.51	2.34	6	1
3:D:624:PCW:O31	3:D:624:PCW:O3P	0.51	2.29	6	1
3:B:208:PCW:H471	3:C:203:PCW:C18	0.51	2.35	6	1
3:B:207:PCW:H11	3:B:207:PCW:O31	0.51	2.06	12	2
3:C:207:PCW:H172	4:C:213:17F:C18	0.51	2.33	7	1
3:D:612:PCW:C8	3:D:625:PCW:C14	0.51	2.89	8	1
3:D:619:PCW:H322	3:D:627:PCW:C12	0.51	2.33	19	2
4:B:211:17F:H47	3:C:204:PCW:C39	0.51	2.27	8	1
3:C:211:PCW:H211	4:C:215:17F:H73	0.51	1.83	8	1
3:D:604:PCW:O1P	3:D:623:PCW:C8	0.51	2.59	13	1
3:D:616:PCW:N	4:D:632:17F:O4	0.51	2.44	13	1
3:D:609:PCW:H451	3:C:206:PCW:C20	0.51	2.35	14	1
3:D:609:PCW:C21	3:D:616:PCW:H372	0.51	2.35	16	1
3:D:603:PCW:H61	3:C:216:PCW:O2P	0.51	2.06	17	1
3:D:627:PCW:H41	3:D:627:PCW:O31	0.51	2.06	18	1
3:B:206:PCW:O31	3:B:206:PCW:O3	0.51	2.29	16	7
3:A:405:PCW:H371	3:A:411:PCW:C46	0.51	2.22	2	2
3:A:419:PCW:H481	3:D:604:PCW:H272	0.51	1.83	2	1
3:B:204:PCW:H472	3:B:207:PCW:H431	0.51	1.82	2	1
4:C:218:17F:HN1	4:C:218:17F:C17	0.51	2.19	2	2
3:A:403:PCW:O11	3:A:403:PCW:H51	0.51	2.06	17	2
4:A:422:17F:C2X	4:C:218:17F:H78	0.51	2.34	4	1
3:A:421:PCW:C6	4:D:630:17F:O8	0.51	2.56	5	2
3:B:208:PCW:H341	3:C:211:PCW:C6	0.51	2.36	5	1
3:B:208:PCW:H412	3:C:203:PCW:C22	0.51	2.36	6	1
3:D:602:PCW:H341	4:C:214:17F:H67	0.51	1.82	7	1
3:C:205:PCW:C33	3:C:209:PCW:C34	0.51	2.88	7	1
3:B:206:PCW:C14	3:B:206:PCW:C39	0.51	2.88	8	1
3:D:602:PCW:C48	4:D:628:17F:H65	0.51	2.36	9	1
3:D:614:PCW:H122	3:D:620:PCW:C39	0.51	2.35	10	1
3:C:211:PCW:C31	3:C:211:PCW:O3	0.51	2.58	10	2

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
3:D:623:PCW:H232	3:B:203:PCW:C48	0.51	2.32	11	1
3:D:603:PCW:H51	4:C:219:17F:O1	0.51	2.06	14	1
3:B:207:PCW:C20	4:B:210:17F:H19A	0.51	2.36	14	2
3:D:608:PCW:H441	3:B:206:PCW:H461	0.51	1.82	16	1
3:C:205:PCW:H441	3:C:212:PCW:H461	0.51	1.83	16	1
3:A:410:PCW:C18	3:A:410:PCW:H231	0.51	2.35	18	1
3:D:604:PCW:H322	3:D:606:PCW:C12	0.51	2.32	19	2
3:D:624:PCW:H451	4:B:209:17F:H76	0.51	1.79	19	1
3:B:205:PCW:C3	3:C:204:PCW:H52	0.51	2.35	19	1
3:C:206:PCW:C13	3:C:207:PCW:H19	0.51	2.31	20	1
1:A:372:ARG:O	1:A:376:LEU:HG	0.50	2.06	12	3
1:A:250:VAL:HG11	3:A:412:PCW:H271	0.50	1.82	2	2
3:B:204:PCW:H382	4:B:210:17F:C24	0.50	2.36	2	1
3:B:207:PCW:H182	3:B:207:PCW:H342	0.50	1.83	2	1
4:C:218:17F:H18	4:C:218:17F:H9A	0.50	1.82	2	1
1:A:379:LEU:O	1:A:383:LYS:HG3	0.50	2.06	4	1
3:C:203:PCW:C45	3:C:204:PCW:H212	0.50	2.36	4	1
3:B:207:PCW:H441	4:B:210:17F:H50	0.50	1.84	5	1
3:C:216:PCW:C46	3:C:217:PCW:H361	0.50	2.21	6	1
3:D:617:PCW:C48	3:C:210:PCW:H271	0.50	2.28	8	1
5:C:201:GSP:O5'	5:C:201:GSP:C2'	0.50	2.59	15	2
3:C:212:PCW:H412	4:C:215:17F:H63	0.50	1.83	10	1
4:C:218:17F:H39	4:C:219:17F:H70	0.50	1.82	13	1
3:A:404:PCW:H172	3:A:404:PCW:H462	0.50	1.82	15	1
3:D:614:PCW:H471	3:D:620:PCW:C43	0.50	2.31	18	2
3:B:203:PCW:C21	4:B:209:17F:H32	0.50	2.36	20	1
3:A:404:PCW:O3	3:A:404:PCW:C31	0.50	2.60	2	8
3:D:615:PCW:C8	3:D:625:PCW:O1P	0.50	2.56	5	2
3:D:619:PCW:H352	3:D:627:PCW:H341	0.50	1.82	10	2
3:C:205:PCW:C1	4:C:214:17F:H10	0.50	2.34	2	1
3:A:418:PCW:H39	3:D:613:PCW:C42	0.50	2.36	8	3
1:A:231:ASN:HA	1:A:234:LYS:HE2	0.50	1.82	9	2
3:A:409:PCW:C33	3:B:206:PCW:H341	0.50	2.36	4	1
3:A:414:PCW:H411	3:A:414:PCW:C37	0.50	2.27	5	1
3:A:409:PCW:H372	3:B:206:PCW:C40	0.50	2.37	7	1
3:A:418:PCW:C40	3:D:613:PCW:H231	0.50	2.36	7	5
3:A:406:PCW:C48	3:D:619:PCW:H261	0.50	2.30	8	1
3:D:604:PCW:C11	3:D:604:PCW:H73	0.50	2.36	8	1
3:A:408:PCW:H481	3:A:413:PCW:H241	0.50	1.84	10	1
3:D:602:PCW:H351	4:C:214:17F:H77	0.50	1.81	14	3
1:D:590:GLU:O	1:D:594:LYS:HD3	0.50	2.07	11	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
3:B:205:PCW:H332	3:B:208:PCW:H61	0.50	1.83	11	1
1:D:502:GLU:HG2	1:D:506:ARG:HE	0.50	1.65	12	1
3:C:207:PCW:C3	4:C:213:17F:H1	0.50	2.36	20	2
3:D:609:PCW:H472	4:D:632:17F:H44	0.50	1.84	14	1
3:D:627:PCW:H63	3:D:627:PCW:O31	0.50	2.05	14	1
3:A:404:PCW:C5	3:A:406:PCW:O2P	0.50	2.60	17	1
3:A:420:PCW:C3	3:D:618:PCW:H411	0.50	2.36	18	1
3:B:205:PCW:H232	3:C:210:PCW:H251	0.50	1.83	18	1
3:C:206:PCW:H261	3:C:208:PCW:C41	0.50	2.32	18	1
3:C:207:PCW:H411	4:C:213:17F:C8	0.50	2.36	20	1
3:A:402:PCW:H122	3:A:407:PCW:H132	0.50	1.81	1	1
3:A:414:PCW:C31	3:A:414:PCW:C35	0.50	2.89	9	11
3:A:418:PCW:C36	3:D:613:PCW:H131	0.50	2.22	19	3
2:C:5:LYS:HA	2:C:54:ASP:HB3	0.50	1.82	4	4
3:C:203:PCW:H181	3:C:203:PCW:C22	0.50	2.34	20	3
3:C:206:PCW:H241	3:C:208:PCW:H431	0.50	1.82	1	1
4:C:214:17F:O8	4:C:214:17F:H5	0.50	2.07	5	2
3:D:603:PCW:H472	3:D:603:PCW:C21	0.50	2.36	2	2
3:D:614:PCW:H281	4:B:209:17F:H35	0.50	1.83	6	2
3:D:619:PCW:O31	3:D:619:PCW:O3P	0.50	2.30	19	7
2:B:17:SER:OG	5:B:201:GSP:O3G	0.50	2.29	3	6
1:D:411:THR:O	1:D:415:LEU:HG	0.50	2.07	11	3
4:D:630:17F:O7	4:D:630:17F:O10	0.50	2.29	6	5
3:B:208:PCW:H352	3:C:204:PCW:H331	0.50	1.81	3	2
3:D:624:PCW:O31	3:D:624:PCW:H61	0.50	2.07	4	1
3:C:211:PCW:H151	4:C:215:17F:H65	0.50	1.82	4	1
3:A:417:PCW:O31	3:A:417:PCW:O4P	0.50	2.29	18	4
3:D:614:PCW:C47	3:D:620:PCW:H231	0.50	2.35	5	2
3:D:608:PCW:C6	3:D:626:PCW:H242	0.50	2.30	6	2
3:A:414:PCW:H121	4:A:415:17F:H69	0.50	1.83	7	1
4:A:422:17F:C11	4:C:218:17F:C38	0.50	2.82	7	2
3:D:605:PCW:C18	3:D:614:PCW:H342	0.50	2.36	7	2
3:A:411:PCW:C11	3:A:411:PCW:O31	0.50	2.59	8	1
3:D:603:PCW:H451	3:D:611:PCW:C43	0.50	2.27	10	1
3:D:608:PCW:H461	4:D:628:17F:C33	0.50	2.37	10	1
3:A:414:PCW:C25	4:A:415:17F:H59	0.50	2.35	19	2
3:C:203:PCW:H281	3:C:211:PCW:C44	0.50	2.37	12	1
3:C:212:PCW:H162	4:C:215:17F:H9A	0.50	1.82	13	2
3:D:604:PCW:H331	4:C:219:17F:O8	0.50	2.06	14	1
3:D:625:PCW:H11	3:D:626:PCW:H12	0.50	1.83	14	1
3:A:404:PCW:H152	3:B:205:PCW:H471	0.50	1.81	16	2

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
3:D:616:PCW:H272	4:D:632:17F:H45	0.50	1.81	17	2
3:A:406:PCW:H471	4:B:211:17F:H33	0.50	1.83	17	1
3:A:405:PCW:H52	3:A:406:PCW:C11	0.50	2.36	20	2
3:A:414:PCW:H212	3:A:414:PCW:C17	0.50	2.17	20	1
3:C:209:PCW:H442	3:C:212:PCW:H271	0.50	1.83	20	1
3:D:609:PCW:O31	3:D:609:PCW:H131	0.50	2.06	12	10
3:D:615:PCW:O31	3:D:615:PCW:C1	0.50	2.57	15	7
3:D:627:PCW:H182	3:D:627:PCW:H221	0.50	1.82	1	6
3:B:206:PCW:O31	3:B:206:PCW:H342	0.50	2.05	16	3
4:B:211:17F:O7	4:B:211:17F:O10	0.50	2.29	17	5
3:C:205:PCW:H432	4:C:215:17F:H37	0.50	1.82	2	1
3:C:207:PCW:C42	4:C:213:17F:C1Y	0.50	2.83	2	1
1:A:335:LEU:O	1:A:339:LYS:HB2	0.50	2.06	5	4
3:A:409:PCW:H382	4:B:210:17F:C35	0.50	2.37	5	1
3:A:413:PCW:H421	3:A:413:PCW:C28	0.50	2.36	5	1
3:D:604:PCW:C5	3:D:604:PCW:O11	0.50	2.59	5	1
3:C:203:PCW:H372	3:C:207:PCW:C8	0.50	2.37	5	1
3:D:603:PCW:H341	3:D:611:PCW:O31	0.50	2.07	6	1
3:D:606:PCW:H62	3:D:626:PCW:H20	0.50	1.84	6	1
2:C:16:LYS:HE2	2:C:57:ASP:OD1	0.50	2.07	10	3
3:D:601:PCW:H61	3:D:602:PCW:H11	0.50	1.83	8	1
3:D:617:PCW:O2P	3:C:216:PCW:C4	0.50	2.57	8	1
3:A:406:PCW:H483	3:D:619:PCW:C25	0.50	2.37	10	1
3:A:408:PCW:H371	3:A:413:PCW:H171	0.50	1.83	10	2
2:B:160:VAL:HA	2:B:163:ILE:HD12	0.50	1.84	11	1
3:B:206:PCW:H42	3:B:206:PCW:O11	0.50	2.05	12	1
3:C:205:PCW:H161	3:C:209:PCW:H221	0.50	1.84	12	1
3:A:411:PCW:H283	3:B:205:PCW:H212	0.50	1.84	13	1
3:A:410:PCW:C3	3:A:410:PCW:O2P	0.50	2.59	14	1
3:C:212:PCW:C39	4:C:215:17F:H59	0.50	2.37	14	1
3:A:401:PCW:H452	3:D:612:PCW:H251	0.50	1.81	15	1
3:C:206:PCW:O4P	4:C:214:17F:H12A	0.50	2.07	15	1
3:C:203:PCW:H471	3:C:210:PCW:H222	0.50	1.83	16	1
3:A:401:PCW:H39	3:B:204:PCW:H241	0.50	1.83	17	1
3:D:604:PCW:C36	4:C:218:17F:H36	0.50	2.36	18	1
3:D:624:PCW:H282	3:C:217:PCW:C26	0.50	2.29	19	1
4:A:416:17F:H18	4:A:416:17F:H9A	0.50	1.83	1	2
3:A:420:PCW:O3	3:A:420:PCW:O31	0.50	2.30	2	13
3:D:609:PCW:O31	3:D:609:PCW:C13	0.50	2.60	18	11
3:D:616:PCW:H472	3:C:208:PCW:H241	0.50	1.82	1	1
3:D:624:PCW:C48	4:B:209:17F:H55	0.50	2.24	12	3

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
3:C:206:PCW:H211	3:C:208:PCW:C38	0.50	2.37	3	1
3:D:609:PCW:C7	3:D:621:PCW:O11	0.50	2.59	13	5
3:A:408:PCW:C35	3:A:413:PCW:C15	0.50	2.89	5	4
3:A:413:PCW:C8	3:C:210:PCW:H2	0.50	2.37	5	2
4:D:631:17F:C8	3:C:217:PCW:C7	0.50	2.86	9	1
3:A:401:PCW:H322	3:B:207:PCW:C24	0.50	2.37	10	1
3:A:421:PCW:O2P	3:D:618:PCW:C8	0.50	2.59	10	2
3:A:403:PCW:H182	3:A:403:PCW:H411	0.50	1.83	11	1
3:D:618:PCW:H51	3:D:618:PCW:O11	0.50	2.06	11	1
3:D:627:PCW:C25	3:C:216:PCW:H451	0.50	2.36	14	2
3:A:419:PCW:H381	3:D:625:PCW:H262	0.50	1.83	12	2
3:A:421:PCW:C7	4:D:630:17F:H4	0.50	2.37	12	1
3:C:203:PCW:C7	3:C:207:PCW:O31	0.50	2.59	14	1
4:A:416:17F:H31	3:B:204:PCW:H151	0.50	1.82	15	1
3:A:410:PCW:H242	4:A:422:17F:C41	0.50	2.27	17	1
3:D:616:PCW:H452	3:C:208:PCW:H262	0.50	1.83	1	1
3:D:614:PCW:C14	3:D:620:PCW:C39	0.50	2.89	15	5
3:D:622:PCW:C14	3:D:622:PCW:C18	0.50	2.88	14	7
3:A:419:PCW:N	3:D:626:PCW:O31	0.50	2.45	3	1
3:A:406:PCW:C40	3:B:205:PCW:H172	0.50	2.36	4	2
3:A:409:PCW:H361	3:B:206:PCW:H361	0.50	1.82	4	1
3:A:410:PCW:H282	4:A:422:17F:H75	0.50	1.82	10	2
4:A:416:17F:H68	3:B:204:PCW:H272	0.50	1.82	5	2
3:B:204:PCW:H39	4:B:210:17F:H8	0.50	1.83	14	2
2:C:17:SER:OG	5:C:201:GSP:O3G	0.50	2.30	7	9
3:D:603:PCW:H432	3:D:611:PCW:C35	0.50	2.36	6	1
3:D:613:PCW:C21	3:D:613:PCW:H171	0.50	2.33	6	1
3:A:414:PCW:H252	4:A:415:17F:H61	0.50	1.83	7	1
3:D:603:PCW:C46	3:D:611:PCW:H412	0.50	2.36	13	3
4:D:628:17F:H36	4:D:629:17F:H77	0.50	1.84	8	1
3:C:206:PCW:H172	3:C:208:PCW:H152	0.50	1.84	8	1
3:C:207:PCW:C40	4:C:213:17F:H8	0.50	2.36	8	1
3:B:203:PCW:C41	3:B:203:PCW:H371	0.50	2.36	9	1
3:C:207:PCW:C17	3:C:208:PCW:H331	0.50	2.36	9	2
3:C:210:PCW:H422	3:C:210:PCW:C16	0.50	2.35	9	1
3:C:211:PCW:C5	3:C:211:PCW:C1	0.50	2.86	9	1
3:A:408:PCW:H222	4:D:631:17F:C30	0.50	2.25	10	1
3:A:404:PCW:H63	4:A:415:17F:H11	0.50	1.82	11	1
3:A:405:PCW:H51	3:A:406:PCW:C12	0.50	2.36	11	1
3:C:211:PCW:H152	4:C:215:17F:H58	0.50	1.82	13	1
3:D:617:PCW:H382	3:D:619:PCW:H142	0.50	1.83	14	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
2:B:135:ARG:HG3	2:C:161:ARG:HB3	0.50	1.82	14	1
3:C:206:PCW:H152	3:C:207:PCW:H241	0.50	1.82	14	1
3:A:408:PCW:C24	3:A:411:PCW:H222	0.50	2.37	15	2
3:C:203:PCW:C1	3:C:203:PCW:O31	0.50	2.53	15	1
3:C:209:PCW:H421	3:C:212:PCW:H283	0.50	1.83	15	1
4:C:215:17F:H36	4:C:215:17F:H65	0.50	1.84	15	1
3:D:608:PCW:C25	4:D:629:17F:H63	0.50	2.36	17	1
2:C:15:GLY:HA3	5:C:201:GSP:C8	0.50	2.42	19	1
3:C:206:PCW:C44	4:C:214:17F:H75	0.50	2.29	19	1
3:D:604:PCW:H283	4:C:213:17F:C29	0.50	2.37	1	1
3:A:406:PCW:H422	3:C:204:PCW:H431	0.50	1.82	2	1
3:D:606:PCW:H31	4:C:218:17F:H1	0.50	1.84	2	1
3:D:610:PCW:C1	4:D:631:17F:H6	0.50	2.31	20	2
2:C:41:ARG:HA	2:C:53:LEU:O	0.50	2.07	12	3
4:A:422:17F:H30	4:A:422:17F:C23	0.50	2.34	4	1
3:D:610:PCW:H121	4:D:631:17F:H18	0.50	1.83	16	2
3:D:602:PCW:C17	3:D:602:PCW:C21	0.50	2.81	18	3
4:D:632:17F:O10	4:D:632:17F:C4	0.50	2.58	6	3
3:C:203:PCW:C41	3:C:204:PCW:H141	0.50	2.32	6	1
3:C:205:PCW:H472	4:C:215:17F:H12A	0.50	1.84	6	1
3:A:408:PCW:C23	3:A:411:PCW:C23	0.50	2.88	13	3
3:D:623:PCW:H161	3:D:624:PCW:H371	0.50	1.83	7	1
3:B:207:PCW:H361	3:B:207:PCW:C22	0.50	2.37	8	3
3:A:404:PCW:H411	3:A:414:PCW:H251	0.50	1.82	8	1
4:D:632:17F:C32	4:D:632:17F:H67	0.50	2.36	8	1
3:A:403:PCW:H52	3:A:404:PCW:O1P	0.50	2.07	9	1
3:D:614:PCW:C20	4:B:209:17F:C27	0.50	2.90	12	5
4:B:210:17F:H30	4:C:215:17F:H10A	0.50	1.84	9	1
3:D:603:PCW:H171	3:C:216:PCW:C13	0.50	2.37	10	1
2:B:117:LYS:HE2	5:B:201:GSP:C8	0.50	2.42	13	1
3:C:206:PCW:H162	3:C:207:PCW:H222	0.50	1.83	13	1
3:A:411:PCW:C6	4:B:211:17F:O5	0.50	2.59	14	1
3:D:619:PCW:C32	3:D:627:PCW:H152	0.50	2.22	16	2
2:B:128:LYS:HD2	2:C:47:ASP:H	0.50	1.65	17	1
3:A:406:PCW:H341	3:B:205:PCW:C32	0.50	2.37	19	1
3:D:610:PCW:C28	4:D:631:17F:H68	0.50	2.36	19	1
3:D:609:PCW:H131	3:D:609:PCW:O31	0.50	2.07	2	1
3:D:619:PCW:H242	3:C:204:PCW:H471	0.50	1.83	2	1
3:B:204:PCW:O31	3:B:204:PCW:H73	0.50	2.06	16	3
2:C:6:LEU:O	2:C:55:ILE:HA	0.50	2.07	14	5
3:C:209:PCW:H141	4:C:214:17F:C8	0.50	2.34	2	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
3:A:411:PCW:O1P	3:C:204:PCW:C7	0.50	2.59	12	2
4:B:210:17F:H36	4:B:210:17F:C24	0.50	2.32	4	1
3:C:212:PCW:O1P	3:C:212:PCW:C31	0.50	2.59	4	2
3:A:402:PCW:C44	3:C:208:PCW:H132	0.50	2.36	5	1
3:A:404:PCW:H241	3:D:618:PCW:H281	0.50	1.83	7	1
3:D:609:PCW:C5	4:D:632:17F:HN1	0.50	2.20	7	2
3:D:607:PCW:H382	3:D:626:PCW:H452	0.50	1.81	20	2
3:C:203:PCW:C15	4:C:213:17F:C21	0.50	2.90	11	1
3:D:608:PCW:H262	4:D:629:17F:H30	0.50	1.82	12	2
3:D:614:PCW:C22	4:B:209:17F:H47	0.50	2.36	12	2
3:A:408:PCW:H152	3:A:411:PCW:H231	0.50	1.83	14	1
4:B:210:17F:C9	3:C:205:PCW:H451	0.50	2.37	15	1
3:B:206:PCW:H52	3:B:206:PCW:O11	0.50	2.06	16	1
3:D:612:PCW:H322	3:D:623:PCW:H352	0.50	1.80	17	1
3:A:414:PCW:C33	4:B:209:17F:O8	0.50	2.59	18	1
3:D:621:PCW:O31	3:D:621:PCW:H52	0.50	2.07	18	1
3:B:208:PCW:C35	3:C:211:PCW:H63	0.50	2.37	18	1
3:B:208:PCW:H462	3:C:203:PCW:H151	0.50	1.83	1	1
3:D:603:PCW:O4P	4:C:219:17F:O1	0.50	2.30	14	7
2:B:144:THR:HG22	2:B:151:GLY:HA3	0.50	1.82	2	2
4:D:628:17F:C31	4:D:629:17F:H51	0.50	2.37	3	3
3:B:208:PCW:H321	3:C:211:PCW:C8	0.50	2.37	3	2
3:C:209:PCW:H422	3:C:212:PCW:H283	0.50	1.83	4	1
3:C:212:PCW:H32	4:C:215:17F:O2	0.50	2.07	4	1
3:A:417:PCW:O11	3:A:417:PCW:C2	0.50	2.58	10	4
3:D:612:PCW:H32	3:D:620:PCW:H31	0.50	1.83	6	2
2:B:13:GLY:HA2	2:B:32:TYR:HE1	0.50	1.67	6	1
3:A:401:PCW:O3	3:A:401:PCW:C31	0.50	2.60	7	3
3:D:606:PCW:C6	3:D:606:PCW:O11	0.50	2.56	7	3
4:B:211:17F:H39	3:C:204:PCW:H381	0.50	1.82	7	1
3:C:209:PCW:O3	4:C:214:17F:H6	0.50	2.07	7	2
3:D:607:PCW:C43	3:D:626:PCW:C48	0.50	2.90	9	1
3:A:404:PCW:H462	3:A:404:PCW:C17	0.50	2.36	10	1
3:A:407:PCW:H331	3:A:410:PCW:H352	0.50	1.84	10	3
3:A:421:PCW:H351	3:D:618:PCW:C15	0.50	2.31	17	4
3:C:205:PCW:H131	3:C:209:PCW:H151	0.50	1.82	11	1
3:C:212:PCW:C34	4:C:213:17F:H9A	0.50	2.36	12	1
3:C:210:PCW:H382	3:C:210:PCW:H422	0.50	1.83	14	1
2:C:131:GLN:HG3	2:C:141:PHE:HD2	0.50	1.67	15	1
2:B:117:LYS:NZ	5:B:201:GSP:N7	0.50	2.58	18	1
4:B:210:17F:H11A	4:C:215:17F:H12A	0.50	1.84	19	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
3:D:606:PCW:H73	3:D:626:PCW:H171	0.49	1.84	16	3
3:D:610:PCW:H152	4:D:631:17F:C33	0.49	2.37	19	6
3:D:622:PCW:H381	4:D:632:17F:C42	0.49	2.37	1	1
3:C:206:PCW:H151	3:C:208:PCW:C16	0.49	2.37	1	1
4:A:422:17F:H40	4:C:219:17F:H62	0.49	1.84	2	1
4:B:210:17F:N1	3:C:212:PCW:O11	0.49	2.45	2	1
1:D:574:LEU:O	1:D:578:GLU:HG2	0.49	2.07	7	4
3:C:217:PCW:H122	4:C:218:17F:C38	0.49	2.37	4	1
3:A:420:PCW:O2P	3:A:420:PCW:C3	0.49	2.59	10	2
3:D:617:PCW:H441	3:D:627:PCW:C26	0.49	2.34	5	2
4:D:632:17F:H65	3:C:208:PCW:H461	0.49	1.84	5	2
3:D:604:PCW:H451	3:D:606:PCW:C14	0.49	2.36	11	2
3:C:203:PCW:C45	3:C:204:PCW:H161	0.49	2.37	7	1
3:A:411:PCW:H262	3:C:210:PCW:C22	0.49	2.37	8	1
4:B:210:17F:H2	4:B:210:17F:C4	0.49	2.37	8	1
3:C:207:PCW:C46	4:C:213:17F:H78	0.49	2.36	8	1
3:C:210:PCW:H52	3:C:210:PCW:C31	0.49	2.37	8	1
3:D:605:PCW:C8	4:D:630:17F:O4	0.49	2.59	9	1
3:D:616:PCW:H281	3:C:206:PCW:H482	0.49	1.83	9	1
3:D:608:PCW:H482	4:D:628:17F:C34	0.49	2.33	10	1
3:D:605:PCW:O2P	3:D:614:PCW:C5	0.49	2.60	11	1
3:C:203:PCW:H281	3:C:211:PCW:C45	0.49	2.37	12	1
3:C:203:PCW:O1P	3:C:211:PCW:C7	0.49	2.59	16	2
3:B:203:PCW:C47	3:C:211:PCW:H232	0.49	2.37	13	1
3:C:203:PCW:H231	3:C:204:PCW:H341	0.49	1.83	16	1
3:C:217:PCW:H462	4:C:219:17F:H55	0.49	1.84	19	1
3:D:614:PCW:H282	4:B:209:17F:H46	0.49	1.84	20	1
3:B:205:PCW:H42	3:C:204:PCW:H63	0.49	1.81	20	1
3:B:207:PCW:C4	3:B:207:PCW:O11	0.49	2.59	18	10
3:A:403:PCW:H41	3:A:403:PCW:C11	0.49	2.37	12	4
3:B:204:PCW:C7	3:B:204:PCW:O31	0.49	2.60	10	4
3:A:407:PCW:O3	3:A:407:PCW:O31	0.49	2.30	5	3
3:C:209:PCW:H451	3:C:212:PCW:H19	0.49	1.84	5	1
4:D:632:17F:H54	3:C:208:PCW:H161	0.49	1.83	6	1
3:D:604:PCW:C25	4:C:215:17F:H52	0.49	2.37	8	1
3:A:421:PCW:C16	4:D:630:17F:H60	0.49	2.36	10	2
3:D:617:PCW:H19	3:D:618:PCW:H482	0.49	1.84	10	1
1:A:376:LEU:O	1:A:380:GLU:HG3	0.49	2.07	19	4
3:A:414:PCW:C11	3:A:414:PCW:C37	0.49	2.90	17	2
3:D:601:PCW:H372	3:D:602:PCW:H171	0.49	1.85	16	1
3:D:603:PCW:H231	3:D:611:PCW:H351	0.49	1.83	16	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
3:A:402:PCW:H322	3:A:402:PCW:H52	0.49	1.83	19	1
3:B:205:PCW:H172	3:C:204:PCW:H342	0.49	1.82	19	1
3:C:206:PCW:H211	3:C:208:PCW:C41	0.49	2.37	19	1
4:D:631:17F:C4	4:D:631:17F:H1A	0.49	2.37	20	1
3:C:206:PCW:C6	3:C:212:PCW:O1P	0.49	2.60	20	1
3:A:405:PCW:O11	3:A:405:PCW:C2	0.49	2.59	1	4
3:A:405:PCW:H63	4:B:211:17F:O4	0.49	2.07	1	1
4:A:422:17F:H44	4:C:219:17F:H61	0.49	1.84	2	1
3:D:608:PCW:C12	3:D:609:PCW:H171	0.49	2.37	2	2
3:B:208:PCW:C37	3:C:204:PCW:H352	0.49	2.38	2	2
4:B:210:17F:C32	3:C:212:PCW:H232	0.49	2.30	2	1
3:D:624:PCW:O11	3:D:624:PCW:H2	0.49	2.08	3	3
3:B:204:PCW:C44	4:B:210:17F:H44	0.49	2.31	4	1
3:B:208:PCW:C34	3:C:211:PCW:H63	0.49	2.37	5	1
3:C:203:PCW:H461	3:C:204:PCW:H141	0.49	1.85	5	1
3:A:405:PCW:H322	3:A:406:PCW:H181	0.49	1.84	6	1
3:D:606:PCW:O11	3:D:606:PCW:N	0.49	2.45	6	1
3:D:620:PCW:O31	3:D:620:PCW:C1	0.49	2.55	6	2
3:C:204:PCW:C48	3:C:216:PCW:H232	0.49	2.27	6	1
3:C:207:PCW:C32	3:C:207:PCW:C6	0.49	2.90	10	3
3:A:402:PCW:H421	3:C:208:PCW:C13	0.49	2.33	13	3
3:C:203:PCW:H451	3:C:204:PCW:H232	0.49	1.83	7	1
3:C:205:PCW:C6	4:C:214:17F:O8	0.49	2.59	8	2
3:C:209:PCW:H132	4:C:214:17F:O7	0.49	2.07	7	2
3:D:603:PCW:H73	3:C:216:PCW:O3P	0.49	2.07	8	1
3:D:617:PCW:H12	3:D:617:PCW:C4	0.49	2.33	8	1
3:C:206:PCW:C15	3:C:207:PCW:H222	0.49	2.37	8	2
3:A:405:PCW:H361	3:A:411:PCW:C46	0.49	2.24	17	2
3:C:203:PCW:C15	4:C:213:17F:H37	0.49	2.36	9	2
4:A:415:17F:C27	4:A:416:17F:H71	0.49	2.32	10	1
3:D:624:PCW:H472	4:B:209:17F:C30	0.49	2.38	13	2
3:A:413:PCW:C36	3:C:210:PCW:H141	0.49	2.36	18	1
3:A:403:PCW:H332	3:A:406:PCW:O4P	0.49	2.07	19	1
3:D:616:PCW:H472	3:C:208:PCW:C20	0.49	2.37	20	1
3:C:206:PCW:H62	3:C:212:PCW:O1P	0.49	2.07	20	1
3:C:207:PCW:H272	4:C:214:17F:H43	0.49	1.84	20	1
3:A:413:PCW:H341	3:A:413:PCW:O31	0.49	2.07	10	3
3:C:203:PCW:H482	3:C:204:PCW:H152	0.49	1.84	1	1
3:D:612:PCW:H181	3:D:620:PCW:C15	0.49	2.37	2	1
3:B:204:PCW:C6	3:B:204:PCW:O31	0.49	2.60	2	1
3:C:205:PCW:H242	3:C:209:PCW:H411	0.49	1.84	2	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
3:C:207:PCW:H452	4:C:213:17F:H75	0.49	1.84	3	1
3:D:603:PCW:C31	3:D:603:PCW:C4	0.49	2.91	8	3
4:D:628:17F:H36	4:D:629:17F:C41	0.49	2.31	4	2
3:D:606:PCW:H63	3:D:606:PCW:H131	0.49	1.83	5	4
2:C:83:ALA:HB1	2:C:85:ASN:OD1	0.49	2.08	5	1
4:A:422:17F:C34	4:D:632:17F:H72	0.49	2.36	6	1
3:A:406:PCW:H331	4:B:211:17F:C8	0.49	2.33	7	1
3:D:614:PCW:H261	4:B:209:17F:H70	0.49	1.85	9	1
3:D:621:PCW:C4	3:D:621:PCW:O31	0.49	2.60	9	1
3:B:203:PCW:H172	4:B:209:17F:H32	0.49	1.82	9	1
3:A:401:PCW:H39	3:A:401:PCW:H282	0.49	1.83	10	1
3:C:217:PCW:C11	4:C:218:17F:H62	0.49	2.37	10	1
3:A:402:PCW:H451	4:D:632:17F:C30	0.49	2.37	11	2
3:A:413:PCW:C31	3:A:413:PCW:H52	0.49	2.36	11	1
3:A:406:PCW:H141	4:B:211:17F:H19A	0.49	1.83	13	1
3:D:601:PCW:O3	3:D:601:PCW:O31	0.49	2.30	13	2
3:D:624:PCW:C11	3:D:624:PCW:O31	0.49	2.61	13	3
2:B:116:ASN:ND2	5:B:201:GSP:N7	0.49	2.60	17	4
3:B:208:PCW:C35	3:C:203:PCW:H221	0.49	2.30	13	1
3:D:623:PCW:C20	4:C:215:17F:H51	0.49	2.38	14	1
3:B:208:PCW:H41	3:B:208:PCW:H2	0.49	1.82	14	1
3:D:615:PCW:H432	3:D:620:PCW:C20	0.49	2.38	16	1
3:A:401:PCW:C32	3:B:207:PCW:H39	0.49	2.36	17	1
3:D:603:PCW:C6	3:C:216:PCW:P	0.49	3.01	17	1
3:A:414:PCW:H232	4:A:415:17F:H59	0.49	1.84	19	1
2:B:46:ILE:HA	2:C:128:LYS:HD2	0.49	1.84	19	1
3:C:203:PCW:H281	3:C:211:PCW:H481	0.49	1.83	19	1
3:A:402:PCW:H40	3:A:407:PCW:H261	0.49	1.85	20	1
3:A:409:PCW:C19	3:A:409:PCW:C15	0.49	2.89	1	15
4:B:210:17F:O2	4:B:210:17F:H2	0.49	2.07	2	1
3:D:623:PCW:H122	3:D:624:PCW:C35	0.49	2.37	4	2
3:A:412:PCW:H462	3:C:210:PCW:C48	0.49	2.36	15	2
3:A:409:PCW:C37	3:B:206:PCW:H332	0.49	2.37	6	1
3:D:625:PCW:O11	3:D:625:PCW:C2	0.49	2.58	16	7
3:C:207:PCW:H172	4:C:213:17F:C20	0.49	2.36	7	1
3:D:606:PCW:H252	4:C:218:17F:H42	0.49	1.84	20	2
3:A:404:PCW:H232	3:D:618:PCW:H283	0.49	1.85	9	1
3:A:420:PCW:H441	3:D:617:PCW:H251	0.49	1.83	10	1
3:A:404:PCW:H471	4:A:415:17F:H52	0.49	1.85	11	1
2:B:89:SER:O	2:B:93:ILE:HG12	0.49	2.07	11	2
3:A:403:PCW:H73	3:A:403:PCW:C12	0.49	2.37	12	3

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
3:A:419:PCW:H381	3:D:625:PCW:H271	0.49	1.84	13	1
3:C:205:PCW:O31	3:C:209:PCW:C3	0.49	2.61	14	1
3:D:612:PCW:O2P	3:D:614:PCW:H61	0.49	2.07	15	1
3:D:626:PCW:C31	3:D:626:PCW:C11	0.49	2.91	15	1
3:A:403:PCW:C8	4:A:415:17F:O4	0.49	2.61	16	1
3:D:612:PCW:H371	3:D:612:PCW:H19	0.49	1.84	16	1
4:D:629:17F:H4	4:D:629:17F:H1A	0.49	1.84	16	1
3:C:207:PCW:H441	4:C:213:17F:H58	0.49	1.84	16	1
4:C:213:17F:H46	4:C:215:17F:H76	0.49	1.83	16	1
3:D:614:PCW:H32	3:D:620:PCW:H32	0.49	1.85	18	1
3:C:207:PCW:C46	3:C:207:PCW:H262	0.49	2.37	19	1
3:A:405:PCW:C6	4:B:211:17F:O4	0.49	2.61	1	1
3:D:603:PCW:C8	3:D:603:PCW:C13	0.49	2.91	19	3
4:A:416:17F:H68	3:B:204:PCW:H283	0.49	1.84	3	1
3:D:602:PCW:H362	4:C:214:17F:C34	0.49	2.37	4	3
3:A:402:PCW:H82	3:A:407:PCW:C11	0.49	2.37	13	2
4:D:630:17F:O6	4:D:630:17F:C17	0.49	2.61	20	7
3:D:604:PCW:H221	3:D:604:PCW:H161	0.49	1.82	6	1
4:A:416:17F:H72	3:D:614:PCW:H241	0.49	1.80	9	1
3:C:203:PCW:C17	3:C:203:PCW:H132	0.49	2.37	11	2
3:B:204:PCW:C45	3:B:207:PCW:H222	0.49	2.37	11	1
2:C:72:MET:SD	2:C:100:ILE:HA	0.49	2.48	12	1
4:A:416:17F:H77	4:B:209:17F:H73	0.49	1.83	13	1
3:D:601:PCW:C45	3:D:601:PCW:H152	0.49	2.38	15	1
1:A:285:GLU:HA	1:A:288:ARG:HD2	0.49	1.84	16	1
2:C:32:TYR:HD1	5:C:201:GSP:C5'	0.49	2.20	17	1
3:C:212:PCW:H332	4:C:215:17F:H20A	0.49	1.85	17	1
1:D:463:TRP:NE1	4:D:629:17F:H77	0.49	2.22	19	1
3:B:204:PCW:H122	3:B:207:PCW:C40	0.49	2.38	19	1
3:B:207:PCW:H462	4:B:210:17F:C28	0.49	2.38	19	1
4:B:210:17F:H8A	4:C:215:17F:H8	0.49	1.85	19	1
3:D:604:PCW:C43	3:D:606:PCW:H181	0.49	2.37	20	1
3:A:409:PCW:H19	3:A:409:PCW:H151	0.49	1.85	1	2
4:A:415:17F:H12	4:B:209:17F:H5	0.49	1.84	1	2
3:D:605:PCW:C31	3:D:614:PCW:C6	0.49	2.90	6	5
3:D:603:PCW:C25	3:D:611:PCW:H171	0.49	2.35	3	2
3:D:603:PCW:H432	3:D:611:PCW:H362	0.49	1.84	3	1
2:C:6:LEU:HD11	2:C:53:LEU:HB3	0.49	1.83	3	1
3:D:602:PCW:C15	4:D:628:17F:H54	0.49	2.37	4	1
3:C:217:PCW:H2	4:C:218:17F:H78	0.49	1.84	6	1
3:A:404:PCW:C20	3:D:611:PCW:H282	0.49	2.38	7	2

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
3:A:408:PCW:H261	4:D:631:17F:H54	0.49	1.85	7	1
3:A:420:PCW:H362	3:D:618:PCW:H381	0.49	1.85	7	1
3:D:621:PCW:C14	4:D:632:17F:C18	0.49	2.91	17	2
3:C:209:PCW:H141	4:C:214:17F:C18	0.49	2.37	7	1
3:B:203:PCW:C19	3:B:204:PCW:H331	0.49	2.38	8	1
4:A:415:17F:C10	4:B:209:17F:H30	0.49	2.38	10	1
3:B:204:PCW:H431	4:B:210:17F:H10	0.49	1.83	10	1
3:D:603:PCW:H361	3:D:611:PCW:H342	0.49	1.83	11	1
3:D:620:PCW:H451	4:B:209:17F:H74	0.49	1.84	19	2
3:B:205:PCW:C48	3:B:208:PCW:H19	0.49	2.38	12	2
3:C:207:PCW:H161	4:C:213:17F:C33	0.49	2.25	12	1
3:D:607:PCW:C36	3:D:626:PCW:H422	0.49	2.35	13	1
3:D:609:PCW:C39	3:D:616:PCW:H421	0.49	2.38	13	2
3:A:410:PCW:C26	3:D:621:PCW:H411	0.49	2.35	14	1
4:A:416:17F:C41	4:B:209:17F:H73	0.49	2.38	15	1
4:A:416:17F:H32	3:B:204:PCW:H211	0.49	1.84	17	1
3:B:203:PCW:H382	3:C:211:PCW:H162	0.49	1.83	17	1
3:A:410:PCW:C12	3:C:208:PCW:H352	0.49	2.38	18	1
3:B:206:PCW:H412	3:C:209:PCW:H39	0.49	1.85	18	1
3:B:208:PCW:C45	4:C:218:17F:H49	0.49	2.35	19	1
3:C:212:PCW:H162	4:C:215:17F:C10	0.49	2.38	20	1
3:A:402:PCW:H411	3:C:208:PCW:C36	0.49	2.37	1	2
3:D:624:PCW:H451	4:B:209:17F:H77	0.49	1.82	19	2
3:B:208:PCW:C45	3:C:203:PCW:H121	0.49	2.38	1	1
3:B:208:PCW:H31	3:C:211:PCW:H452	0.49	1.83	1	1
3:A:411:PCW:O3	3:A:411:PCW:O31	0.49	2.30	7	12
3:A:408:PCW:H252	4:D:631:17F:H54	0.49	1.83	3	1
3:D:610:PCW:O4P	4:D:631:17F:O8	0.49	2.31	3	1
3:A:404:PCW:O2P	3:A:406:PCW:C5	0.49	2.54	4	1
3:A:405:PCW:C7	4:B:211:17F:O5	0.49	2.60	4	1
1:D:443:LYS:O	1:D:447:GLU:HB2	0.49	2.08	4	3
1:D:495:LYS:O	1:D:499:LEU:HB2	0.49	2.08	14	10
3:C:203:PCW:C45	3:C:210:PCW:H20	0.49	2.36	4	1
4:A:416:17F:H57	3:B:204:PCW:H162	0.49	1.83	5	1
2:B:18:ALA:HB3	5:B:201:GSP:C8	0.49	2.43	5	1
3:B:208:PCW:C34	3:C:211:PCW:H12	0.49	2.38	5	1
3:A:402:PCW:H431	3:C:206:PCW:H231	0.49	1.83	6	2
3:D:608:PCW:H63	3:D:626:PCW:H222	0.49	1.84	12	3
3:B:203:PCW:C22	4:B:209:17F:H56	0.49	2.38	9	1
3:A:407:PCW:C33	3:A:410:PCW:H352	0.49	2.38	15	2
4:C:215:17F:H77	4:C:215:17F:C28	0.49	2.38	12	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
3:A:403:PCW:H381	3:A:403:PCW:C15	0.49	2.38	13	1
3:C:203:PCW:H11	3:C:203:PCW:O31	0.49	2.07	13	2
3:B:207:PCW:H342	3:B:207:PCW:C18	0.49	2.31	19	2
3:B:206:PCW:H231	3:C:205:PCW:H132	0.49	1.83	18	1
3:A:417:PCW:H442	3:D:618:PCW:C21	0.49	2.38	1	1
3:A:413:PCW:H382	3:C:210:PCW:C14	0.49	2.37	9	2
1:D:496:LEU:O	1:D:500:GLY:HA3	0.49	2.08	4	9
2:B:165:LYS:HB2	2:C:135:ARG:HD3	0.49	1.85	17	2
3:C:211:PCW:H283	4:C:215:17F:H52	0.49	1.83	2	1
4:A:415:17F:O10	4:A:415:17F:O7	0.49	2.30	10	2
3:D:627:PCW:H82	3:D:627:PCW:O4P	0.49	2.08	3	1
3:D:612:PCW:H181	3:D:620:PCW:H172	0.49	1.83	7	1
3:D:608:PCW:H52	3:D:626:PCW:H222	0.49	1.83	9	1
3:B:203:PCW:C47	3:C:211:PCW:H251	0.49	2.30	16	3
3:D:612:PCW:P	3:D:614:PCW:H61	0.49	2.48	15	3
3:D:619:PCW:H151	3:D:627:PCW:C14	0.49	2.34	11	1
3:A:406:PCW:C27	4:B:211:17F:H57	0.49	2.37	13	2
3:D:603:PCW:H462	3:D:611:PCW:C43	0.49	2.37	13	1
4:C:215:17F:H48	4:C:215:17F:C42	0.49	2.38	13	1
3:A:417:PCW:C6	4:D:630:17F:O4	0.49	2.61	15	1
3:C:211:PCW:H171	3:C:211:PCW:H482	0.49	1.84	15	1
3:C:206:PCW:H162	3:C:208:PCW:H321	0.49	1.85	16	1
3:A:417:PCW:H172	3:A:420:PCW:C41	0.49	2.35	18	1
3:A:406:PCW:O11	3:A:406:PCW:C2	0.49	2.59	1	1
3:A:408:PCW:O2P	3:A:411:PCW:C14	0.49	2.60	1	1
3:B:207:PCW:H381	3:B:207:PCW:H232	0.49	1.84	1	1
4:B:211:17F:H19	4:B:211:17F:H8A	0.49	1.84	1	1
3:B:208:PCW:H12	3:C:211:PCW:C34	0.49	2.38	2	1
2:C:146:ALA:N	5:C:201:GSP:O6	0.49	2.45	2	9
3:D:604:PCW:O3	3:D:604:PCW:C31	0.49	2.61	10	11
2:B:57:ASP:OD2	5:B:201:GSP:O3G	0.49	2.31	8	3
3:B:203:PCW:H411	3:C:211:PCW:H221	0.49	1.84	3	1
3:D:610:PCW:H132	3:D:610:PCW:C34	0.49	2.35	4	2
3:D:626:PCW:H182	3:D:626:PCW:H82	0.49	1.85	5	1
3:C:209:PCW:H481	3:C:209:PCW:H282	0.49	1.83	19	2
3:C:211:PCW:O4P	3:C:211:PCW:H62	0.49	2.07	5	1
3:B:204:PCW:H471	3:B:207:PCW:H271	0.49	1.85	6	1
3:C:217:PCW:C2	4:C:218:17F:H78	0.49	2.38	6	1
3:A:405:PCW:C23	3:A:418:PCW:H262	0.49	2.38	7	1
3:A:411:PCW:H262	3:C:210:PCW:H231	0.49	1.82	8	1
3:A:413:PCW:H442	3:C:210:PCW:H212	0.49	1.83	8	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
3:A:404:PCW:H382	3:A:404:PCW:C14	0.49	2.28	9	3
4:C:218:17F:H42	4:C:219:17F:C41	0.49	2.37	10	1
3:A:406:PCW:H222	4:B:211:17F:C1Y	0.49	2.38	13	1
3:C:212:PCW:C39	4:C:213:17F:H55	0.49	2.37	13	1
3:D:614:PCW:H251	4:B:209:17F:C25	0.49	2.36	14	1
3:A:418:PCW:C38	3:D:613:PCW:H432	0.49	2.38	16	1
3:B:206:PCW:C38	3:C:205:PCW:H283	0.49	2.38	16	1
3:D:614:PCW:C24	4:B:209:17F:H71	0.49	2.38	19	1
3:A:403:PCW:C36	3:A:403:PCW:C32	0.48	2.65	9	3
3:D:626:PCW:C31	3:D:626:PCW:O3	0.48	2.61	8	11
3:C:206:PCW:H61	3:C:212:PCW:P	0.48	2.47	1	1
3:C:209:PCW:C45	3:C:212:PCW:H212	0.48	2.35	1	1
3:A:409:PCW:H321	3:B:206:PCW:H73	0.48	1.85	2	1
3:C:211:PCW:H2	4:C:215:17F:H19A	0.48	1.85	2	1
3:A:413:PCW:C8	3:C:210:PCW:O2P	0.48	2.60	3	2
3:D:603:PCW:C16	3:D:624:PCW:C22	0.48	2.91	11	4
2:C:37:GLU:HG3	2:C:58:THR:HG22	0.48	1.85	3	2
3:A:408:PCW:H42	3:A:408:PCW:H12	0.48	1.85	4	1
3:B:207:PCW:C6	4:B:210:17F:H11	0.48	2.38	4	1
3:C:206:PCW:O31	3:C:206:PCW:O3P	0.48	2.30	8	2
3:A:409:PCW:C39	4:B:210:17F:H65	0.48	2.37	5	1
3:A:414:PCW:H452	4:B:209:17F:H12A	0.48	1.85	6	1
3:B:205:PCW:H63	3:B:205:PCW:O3P	0.48	2.08	7	1
3:A:418:PCW:H341	3:D:613:PCW:C15	0.48	2.38	10	2
2:B:16:LYS:HG2	5:B:201:GSP:PB	0.48	2.48	17	2
3:A:403:PCW:H63	3:A:403:PCW:H121	0.48	1.85	13	1
4:A:416:17F:H72	4:B:209:17F:H68	0.48	1.85	13	1
1:A:276:VAL:O	1:A:280:ARG:HB2	0.48	2.07	14	2
3:A:418:PCW:O31	3:A:418:PCW:C4	0.48	2.61	16	1
3:D:608:PCW:C42	3:B:206:PCW:H472	0.48	2.37	16	1
3:A:414:PCW:H162	4:A:415:17F:H31	0.48	1.84	17	1
4:A:422:17F:H55	3:D:606:PCW:C41	0.48	2.34	20	1
3:A:421:PCW:H11	3:A:421:PCW:H41	0.48	1.84	1	2
3:D:605:PCW:O1P	3:D:605:PCW:H2	0.48	2.08	18	8
2:C:35:THR:OG1	5:C:201:GSP:O3G	0.48	2.31	19	9
3:B:208:PCW:C37	3:C:204:PCW:H331	0.48	2.38	2	2
3:C:205:PCW:H242	3:C:209:PCW:C41	0.48	2.38	2	1
3:C:205:PCW:H412	3:C:212:PCW:H211	0.48	1.83	2	1
3:A:403:PCW:H321	3:A:404:PCW:C1	0.48	2.35	3	1
3:B:204:PCW:C41	3:B:207:PCW:H61	0.48	2.38	3	1
3:A:418:PCW:H352	3:D:613:PCW:C13	0.48	2.38	4	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
3:A:418:PCW:C34	3:D:613:PCW:H161	0.48	2.36	5	1
3:C:206:PCW:C24	3:C:208:PCW:H381	0.48	2.37	5	1
2:C:147:LYS:HB2	5:C:201:GSP:N1	0.48	2.24	7	1
3:D:623:PCW:O31	3:D:623:PCW:O3	0.48	2.30	9	2
3:B:208:PCW:O11	3:B:208:PCW:O4P	0.48	2.30	11	1
1:A:341:ASN:O	1:A:345:ARG:HG3	0.48	2.08	19	2
3:A:408:PCW:H482	3:A:413:PCW:H232	0.48	1.85	12	1
4:A:416:17F:C36	3:B:204:PCW:H252	0.48	2.38	12	1
2:C:13:GLY:CA	5:C:201:GSP:H5'1	0.48	2.38	13	1
3:A:405:PCW:O2P	3:A:406:PCW:H171	0.48	2.08	14	2
1:D:415:LEU:O	1:D:419:LEU:HG	0.48	2.08	15	2
3:D:624:PCW:H471	4:B:209:17F:H54	0.48	1.79	15	1
3:A:408:PCW:C18	3:A:413:PCW:H262	0.48	2.37	16	1
3:D:616:PCW:H122	4:D:632:17F:C7	0.48	2.38	16	1
3:D:607:PCW:O3	3:D:626:PCW:H421	0.48	2.07	18	1
3:C:207:PCW:C15	4:C:213:17F:H20A	0.48	2.38	3	3
3:B:203:PCW:C8	3:B:203:PCW:O4P	0.48	2.61	7	4
3:C:216:PCW:O2	3:C:216:PCW:C11	0.48	2.62	8	11
3:A:402:PCW:O2	3:A:402:PCW:P	0.48	2.71	4	2
3:A:402:PCW:H412	3:C:206:PCW:H272	0.48	1.84	4	1
3:C:211:PCW:P	3:C:211:PCW:C6	0.48	2.90	4	1
4:C:213:17F:H39	4:C:218:17F:H55	0.48	1.85	4	1
3:D:604:PCW:C16	3:D:604:PCW:H211	0.48	2.38	18	2
3:D:607:PCW:H472	3:C:209:PCW:C48	0.48	2.38	6	2
1:A:263:LYS:O	1:A:267:GLU:HG3	0.48	2.09	7	1
3:D:602:PCW:C33	4:C:214:17F:H61	0.48	2.38	7	1
3:B:204:PCW:C42	3:B:207:PCW:H411	0.48	2.39	7	1
3:D:616:PCW:H432	3:C:208:PCW:C26	0.48	2.26	9	1
3:D:617:PCW:O4P	3:D:617:PCW:C3	0.48	2.62	18	4
3:A:402:PCW:C12	3:A:407:PCW:H132	0.48	2.37	11	2
4:B:211:17F:H40	3:C:204:PCW:C42	0.48	2.37	11	1
3:D:609:PCW:C25	4:D:628:17F:H70	0.48	2.34	15	2
4:A:422:17F:H48	4:C:218:17F:H12	0.48	1.83	13	1
3:D:609:PCW:C46	3:C:208:PCW:H451	0.48	2.34	19	2
3:B:208:PCW:H131	3:C:203:PCW:H283	0.48	1.84	14	1
4:C:218:17F:H20A	4:C:218:17F:C9	0.48	2.36	14	1
3:C:206:PCW:H41	4:C:214:17F:H10A	0.48	1.84	16	1
3:C:209:PCW:C12	4:C:214:17F:H18	0.48	2.38	16	1
3:D:624:PCW:H472	4:B:209:17F:H55	0.48	1.83	17	1
4:B:210:17F:H36	4:C:215:17F:C21	0.48	2.38	19	2
3:B:208:PCW:C36	3:C:211:PCW:H63	0.48	2.38	18	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
3:C:210:PCW:H461	3:C:210:PCW:C18	0.48	2.39	18	1
3:A:402:PCW:C42	3:C:208:PCW:H361	0.48	2.37	19	1
3:C:206:PCW:H152	3:C:207:PCW:H181	0.48	1.83	19	1
3:D:610:PCW:O11	4:D:631:17F:H18A	0.48	2.07	20	1
3:A:402:PCW:C44	3:C:208:PCW:H172	0.48	2.38	1	1
3:A:409:PCW:H131	4:B:210:17F:C1Y	0.48	2.38	1	1
3:C:206:PCW:C17	3:C:207:PCW:C20	0.48	2.92	1	1
1:A:233:GLU:HA	1:A:236:THR:OG1	0.48	2.09	2	4
3:A:417:PCW:C41	3:A:417:PCW:C37	0.48	2.89	2	2
3:C:211:PCW:C15	4:C:215:17F:H61	0.48	2.35	2	1
3:A:413:PCW:H462	3:D:627:PCW:H281	0.48	1.84	3	1
4:B:210:17F:C38	3:C:209:PCW:H421	0.48	2.37	3	1
3:C:211:PCW:H242	4:C:215:17F:C40	0.48	2.38	3	1
3:A:408:PCW:H31	3:A:413:PCW:H121	0.48	1.84	4	1
2:B:84:ILE:HD13	2:B:118:CYS:HA	0.48	1.84	6	4
3:B:204:PCW:C3	3:B:207:PCW:H351	0.48	2.32	4	1
3:B:208:PCW:C4	3:C:211:PCW:H82	0.48	2.38	4	1
3:A:404:PCW:C11	3:B:205:PCW:H452	0.48	2.38	5	1
3:D:605:PCW:C48	3:D:614:PCW:H162	0.48	2.39	5	2
3:D:616:PCW:H483	3:C:207:PCW:H241	0.48	1.85	12	2
3:C:207:PCW:C42	4:C:213:17F:H33	0.48	2.37	14	2
3:A:410:PCW:H252	4:A:422:17F:C41	0.48	2.38	10	1
3:D:602:PCW:H371	4:C:214:17F:H70	0.48	1.84	17	2
3:A:405:PCW:H82	3:A:405:PCW:O4P	0.48	2.09	11	1
3:B:203:PCW:H451	3:C:211:PCW:C25	0.48	2.39	11	1
3:B:206:PCW:O11	3:C:209:PCW:C33	0.48	2.62	14	2
3:C:206:PCW:O31	3:C:208:PCW:H63	0.48	2.08	14	1
3:A:404:PCW:H172	3:A:404:PCW:C45	0.48	2.38	15	1
3:D:622:PCW:H411	3:D:622:PCW:C37	0.48	2.31	15	1
3:D:608:PCW:C17	4:D:629:17F:H18A	0.48	2.36	16	1
3:D:604:PCW:H231	4:C:215:17F:H75	0.48	1.84	17	1
3:C:205:PCW:C1	4:C:214:17F:O7	0.48	2.61	17	1
3:B:204:PCW:H422	3:B:207:PCW:H451	0.48	1.85	19	1
3:D:616:PCW:H121	4:D:632:17F:C8	0.48	2.38	20	1
3:D:624:PCW:O31	3:D:624:PCW:C11	0.48	2.61	9	6
3:B:208:PCW:H39	3:C:204:PCW:H352	0.48	1.86	1	1
3:C:217:PCW:O4P	3:C:217:PCW:H62	0.48	2.06	1	2
3:A:410:PCW:H381	3:A:410:PCW:C18	0.48	2.38	2	1
3:B:208:PCW:C37	3:C:203:PCW:H221	0.48	2.37	2	1
5:C:201:GSP:O2B	5:C:201:GSP:O1A	0.48	2.30	12	4
3:C:203:PCW:H361	3:C:204:PCW:C12	0.48	2.39	2	2

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
3:A:404:PCW:C15	3:B:205:PCW:C45	0.48	2.87	4	1
3:D:619:PCW:H462	3:B:205:PCW:H232	0.48	1.84	6	1
3:C:216:PCW:H483	3:C:217:PCW:H381	0.48	1.85	6	1
3:D:616:PCW:C5	4:D:632:17F:O5	0.48	2.59	7	1
3:C:205:PCW:C33	3:C:209:PCW:H342	0.48	2.38	7	1
4:A:416:17F:H20	4:A:416:17F:O10	0.48	2.09	9	1
3:D:609:PCW:O11	3:D:616:PCW:C8	0.48	2.61	18	4
3:A:401:PCW:C45	3:D:612:PCW:H271	0.48	2.27	11	1
3:D:627:PCW:O31	3:D:627:PCW:C5	0.48	2.61	12	2
3:C:212:PCW:H371	4:C:215:17F:C32	0.48	2.36	12	1
3:D:616:PCW:H471	3:C:208:PCW:H222	0.48	1.83	13	1
3:C:211:PCW:H152	4:C:215:17F:H62	0.48	1.84	13	1
3:A:402:PCW:H181	3:A:407:PCW:C21	0.48	2.25	19	1
3:A:402:PCW:C38	3:C:208:PCW:H31	0.48	2.36	19	1
3:C:207:PCW:H412	4:C:213:17F:H8A	0.48	1.84	19	1
3:A:406:PCW:H122	4:B:211:17F:H9A	0.48	1.86	1	1
3:A:413:PCW:H442	3:C:210:PCW:H483	0.48	1.83	6	2
2:B:84:ILE:CD1	2:B:118:CYS:HA	0.48	2.38	1	3
3:C:209:PCW:C46	3:C:212:PCW:H452	0.48	2.39	1	1
3:C:212:PCW:H222	3:C:212:PCW:H421	0.48	1.85	1	1
3:D:606:PCW:C7	3:D:626:PCW:H281	0.48	2.32	14	2
3:D:605:PCW:H461	3:D:620:PCW:C48	0.48	2.38	3	1
3:D:617:PCW:H341	3:C:216:PCW:C35	0.48	2.39	16	3
3:C:204:PCW:H282	3:C:217:PCW:H421	0.48	1.85	15	2
3:A:401:PCW:H51	3:B:207:PCW:H321	0.48	1.85	4	1
3:B:204:PCW:H441	4:B:210:17F:C25	0.48	2.32	4	1
3:B:205:PCW:H31	4:B:211:17F:H4	0.48	1.84	4	2
3:A:405:PCW:H342	3:A:406:PCW:H232	0.48	1.85	5	1
3:A:408:PCW:H242	3:A:411:PCW:C25	0.48	2.39	13	4
3:C:210:PCW:H432	3:C:210:PCW:C16	0.48	2.38	5	1
3:D:605:PCW:H471	3:D:614:PCW:C16	0.48	2.38	6	1
3:D:615:PCW:C43	3:D:620:PCW:H20	0.48	2.37	6	2
2:B:126:ASP:O	2:B:129:GLN:HG2	0.48	2.08	6	2
3:D:605:PCW:C23	3:D:614:PCW:H382	0.48	2.35	7	1
3:D:624:PCW:O1P	3:D:624:PCW:H51	0.48	2.08	14	2
1:A:264:LYS:NZ	1:D:513:ALA:HB2	0.48	2.23	9	1
3:B:208:PCW:C36	3:C:203:PCW:H172	0.48	2.36	11	2
3:A:421:PCW:O3	4:D:630:17F:H8A	0.48	2.08	11	1
3:B:203:PCW:C22	4:B:209:17F:H18	0.48	2.38	12	1
1:D:475:GLU:O	1:D:478:ARG:HB2	0.48	2.09	13	1
4:A:422:17F:H63	3:D:622:PCW:C47	0.48	2.38	16	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
3:C:211:PCW:H261	4:C:215:17F:C40	0.48	2.37	17	1
3:A:406:PCW:C45	4:B:211:17F:H30	0.48	2.38	19	1
4:A:422:17F:H12	3:D:622:PCW:C48	0.48	2.32	19	1
3:C:206:PCW:H242	3:C:208:PCW:C41	0.48	2.22	19	1
3:D:611:PCW:C11	3:D:611:PCW:C31	0.48	2.92	1	1
3:A:411:PCW:C17	3:A:411:PCW:C21	0.48	2.75	2	1
3:A:418:PCW:H431	3:D:613:PCW:H212	0.48	1.85	4	2
3:D:604:PCW:O31	3:D:606:PCW:C8	0.48	2.62	19	6
3:C:203:PCW:H82	3:C:211:PCW:O2P	0.48	2.09	4	1
3:C:203:PCW:C7	3:C:212:PCW:H321	0.48	2.38	4	1
3:D:614:PCW:C16	3:D:620:PCW:H412	0.48	2.38	5	1
3:D:616:PCW:H483	3:C:206:PCW:H122	0.48	1.85	5	1
4:B:211:17F:H50	3:C:204:PCW:H483	0.48	1.85	5	1
3:D:612:PCW:O2P	3:D:620:PCW:C5	0.48	2.61	6	2
3:B:203:PCW:C6	3:C:211:PCW:O2P	0.48	2.62	6	1
3:C:206:PCW:C8	3:C:212:PCW:C32	0.48	2.81	8	1
3:C:211:PCW:H261	4:C:215:17F:H78	0.48	1.86	8	1
4:C:215:17F:N1	4:C:215:17F:C4	0.48	2.76	8	1
4:C:215:17F:H2	4:C:215:17F:H4	0.48	1.85	8	1
3:B:203:PCW:H422	4:C:215:17F:H43	0.48	1.84	9	1
3:A:401:PCW:H442	3:D:615:PCW:H242	0.48	1.84	10	1
3:A:420:PCW:H441	3:D:617:PCW:C23	0.48	2.34	10	1
3:A:410:PCW:O4P	3:A:410:PCW:C7	0.48	2.61	12	1
4:C:215:17F:H18	4:C:215:17F:O1	0.48	2.09	14	1
3:B:206:PCW:H441	3:C:205:PCW:H282	0.48	1.84	15	1
3:A:419:PCW:C32	3:D:625:PCW:H342	0.48	2.36	16	1
3:A:406:PCW:H372	4:B:211:17F:H8A	0.48	1.84	17	1
3:D:623:PCW:H281	3:D:624:PCW:C45	0.48	2.39	17	1
3:B:206:PCW:H31	3:B:206:PCW:H51	0.48	1.84	17	1
4:B:210:17F:H68	3:C:209:PCW:C40	0.48	2.38	17	1
4:B:210:17F:C1X	4:C:215:17F:C21	0.48	2.92	19	1
1:A:255:GLN:HB2	1:A:256:PRO:CD	0.48	2.39	1	14
3:A:409:PCW:H352	4:B:210:17F:H62	0.48	1.86	7	2
3:A:411:PCW:H41	3:A:411:PCW:C32	0.48	2.37	1	1
3:A:402:PCW:O11	3:A:402:PCW:O2	0.48	2.31	7	4
3:C:204:PCW:C17	3:C:216:PCW:H281	0.48	2.38	2	1
3:B:206:PCW:H261	4:C:214:17F:C18	0.48	2.38	3	1
4:C:218:17F:C24	4:C:219:17F:H70	0.48	2.38	3	1
3:A:404:PCW:O31	3:A:404:PCW:H362	0.48	2.09	5	1
3:D:622:PCW:O31	3:D:622:PCW:C1	0.48	2.58	5	2
3:B:205:PCW:H131	3:C:204:PCW:H42	0.48	1.86	5	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
3:A:409:PCW:H172	3:B:207:PCW:H271	0.48	1.85	6	1
3:D:611:PCW:O11	3:D:611:PCW:O2	0.48	2.31	12	4
3:A:405:PCW:H322	3:A:406:PCW:H182	0.48	1.85	16	3
3:D:602:PCW:C46	4:D:628:17F:C36	0.48	2.88	7	1
3:A:413:PCW:C44	3:C:210:PCW:H232	0.48	2.39	8	1
3:B:203:PCW:C6	3:C:211:PCW:O31	0.48	2.62	8	3
4:B:211:17F:H65	4:B:211:17F:H59	0.48	1.86	17	2
4:C:215:17F:H20A	4:C:215:17F:O10	0.48	2.08	17	2
3:A:404:PCW:H20	3:D:611:PCW:C26	0.48	2.38	10	1
3:B:207:PCW:H61	4:B:210:17F:C8	0.48	2.37	10	1
3:C:209:PCW:H271	3:C:209:PCW:H431	0.48	1.84	11	1
3:A:406:PCW:C32	3:B:205:PCW:H342	0.48	2.37	14	2
1:D:554:HIS:O	1:D:558:LEU:HG	0.48	2.08	14	1
3:C:210:PCW:H121	3:C:210:PCW:H341	0.48	1.86	14	1
3:A:414:PCW:H121	4:A:415:17F:C35	0.48	2.38	15	1
3:C:205:PCW:H212	3:C:209:PCW:H271	0.48	1.85	15	1
3:B:208:PCW:C7	3:B:208:PCW:H121	0.48	2.39	16	1
2:B:39:SER:HB2	2:B:41:ARG:NH1	0.48	2.24	17	1
3:D:620:PCW:H452	4:B:209:17F:H74	0.48	1.86	19	1
3:D:621:PCW:C28	4:D:632:17F:C21	0.48	2.91	19	1
3:D:627:PCW:H221	3:D:627:PCW:C18	0.48	2.39	1	2
3:C:203:PCW:O2	3:C:207:PCW:H382	0.48	2.09	17	3
3:D:601:PCW:O31	3:D:601:PCW:O3P	0.48	2.31	5	5
3:D:617:PCW:C48	3:C:210:PCW:H283	0.48	2.34	2	1
2:B:2:THR:HB	2:B:4:TYR:CE2	0.48	2.44	8	3
3:D:617:PCW:H281	3:D:619:PCW:H282	0.48	1.85	3	1
3:B:206:PCW:H122	3:C:209:PCW:C37	0.48	2.38	3	1
1:D:546:GLU:O	1:D:550:LYS:HD2	0.48	2.09	10	3
3:D:619:PCW:H381	3:D:627:PCW:C18	0.48	2.37	5	3
3:D:605:PCW:H382	3:D:612:PCW:C3	0.48	2.38	5	1
3:B:204:PCW:H73	3:B:204:PCW:C1	0.48	2.39	17	2
3:B:208:PCW:H481	3:C:211:PCW:H152	0.48	1.85	5	1
3:D:606:PCW:H62	3:D:626:PCW:C20	0.48	2.38	6	1
3:B:208:PCW:H452	3:C:203:PCW:H152	0.48	1.85	6	1
3:A:401:PCW:C40	3:B:204:PCW:H282	0.48	2.39	7	1
3:D:608:PCW:H282	4:D:629:17F:C36	0.48	2.33	7	1
3:D:618:PCW:O3P	3:D:618:PCW:H51	0.48	2.09	7	1
3:C:204:PCW:C21	3:C:204:PCW:H172	0.48	2.39	19	2
3:A:418:PCW:C44	3:D:613:PCW:H272	0.48	2.37	8	2
1:A:327:LEU:HD23	1:A:330:ARG:HD2	0.48	1.85	9	2
1:A:362:GLU:HA	1:A:366:PRO:HD2	0.48	1.84	9	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
3:B:203:PCW:H42	4:C:215:17F:C6	0.48	2.39	9	1
4:B:210:17F:C2X	4:C:215:17F:H10A	0.48	2.39	9	1
4:C:214:17F:H36	4:C:214:17F:C24	0.48	2.30	9	1
3:A:403:PCW:H63	3:A:403:PCW:C12	0.48	2.39	13	1
3:B:206:PCW:H411	4:B:210:17F:C38	0.48	2.38	13	1
3:C:211:PCW:C13	4:C:215:17F:H58	0.48	2.36	13	1
3:D:605:PCW:H451	3:D:624:PCW:H442	0.48	1.84	14	1
4:A:415:17F:H45	3:B:205:PCW:H483	0.48	1.86	18	1
3:A:403:PCW:O4P	3:A:403:PCW:O11	0.48	2.32	19	1
3:C:209:PCW:H341	3:C:212:PCW:C26	0.48	2.38	19	1
3:A:406:PCW:H242	3:A:411:PCW:H452	0.48	1.83	20	1
3:C:206:PCW:C6	3:C:212:PCW:C32	0.48	2.91	20	1
3:C:206:PCW:O3	3:C:206:PCW:O31	0.48	2.32	10	4
3:C:203:PCW:H272	3:C:211:PCW:C47	0.48	2.34	17	3
3:A:402:PCW:H412	3:C:206:PCW:C27	0.48	2.39	4	1
3:A:414:PCW:H142	4:A:415:17F:H67	0.48	1.86	5	1
2:B:6:LEU:O	2:B:55:ILE:HA	0.48	2.09	5	5
3:C:211:PCW:H182	4:C:215:17F:C34	0.48	2.39	5	1
3:B:203:PCW:N	3:C:211:PCW:O31	0.48	2.46	12	4
3:B:208:PCW:H412	3:C:203:PCW:C23	0.48	2.39	6	1
3:C:207:PCW:C17	4:C:213:17F:H20A	0.48	2.38	7	1
3:C:205:PCW:H231	3:C:209:PCW:C28	0.48	2.39	8	1
3:B:208:PCW:H372	3:C:204:PCW:H352	0.48	1.86	9	1
3:C:204:PCW:O31	3:C:204:PCW:H12	0.48	2.08	17	3
4:A:415:17F:H47	4:A:416:17F:C39	0.48	2.31	10	1
2:C:47:ASP:HB2	2:C:164:ARG:HH12	0.48	1.68	16	2
3:A:409:PCW:H171	3:B:207:PCW:C28	0.48	2.38	12	1
3:B:206:PCW:H211	3:C:205:PCW:H171	0.48	1.85	12	1
3:C:205:PCW:H441	3:C:212:PCW:H231	0.48	1.85	13	1
3:A:403:PCW:C32	3:A:406:PCW:H51	0.48	2.21	14	1
3:A:414:PCW:H121	4:A:415:17F:C36	0.48	2.38	15	1
3:D:607:PCW:C3	3:D:626:PCW:H381	0.48	2.09	15	1
3:C:211:PCW:H461	3:C:211:PCW:H141	0.48	1.84	15	1
3:A:409:PCW:H261	3:A:409:PCW:C48	0.48	2.38	16	1
4:A:422:17F:H66	3:D:622:PCW:H421	0.48	1.84	16	1
3:C:206:PCW:H161	3:C:207:PCW:C18	0.48	2.38	16	1
3:A:410:PCW:H232	4:A:422:17F:C42	0.48	2.38	17	1
3:D:621:PCW:C7	3:D:621:PCW:H11	0.48	2.38	17	1
3:A:403:PCW:H342	3:A:404:PCW:O11	0.48	2.08	20	1
3:A:414:PCW:C36	4:B:209:17F:H11	0.48	2.32	20	1
1:A:365:LYS:CB	1:A:366:PRO:HD3	0.47	2.35	16	8

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
3:D:614:PCW:C48	3:D:620:PCW:H161	0.47	2.39	1	1
3:D:619:PCW:O1P	3:D:627:PCW:C6	0.47	2.62	5	5
3:C:205:PCW:C14	3:C:209:PCW:C34	0.47	2.88	3	1
3:A:406:PCW:C22	4:B:211:17F:H31	0.47	2.38	19	2
3:D:604:PCW:H211	3:D:604:PCW:H162	0.47	1.86	4	5
3:D:627:PCW:O31	3:D:627:PCW:H62	0.47	2.08	4	2
2:C:84:ILE:HD13	2:C:118:CYS:HA	0.47	1.86	11	5
3:A:411:PCW:C26	3:B:205:PCW:H231	0.47	2.39	6	1
3:A:414:PCW:H471	4:B:209:17F:H65	0.47	1.85	6	1
3:B:204:PCW:C44	3:C:205:PCW:H483	0.47	2.39	6	1
3:B:206:PCW:C27	3:C:205:PCW:H171	0.47	2.39	6	1
3:C:203:PCW:O11	3:C:203:PCW:C2	0.47	2.60	6	6
3:D:616:PCW:H483	3:C:207:PCW:C22	0.47	2.39	7	1
3:A:410:PCW:H122	3:C:207:PCW:C15	0.47	2.29	8	1
4:A:415:17F:O2	4:A:415:17F:C17	0.47	2.61	15	2
3:D:623:PCW:C39	3:D:623:PCW:H151	0.47	2.39	8	1
3:D:603:PCW:H142	3:D:624:PCW:H182	0.47	1.85	9	1
3:C:207:PCW:C42	4:C:213:17F:H12	0.47	2.39	9	1
3:A:401:PCW:H462	3:D:615:PCW:H222	0.47	1.85	10	1
3:A:402:PCW:O2P	3:A:410:PCW:C6	0.47	2.61	10	1
3:D:603:PCW:H252	3:D:611:PCW:C19	0.47	2.39	10	1
3:A:406:PCW:H272	4:B:211:17F:H57	0.47	1.85	13	1
4:A:415:17F:C23	4:A:415:17F:H29	0.47	2.39	13	1
4:B:210:17F:H78	3:C:209:PCW:H412	0.47	1.84	13	1
3:A:407:PCW:H122	3:A:410:PCW:C32	0.47	2.39	14	1
3:A:408:PCW:H452	3:A:412:PCW:H283	0.47	1.85	14	1
3:A:401:PCW:C45	3:D:612:PCW:H251	0.47	2.39	15	1
3:D:605:PCW:O31	3:D:614:PCW:H63	0.47	2.09	18	2
2:C:73:ARG:HG3	2:C:103:VAL:HG12	0.47	1.85	16	2
3:C:206:PCW:H41	4:C:214:17F:H12A	0.47	1.84	17	1
3:D:625:PCW:C44	3:D:626:PCW:H482	0.47	2.39	18	1
3:B:205:PCW:H232	3:C:210:PCW:C25	0.47	2.39	18	1
4:C:219:17F:H11	4:C:219:17F:C31	0.47	2.37	18	1
3:A:406:PCW:C39	3:B:205:PCW:H122	0.47	2.39	19	1
3:D:602:PCW:C35	4:C:214:17F:H67	0.47	2.38	19	1
3:D:621:PCW:H2	3:D:621:PCW:O4P	0.47	2.08	19	1
3:D:623:PCW:H262	3:B:208:PCW:C28	0.47	2.35	19	1
1:A:228:PHE:O	1:A:232:LEU:HG	0.47	2.09	20	1
4:A:416:17F:H75	4:B:209:17F:H68	0.47	1.85	20	1
4:B:211:17F:O10	4:B:211:17F:C6	0.47	2.56	20	1
3:A:408:PCW:C6	3:A:413:PCW:H32	0.47	2.39	1	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
3:B:203:PCW:H372	3:C:211:PCW:H422	0.47	1.86	1	1
2:C:17:SER:HB2	5:C:201:GSP:O1A	0.47	2.09	1	3
3:D:604:PCW:H51	3:D:604:PCW:O11	0.47	2.08	2	1
3:D:604:PCW:C19	4:C:215:17F:H53	0.47	2.39	3	1
3:C:207:PCW:H151	4:C:213:17F:C31	0.47	2.22	3	2
1:A:327:LEU:CD1	3:D:601:PCW:H20	0.47	2.39	4	1
3:A:421:PCW:H321	3:D:618:PCW:C5	0.47	2.34	4	1
2:C:68:ARG:HA	2:C:71:TYR:CE2	0.47	2.43	10	3
3:D:605:PCW:H321	3:D:612:PCW:H12	0.47	1.85	18	2
1:D:426:PHE:O	1:D:430:LEU:HG	0.47	2.09	10	6
3:D:621:PCW:H20	4:D:632:17F:H10A	0.47	1.84	6	1
3:D:627:PCW:H20	3:C:217:PCW:C37	0.47	2.40	6	1
3:D:623:PCW:H261	4:B:209:17F:H75	0.47	1.85	7	1
1:A:363:LYS:HE2	1:D:411:THR:HG23	0.47	1.86	9	2
3:A:403:PCW:H131	3:A:404:PCW:O2	0.47	2.08	13	1
3:A:418:PCW:H361	3:D:613:PCW:H152	0.47	1.83	15	1
3:A:419:PCW:O1P	3:D:615:PCW:C8	0.47	2.62	15	1
3:B:206:PCW:H131	3:C:209:PCW:H352	0.47	1.86	15	1
3:C:205:PCW:H132	3:C:209:PCW:O3	0.47	2.09	15	1
3:D:618:PCW:C1	3:D:618:PCW:O31	0.47	2.56	16	2
3:A:407:PCW:O3P	3:A:412:PCW:C1	0.47	2.60	18	1
3:C:207:PCW:C14	4:C:213:17F:H18	0.47	2.37	18	1
3:A:411:PCW:H252	3:C:210:PCW:H241	0.47	1.85	19	1
3:D:605:PCW:H462	3:D:624:PCW:H471	0.47	1.86	19	1
3:B:205:PCW:C4	3:B:205:PCW:C1	0.47	2.90	2	1
3:B:208:PCW:H362	3:C:203:PCW:C19	0.47	2.39	18	2
3:D:627:PCW:H262	3:C:210:PCW:H272	0.47	1.86	3	1
4:C:215:17F:H67	4:C:215:17F:H36	0.47	1.85	3	1
3:D:610:PCW:C31	3:D:610:PCW:O3	0.47	2.62	5	3
3:D:626:PCW:O3	3:D:626:PCW:C31	0.47	2.62	10	5
2:B:7:VAL:HG11	2:B:71:TYR:CD2	0.47	2.44	13	2
3:C:206:PCW:H32	3:C:207:PCW:H261	0.47	1.86	6	1
3:A:408:PCW:O2P	3:A:408:PCW:H63	0.47	2.09	7	1
3:C:212:PCW:H181	3:C:212:PCW:H411	0.47	1.86	11	2
3:D:603:PCW:H171	3:C:216:PCW:H132	0.47	1.84	10	1
3:D:621:PCW:H252	4:D:632:17F:H12A	0.47	1.85	13	3
3:C:207:PCW:C6	3:C:207:PCW:C32	0.47	2.92	11	1
3:A:419:PCW:C6	3:D:626:PCW:C31	0.47	2.92	18	2
1:D:471:ARG:HA	1:D:475:GLU:CG	0.47	2.38	13	2
3:C:208:PCW:H61	4:C:213:17F:C3	0.47	2.39	16	2
3:D:609:PCW:O31	3:D:616:PCW:H61	0.47	2.08	14	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
3:D:621:PCW:H461	3:C:208:PCW:C47	0.47	2.30	14	1
2:C:1:SER:N	2:C:50:THR:HB	0.47	2.23	14	1
3:C:209:PCW:H272	3:C:209:PCW:C40	0.47	2.39	15	1
2:C:46:ILE:HD13	2:C:160:VAL:HG21	0.47	1.85	19	2
3:D:613:PCW:C32	3:D:619:PCW:C13	0.47	2.88	19	1
3:C:204:PCW:C27	3:C:217:PCW:H472	0.47	2.39	1	1
3:C:206:PCW:C15	3:C:208:PCW:C16	0.47	2.92	1	3
2:B:58:THR:HG21	2:B:71:TYR:CE1	0.47	2.44	9	3
3:A:414:PCW:O3	3:A:414:PCW:C35	0.47	2.55	3	4
3:D:618:PCW:H2	3:D:618:PCW:H51	0.47	1.86	6	2
3:C:204:PCW:H242	3:C:210:PCW:H221	0.47	1.85	4	1
3:A:405:PCW:O2	3:A:405:PCW:O2P	0.47	2.33	5	1
3:A:410:PCW:H40	3:A:412:PCW:H351	0.47	1.86	5	1
4:A:416:17F:O5	3:B:204:PCW:C8	0.47	2.60	5	1
3:A:417:PCW:H39	3:A:417:PCW:H151	0.47	1.87	5	1
3:D:603:PCW:H231	3:D:603:PCW:H442	0.47	1.86	5	1
3:A:406:PCW:H252	4:B:211:17F:H60	0.47	1.84	7	1
3:C:205:PCW:C8	3:C:205:PCW:O4P	0.47	2.62	8	3
1:A:331:LEU:O	1:A:335:LEU:HG	0.47	2.10	8	1
4:A:416:17F:C42	3:D:620:PCW:H471	0.47	2.40	9	1
3:D:608:PCW:C25	4:D:629:17F:H62	0.47	2.39	9	1
3:C:217:PCW:C36	4:C:218:17F:H77	0.47	2.40	10	1
3:A:410:PCW:H222	4:A:422:17F:C41	0.47	2.34	11	1
3:A:407:PCW:O31	3:A:407:PCW:O4P	0.47	2.32	12	2
4:C:219:17F:C12	4:C:219:17F:H59	0.47	2.39	13	1
3:A:413:PCW:C46	3:C:204:PCW:H283	0.47	2.30	15	1
3:C:207:PCW:C23	3:C:207:PCW:C28	0.47	2.60	18	1
1:A:250:VAL:HG21	3:A:412:PCW:H252	0.47	1.86	19	1
2:B:32:TYR:CE1	5:B:201:GSP:S1G	0.47	3.08	19	1
3:A:403:PCW:C23	3:A:403:PCW:C18	0.47	2.87	1	1
3:D:604:PCW:C18	4:C:215:17F:H52	0.47	2.39	1	1
4:D:631:17F:O7	4:D:631:17F:C17	0.47	2.63	12	11
3:B:208:PCW:O31	3:B:208:PCW:P	0.47	2.72	1	4
3:D:610:PCW:H171	4:D:631:17F:H65	0.47	1.87	3	1
3:D:613:PCW:O11	3:D:613:PCW:C2	0.47	2.57	17	6
3:D:615:PCW:H52	3:D:625:PCW:C4	0.47	2.39	3	1
3:C:206:PCW:C4	4:C:213:17F:O1	0.47	2.62	3	1
3:D:616:PCW:H481	3:C:208:PCW:H20	0.47	1.85	4	1
3:C:206:PCW:C1	4:C:214:17F:H35	0.47	2.39	4	1
4:B:211:17F:H4A	4:B:211:17F:O10	0.47	2.08	5	1
3:A:421:PCW:P	3:D:618:PCW:C4	0.47	2.98	20	3

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
2:B:123:ARG:HD3	2:B:125:VAL:O	0.47	2.09	14	2
3:A:418:PCW:O3P	3:A:418:PCW:C31	0.47	2.62	7	3
3:D:601:PCW:H451	3:D:601:PCW:H151	0.47	1.86	7	1
3:C:207:PCW:H361	4:C:213:17F:H5	0.47	1.87	8	1
3:D:604:PCW:H212	3:C:211:PCW:C28	0.47	2.40	9	1
3:C:209:PCW:C47	3:C:209:PCW:H281	0.47	2.38	10	2
3:C:212:PCW:H351	4:C:215:17F:H20A	0.47	1.85	9	1
3:A:402:PCW:C44	3:C:206:PCW:H282	0.47	2.38	12	1
3:C:207:PCW:C12	4:C:213:17F:O10	0.47	2.62	12	1
3:A:414:PCW:H161	4:A:415:17F:H34	0.47	1.83	13	2
3:A:419:PCW:C48	3:C:212:PCW:H472	0.47	2.39	13	1
3:D:621:PCW:O1P	3:D:622:PCW:N	0.47	2.48	13	1
1:A:338:LEU:O	1:A:342:GLY:HA3	0.47	2.09	14	1
3:D:623:PCW:H39	3:D:623:PCW:H132	0.47	1.84	14	1
1:A:362:GLU:OE2	1:D:414:LYS:HE3	0.47	2.09	15	1
3:A:407:PCW:O31	3:A:407:PCW:H51	0.47	2.09	15	3
3:A:414:PCW:C12	4:A:415:17F:H62	0.47	2.38	15	1
3:C:204:PCW:H222	3:C:210:PCW:C28	0.47	2.40	16	1
3:C:206:PCW:H162	3:C:208:PCW:C33	0.47	2.38	16	1
3:A:411:PCW:C27	3:C:203:PCW:H472	0.47	2.40	17	1
4:A:422:17F:H34	3:D:622:PCW:H483	0.47	1.85	18	1
3:D:605:PCW:H322	3:D:612:PCW:C1	0.47	2.40	18	1
3:B:206:PCW:H42	3:B:206:PCW:C11	0.47	2.39	1	1
3:D:604:PCW:H2	3:D:606:PCW:C6	0.47	2.39	2	1
3:B:206:PCW:H241	3:C:205:PCW:H19	0.47	1.86	2	1
3:C:207:PCW:H142	4:C:213:17F:C18	0.47	2.38	18	2
3:A:412:PCW:H442	3:C:203:PCW:H412	0.47	1.86	4	1
3:A:417:PCW:O11	3:D:618:PCW:H332	0.47	2.10	4	1
3:D:617:PCW:C48	3:B:205:PCW:C22	0.47	2.89	14	2
3:D:624:PCW:C6	3:D:624:PCW:O31	0.47	2.62	4	1
3:C:212:PCW:C34	4:C:213:17F:O8	0.47	2.62	4	1
3:A:402:PCW:P	3:A:410:PCW:H41	0.47	2.50	13	3
3:D:605:PCW:C41	3:D:605:PCW:H372	0.47	2.39	5	2
3:D:621:PCW:O31	3:D:621:PCW:H41	0.47	2.09	9	2
4:C:213:17F:H2	4:C:213:17F:O2	0.47	2.10	5	2
3:A:401:PCW:H322	3:B:207:PCW:H371	0.47	1.85	6	1
3:A:401:PCW:H482	3:D:612:PCW:H241	0.47	1.86	6	1
3:C:207:PCW:C42	4:C:213:17F:H34	0.47	2.39	8	1
4:B:210:17F:H12	4:B:210:17F:C23	0.47	2.40	12	1
3:A:406:PCW:H161	4:B:211:17F:H18	0.47	1.86	13	1
3:C:206:PCW:H242	3:C:208:PCW:H382	0.47	1.86	14	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
3:A:405:PCW:H382	3:A:411:PCW:H40	0.47	1.86	15	1
3:A:404:PCW:C16	3:A:404:PCW:C42	0.47	2.76	16	1
3:B:206:PCW:H211	3:C:205:PCW:H151	0.47	1.86	18	1
3:C:206:PCW:H242	3:C:208:PCW:C43	0.47	2.23	18	1
3:A:402:PCW:H381	3:C:208:PCW:C3	0.47	2.36	19	1
3:B:205:PCW:H221	3:C:204:PCW:H362	0.47	1.86	19	1
3:B:208:PCW:H142	3:C:203:PCW:H261	0.47	1.87	19	1
3:A:404:PCW:H52	3:B:205:PCW:H39	0.47	1.86	1	1
1:D:510:HIS:O	1:D:514:LEU:HG	0.47	2.09	19	9
3:D:606:PCW:C32	3:D:608:PCW:C8	0.47	2.89	1	1
3:A:401:PCW:C47	3:D:612:PCW:H241	0.47	2.37	2	1
3:A:407:PCW:H82	3:A:410:PCW:H371	0.47	1.86	2	1
4:A:416:17F:C32	3:B:204:PCW:H222	0.47	2.39	2	1
3:A:418:PCW:H39	3:D:613:PCW:C45	0.47	2.40	18	2
3:C:204:PCW:O31	3:C:204:PCW:C1	0.47	2.53	2	3
4:C:214:17F:H2	4:C:214:17F:O1	0.47	2.09	2	1
3:D:604:PCW:H283	4:C:213:17F:H50	0.47	1.84	3	1
3:D:605:PCW:H362	3:D:624:PCW:H362	0.47	1.85	3	1
2:B:13:GLY:HA2	5:B:201:GSP:C5'	0.47	2.40	4	4
3:C:203:PCW:C4	3:C:211:PCW:O1P	0.47	2.61	10	3
2:B:68:ARG:HB3	2:B:99:GLN:HE22	0.47	1.70	10	2
3:C:206:PCW:H12	4:C:214:17F:H35	0.47	1.85	4	1
3:A:404:PCW:H431	4:A:415:17F:H44	0.47	1.86	5	1
3:D:616:PCW:C22	3:C:208:PCW:H251	0.47	2.40	14	2
3:B:203:PCW:C45	4:C:215:17F:H42	0.47	2.40	5	1
3:B:205:PCW:O31	3:B:208:PCW:H82	0.47	2.08	5	2
3:B:206:PCW:O4P	3:B:206:PCW:C3	0.47	2.56	20	2
3:B:208:PCW:C32	3:C:211:PCW:H12	0.47	2.40	5	1
3:C:206:PCW:H20	3:C:208:PCW:H431	0.47	1.86	5	1
3:C:212:PCW:H452	3:C:212:PCW:H212	0.47	1.87	10	2
3:A:414:PCW:H321	4:A:415:17F:C19	0.47	2.33	6	1
3:A:414:PCW:H431	4:B:209:17F:H12A	0.47	1.86	6	2
3:B:204:PCW:H422	4:B:210:17F:H44	0.47	1.87	6	1
4:B:210:17F:H40	4:C:215:17F:C1X	0.47	2.39	6	1
3:C:207:PCW:H211	4:C:213:17F:H19	0.47	1.86	6	1
3:D:604:PCW:O1P	3:D:604:PCW:H32	0.47	2.10	16	2
3:D:621:PCW:C46	3:C:208:PCW:H481	0.47	2.39	7	1
3:A:401:PCW:H471	3:D:612:PCW:H251	0.47	1.85	8	1
3:B:204:PCW:H442	3:C:205:PCW:H483	0.47	1.86	8	1
3:B:205:PCW:H11	3:B:208:PCW:C6	0.47	2.39	8	1
3:C:206:PCW:C16	3:C:208:PCW:H342	0.47	2.30	17	2

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
3:C:212:PCW:C35	4:C:213:17F:H9	0.47	2.39	8	1
3:A:402:PCW:H431	3:C:206:PCW:C25	0.47	2.29	9	1
3:A:414:PCW:H351	3:A:414:PCW:O2	0.47	2.09	9	1
4:A:415:17F:H50	3:B:208:PCW:H20	0.47	1.86	9	1
3:A:403:PCW:O11	3:A:403:PCW:H52	0.47	2.10	10	1
3:A:421:PCW:H162	4:D:630:17F:H60	0.47	1.86	10	1
3:B:205:PCW:H232	3:C:204:PCW:H231	0.47	1.86	10	1
3:C:207:PCW:H412	4:C:213:17F:C1X	0.47	2.39	10	1
3:A:409:PCW:O31	3:B:206:PCW:H41	0.47	2.09	12	1
3:D:616:PCW:H231	3:C:208:PCW:H272	0.47	1.87	12	1
2:C:41:ARG:HD2	2:C:54:ASP:OD1	0.47	2.08	12	1
3:A:403:PCW:H51	3:A:404:PCW:O2P	0.47	2.10	13	1
3:A:411:PCW:H11	3:B:205:PCW:C13	0.47	2.39	13	1
3:D:614:PCW:C27	4:B:209:17F:H50	0.47	2.40	13	1
3:C:205:PCW:H11	4:C:214:17F:C8	0.47	2.40	13	2
1:A:315:ALA:O	1:A:319:HIS:HB2	0.47	2.10	14	1
3:D:608:PCW:H121	3:D:609:PCW:H171	0.47	1.86	14	1
3:C:207:PCW:C35	4:C:213:17F:H59	0.47	2.39	14	1
3:C:216:PCW:C14	3:C:216:PCW:H372	0.47	2.39	14	1
3:D:625:PCW:H382	3:D:626:PCW:H371	0.47	1.87	15	1
3:C:203:PCW:H242	3:C:204:PCW:H352	0.47	1.87	15	1
3:C:206:PCW:O2P	4:C:213:17F:N1	0.47	2.47	15	1
3:A:406:PCW:H272	4:B:211:17F:C34	0.47	2.39	16	1
3:D:616:PCW:H281	3:C:206:PCW:H472	0.47	1.87	16	1
3:A:403:PCW:C48	3:A:404:PCW:H281	0.47	2.39	17	1
3:B:207:PCW:O31	3:B:207:PCW:H131	0.47	2.10	17	1
3:D:604:PCW:H361	4:C:218:17F:C2X	0.47	2.40	18	1
3:C:211:PCW:H132	4:C:215:17F:H61	0.47	1.85	18	1
3:A:409:PCW:C33	3:B:206:PCW:H352	0.47	2.38	19	1
3:D:614:PCW:H20	4:B:209:17F:H51	0.47	1.86	19	1
4:B:211:17F:C30	3:C:216:PCW:H232	0.47	2.39	19	1
1:A:292:HIS:O	1:A:296:GLU:HG2	0.47	2.10	20	1
3:A:410:PCW:H222	4:A:422:17F:H76	0.47	1.86	20	1
3:B:204:PCW:H482	3:C:205:PCW:H471	0.47	1.86	20	1
3:C:207:PCW:C27	4:C:214:17F:H43	0.47	2.40	20	1
1:A:348:GLU:OE2	1:D:429:ASN:HB2	0.47	2.10	1	1
3:D:602:PCW:C5	4:C:214:17F:O10	0.47	2.49	1	1
3:D:604:PCW:O1P	3:D:623:PCW:C7	0.47	2.63	13	3
3:A:411:PCW:H132	3:B:205:PCW:C28	0.47	2.40	2	1
4:A:415:17F:H50	4:B:209:17F:H62	0.47	1.87	2	1
3:D:603:PCW:H472	3:D:603:PCW:H231	0.47	1.87	2	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
3:C:205:PCW:H11	4:C:214:17F:C10	0.47	2.35	2	1
3:C:206:PCW:C35	3:C:208:PCW:H121	0.47	2.40	2	1
3:A:406:PCW:H20	4:B:211:17F:C1Y	0.47	2.38	3	2
3:D:612:PCW:H32	3:D:620:PCW:H63	0.47	1.86	3	1
2:C:17:SER:N	5:C:201:GSP:O1A	0.47	2.48	3	2
3:C:211:PCW:H221	3:C:211:PCW:H181	0.47	1.86	3	2
3:A:408:PCW:C16	3:A:413:PCW:H261	0.47	2.39	4	1
3:A:409:PCW:O31	3:A:409:PCW:H11	0.47	2.09	4	2
1:D:502:GLU:O	1:D:506:ARG:HG3	0.47	2.09	9	8
1:A:251:LYS:O	1:A:254:VAL:HG12	0.47	2.09	5	3
3:D:614:PCW:H282	4:B:209:17F:C2X	0.47	2.31	5	1
4:C:215:17F:H72	4:C:215:17F:H44	0.47	1.85	5	1
3:D:604:PCW:C21	3:D:604:PCW:C16	0.47	2.92	6	1
3:B:208:PCW:H482	3:C:216:PCW:H20	0.47	1.85	6	2
3:A:401:PCW:C31	3:B:207:PCW:H232	0.47	2.40	7	1
3:B:208:PCW:H462	4:C:218:17F:H54	0.47	1.85	16	3
3:D:604:PCW:C4	3:D:604:PCW:O11	0.47	2.63	8	1
3:C:203:PCW:C14	4:C:213:17F:C21	0.47	2.90	9	1
3:C:206:PCW:H152	3:C:208:PCW:C16	0.47	2.38	13	2
3:A:421:PCW:O11	3:A:421:PCW:H62	0.47	2.09	10	1
3:D:624:PCW:H261	3:C:217:PCW:H251	0.47	1.85	10	1
3:C:211:PCW:C13	4:C:215:17F:H56	0.47	2.40	20	3
1:D:440:GLU:O	1:D:444:ASP:HB2	0.47	2.10	14	3
4:A:415:17F:C36	4:B:209:17F:H29	0.47	2.40	12	1
4:A:422:17F:H9	4:A:422:17F:H19A	0.47	1.85	12	1
3:D:614:PCW:C43	3:D:620:PCW:C39	0.47	2.90	12	1
3:B:205:PCW:H42	3:C:204:PCW:H73	0.47	1.86	12	1
3:A:419:PCW:O2P	3:A:419:PCW:C2	0.47	2.56	13	1
3:A:401:PCW:H411	3:B:204:PCW:H261	0.47	1.86	14	1
4:A:422:17F:H73	3:D:622:PCW:H441	0.47	1.87	15	1
3:D:624:PCW:C22	3:C:217:PCW:H232	0.47	2.35	16	1
4:C:218:17F:H64	4:C:219:17F:C35	0.47	2.39	16	1
3:A:403:PCW:H322	3:A:404:PCW:O3P	0.47	2.10	17	1
3:A:406:PCW:H451	4:B:211:17F:H11A	0.47	1.87	19	1
3:A:402:PCW:H411	3:C:208:PCW:C38	0.47	2.38	1	1
3:A:404:PCW:C35	3:A:404:PCW:C31	0.47	2.90	11	2
3:A:412:PCW:H412	3:C:210:PCW:H412	0.47	1.86	1	1
3:A:413:PCW:H332	3:C:210:PCW:H132	0.47	1.87	1	1
3:D:609:PCW:C8	3:D:609:PCW:O4P	0.47	2.62	5	18
3:B:208:PCW:H411	3:C:203:PCW:H221	0.47	1.86	1	1
2:C:97:ARG:HD3	2:C:98:GLU:OE1	0.47	2.09	2	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
3:D:606:PCW:H451	4:D:632:17F:H31	0.47	1.86	4	1
3:D:612:PCW:H241	3:D:612:PCW:C45	0.47	2.39	4	1
3:B:203:PCW:H461	4:C:215:17F:H50	0.47	1.87	17	2
2:C:60:GLY:HA3	5:C:201:GSP:S1G	0.47	2.50	4	1
3:A:419:PCW:H412	3:D:625:PCW:H271	0.47	1.85	6	1
3:D:603:PCW:C21	3:D:603:PCW:C17	0.47	2.86	13	2
4:D:628:17F:O8	4:D:628:17F:C5	0.47	2.53	7	1
2:C:46:ILE:HD11	2:C:53:LEU:HD11	0.47	1.87	7	1
3:A:411:PCW:H252	3:A:413:PCW:H39	0.47	1.86	17	2
3:D:621:PCW:O31	3:D:621:PCW:H342	0.47	2.10	18	2
4:C:213:17F:H29	4:C:215:17F:H57	0.47	1.82	9	1
3:A:420:PCW:P	3:A:420:PCW:C3	0.47	3.03	10	1
3:B:205:PCW:H212	3:C:203:PCW:H481	0.47	1.85	10	1
3:A:413:PCW:H321	3:A:413:PCW:C7	0.47	2.39	11	1
3:D:605:PCW:C48	3:D:620:PCW:H432	0.47	2.39	12	1
3:C:205:PCW:H32	3:C:209:PCW:H131	0.47	1.87	12	1
4:C:219:17F:H65	4:C:219:17F:H12A	0.47	1.86	13	1
3:A:402:PCW:C44	3:C:206:PCW:H251	0.47	2.40	14	1
3:A:419:PCW:H482	3:D:604:PCW:H272	0.47	1.86	14	1
3:C:210:PCW:H352	3:C:210:PCW:C12	0.47	2.40	14	1
3:C:205:PCW:H212	3:C:209:PCW:C26	0.47	2.40	15	1
3:C:216:PCW:H471	3:C:217:PCW:H381	0.47	1.85	15	1
3:D:612:PCW:O1P	3:D:614:PCW:C7	0.47	2.62	19	1
3:D:603:PCW:C14	3:D:624:PCW:H182	0.47	2.40	9	2
3:D:615:PCW:C4	3:D:625:PCW:C4	0.47	2.81	1	1
3:C:204:PCW:H32	3:C:204:PCW:P	0.47	2.50	13	6
1:A:245:LYS:O	1:A:249:GLU:HB2	0.47	2.10	2	2
3:A:401:PCW:H221	3:A:401:PCW:H181	0.47	1.87	2	1
4:A:415:17F:H39	4:A:415:17F:C1X	0.47	2.39	2	1
3:C:203:PCW:C24	3:C:204:PCW:H361	0.47	2.41	2	1
3:C:216:PCW:C8	3:C:216:PCW:O4P	0.47	2.62	3	13
4:D:628:17F:O10	4:D:628:17F:O7	0.47	2.33	13	7
4:A:416:17F:H32	3:B:204:PCW:H162	0.47	1.87	4	1
3:D:627:PCW:O31	3:D:627:PCW:O3	0.47	2.33	16	3
3:A:412:PCW:H462	3:C:210:PCW:H483	0.47	1.86	5	1
3:D:603:PCW:C16	3:D:624:PCW:C21	0.47	2.93	5	1
3:D:616:PCW:H282	4:D:632:17F:C26	0.47	2.40	5	1
3:C:203:PCW:H361	3:C:204:PCW:C11	0.47	2.40	5	1
3:A:401:PCW:H322	3:B:207:PCW:C37	0.47	2.40	6	1
3:A:401:PCW:C48	3:D:615:PCW:H242	0.47	2.39	6	1
1:D:544:LEU:O	1:D:548:HIS:HB2	0.47	2.10	6	2

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
3:D:617:PCW:H342	3:C:216:PCW:H362	0.47	1.87	10	2
3:A:419:PCW:H381	3:D:625:PCW:C24	0.47	2.39	8	1
3:C:203:PCW:C24	3:C:204:PCW:H372	0.47	2.39	8	1
1:A:224:VAL:HG22	1:D:550:LYS:HD3	0.47	1.86	18	3
3:A:414:PCW:O4P	3:A:414:PCW:H82	0.47	2.09	9	1
1:D:433:GLU:O	1:D:437:LEU:HG	0.47	2.10	9	3
3:A:407:PCW:C31	3:A:410:PCW:H352	0.47	2.39	11	1
3:A:409:PCW:H461	3:A:419:PCW:H272	0.47	1.86	11	2
3:D:614:PCW:H32	3:D:620:PCW:C3	0.47	2.39	19	2
3:D:625:PCW:O11	3:D:625:PCW:H51	0.47	2.10	11	2
1:A:359:THR:HG22	1:D:414:LYS:HD2	0.47	1.87	12	1
3:D:623:PCW:H232	3:B:203:PCW:H472	0.47	1.85	12	1
3:A:402:PCW:H412	3:A:407:PCW:H152	0.47	1.85	14	1
3:C:207:PCW:C37	4:C:213:17F:H34	0.47	2.35	14	1
3:A:405:PCW:H283	3:A:418:PCW:H482	0.47	1.87	15	1
3:C:206:PCW:H52	4:C:214:17F:H9	0.47	1.85	16	1
3:C:217:PCW:C18	4:C:219:17F:H29	0.47	2.40	16	1
3:D:609:PCW:C26	3:D:616:PCW:H411	0.47	2.40	20	1
3:D:603:PCW:H242	3:D:611:PCW:H351	0.46	1.83	18	2
3:D:620:PCW:O4P	3:D:620:PCW:C8	0.46	2.64	5	18
3:A:404:PCW:C14	3:B:205:PCW:H451	0.46	2.38	2	2
4:A:416:17F:O9	4:A:416:17F:O8	0.46	2.33	7	4
3:C:205:PCW:C25	3:C:209:PCW:H283	0.46	2.35	2	1
3:C:205:PCW:C17	3:C:209:PCW:H361	0.46	2.39	2	1
4:C:218:17F:H9A	4:C:218:17F:C18	0.46	2.40	2	1
3:D:617:PCW:H471	3:C:204:PCW:H472	0.46	1.86	3	1
3:D:623:PCW:C11	3:D:624:PCW:H332	0.46	2.40	4	1
3:B:205:PCW:H132	3:C:204:PCW:H42	0.46	1.81	5	1
3:A:411:PCW:P	4:B:211:17F:O3	0.46	2.73	7	1
3:A:412:PCW:H422	3:C:210:PCW:H182	0.46	1.87	7	1
3:C:205:PCW:C1	3:C:209:PCW:H152	0.46	2.29	7	1
4:C:215:17F:C42	4:C:215:17F:H52	0.46	2.39	12	1
4:B:210:17F:H43	4:C:215:17F:C21	0.46	2.40	13	1
4:A:416:17F:H74	4:B:209:17F:H70	0.46	1.87	15	1
4:A:422:17F:O10	4:A:422:17F:O1	0.46	2.31	16	1
2:B:131:GLN:HG3	2:B:141:PHE:CD2	0.46	2.44	17	1
3:C:203:PCW:H73	3:C:212:PCW:H11	0.46	1.86	17	1
3:A:401:PCW:H483	3:D:615:PCW:H481	0.46	1.86	18	1
3:A:418:PCW:H442	3:D:613:PCW:C27	0.46	2.40	18	1
4:B:210:17F:H72	3:C:209:PCW:H441	0.46	1.86	20	1
3:A:402:PCW:C44	3:C:206:PCW:H231	0.46	2.41	9	2

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
3:D:619:PCW:H362	4:D:631:17F:C21	0.46	2.39	1	1
2:C:120:LEU:HD11	5:C:201:GSP:N2	0.46	2.25	1	3
3:C:206:PCW:H241	3:C:208:PCW:C42	0.46	2.41	1	1
3:D:622:PCW:H182	4:D:631:17F:H20	0.46	1.87	9	2
4:B:210:17F:C38	3:C:209:PCW:H441	0.46	2.40	3	1
4:C:213:17F:C22	4:C:218:17F:H55	0.46	2.40	4	2
3:A:401:PCW:C24	3:D:615:PCW:H281	0.46	2.41	5	1
3:A:408:PCW:H232	3:A:408:PCW:C18	0.46	2.40	8	2
3:A:418:PCW:O3	3:A:418:PCW:O31	0.46	2.33	5	3
2:B:32:TYR:CD1	5:B:201:GSP:H3'	0.46	2.46	5	1
2:B:116:ASN:HA	2:B:144:THR:O	0.46	2.11	5	1
3:B:206:PCW:C25	3:C:205:PCW:H19	0.46	2.35	8	2
3:B:208:PCW:H471	3:C:203:PCW:C17	0.46	2.40	6	1
3:A:407:PCW:O31	3:A:410:PCW:H351	0.46	2.10	16	2
3:D:608:PCW:H472	4:D:628:17F:C33	0.46	2.39	7	1
3:D:605:PCW:C48	3:D:620:PCW:H441	0.46	2.40	8	1
4:B:210:17F:H4	4:B:210:17F:C2	0.46	2.40	8	1
4:B:210:17F:H11A	3:C:205:PCW:C45	0.46	2.40	8	1
3:B:208:PCW:O1P	3:C:211:PCW:C8	0.46	2.63	19	2
3:A:404:PCW:C6	3:B:205:PCW:H40	0.46	2.36	12	1
3:D:603:PCW:C6	3:C:216:PCW:O2P	0.46	2.63	15	2
1:A:310:ARG:O	1:A:314:ASP:HB2	0.46	2.11	14	2
3:A:421:PCW:H442	3:D:618:PCW:C21	0.46	2.40	14	1
3:C:206:PCW:H73	4:C:213:17F:C18	0.46	2.40	14	1
3:C:209:PCW:H121	4:C:214:17F:H4	0.46	1.86	19	1
3:B:203:PCW:H472	3:C:211:PCW:C27	0.46	2.32	20	1
3:A:406:PCW:C28	3:D:619:PCW:H262	0.46	2.39	1	1
3:A:409:PCW:C8	3:A:409:PCW:O4P	0.46	2.63	1	7
3:D:606:PCW:C17	3:D:606:PCW:C21	0.46	2.78	4	10
3:D:609:PCW:H172	3:D:616:PCW:H331	0.46	1.85	1	2
3:D:624:PCW:C7	3:D:624:PCW:H321	0.46	2.41	1	2
3:B:206:PCW:C43	3:C:209:PCW:H39	0.46	2.41	1	1
3:A:413:PCW:O31	3:A:413:PCW:O3	0.46	2.33	16	3
3:A:418:PCW:C39	3:D:613:PCW:H432	0.46	2.39	3	2
3:B:208:PCW:O11	3:B:208:PCW:C2	0.46	2.57	15	5
3:A:401:PCW:H51	3:B:204:PCW:O2P	0.46	2.11	5	1
3:C:210:PCW:O11	3:C:210:PCW:O2	0.46	2.34	5	1
3:D:616:PCW:O2	3:D:616:PCW:C11	0.46	2.63	6	1
3:D:606:PCW:C33	3:D:608:PCW:H61	0.46	2.39	7	1
3:C:203:PCW:H472	3:C:210:PCW:H282	0.46	1.86	7	1
3:A:408:PCW:O11	3:A:411:PCW:H142	0.46	2.09	9	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
3:B:203:PCW:H42	4:C:215:17F:H6A	0.46	1.87	9	1
4:B:211:17F:H69	4:B:211:17F:C11	0.46	2.36	9	2
3:D:619:PCW:H362	4:D:631:17F:H40	0.46	1.87	11	1
3:D:605:PCW:O1P	3:D:605:PCW:O31	0.46	2.32	20	2
3:A:406:PCW:C35	4:B:211:17F:C8	0.46	2.90	14	1
3:A:414:PCW:C22	3:A:414:PCW:C18	0.46	2.86	15	1
3:D:604:PCW:H272	4:C:215:17F:H77	0.46	1.87	15	1
3:A:420:PCW:O2	3:A:420:PCW:H342	0.46	2.11	18	2
3:B:206:PCW:O11	3:B:206:PCW:C5	0.46	2.64	16	1
3:D:617:PCW:C46	3:D:627:PCW:H251	0.46	2.39	17	1
3:A:418:PCW:C33	3:D:613:PCW:C13	0.46	2.93	18	1
3:A:419:PCW:C43	3:D:625:PCW:H442	0.46	2.38	19	1
3:D:608:PCW:H262	4:D:629:17F:H36	0.46	1.83	19	1
3:D:625:PCW:O31	3:D:625:PCW:C11	0.46	2.63	20	1
2:B:126:ASP:OD1	2:B:128:LYS:HG2	0.46	2.11	1	1
3:C:206:PCW:C19	3:C:208:PCW:H19	0.46	2.38	1	1
3:C:210:PCW:H181	3:C:210:PCW:C46	0.46	2.33	1	1
2:B:64:TYR:O	2:B:68:ARG:HB2	0.46	2.10	7	3
4:B:210:17F:H41	4:B:210:17F:C2X	0.46	2.40	4	1
3:C:204:PCW:C48	3:C:216:PCW:C23	0.46	2.90	6	1
3:D:606:PCW:H42	3:D:626:PCW:H19	0.46	1.87	7	1
3:A:403:PCW:C48	3:A:404:PCW:H211	0.46	2.40	11	1
3:D:609:PCW:H452	3:C:208:PCW:C19	0.46	2.41	14	1
3:D:616:PCW:H342	3:C:208:PCW:C28	0.46	2.41	14	1
3:C:207:PCW:H122	4:C:213:17F:C20	0.46	2.38	14	1
3:D:617:PCW:C36	3:C:216:PCW:H382	0.46	2.40	15	1
3:C:209:PCW:C28	3:C:209:PCW:C40	0.46	2.94	15	1
3:D:603:PCW:H161	3:D:624:PCW:C21	0.46	2.40	17	1
3:D:614:PCW:H481	3:D:620:PCW:H211	0.46	1.87	17	1
3:B:208:PCW:H52	3:B:208:PCW:O31	0.46	2.08	18	1
3:C:203:PCW:C44	3:C:204:PCW:H232	0.46	2.41	18	1
3:B:205:PCW:O4P	3:B:205:PCW:C8	0.46	2.64	11	5
3:C:212:PCW:C8	3:C:212:PCW:O4P	0.46	2.64	4	7
3:A:401:PCW:H442	3:D:615:PCW:H261	0.46	1.87	2	1
3:A:410:PCW:C21	3:A:410:PCW:H171	0.46	2.40	2	1
3:D:616:PCW:C48	3:C:207:PCW:H271	0.46	2.39	2	1
3:A:406:PCW:H451	4:B:211:17F:C1Z	0.46	2.35	3	1
1:D:445:LEU:O	1:D:448:VAL:HG12	0.46	2.11	8	2
4:A:416:17F:H64	3:B:204:PCW:H272	0.46	1.86	4	1
3:D:610:PCW:O3	3:D:610:PCW:O31	0.46	2.33	5	1
3:C:209:PCW:H451	3:C:212:PCW:H172	0.46	1.86	5	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
3:C:211:PCW:C23	4:C:213:17F:H43	0.46	2.40	5	1
3:A:418:PCW:C36	3:D:613:PCW:C15	0.46	2.92	6	1
3:D:606:PCW:O4P	3:D:606:PCW:H2	0.46	2.09	6	1
3:D:612:PCW:H82	3:D:623:PCW:H321	0.46	1.87	6	1
1:A:259:ASP:O	1:A:263:LYS:HB2	0.46	2.11	8	3
3:A:404:PCW:H40	4:A:415:17F:H41	0.46	1.86	11	1
3:D:619:PCW:H442	3:D:627:PCW:C28	0.46	2.38	11	1
1:A:386:PHE:CE2	4:A:415:17F:H76	0.46	2.46	12	1
3:A:408:PCW:H63	3:A:408:PCW:O2P	0.46	2.10	13	2
3:C:209:PCW:O31	3:C:209:PCW:P	0.46	2.73	12	2
3:D:625:PCW:H412	3:D:626:PCW:C39	0.46	2.41	13	1
3:A:402:PCW:H412	3:A:407:PCW:C15	0.46	2.41	14	1
3:D:617:PCW:C42	3:D:627:PCW:H232	0.46	2.35	14	1
4:B:211:17F:O7	4:B:211:17F:C17	0.46	2.63	17	1
3:D:617:PCW:C39	3:D:619:PCW:C14	0.46	2.85	20	2
1:D:447:GLU:O	1:D:451:LYS:HB2	0.46	2.11	19	1
3:C:205:PCW:H441	4:C:215:17F:H71	0.46	1.87	19	1
4:A:416:17F:H76	4:B:209:17F:H73	0.46	1.87	20	1
3:D:609:PCW:H442	3:C:208:PCW:H231	0.46	1.86	20	1
2:C:142:ILE:HD12	2:C:155:ALA:HA	0.46	1.88	1	1
2:B:47:ASP:HA	2:C:128:LYS:HB3	0.46	1.88	9	3
2:C:92:ASP:HA	2:C:95:HIS:HD2	0.46	1.70	18	3
1:A:297:LYS:O	1:A:301:LEU:HB2	0.46	2.10	11	7
3:A:406:PCW:H352	3:B:205:PCW:C3	0.46	2.40	5	1
3:B:208:PCW:H481	3:C:211:PCW:C15	0.46	2.40	5	1
4:A:416:17F:O9	4:A:416:17F:C7	0.46	2.63	7	1
3:C:208:PCW:C8	4:C:213:17F:O5	0.46	2.64	9	1
3:B:208:PCW:H2	3:B:208:PCW:O4P	0.46	2.10	10	1
3:D:621:PCW:P	3:D:622:PCW:H52	0.46	2.47	11	1
3:B:207:PCW:H51	3:B:207:PCW:O11	0.46	2.11	13	1
4:B:211:17F:H56	4:B:211:17F:C35	0.46	2.16	13	1
3:C:207:PCW:C43	4:C:213:17F:H32	0.46	2.41	13	1
3:A:408:PCW:C45	3:A:412:PCW:H283	0.46	2.41	14	1
4:C:215:17F:O1	4:C:215:17F:C18	0.46	2.64	14	1
3:B:204:PCW:H31	3:B:207:PCW:H322	0.46	1.87	17	1
3:C:212:PCW:C44	4:C:215:17F:H78	0.46	2.40	19	1
3:A:409:PCW:O31	3:A:409:PCW:H342	0.46	2.10	20	1
3:A:404:PCW:H62	3:A:404:PCW:C36	0.46	2.41	1	1
3:C:205:PCW:O4P	3:C:205:PCW:C8	0.46	2.64	3	8
3:C:206:PCW:H42	4:C:213:17F:O1	0.46	2.10	10	4
1:A:217:LEU:O	1:A:221:LEU:HG	0.46	2.11	13	5

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
3:C:203:PCW:C1	3:C:211:PCW:C6	0.46	2.92	16	3
3:A:420:PCW:H372	3:D:618:PCW:C41	0.46	2.41	3	1
3:D:616:PCW:H171	3:D:616:PCW:H212	0.46	1.86	3	1
3:A:408:PCW:C13	3:A:411:PCW:H211	0.46	2.39	4	1
3:D:617:PCW:H483	3:B:205:PCW:H242	0.46	1.87	5	1
3:B:207:PCW:H231	3:B:207:PCW:C36	0.46	2.38	5	1
3:A:403:PCW:O31	3:A:403:PCW:C35	0.46	2.63	13	4
3:D:603:PCW:C44	3:D:611:PCW:H371	0.46	2.38	6	2
2:C:72:MET:HE1	2:C:100:ILE:HG13	0.46	1.86	6	1
3:C:205:PCW:H412	3:C:212:PCW:H261	0.46	1.87	7	1
3:C:211:PCW:H231	4:C:213:17F:C25	0.46	2.41	7	1
3:A:418:PCW:H341	3:D:613:PCW:H152	0.46	1.88	10	2
3:D:619:PCW:O1P	3:D:627:PCW:C5	0.46	2.62	8	1
2:C:34:PRO:HA	5:C:201:GSP:S1G	0.46	2.50	8	1
3:A:406:PCW:O3	4:B:211:17F:H71	0.46	2.10	9	1
3:A:411:PCW:H252	3:C:210:PCW:C24	0.46	2.41	19	3
3:D:603:PCW:H142	3:D:624:PCW:C18	0.46	2.40	9	1
4:B:211:17F:H19	4:B:211:17F:H8	0.46	1.88	9	1
3:A:410:PCW:H283	4:A:422:17F:H76	0.46	1.87	10	1
3:D:608:PCW:C22	4:D:628:17F:H10A	0.46	2.41	10	2
2:C:123:ARG:HD3	2:C:125:VAL:O	0.46	2.10	10	2
3:C:206:PCW:O4P	3:C:206:PCW:C7	0.46	2.63	10	1
3:D:609:PCW:H41	4:D:632:17F:O10	0.46	2.10	12	1
3:A:406:PCW:C38	3:B:205:PCW:H121	0.46	2.40	14	1
4:A:422:17F:C37	3:D:622:PCW:H421	0.46	2.40	16	1
3:A:406:PCW:H131	4:B:211:17F:H75	0.46	1.87	17	1
2:C:97:ARG:O	2:C:101:LYS:HG3	0.46	2.10	17	1
3:D:604:PCW:C38	4:C:218:17F:H40	0.46	2.40	18	1
3:D:619:PCW:H281	4:B:211:17F:C2X	0.46	2.41	18	1
3:C:216:PCW:C14	3:C:216:PCW:C37	0.46	2.91	18	1
3:A:406:PCW:H422	3:B:205:PCW:C22	0.46	2.40	19	1
3:C:212:PCW:O3	4:C:215:17F:H32	0.46	2.10	19	1
3:A:410:PCW:C22	4:A:422:17F:C42	0.46	2.86	20	1
3:A:402:PCW:H442	3:C:206:PCW:H231	0.46	1.88	1	1
3:B:204:PCW:O1P	3:B:207:PCW:H11	0.46	2.11	1	1
3:D:604:PCW:P	3:D:604:PCW:H31	0.46	2.50	2	2
3:D:605:PCW:H61	4:D:630:17F:O4	0.46	2.11	3	1
3:D:619:PCW:C37	3:D:627:PCW:H161	0.46	2.41	5	4
3:A:408:PCW:H271	4:D:631:17F:C30	0.46	2.41	4	1
2:B:146:ALA:N	5:B:201:GSP:O6	0.46	2.48	9	5
3:A:414:PCW:C45	4:B:209:17F:H36	0.46	2.40	6	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
3:D:622:PCW:H362	4:D:631:17F:H59	0.46	1.87	6	2
3:A:403:PCW:C14	3:A:403:PCW:C38	0.46	2.94	7	1
3:A:409:PCW:H372	3:B:206:PCW:C41	0.46	2.41	7	1
2:C:12:ASP:HA	5:C:201:GSP:O1B	0.46	2.10	7	1
3:A:420:PCW:C39	3:D:618:PCW:H451	0.46	2.41	9	1
3:D:619:PCW:H362	4:D:631:17F:C23	0.46	2.41	11	1
3:B:206:PCW:H422	3:C:209:PCW:C40	0.46	2.40	11	1
3:A:405:PCW:C34	3:A:411:PCW:H421	0.46	2.40	12	1
4:B:210:17F:H40	4:B:210:17F:C12	0.46	2.40	12	1
3:C:203:PCW:H351	3:C:207:PCW:C33	0.46	2.41	12	1
3:D:602:PCW:H471	4:D:629:17F:H44	0.46	1.88	13	1
3:C:206:PCW:H152	3:C:207:PCW:C22	0.46	2.41	14	1
3:A:410:PCW:C25	4:A:422:17F:H76	0.46	2.40	15	1
3:A:409:PCW:C14	3:A:419:PCW:H231	0.46	2.38	16	1
3:A:406:PCW:H271	4:B:211:17F:H57	0.46	1.88	20	2
3:D:608:PCW:C22	4:D:628:17F:H8A	0.46	2.41	17	1
3:D:615:PCW:H52	3:D:625:PCW:O31	0.46	2.11	17	1
3:C:212:PCW:H332	4:C:215:17F:H20	0.46	1.86	17	1
4:A:416:17F:H57	3:B:204:PCW:C17	0.46	2.40	18	1
3:D:623:PCW:H232	3:B:203:PCW:H483	0.46	1.87	18	1
3:C:217:PCW:C17	4:C:219:17F:H32	0.46	2.38	20	1
3:A:402:PCW:C40	3:A:407:PCW:H261	0.46	2.41	1	1
3:A:412:PCW:H381	3:C:210:PCW:H361	0.46	1.87	15	2
3:A:419:PCW:C48	3:D:604:PCW:H272	0.46	2.40	2	2
3:C:205:PCW:C16	3:C:209:PCW:H211	0.46	2.41	2	1
3:C:209:PCW:H372	3:C:209:PCW:H422	0.46	1.87	2	1
3:D:617:PCW:O3	3:D:617:PCW:C31	0.46	2.64	20	6
3:B:204:PCW:H411	3:B:207:PCW:C6	0.46	2.40	3	1
4:C:215:17F:H63	4:C:215:17F:C1X	0.46	2.35	3	1
3:A:401:PCW:H51	3:B:207:PCW:C32	0.46	2.41	4	2
1:D:550:LYS:O	1:D:554:HIS:HB2	0.46	2.10	4	1
3:C:204:PCW:H221	3:C:217:PCW:C47	0.46	2.41	4	1
4:A:416:17F:C33	3:B:203:PCW:H241	0.46	2.41	5	1
3:C:209:PCW:C45	3:C:212:PCW:H172	0.46	2.41	5	1
4:C:219:17F:O6	4:C:219:17F:H2	0.46	2.11	7	3
3:C:206:PCW:C36	3:C:208:PCW:H122	0.46	2.40	7	1
3:C:217:PCW:H461	4:C:219:17F:H55	0.46	1.86	7	1
3:D:623:PCW:C12	3:D:624:PCW:C33	0.46	2.94	8	1
3:B:203:PCW:H221	4:B:209:17F:H56	0.46	1.88	9	1
3:B:207:PCW:C17	4:B:210:17F:H19	0.46	2.41	10	1
3:D:609:PCW:C5	3:D:621:PCW:O11	0.46	2.63	11	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
3:D:621:PCW:O1P	3:D:622:PCW:H41	0.46	2.11	14	1
3:A:406:PCW:C13	4:B:211:17F:H75	0.46	2.41	15	1
3:D:614:PCW:H471	3:D:620:PCW:H422	0.46	1.86	15	1
3:C:205:PCW:C24	3:C:209:PCW:H283	0.46	2.41	15	1
3:A:413:PCW:H371	3:C:210:PCW:H141	0.46	1.87	16	1
3:A:421:PCW:H322	3:D:618:PCW:H52	0.46	1.88	16	1
3:C:205:PCW:H181	3:C:209:PCW:C26	0.46	2.39	16	1
4:A:422:17F:O9	4:A:422:17F:O8	0.46	2.33	18	1
3:D:602:PCW:H142	3:D:602:PCW:C39	0.46	2.39	18	1
3:A:409:PCW:H332	3:B:206:PCW:H352	0.46	1.87	19	1
3:D:610:PCW:C5	4:D:631:17F:O1	0.46	2.64	20	1
1:A:255:GLN:HB2	1:A:256:PRO:HD3	0.46	1.88	1	6
3:A:406:PCW:C27	3:D:619:PCW:H262	0.46	2.40	1	1
3:A:413:PCW:C45	4:D:631:17F:H52	0.46	2.41	18	3
3:D:605:PCW:H461	3:D:620:PCW:H471	0.46	1.86	1	2
3:B:204:PCW:H62	3:B:204:PCW:O4P	0.46	2.10	2	1
3:C:207:PCW:H483	3:C:207:PCW:C28	0.46	2.40	2	1
3:A:405:PCW:P	3:A:406:PCW:H171	0.46	2.51	3	1
3:D:604:PCW:C23	4:C:215:17F:H54	0.46	2.41	3	1
3:C:205:PCW:H382	3:C:205:PCW:H422	0.46	1.86	3	1
3:A:408:PCW:H121	3:A:413:PCW:H352	0.46	1.87	5	1
3:D:611:PCW:H82	3:C:216:PCW:C7	0.46	2.41	6	3
3:A:402:PCW:H441	4:D:632:17F:H53	0.46	1.87	6	1
3:C:217:PCW:H2	4:C:218:17F:C42	0.46	2.41	6	1
3:D:604:PCW:C5	4:C:219:17F:H4A	0.46	2.40	7	1
3:A:421:PCW:H122	4:D:630:17F:H11A	0.46	1.86	9	2
3:A:404:PCW:H121	3:A:404:PCW:C38	0.46	2.39	10	1
3:A:406:PCW:H39	3:B:205:PCW:C17	0.46	2.40	10	1
3:A:405:PCW:H362	3:A:411:PCW:H421	0.46	1.88	11	1
4:A:416:17F:C31	3:B:204:PCW:H211	0.46	2.39	11	2
3:D:602:PCW:H252	4:D:628:17F:H44	0.46	1.88	12	1
4:D:632:17F:H62	3:C:208:PCW:H461	0.46	1.88	12	1
3:A:417:PCW:H451	3:D:618:PCW:H251	0.46	1.86	14	1
3:D:609:PCW:H362	4:D:632:17F:H31	0.46	1.88	14	1
3:B:208:PCW:H73	3:B:208:PCW:H121	0.46	1.86	16	1
4:A:422:17F:H40	4:A:422:17F:C1X	0.46	2.39	17	1
2:C:14:VAL:HG23	2:C:16:LYS:HG3	0.46	1.89	17	1
3:D:619:PCW:O2P	3:D:627:PCW:C8	0.46	2.63	18	1
3:B:205:PCW:H221	3:C:210:PCW:H262	0.46	1.87	18	1
4:C:219:17F:C32	4:C:219:17F:C12	0.46	2.90	18	1
3:A:412:PCW:O3	3:A:412:PCW:C31	0.45	2.63	11	8

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
3:D:614:PCW:H462	3:D:620:PCW:H372	0.45	1.88	17	2
3:D:611:PCW:H483	3:B:208:PCW:H262	0.45	1.88	2	1
1:A:305:MET:SD	1:D:473:LYS:HE3	0.45	2.51	3	1
3:A:402:PCW:C39	3:A:407:PCW:H272	0.45	2.36	3	2
4:B:210:17F:H60	3:C:205:PCW:H442	0.45	1.87	3	1
3:C:206:PCW:C8	3:C:206:PCW:O4P	0.45	2.64	14	4
4:C:215:17F:H77	4:C:215:17F:H49	0.45	1.87	12	3
3:C:206:PCW:H61	4:C:213:17F:O1	0.45	2.10	4	1
3:C:211:PCW:H242	4:C:215:17F:C27	0.45	2.40	4	1
3:D:603:PCW:O3	3:D:603:PCW:C31	0.45	2.63	9	2
3:D:612:PCW:O4P	3:D:620:PCW:C6	0.45	2.63	5	1
3:D:626:PCW:O2	3:D:626:PCW:P	0.45	2.74	5	6
3:B:208:PCW:C45	4:C:213:17F:H37	0.45	2.40	5	1
1:A:386:PHE:HZ	4:A:415:17F:H75	0.45	1.71	6	1
3:D:606:PCW:H232	4:C:218:17F:H38	0.45	1.87	20	2
3:A:408:PCW:C11	3:A:413:PCW:O3	0.45	2.64	8	1
3:D:613:PCW:H471	3:D:613:PCW:C23	0.45	2.22	8	1
3:D:617:PCW:H362	3:C:216:PCW:H362	0.45	1.87	9	2
3:B:203:PCW:H431	4:C:215:17F:H42	0.45	1.87	9	1
3:A:402:PCW:H451	4:D:632:17F:H55	0.45	1.88	11	1
3:C:212:PCW:H211	3:C:212:PCW:H421	0.45	1.87	12	1
3:A:414:PCW:H121	4:A:415:17F:C1Y	0.45	2.41	14	1
3:A:404:PCW:H172	3:A:404:PCW:C44	0.45	2.40	15	1
2:C:32:TYR:HD1	5:C:201:GSP:C4'	0.45	2.24	15	1
2:B:38:ASP:HB3	2:B:57:ASP:HB3	0.45	1.88	16	1
4:C:213:17F:C17	4:C:213:17F:O7	0.45	2.64	17	2
3:D:616:PCW:H282	4:D:632:17F:H50	0.45	1.88	18	1
3:C:212:PCW:H171	3:C:212:PCW:H382	0.45	1.88	19	1
3:D:610:PCW:C7	4:D:631:17F:O1	0.45	2.65	20	1
3:A:402:PCW:H42	3:A:410:PCW:O4P	0.45	2.11	1	2
3:A:409:PCW:H131	4:B:210:17F:H31	0.45	1.88	6	2
3:D:613:PCW:O4P	3:D:613:PCW:O2	0.45	2.33	1	2
3:D:615:PCW:H62	3:D:625:PCW:O1P	0.45	2.11	2	1
3:C:212:PCW:H422	4:C:215:17F:C36	0.45	2.40	2	1
3:C:206:PCW:H51	4:C:213:17F:O1	0.45	2.11	3	1
2:C:82:PHE:HB3	2:C:93:ILE:HD11	0.45	1.88	4	1
3:A:404:PCW:C31	3:A:404:PCW:O3	0.45	2.65	10	3
3:A:412:PCW:H411	3:C:210:PCW:H382	0.45	1.87	5	1
3:D:612:PCW:H161	3:D:620:PCW:H151	0.45	1.87	5	2
3:C:207:PCW:H252	3:C:208:PCW:C19	0.45	2.31	8	1
3:C:209:PCW:C46	3:C:212:PCW:H271	0.45	2.41	9	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
4:A:415:17F:H55	3:D:624:PCW:H442	0.45	1.87	10	1
3:C:212:PCW:H441	4:C:215:17F:C22	0.45	2.41	10	1
3:A:413:PCW:H442	3:C:210:PCW:C48	0.45	2.41	11	1
3:A:413:PCW:C38	3:C:210:PCW:H161	0.45	2.42	16	2
3:D:601:PCW:H151	3:D:601:PCW:H471	0.45	1.89	17	3
2:C:40:TYR:HB2	2:C:55:ILE:HB	0.45	1.88	16	2
3:D:627:PCW:O31	3:D:627:PCW:H51	0.45	2.11	12	1
2:B:46:ILE:HD13	2:B:157:TYR:HA	0.45	1.87	15	2
3:A:410:PCW:C23	3:A:410:PCW:H181	0.45	2.42	18	1
3:A:410:PCW:H122	3:C:208:PCW:C35	0.45	2.41	18	1
3:A:413:PCW:H283	3:A:413:PCW:H411	0.45	1.87	18	1
3:A:406:PCW:O3P	3:A:406:PCW:C31	0.45	2.64	19	1
3:B:203:PCW:H39	3:C:211:PCW:H442	0.45	1.89	1	1
3:C:206:PCW:H52	4:C:214:17F:H10	0.45	1.89	1	1
3:A:417:PCW:C8	4:D:630:17F:C3	0.45	2.94	2	1
3:B:203:PCW:H182	4:B:210:17F:H37	0.45	1.87	2	1
3:B:208:PCW:O31	3:B:208:PCW:C1	0.45	2.63	3	1
3:C:203:PCW:H19	3:C:211:PCW:C3	0.45	2.34	5	1
3:D:610:PCW:H362	3:D:610:PCW:C13	0.45	2.39	6	1
3:C:212:PCW:O1P	3:C:212:PCW:O2	0.45	2.34	8	1
3:A:403:PCW:O1P	3:A:403:PCW:H32	0.45	2.11	9	1
3:C:217:PCW:C19	4:C:219:17F:C1X	0.45	2.94	9	1
1:A:334:ARG:HD2	1:D:440:GLU:OE1	0.45	2.11	13	1
3:D:603:PCW:H472	3:D:603:PCW:C23	0.45	2.38	14	1
3:D:601:PCW:H152	3:D:601:PCW:H451	0.45	1.87	15	1
3:A:418:PCW:H442	3:D:613:PCW:H271	0.45	1.87	18	1
3:D:619:PCW:C48	3:B:205:PCW:H242	0.45	2.41	18	1
3:D:610:PCW:N	4:D:631:17F:O1	0.45	2.50	20	1
3:A:413:PCW:H51	3:A:413:PCW:O3P	0.45	2.12	1	1
1:A:291:LEU:HD23	1:A:294:LEU:HD12	0.45	1.88	14	2
2:B:161:ARG:CZ	2:C:131:GLN:HB3	0.45	2.41	3	2
3:A:403:PCW:C5	3:A:404:PCW:O1P	0.45	2.65	12	2
3:C:205:PCW:C31	4:C:214:17F:N1	0.45	2.80	4	1
1:A:277:GLU:HB2	1:A:278:PRO:CD	0.45	2.41	12	2
1:A:363:LYS:HA	1:A:367:ALA:CB	0.45	2.41	18	2
3:D:611:PCW:O31	3:D:611:PCW:O3	0.45	2.33	5	2
3:D:612:PCW:H272	3:B:204:PCW:H283	0.45	1.89	5	1
3:D:616:PCW:H121	4:D:632:17F:O7	0.45	2.11	5	1
3:D:622:PCW:O31	3:D:622:PCW:H11	0.45	2.12	5	1
3:D:606:PCW:H252	4:C:218:17F:C21	0.45	2.42	6	1
3:B:208:PCW:C47	3:C:203:PCW:H232	0.45	2.40	6	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
3:B:208:PCW:H452	3:C:203:PCW:H161	0.45	1.88	6	1
3:C:216:PCW:H462	3:C:217:PCW:C36	0.45	2.24	6	1
3:D:612:PCW:H181	3:D:620:PCW:C17	0.45	2.41	7	1
3:A:403:PCW:C23	3:A:403:PCW:C27	0.45	2.93	9	1
3:D:606:PCW:C40	3:D:609:PCW:H31	0.45	2.42	9	1
3:B:205:PCW:H231	3:C:203:PCW:H472	0.45	1.88	10	1
3:D:614:PCW:H142	3:D:620:PCW:H382	0.45	1.88	11	1
3:A:421:PCW:H73	4:D:630:17F:H4	0.45	1.88	12	1
3:A:410:PCW:C22	3:D:622:PCW:H40	0.45	2.40	14	1
3:B:207:PCW:C36	3:B:207:PCW:H231	0.45	2.40	14	1
3:A:413:PCW:H431	3:C:210:PCW:H212	0.45	1.89	15	1
3:A:412:PCW:C46	3:C:210:PCW:H19	0.45	2.41	16	1
3:C:203:PCW:C37	4:C:213:17F:H75	0.45	2.41	17	1
3:C:209:PCW:H121	4:C:214:17F:H18	0.45	1.89	20	2
3:A:414:PCW:H161	4:A:415:17F:C1Z	0.45	2.41	18	1
2:B:117:LYS:NZ	5:B:201:GSP:C5	0.45	2.85	18	1
3:B:206:PCW:H232	3:C:205:PCW:H132	0.45	1.87	18	1
3:D:604:PCW:H283	4:C:213:17F:H52	0.45	1.89	19	1
3:C:207:PCW:O2P	3:C:207:PCW:C3	0.45	2.63	19	1
3:A:410:PCW:H222	4:A:422:17F:H78	0.45	1.87	1	2
3:C:206:PCW:H11	3:C:206:PCW:H41	0.45	1.88	1	1
3:B:206:PCW:H272	3:C:209:PCW:H19	0.45	1.88	3	1
3:D:607:PCW:C8	4:D:628:17F:O4	0.45	2.64	4	1
3:C:204:PCW:H231	3:C:210:PCW:C26	0.45	2.42	4	1
1:D:404:ASN:O	1:D:408:VAL:HG23	0.45	2.11	6	1
1:A:215:SER:O	1:A:219:GLU:HG3	0.45	2.11	7	3
3:A:404:PCW:H141	3:B:205:PCW:H452	0.45	1.87	8	1
3:A:409:PCW:H331	4:B:210:17F:H58	0.45	1.88	8	1
3:A:405:PCW:H231	3:A:418:PCW:H283	0.45	1.86	9	1
2:B:17:SER:N	5:B:201:GSP:O1A	0.45	2.48	9	1
3:D:622:PCW:H381	4:D:632:17F:H76	0.45	1.87	10	1
3:B:206:PCW:C24	3:C:205:PCW:H151	0.45	2.41	10	1
3:D:609:PCW:O3	3:D:609:PCW:C31	0.45	2.65	11	1
3:D:618:PCW:H62	3:D:618:PCW:C2	0.45	2.33	12	1
2:B:47:ASP:OD1	2:B:161:ARG:HD2	0.45	2.12	12	1
3:A:404:PCW:C16	3:A:404:PCW:H442	0.45	2.41	15	1
1:D:463:TRP:HE1	4:D:629:17F:H75	0.45	1.71	15	1
3:A:405:PCW:C7	4:B:211:17F:O1	0.45	2.63	17	1
3:C:203:PCW:H2	3:C:203:PCW:O11	0.45	2.11	18	1
3:A:417:PCW:C15	3:D:603:PCW:H272	0.45	2.42	11	2
3:B:208:PCW:H131	3:C:211:PCW:C47	0.45	2.41	1	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
4:C:213:17F:O7	4:C:213:17F:C17	0.45	2.65	11	7
3:D:605:PCW:H52	3:D:605:PCW:O1P	0.45	2.11	3	1
3:D:622:PCW:C41	4:D:632:17F:H75	0.45	2.27	3	1
2:B:126:ASP:OD1	2:B:128:LYS:HD3	0.45	2.10	3	1
3:B:206:PCW:H142	3:C:209:PCW:C38	0.45	2.41	3	1
3:A:409:PCW:H52	3:B:206:PCW:H321	0.45	1.88	4	1
3:C:207:PCW:H42	3:C:207:PCW:O11	0.45	2.12	4	1
3:C:207:PCW:C47	3:C:207:PCW:H262	0.45	2.42	5	1
3:A:401:PCW:H411	3:B:204:PCW:H231	0.45	1.89	6	1
3:B:203:PCW:H381	3:C:211:PCW:C46	0.45	2.41	6	1
4:A:416:17F:H53	3:D:614:PCW:H451	0.45	1.87	7	1
2:C:118:CYS:SG	2:C:143:GLU:HB3	0.45	2.51	7	2
2:C:158:THR:HA	2:C:161:ARG:HE	0.45	1.72	18	2
3:A:408:PCW:H272	3:B:205:PCW:H241	0.45	1.88	9	1
3:A:408:PCW:H232	3:A:411:PCW:C22	0.45	2.39	18	3
3:A:421:PCW:O31	3:A:421:PCW:O1P	0.45	2.35	10	1
1:D:492:LEU:O	1:D:496:LEU:HG	0.45	2.12	20	2
3:D:612:PCW:C1	3:D:620:PCW:O11	0.45	2.65	10	1
3:B:205:PCW:H232	3:C:210:PCW:C28	0.45	2.39	10	1
4:A:422:17F:C7	3:D:622:PCW:H141	0.45	2.41	11	1
3:C:209:PCW:H441	3:C:212:PCW:C27	0.45	2.39	11	1
3:C:205:PCW:C40	3:C:212:PCW:H252	0.45	2.42	12	1
3:D:607:PCW:H471	3:C:209:PCW:H462	0.45	1.88	13	1
3:D:627:PCW:H211	3:C:217:PCW:C37	0.45	2.39	14	1
3:B:204:PCW:H73	3:B:204:PCW:C2	0.45	2.40	18	2
3:A:401:PCW:H481	3:D:620:PCW:H271	0.45	1.88	18	1
3:C:203:PCW:H19	3:C:211:PCW:O11	0.45	2.12	18	1
3:C:211:PCW:C15	4:C:215:17F:C36	0.45	2.94	18	1
3:A:402:PCW:H39	3:A:407:PCW:H252	0.45	1.87	20	1
3:B:204:PCW:C39	3:B:207:PCW:H63	0.45	2.41	20	1
3:A:404:PCW:C7	4:A:415:17F:C3	0.45	2.95	1	1
3:D:603:PCW:H442	3:D:611:PCW:C36	0.45	2.40	1	3
3:D:623:PCW:C31	3:D:623:PCW:O3	0.45	2.65	1	1
3:A:413:PCW:H362	3:C:210:PCW:C13	0.45	2.42	2	1
4:A:416:17F:C32	3:B:204:PCW:H271	0.45	2.41	3	1
3:D:603:PCW:H442	3:D:611:PCW:C37	0.45	2.42	13	3
3:D:604:PCW:C19	4:C:215:17F:C30	0.45	2.95	3	1
3:D:612:PCW:H241	3:D:612:PCW:H461	0.45	1.88	4	1
3:D:621:PCW:O31	3:D:621:PCW:P	0.45	2.75	4	2
3:C:212:PCW:H411	3:C:212:PCW:H181	0.45	1.88	4	1
1:A:254:VAL:O	1:A:258:LEU:HB2	0.45	2.12	5	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
3:D:606:PCW:H131	3:D:606:PCW:C6	0.45	2.42	5	1
3:D:603:PCW:H82	3:D:603:PCW:O3	0.45	2.12	6	1
3:D:604:PCW:H41	3:D:604:PCW:C3	0.45	2.32	6	1
3:D:616:PCW:H281	4:D:632:17F:H46	0.45	1.89	6	1
3:A:406:PCW:H361	3:B:205:PCW:O2	0.45	2.11	8	2
3:C:216:PCW:H122	3:C:217:PCW:H152	0.45	1.87	8	1
3:C:208:PCW:O3	3:C:208:PCW:C31	0.45	2.64	15	3
3:A:408:PCW:C25	3:A:411:PCW:H221	0.45	2.41	10	1
2:B:14:VAL:CG2	2:B:16:LYS:HG3	0.45	2.42	10	1
3:C:206:PCW:C8	4:C:214:17F:C10	0.45	2.95	10	1
3:A:404:PCW:C14	3:B:205:PCW:H452	0.45	2.41	13	1
3:D:618:PCW:O31	3:D:618:PCW:O3	0.45	2.35	13	1
3:C:206:PCW:C7	3:C:212:PCW:P	0.45	3.04	13	1
1:A:272:TYR:O	1:A:276:VAL:HB	0.45	2.11	15	2
1:A:326:GLU:O	1:A:330:ARG:HG3	0.45	2.10	16	1
3:C:217:PCW:H181	4:C:219:17F:H29	0.45	1.89	16	1
3:A:402:PCW:H412	3:C:206:PCW:C25	0.45	2.42	17	1
3:D:621:PCW:P	3:D:622:PCW:H42	0.45	2.51	17	1
3:A:420:PCW:H31	3:D:618:PCW:H411	0.45	1.88	18	1
3:B:205:PCW:C28	4:B:211:17F:H20A	0.45	2.41	18	1
3:A:408:PCW:H231	3:A:411:PCW:H222	0.45	1.89	19	1
3:A:414:PCW:C12	4:A:415:17F:H58	0.45	2.41	2	1
3:C:206:PCW:C34	3:C:208:PCW:H121	0.45	2.42	2	1
3:D:607:PCW:H261	3:B:206:PCW:C48	0.45	2.42	3	1
3:A:409:PCW:H321	3:B:206:PCW:H41	0.45	1.89	4	1
3:C:211:PCW:H62	3:C:211:PCW:O4P	0.45	2.11	4	1
3:C:205:PCW:C6	4:C:214:17F:H2	0.45	2.37	5	1
3:A:408:PCW:C35	3:A:413:PCW:H151	0.45	2.42	6	1
3:D:602:PCW:H362	4:C:214:17F:H60	0.45	1.89	6	1
3:B:203:PCW:H11	3:C:211:PCW:H372	0.45	1.88	7	1
3:C:205:PCW:H381	3:C:212:PCW:C23	0.45	2.41	7	1
4:A:416:17F:H1A	4:A:416:17F:H4	0.45	1.89	9	2
3:B:203:PCW:H411	4:C:215:17F:H39	0.45	1.88	9	1
1:D:574:LEU:HB2	1:D:575:PRO:HD3	0.45	1.88	10	1
3:C:209:PCW:O31	3:C:209:PCW:C1	0.45	2.60	18	2
3:A:414:PCW:H442	4:A:415:17F:H64	0.45	1.88	11	1
3:A:409:PCW:H171	3:B:207:PCW:H281	0.45	1.88	12	1
3:A:410:PCW:O4P	3:A:410:PCW:H73	0.45	2.12	12	1
2:C:68:ARG:HB3	2:C:99:GLN:HE22	0.45	1.72	12	1
3:A:412:PCW:C31	3:A:412:PCW:O3	0.45	2.64	13	2
3:C:207:PCW:H341	3:C:207:PCW:H62	0.45	1.89	13	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
3:D:627:PCW:C20	3:C:217:PCW:H351	0.45	2.40	14	1
3:A:403:PCW:O11	3:A:403:PCW:C7	0.45	2.61	15	1
3:C:212:PCW:C2	4:C:215:17F:O1	0.45	2.65	15	1
3:C:203:PCW:C8	3:C:211:PCW:O1P	0.45	2.64	17	1
3:D:604:PCW:H181	4:C:215:17F:H52	0.45	1.89	1	1
3:D:624:PCW:C19	3:C:217:PCW:H232	0.45	2.42	17	2
3:B:207:PCW:H251	3:B:207:PCW:H451	0.45	1.88	1	1
2:C:33:ASP:O	5:C:201:GSP:S1G	0.45	2.75	9	4
3:D:603:PCW:H222	3:D:603:PCW:H441	0.45	1.89	3	2
3:D:612:PCW:H241	3:D:612:PCW:H452	0.45	1.87	4	1
3:D:616:PCW:C48	3:C:208:PCW:H20	0.45	2.41	4	1
3:C:203:PCW:H82	3:C:211:PCW:H41	0.45	1.88	5	1
3:A:412:PCW:H482	3:C:217:PCW:H481	0.45	1.89	6	1
1:D:469:LEU:HD22	1:D:473:LYS:HE3	0.45	1.89	6	1
4:D:632:17F:H59	4:D:632:17F:H66	0.45	1.86	6	1
3:C:205:PCW:H472	4:C:215:17F:C12	0.45	2.41	6	1
3:C:211:PCW:H261	4:C:215:17F:C42	0.45	2.42	8	1
3:C:216:PCW:C12	3:C:217:PCW:H152	0.45	2.42	8	1
3:A:406:PCW:H441	3:C:204:PCW:C43	0.45	2.42	9	2
3:A:414:PCW:H442	4:A:415:17F:H68	0.45	1.89	10	1
3:A:420:PCW:H131	3:A:420:PCW:C32	0.45	2.42	10	1
3:D:605:PCW:P	3:D:614:PCW:C5	0.45	3.05	17	2
2:B:14:VAL:HA	2:B:83:ALA:HB2	0.45	1.89	11	1
2:B:72:MET:SD	2:B:99:GLN:HG2	0.45	2.52	11	1
3:C:206:PCW:C7	3:C:206:PCW:O4P	0.45	2.63	13	3
3:C:211:PCW:H242	4:C:215:17F:H74	0.45	1.88	13	1
4:C:215:17F:P1	4:C:215:17F:C18	0.45	3.05	14	1
3:D:601:PCW:H39	4:D:628:17F:H54	0.45	1.89	16	1
3:C:203:PCW:O2P	3:C:207:PCW:H331	0.45	2.12	17	1
3:D:609:PCW:C11	3:D:616:PCW:H61	0.45	2.42	18	1
3:B:203:PCW:C19	4:B:210:17F:H38	0.45	2.42	20	1
3:B:205:PCW:H132	3:C:204:PCW:H52	0.45	1.88	20	1
1:D:469:LEU:O	1:D:473:LYS:HB2	0.45	2.12	1	3
3:D:603:PCW:C21	3:D:603:PCW:H441	0.45	2.42	1	1
3:D:605:PCW:H231	3:D:614:PCW:H381	0.45	1.87	8	2
3:D:623:PCW:H242	3:B:203:PCW:C44	0.45	2.41	1	1
3:D:627:PCW:H2	3:D:627:PCW:O4P	0.45	2.11	1	1
3:A:403:PCW:H51	3:A:404:PCW:O1P	0.45	2.11	6	3
3:A:410:PCW:O31	3:A:410:PCW:H11	0.45	2.12	4	3
4:A:416:17F:O7	4:A:416:17F:O10	0.45	2.35	3	3
3:D:603:PCW:H161	3:D:624:PCW:C22	0.45	2.41	3	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
3:D:619:PCW:H241	3:C:204:PCW:C44	0.45	2.35	4	1
3:A:405:PCW:C8	4:B:211:17F:H2	0.45	2.43	6	1
3:A:407:PCW:C6	3:A:412:PCW:H372	0.45	2.42	6	1
3:D:612:PCW:H63	3:D:623:PCW:C33	0.45	2.41	6	1
3:D:619:PCW:C48	3:B:205:PCW:H222	0.45	2.42	6	1
3:D:616:PCW:O1P	3:D:616:PCW:C5	0.45	2.64	15	3
3:C:203:PCW:H122	3:C:207:PCW:C38	0.45	2.41	7	1
3:A:413:PCW:C38	3:C:210:PCW:H141	0.45	2.42	18	4
3:D:607:PCW:H431	3:D:626:PCW:C48	0.45	2.42	9	2
3:C:212:PCW:H483	4:C:215:17F:H72	0.45	1.89	9	1
3:C:212:PCW:H11	3:C:212:PCW:O31	0.45	2.10	10	1
3:D:602:PCW:H321	4:C:214:17F:H59	0.45	1.88	12	1
2:B:79:LEU:HD12	2:B:112:VAL:HB	0.45	1.88	12	1
2:C:58:THR:HG21	2:C:71:TYR:CE1	0.45	2.47	12	2
3:C:209:PCW:C28	3:C:209:PCW:H421	0.45	2.42	12	1
4:A:422:17F:H65	4:D:632:17F:C37	0.45	2.33	13	1
1:A:242:GLU:OE1	1:D:528:ARG:HB3	0.45	2.11	15	1
3:A:405:PCW:H322	3:A:406:PCW:C18	0.45	2.41	16	1
3:A:419:PCW:H421	4:B:210:17F:H74	0.45	1.87	16	1
3:D:604:PCW:C48	3:D:626:PCW:C28	0.45	2.85	17	1
2:B:131:GLN:HG3	2:B:141:PHE:HD2	0.45	1.72	17	1
3:A:421:PCW:P	3:D:618:PCW:H82	0.45	2.52	19	1
3:D:619:PCW:O2P	3:D:627:PCW:C4	0.45	2.65	19	1
4:A:422:17F:O9	4:A:422:17F:C7	0.44	2.65	19	3
3:B:205:PCW:C8	3:B:208:PCW:H62	0.44	2.42	3	1
3:A:408:PCW:C24	3:A:411:PCW:C23	0.44	2.91	13	3
3:A:405:PCW:H362	3:A:406:PCW:C23	0.44	2.41	6	1
3:A:419:PCW:C48	3:D:625:PCW:H483	0.44	2.41	6	2
3:A:420:PCW:H342	3:D:618:PCW:H381	0.44	1.89	6	1
4:C:214:17F:H39	4:C:214:17F:C1X	0.44	2.38	6	1
3:C:206:PCW:H42	4:C:213:17F:O6	0.44	2.12	7	1
3:B:203:PCW:H461	3:C:211:PCW:H251	0.44	1.86	8	1
3:B:206:PCW:O11	3:B:206:PCW:O2	0.44	2.35	8	1
3:A:419:PCW:H82	3:D:626:PCW:C33	0.44	2.43	9	1
3:A:420:PCW:H461	3:D:617:PCW:H251	0.44	1.87	10	1
4:C:218:17F:H18A	4:C:218:17F:C6	0.44	2.36	10	1
2:C:139:ILE:HB	2:C:140:PRO:HD2	0.44	1.88	11	1
3:C:203:PCW:O3	3:C:207:PCW:H382	0.44	2.12	12	1
3:C:206:PCW:O3P	4:C:214:17F:H12A	0.44	2.11	12	1
3:A:412:PCW:C38	3:C:210:PCW:H381	0.44	2.42	14	1
3:A:413:PCW:H132	3:A:413:PCW:O31	0.44	2.12	14	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
3:B:207:PCW:H20	4:B:210:17F:H19A	0.44	1.89	14	1
3:D:625:PCW:C1	3:D:626:PCW:H32	0.44	2.24	15	1
3:C:206:PCW:H162	3:C:208:PCW:C32	0.44	2.42	16	1
3:A:407:PCW:H482	3:A:410:PCW:C26	0.44	2.42	18	1
3:A:403:PCW:H461	3:D:618:PCW:C28	0.44	2.41	20	1
3:C:212:PCW:H73	4:C:213:17F:C2	0.44	2.41	20	1
3:A:408:PCW:C18	3:A:408:PCW:H232	0.44	2.41	2	1
1:D:533:LEU:HD23	1:D:536:LEU:HD12	0.44	1.87	10	2
3:A:403:PCW:H141	3:A:404:PCW:C32	0.44	2.32	4	1
3:A:403:PCW:C8	4:A:415:17F:O5	0.44	2.65	4	2
3:D:608:PCW:H20	4:D:629:17F:H47	0.44	1.89	5	1
4:D:630:17F:O8	4:D:630:17F:H5	0.44	2.11	5	2
5:B:201:GSP:O3B	5:B:201:GSP:O2A	0.44	2.35	5	1
4:D:628:17F:C21	4:D:629:17F:H70	0.44	2.42	8	2
4:B:209:17F:O10	4:B:209:17F:O7	0.44	2.35	19	2
3:C:206:PCW:C12	3:C:208:PCW:C17	0.44	2.95	6	1
3:D:604:PCW:H262	4:C:213:17F:H51	0.44	1.89	8	1
3:C:207:PCW:O11	3:C:207:PCW:H63	0.44	2.12	8	1
3:D:618:PCW:H2	3:D:618:PCW:C5	0.44	2.41	9	1
3:D:626:PCW:C31	3:D:626:PCW:O2P	0.44	2.65	9	1
3:A:406:PCW:C46	3:D:619:PCW:H251	0.44	2.37	10	1
4:A:415:17F:H10A	4:B:209:17F:H30	0.44	1.88	10	1
3:D:602:PCW:C27	4:D:629:17F:H78	0.44	2.42	10	1
3:C:211:PCW:O3	3:C:211:PCW:O31	0.44	2.35	10	2
3:D:605:PCW:H63	4:D:630:17F:O4	0.44	2.12	14	1
3:C:208:PCW:H51	3:C:208:PCW:O31	0.44	2.11	14	1
3:A:401:PCW:C39	3:B:204:PCW:H262	0.44	2.41	17	1
3:C:212:PCW:H411	3:C:212:PCW:H171	0.44	1.88	17	1
3:A:417:PCW:C8	4:D:630:17F:O5	0.44	2.65	18	1
3:D:619:PCW:O2P	3:D:627:PCW:C5	0.44	2.65	18	1
4:C:219:17F:H56	4:C:219:17F:C10	0.44	2.42	18	1
2:B:32:TYR:HE1	5:B:201:GSP:S1G	0.44	2.35	19	1
3:D:623:PCW:H261	3:B:203:PCW:H422	0.44	1.89	1	1
1:D:497:SER:HB2	1:D:498:PRO:CD	0.44	2.43	7	5
3:D:606:PCW:H442	3:D:609:PCW:C2	0.44	2.43	2	1
3:D:613:PCW:O3P	3:D:613:PCW:C31	0.44	2.64	5	6
4:B:211:17F:H62	4:B:211:17F:C12	0.44	2.42	2	1
3:C:205:PCW:C11	3:C:209:PCW:H161	0.44	2.42	2	1
3:C:207:PCW:H282	3:C:207:PCW:H462	0.44	1.88	2	1
3:C:208:PCW:H61	4:C:213:17F:HN1	0.44	1.73	2	1
3:C:209:PCW:O2P	4:C:214:17F:N1	0.44	2.45	2	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
4:C:219:17F:O7	4:C:219:17F:C17	0.44	2.65	8	6
3:A:403:PCW:C7	3:A:404:PCW:O1P	0.44	2.64	3	1
3:B:205:PCW:C48	3:B:208:PCW:C20	0.44	2.94	4	1
3:A:406:PCW:H352	3:B:205:PCW:H31	0.44	1.87	5	1
3:D:605:PCW:O31	3:D:614:PCW:H73	0.44	2.11	6	1
3:D:624:PCW:O3P	3:D:624:PCW:C31	0.44	2.64	6	1
3:D:627:PCW:C26	3:C:210:PCW:H271	0.44	2.38	6	1
3:C:216:PCW:H322	3:C:216:PCW:C5	0.44	2.41	17	3
3:C:205:PCW:H141	3:C:209:PCW:C36	0.44	2.40	7	1
3:D:602:PCW:O2	4:C:214:17F:C33	0.44	2.65	8	1
1:A:308:ARG:HG3	1:D:469:LEU:HD21	0.44	1.89	9	2
3:D:614:PCW:H483	3:D:620:PCW:H381	0.44	1.88	9	1
3:D:622:PCW:C20	4:D:631:17F:H19A	0.44	2.42	9	1
3:A:401:PCW:C41	3:B:207:PCW:H482	0.44	2.42	10	1
3:A:420:PCW:O2P	3:A:420:PCW:H31	0.44	2.12	10	1
3:A:420:PCW:C35	3:D:618:PCW:C41	0.44	2.93	11	1
3:D:608:PCW:H431	4:D:628:17F:C33	0.44	2.42	13	3
3:C:216:PCW:O31	3:C:216:PCW:H52	0.44	2.12	11	1
3:B:206:PCW:H131	3:C:209:PCW:H372	0.44	1.89	12	1
3:D:605:PCW:C6	4:D:630:17F:O4	0.44	2.65	14	1
3:D:605:PCW:H261	3:D:614:PCW:H412	0.44	1.89	14	1
3:D:607:PCW:H431	3:D:626:PCW:H481	0.44	1.89	14	1
3:D:614:PCW:H20	4:B:209:17F:H47	0.44	1.86	15	1
3:C:203:PCW:H31	3:C:207:PCW:C38	0.44	2.42	15	1
3:D:609:PCW:H122	3:D:616:PCW:H73	0.44	1.89	16	1
3:C:217:PCW:H19	4:C:219:17F:C19	0.44	2.43	17	1
3:C:203:PCW:H431	3:C:204:PCW:H161	0.44	1.90	18	1
3:A:406:PCW:C26	3:A:411:PCW:H481	0.44	2.42	19	1
3:D:603:PCW:O3P	4:C:219:17F:O1	0.44	2.35	19	1
3:D:621:PCW:H272	4:D:632:17F:C2X	0.44	2.27	20	1
4:C:218:17F:P1	4:C:218:17F:O9	0.44	2.76	20	1
3:A:407:PCW:P	3:A:412:PCW:H11	0.44	2.53	1	1
3:A:408:PCW:P	3:A:408:PCW:C3	0.44	3.05	3	1
3:D:602:PCW:C34	4:C:214:17F:H60	0.44	2.39	3	1
3:D:604:PCW:C20	4:C:215:17F:C30	0.44	2.95	3	1
4:C:219:17F:H10A	4:C:219:17F:H56	0.44	1.90	6	2
3:A:407:PCW:H261	3:C:206:PCW:H271	0.44	1.90	5	1
3:D:605:PCW:H372	3:D:605:PCW:H411	0.44	1.87	5	1
3:A:407:PCW:H40	3:A:407:PCW:C18	0.44	2.43	6	1
3:B:203:PCW:C36	3:C:211:PCW:H422	0.44	2.41	7	1
3:C:205:PCW:H42	4:C:214:17F:N1	0.44	2.26	7	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
3:C:207:PCW:C42	4:C:213:17F:C1Z	0.44	2.95	7	1
3:A:413:PCW:O31	3:A:413:PCW:C5	0.44	2.63	8	1
3:D:604:PCW:H381	4:C:218:17F:C22	0.44	2.41	8	1
3:D:621:PCW:H141	4:D:632:17F:C5	0.44	2.42	9	1
3:D:623:PCW:O3	3:D:623:PCW:C31	0.44	2.65	17	2
3:C:216:PCW:H483	3:C:217:PCW:H431	0.44	1.83	9	1
3:A:421:PCW:H332	4:D:630:17F:H10A	0.44	1.89	10	1
3:C:203:PCW:C40	4:C:213:17F:H66	0.44	2.41	11	2
4:C:215:17F:C7	4:C:215:17F:O9	0.44	2.65	11	1
4:A:422:17F:H62	3:D:622:PCW:C41	0.44	2.42	13	2
3:D:617:PCW:H452	3:C:204:PCW:H452	0.44	1.88	14	1
3:D:608:PCW:C26	4:D:629:17F:C35	0.44	2.96	17	1
3:B:208:PCW:H12	3:B:208:PCW:O31	0.44	2.11	18	1
3:A:406:PCW:C36	3:B:205:PCW:H322	0.44	2.33	19	1
3:C:207:PCW:H462	3:C:207:PCW:H262	0.44	1.89	19	1
3:A:405:PCW:H371	3:A:411:PCW:C44	0.44	2.43	20	1
3:A:413:PCW:H421	3:A:413:PCW:H283	0.44	1.89	20	1
3:A:418:PCW:C43	3:D:613:PCW:H162	0.44	2.42	2	1
3:C:209:PCW:H461	3:C:212:PCW:H283	0.44	1.90	2	1
3:A:408:PCW:C15	3:A:413:PCW:H352	0.44	2.28	3	1
3:B:203:PCW:O31	3:B:203:PCW:H11	0.44	2.12	5	2
4:B:210:17F:O2	4:B:210:17F:C2	0.44	2.65	4	2
1:D:455:TYR:O	1:D:459:PHE:HB2	0.44	2.13	5	1
3:B:208:PCW:C45	4:C:219:17F:H42	0.44	2.41	6	1
4:A:422:17F:C2X	4:C:219:17F:H62	0.44	2.33	8	1
3:A:401:PCW:C25	3:D:615:PCW:C27	0.44	2.94	10	1
3:A:403:PCW:H382	3:A:403:PCW:C15	0.44	2.37	11	1
3:A:412:PCW:O3	3:A:412:PCW:O31	0.44	2.35	20	2
3:A:406:PCW:H381	3:B:205:PCW:H121	0.44	1.88	14	1
3:C:203:PCW:H321	3:C:207:PCW:C34	0.44	2.43	14	1
3:C:203:PCW:H441	3:C:210:PCW:H19	0.44	1.88	14	1
3:C:207:PCW:H351	4:C:213:17F:H59	0.44	1.90	14	1
3:A:401:PCW:C38	3:B:204:PCW:H281	0.44	2.41	15	1
3:C:205:PCW:O11	3:C:212:PCW:C15	0.44	2.65	15	1
1:D:515:ARG:O	1:D:519:ALA:HB3	0.44	2.12	16	1
3:C:203:PCW:H371	3:C:207:PCW:H382	0.44	1.89	16	1
2:B:17:SER:N	5:B:201:GSP:O2B	0.44	2.50	17	1
3:A:401:PCW:H442	3:D:615:PCW:H272	0.44	1.90	18	1
3:D:604:PCW:C32	3:D:606:PCW:H122	0.44	2.43	18	1
3:B:203:PCW:H41	3:C:211:PCW:H352	0.44	1.88	2	1
3:B:208:PCW:C39	3:C:204:PCW:H352	0.44	2.43	2	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
3:B:208:PCW:H82	3:B:208:PCW:O11	0.44	2.13	3	1
1:A:264:LYS:HE3	1:D:509:ALA:HB1	0.44	1.88	4	1
3:D:610:PCW:O4P	4:D:631:17F:O1	0.44	2.35	4	1
3:C:205:PCW:O2	3:C:205:PCW:O2P	0.44	2.36	15	4
3:D:606:PCW:H232	4:C:218:17F:H37	0.44	1.89	5	3
3:D:616:PCW:O2	3:D:616:PCW:O11	0.44	2.35	6	1
3:A:401:PCW:C41	3:B:204:PCW:H282	0.44	2.43	7	1
3:A:406:PCW:H39	3:B:205:PCW:H141	0.44	1.88	7	1
3:D:604:PCW:H73	3:D:604:PCW:C11	0.44	2.42	7	1
3:D:604:PCW:H251	4:C:215:17F:C29	0.44	2.41	8	1
2:B:55:ILE:HG12	2:B:156:PHE:HE1	0.44	1.71	8	1
3:C:203:PCW:H381	3:C:203:PCW:H411	0.44	1.50	10	5
4:C:215:17F:H35	4:C:215:17F:C36	0.44	2.42	8	1
3:D:610:PCW:H283	4:D:631:17F:H73	0.44	1.89	10	1
3:D:602:PCW:H371	4:C:214:17F:C42	0.44	2.42	11	1
3:D:619:PCW:H321	3:D:627:PCW:H62	0.44	1.88	12	1
3:B:205:PCW:C18	3:C:203:PCW:H481	0.44	2.41	13	1
3:A:401:PCW:C42	3:B:204:PCW:H283	0.44	2.43	14	1
3:A:418:PCW:O4P	3:A:418:PCW:C8	0.44	2.66	14	1
3:D:621:PCW:H141	4:D:632:17F:H5	0.44	1.90	14	1
3:A:413:PCW:C41	3:C:210:PCW:H442	0.44	2.42	15	1
3:A:406:PCW:C20	3:A:411:PCW:H452	0.44	2.43	16	1
3:D:622:PCW:H32	3:D:622:PCW:O4P	0.44	2.13	16	1
3:A:402:PCW:H422	3:C:208:PCW:C15	0.44	2.37	17	1
3:D:606:PCW:H352	4:C:218:17F:O7	0.44	2.11	17	1
3:B:204:PCW:O11	3:B:204:PCW:C2	0.44	2.59	18	2
3:C:205:PCW:C1	4:C:214:17F:C7	0.44	2.96	18	1
4:C:213:17F:H51	4:C:215:17F:H74	0.44	1.89	18	1
1:A:249:GLU:O	1:A:253:LYS:HB2	0.44	2.12	19	1
3:A:408:PCW:H242	3:A:411:PCW:H222	0.44	1.89	19	1
3:A:402:PCW:H62	3:A:410:PCW:O2P	0.44	2.13	20	1
3:B:203:PCW:H431	3:C:211:PCW:H222	0.44	1.89	20	1
3:C:203:PCW:H142	4:C:213:17F:C1X	0.44	2.42	1	1
3:C:207:PCW:O3	3:C:208:PCW:H62	0.44	2.12	1	1
3:A:406:PCW:H422	3:C:204:PCW:C43	0.44	2.43	2	1
3:D:621:PCW:C8	3:D:621:PCW:C3	0.44	2.95	2	1
3:C:211:PCW:O2	3:C:211:PCW:C11	0.44	2.66	12	2
3:C:212:PCW:C41	4:C:215:17F:H59	0.44	2.24	2	1
3:A:420:PCW:C36	3:D:618:PCW:C42	0.44	2.95	3	1
3:D:615:PCW:H52	3:D:625:PCW:H42	0.44	1.89	3	1
3:D:606:PCW:H151	4:C:218:17F:H8	0.44	1.89	5	2

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
3:D:616:PCW:C19	4:D:632:17F:C22	0.44	2.95	4	1
2:C:70:GLN:HA	2:C:73:ARG:NH2	0.44	2.28	4	1
3:A:405:PCW:H52	3:A:406:PCW:C12	0.44	2.43	20	2
3:A:418:PCW:O4P	3:A:418:PCW:H2	0.44	2.13	5	1
4:D:628:17F:C37	4:D:629:17F:H52	0.44	2.36	5	1
3:C:211:PCW:H272	4:C:215:17F:H47	0.44	1.89	5	1
3:D:601:PCW:C42	4:D:628:17F:H52	0.44	2.37	6	1
4:B:210:17F:H36	4:C:215:17F:C1X	0.44	2.42	6	1
3:A:403:PCW:H141	3:A:403:PCW:C38	0.44	2.39	7	1
3:A:406:PCW:C25	4:B:211:17F:C33	0.44	2.96	7	1
3:D:622:PCW:C20	4:D:631:17F:O10	0.44	2.66	7	2
3:C:207:PCW:H422	4:C:213:17F:H33	0.44	1.87	7	1
3:D:609:PCW:H271	4:D:628:17F:H71	0.44	1.90	8	1
3:A:409:PCW:C41	3:A:419:PCW:H282	0.44	2.41	9	1
4:C:213:17F:H40	4:C:215:17F:C32	0.44	2.33	9	1
3:D:619:PCW:H442	3:D:627:PCW:H261	0.44	1.90	20	2
3:D:609:PCW:H271	4:D:628:17F:H70	0.44	1.90	14	1
3:C:212:PCW:H431	4:C:215:17F:H68	0.44	1.89	15	1
3:A:403:PCW:H331	3:A:406:PCW:C1	0.44	2.42	16	1
3:D:627:PCW:O4P	3:D:627:PCW:H2	0.44	2.12	17	1
3:B:207:PCW:O11	3:B:207:PCW:H51	0.44	2.12	17	2
3:C:203:PCW:C36	3:C:204:PCW:H122	0.44	2.42	19	2
3:D:609:PCW:H431	3:C:208:PCW:H241	0.44	1.88	18	1
3:C:206:PCW:N	4:C:213:17F:O1	0.44	2.51	20	1
3:B:203:PCW:O31	3:B:203:PCW:O3	0.44	2.36	1	1
3:A:404:PCW:H442	3:A:404:PCW:C19	0.44	2.43	2	1
4:D:632:17F:C36	3:C:208:PCW:H482	0.44	2.43	2	1
3:C:217:PCW:H19	4:C:219:17F:C20	0.44	2.43	20	2
3:A:406:PCW:H471	4:B:211:17F:C1Y	0.44	2.42	20	2
3:A:413:PCW:H442	3:C:210:PCW:H482	0.44	1.88	4	1
3:D:604:PCW:O11	3:D:604:PCW:C4	0.44	2.66	5	1
3:B:208:PCW:H41	3:C:211:PCW:C5	0.44	2.39	5	1
3:A:417:PCW:H431	3:A:421:PCW:H40	0.44	1.90	6	1
3:D:604:PCW:H362	4:C:219:17F:H9A	0.44	1.89	6	1
3:D:606:PCW:H62	3:D:626:PCW:C19	0.44	2.42	6	1
2:C:126:ASP:O	2:C:129:GLN:HG2	0.44	2.13	6	2
1:A:225:THR:O	1:A:229:TRP:HB2	0.44	2.13	14	2
3:C:203:PCW:C47	3:C:210:PCW:H282	0.44	2.43	7	1
3:C:206:PCW:H121	3:C:208:PCW:H151	0.44	1.89	8	1
3:D:606:PCW:C6	3:D:606:PCW:H131	0.44	2.43	9	1
2:B:72:MET:HE2	2:B:100:ILE:HG13	0.44	1.90	10	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
3:B:203:PCW:C7	4:C:215:17F:H19A	0.44	2.42	12	1
3:C:206:PCW:C6	3:C:212:PCW:H322	0.44	2.43	12	1
3:C:203:PCW:H141	3:C:207:PCW:C39	0.44	2.43	14	1
3:C:203:PCW:H152	4:C:213:17F:C1X	0.44	2.42	14	1
3:C:204:PCW:H262	3:C:210:PCW:C48	0.44	2.43	14	1
3:A:419:PCW:C5	3:D:626:PCW:O31	0.44	2.65	15	1
4:C:215:17F:H30	4:C:215:17F:C34	0.44	2.43	15	1
3:A:404:PCW:H52	3:A:406:PCW:O2P	0.44	2.13	17	1
3:A:409:PCW:H182	3:A:419:PCW:H283	0.44	1.89	20	1
3:A:409:PCW:H482	3:A:419:PCW:H212	0.44	1.89	20	1
3:A:406:PCW:O1P	3:B:205:PCW:H342	0.44	2.12	1	1
1:D:434:THR:O	1:D:438:ARG:HB2	0.44	2.13	1	1
3:D:613:PCW:C5	3:D:613:PCW:H322	0.44	2.43	1	1
4:D:632:17F:H48	3:C:208:PCW:H211	0.44	1.89	1	1
2:C:94:HIS:HA	2:C:137:TYR:OH	0.44	2.12	1	1
3:A:418:PCW:H352	3:D:613:PCW:H131	0.44	1.90	16	2
3:D:608:PCW:H121	3:D:609:PCW:C16	0.44	2.43	2	2
4:B:210:17F:C24	4:B:210:17F:H12	0.44	2.43	3	1
3:A:404:PCW:H171	3:B:205:PCW:H471	0.44	1.89	4	1
3:D:613:PCW:C32	3:D:619:PCW:H152	0.44	2.39	4	1
3:D:617:PCW:C48	3:B:205:PCW:H242	0.44	2.43	5	2
3:C:207:PCW:C14	4:C:213:17F:H56	0.44	2.38	5	1
3:A:407:PCW:H61	3:A:412:PCW:H372	0.44	1.89	18	2
3:A:419:PCW:H372	3:D:625:PCW:H381	0.44	1.90	6	1
3:B:204:PCW:H372	3:B:207:PCW:H63	0.44	1.90	6	1
3:C:204:PCW:C26	3:C:217:PCW:H421	0.44	2.43	7	1
3:C:207:PCW:H19	4:C:213:17F:C31	0.44	2.42	8	2
3:A:401:PCW:H361	3:B:204:PCW:H172	0.44	1.90	8	1
3:A:413:PCW:H381	3:A:413:PCW:H412	0.44	1.55	9	3
3:C:207:PCW:C32	3:C:207:PCW:H63	0.44	2.43	11	1
3:C:209:PCW:C7	4:C:214:17F:O2	0.44	2.65	11	1
3:D:614:PCW:H141	3:D:620:PCW:C38	0.44	2.43	12	1
3:D:605:PCW:H39	3:D:612:PCW:H322	0.44	1.90	13	1
3:D:606:PCW:C37	4:C:218:17F:O8	0.44	2.65	13	2
2:B:131:GLN:HB3	2:C:161:ARG:CZ	0.44	2.43	14	1
3:C:206:PCW:C7	4:C:213:17F:H18A	0.44	2.42	14	1
3:A:421:PCW:H2	3:A:421:PCW:H41	0.44	1.89	15	1
3:D:622:PCW:C36	4:D:631:17F:C34	0.44	2.95	15	1
3:C:209:PCW:H152	4:C:214:17F:H18A	0.44	1.89	15	1
4:A:416:17F:C42	3:D:612:PCW:H471	0.44	2.41	16	1
3:C:204:PCW:H221	3:C:217:PCW:H442	0.44	1.90	16	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
4:C:218:17F:H64	4:C:219:17F:C33	0.44	2.43	16	1
3:B:208:PCW:O3	3:C:203:PCW:H281	0.44	2.13	17	1
3:D:622:PCW:C28	4:D:631:17F:H12	0.44	2.43	18	1
3:B:206:PCW:H231	3:C:205:PCW:C13	0.44	2.43	18	1
3:C:205:PCW:C42	3:C:212:PCW:C26	0.44	2.92	18	1
3:D:605:PCW:C18	3:D:614:PCW:C36	0.44	2.86	19	1
2:B:6:LEU:HD22	2:B:159:LEU:HD23	0.44	1.90	19	1
3:D:603:PCW:C7	3:D:603:PCW:H131	0.43	2.43	1	1
3:D:604:PCW:H171	4:C:215:17F:H53	0.43	1.88	1	1
4:B:210:17F:H1	4:B:210:17F:C4	0.43	2.42	2	1
3:B:206:PCW:H141	3:B:206:PCW:H412	0.43	1.90	3	1
3:D:605:PCW:H482	3:D:620:PCW:H451	0.43	1.89	5	1
3:B:208:PCW:O31	3:B:208:PCW:H51	0.43	2.13	6	1
3:A:413:PCW:H442	3:C:210:PCW:C23	0.43	2.43	7	1
2:C:62:GLU:HG3	2:C:63:GLU:H	0.43	1.73	7	2
3:A:421:PCW:C8	4:D:630:17F:H4	0.43	2.43	9	1
3:D:609:PCW:C11	3:D:616:PCW:C7	0.43	2.96	9	1
3:B:203:PCW:H73	4:C:215:17F:H6A	0.43	1.90	9	1
3:A:402:PCW:O2P	3:A:410:PCW:H52	0.43	2.12	10	1
1:A:394:THR:O	1:A:398:ASN:HB3	0.43	2.13	11	1
3:A:406:PCW:C21	3:A:406:PCW:C16	0.43	2.95	11	1
3:A:418:PCW:H382	3:D:613:PCW:H221	0.43	1.89	11	1
3:A:407:PCW:O31	3:A:407:PCW:P	0.43	2.76	17	3
3:D:621:PCW:C7	3:D:621:PCW:C2	0.43	2.96	12	1
3:A:405:PCW:H61	4:B:211:17F:O2	0.43	2.13	13	1
3:A:414:PCW:C14	4:A:415:17F:H67	0.43	2.43	17	1
4:A:416:17F:C41	3:D:614:PCW:H241	0.43	2.42	17	1
3:D:603:PCW:C5	4:C:219:17F:O1	0.43	2.65	17	1
3:D:627:PCW:O2	3:D:627:PCW:O11	0.43	2.36	17	1
3:C:206:PCW:H351	3:C:208:PCW:H122	0.43	1.89	17	1
3:D:621:PCW:H132	4:D:632:17F:H18A	0.43	1.88	18	1
3:A:411:PCW:H121	3:A:411:PCW:H342	0.43	1.90	19	1
3:A:413:PCW:O31	3:A:413:PCW:H341	0.43	2.13	19	1
3:D:612:PCW:H11	3:D:614:PCW:H61	0.43	1.90	19	1
3:C:207:PCW:H182	3:C:208:PCW:C33	0.43	2.42	20	1
1:A:349:TYR:HE1	3:A:401:PCW:C19	0.43	2.26	1	1
3:A:401:PCW:H422	3:B:204:PCW:H282	0.43	1.90	1	1
3:B:208:PCW:H281	3:C:217:PCW:H271	0.43	1.89	1	1
3:A:417:PCW:H32	3:D:611:PCW:O3	0.43	2.13	3	1
3:C:206:PCW:O11	3:C:206:PCW:O2	0.43	2.35	18	2
3:C:212:PCW:H352	4:C:213:17F:H9A	0.43	1.84	4	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
3:A:409:PCW:O2P	3:B:206:PCW:C6	0.43	2.65	5	1
3:D:604:PCW:O11	3:D:604:PCW:H51	0.43	2.12	5	1
3:B:206:PCW:H232	3:C:205:PCW:H151	0.43	1.84	20	2
3:A:421:PCW:H61	4:D:630:17F:C6	0.43	2.40	6	1
3:B:206:PCW:C6	3:B:206:PCW:O2	0.43	2.66	6	2
3:B:208:PCW:C46	4:C:219:17F:H42	0.43	2.43	6	1
4:B:210:17F:H18	4:B:210:17F:H5	0.43	1.63	6	3
4:B:211:17F:H51	3:C:203:PCW:H262	0.43	1.90	6	1
3:A:411:PCW:H31	3:C:204:PCW:H51	0.43	1.90	7	1
3:C:209:PCW:H141	4:C:214:17F:C17	0.43	2.43	7	1
3:A:414:PCW:H283	4:B:209:17F:C22	0.43	2.43	8	1
3:D:610:PCW:H162	4:D:631:17F:H61	0.43	1.89	8	1
3:C:207:PCW:H131	3:C:207:PCW:C6	0.43	2.44	8	1
3:B:203:PCW:H342	4:B:210:17F:H39	0.43	1.88	9	1
3:C:203:PCW:H411	3:C:203:PCW:H381	0.43	1.52	9	1
1:A:299:SER:HB2	1:A:300:PRO:CD	0.43	2.43	15	3
4:B:211:17F:C22	3:C:204:PCW:H441	0.43	2.43	10	1
3:A:405:PCW:O1P	3:A:405:PCW:C31	0.43	2.66	11	1
1:D:474:VAL:O	1:D:478:ARG:HB2	0.43	2.12	14	2
3:A:403:PCW:C33	3:A:406:PCW:C1	0.43	2.92	12	1
3:C:212:PCW:H221	4:C:215:17F:H10	0.43	1.90	12	1
1:D:461:LYS:O	1:D:465:GLU:HG3	0.43	2.13	13	1
3:B:203:PCW:H332	4:B:210:17F:H29	0.43	1.90	16	1
3:C:207:PCW:O2	3:C:207:PCW:C11	0.43	2.66	16	1
3:C:206:PCW:C4	4:C:214:17F:H12A	0.43	2.43	17	1
2:C:35:THR:CG2	2:C:38:ASP:HB2	0.43	2.43	20	1
3:C:212:PCW:H122	4:C:215:17F:H6	0.43	1.90	20	1
3:A:418:PCW:H481	3:D:613:PCW:H281	0.43	1.88	2	1
3:D:603:PCW:H271	3:D:611:PCW:C18	0.43	2.40	2	1
3:D:616:PCW:H212	3:D:616:PCW:H182	0.43	1.53	2	4
3:B:206:PCW:O31	3:B:206:PCW:C1	0.43	2.63	3	1
4:A:422:17F:C34	4:D:632:17F:H74	0.43	2.43	4	2
3:D:611:PCW:H462	3:B:208:PCW:H241	0.43	1.89	4	1
3:D:627:PCW:C24	3:C:216:PCW:H451	0.43	2.43	11	2
4:A:416:17F:C38	3:B:204:PCW:C27	0.43	2.91	5	1
1:D:438:ARG:HA	1:D:441:MET:HB2	0.43	1.90	6	1
3:D:601:PCW:C7	4:C:214:17F:O2	0.43	2.66	6	1
3:A:408:PCW:H261	4:D:631:17F:C30	0.43	2.43	7	1
3:A:414:PCW:H481	4:B:209:17F:H10A	0.43	1.89	7	1
3:D:616:PCW:H412	3:C:208:PCW:H283	0.43	1.89	7	1
4:D:629:17F:C1	4:D:629:17F:C4	0.43	2.92	7	2

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
4:D:628:17F:C2X	4:D:629:17F:H77	0.43	2.43	8	1
3:C:206:PCW:H63	4:C:213:17F:C6	0.43	2.43	8	1
3:D:604:PCW:C7	4:C:219:17F:O2	0.43	2.66	9	1
3:B:207:PCW:C17	4:B:210:17F:O10	0.43	2.67	11	1
3:C:207:PCW:H181	3:C:207:PCW:H212	0.43	1.60	11	1
3:D:609:PCW:H281	4:C:214:17F:C28	0.43	2.44	12	1
3:D:617:PCW:H52	3:D:617:PCW:O3P	0.43	2.13	12	1
1:A:294:LEU:O	1:A:298:LEU:HG	0.43	2.13	14	1
3:A:419:PCW:H483	3:C:212:PCW:C47	0.43	2.44	14	1
3:A:406:PCW:H131	4:B:211:17F:C40	0.43	2.43	15	1
3:B:208:PCW:O11	3:B:208:PCW:C6	0.43	2.63	15	1
3:A:404:PCW:C15	3:B:205:PCW:H471	0.43	2.43	16	1
4:D:630:17F:O10	4:D:630:17F:C7	0.43	2.66	16	1
3:D:603:PCW:C22	3:D:611:PCW:C33	0.43	2.96	17	1
3:A:406:PCW:H372	3:B:205:PCW:C12	0.43	2.42	18	1
3:B:203:PCW:H472	4:C:215:17F:C29	0.43	2.43	18	1
3:A:420:PCW:H342	3:A:420:PCW:O2	0.43	2.14	20	1
3:D:616:PCW:H122	4:D:632:17F:O7	0.43	2.13	20	1
3:A:408:PCW:O31	3:A:408:PCW:C1	0.43	2.59	1	1
3:A:408:PCW:H63	3:A:413:PCW:H32	0.43	1.90	1	1
3:A:420:PCW:C3	3:D:618:PCW:C42	0.43	2.97	1	2
3:D:627:PCW:O4P	3:D:627:PCW:C8	0.43	2.66	9	5
3:B:203:PCW:H212	4:B:209:17F:H20A	0.43	1.90	3	1
3:C:205:PCW:C11	3:C:209:PCW:C15	0.43	2.96	11	2
2:B:16:LYS:HB2	5:B:201:GSP:O2B	0.43	2.14	5	1
2:C:6:LEU:HD22	2:C:159:LEU:HG	0.43	1.90	5	1
3:A:411:PCW:C4	3:A:411:PCW:O2	0.43	2.66	6	1
3:D:607:PCW:H12	3:D:626:PCW:H362	0.43	1.90	6	3
3:C:206:PCW:C5	4:C:214:17F:H35	0.43	2.36	6	1
3:A:407:PCW:C33	3:A:410:PCW:H372	0.43	2.43	7	1
3:A:411:PCW:O2	3:A:411:PCW:O4P	0.43	2.36	7	1
3:D:601:PCW:H151	3:D:601:PCW:C45	0.43	2.44	7	1
4:D:628:17F:O9	4:D:628:17F:C20	0.43	2.63	7	1
3:B:203:PCW:H472	3:C:211:PCW:H252	0.43	1.88	7	1
3:C:207:PCW:H19	4:C:213:17F:C1Y	0.43	2.44	8	1
1:A:298:LEU:O	1:A:302:GLY:HA3	0.43	2.12	9	4
3:D:606:PCW:H352	4:C:218:17F:C7	0.43	2.44	9	1
3:D:607:PCW:O3	3:D:626:PCW:H422	0.43	2.12	9	1
3:A:406:PCW:H483	3:D:619:PCW:H251	0.43	1.90	10	1
3:A:417:PCW:C31	3:A:417:PCW:O3	0.43	2.67	11	1
3:D:602:PCW:C7	4:C:214:17F:O2	0.43	2.66	11	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
3:B:204:PCW:H451	3:B:207:PCW:H222	0.43	1.89	11	1
1:D:453:GLN:HB2	1:D:454:PRO:CD	0.43	2.43	12	1
3:A:406:PCW:H351	4:B:211:17F:C7	0.43	2.43	14	1
3:C:209:PCW:O11	3:C:209:PCW:C7	0.43	2.65	15	1
3:C:212:PCW:C7	3:C:212:PCW:O4P	0.43	2.66	15	1
3:A:407:PCW:H12	3:A:412:PCW:H11	0.43	1.88	18	2
3:A:409:PCW:H262	3:A:409:PCW:H472	0.43	1.91	18	1
3:A:413:PCW:C8	3:C:210:PCW:H73	0.43	2.44	18	1
3:B:203:PCW:H412	4:B:210:17F:C21	0.43	2.42	18	1
3:B:206:PCW:H283	4:C:214:17F:H32	0.43	1.89	18	1
4:C:218:17F:H70	4:C:219:17F:H63	0.43	1.90	19	1
3:A:401:PCW:C40	3:B:204:PCW:H262	0.43	2.44	20	1
4:B:211:17F:H65	4:B:211:17F:C11	0.43	2.41	20	1
3:C:203:PCW:C8	4:C:213:17F:H6A	0.43	2.44	1	1
3:D:626:PCW:H181	3:D:626:PCW:H211	0.43	1.52	2	4
3:C:217:PCW:C46	4:C:219:17F:H55	0.43	2.43	3	1
3:D:605:PCW:C21	3:D:614:PCW:H152	0.43	2.38	4	1
3:A:409:PCW:H483	3:A:419:PCW:C20	0.43	2.42	5	1
3:D:626:PCW:H182	3:D:626:PCW:C8	0.43	2.43	5	1
3:B:208:PCW:H442	3:C:207:PCW:H331	0.43	1.90	5	1
4:B:211:17F:H50	3:C:204:PCW:C46	0.43	2.38	5	1
3:A:406:PCW:H262	3:A:411:PCW:H472	0.43	1.91	6	1
3:B:208:PCW:C41	3:C:203:PCW:H231	0.43	2.43	6	1
3:D:612:PCW:O11	3:D:620:PCW:H63	0.43	2.14	9	2
2:B:135:ARG:HD3	2:C:161:ARG:CG	0.43	2.44	7	1
3:A:419:PCW:H342	3:D:623:PCW:H472	0.43	1.90	8	1
4:B:210:17F:H11A	3:C:205:PCW:H451	0.43	1.91	8	1
3:A:409:PCW:H462	3:A:419:PCW:H221	0.43	1.91	14	2
3:A:409:PCW:H39	4:B:210:17F:H70	0.43	1.90	12	1
3:D:612:PCW:H381	3:D:623:PCW:H442	0.43	1.89	12	1
3:A:407:PCW:H122	3:A:410:PCW:H322	0.43	1.89	14	1
3:A:407:PCW:H172	3:C:206:PCW:H281	0.43	1.90	14	1
3:D:619:PCW:H321	3:D:627:PCW:H332	0.43	1.89	14	1
3:B:204:PCW:C39	4:B:210:17F:H8	0.43	2.44	14	1
3:A:401:PCW:H452	3:D:612:PCW:C25	0.43	2.43	15	1
3:A:411:PCW:H251	3:B:205:PCW:H242	0.43	1.90	15	1
3:C:209:PCW:C41	3:C:212:PCW:H262	0.43	2.44	15	1
4:B:211:17F:H11	4:B:211:17F:C36	0.43	2.42	20	1
3:C:205:PCW:H82	4:C:214:17F:O8	0.43	2.14	20	1
3:A:404:PCW:H73	4:A:415:17F:C3	0.43	2.42	1	1
3:D:605:PCW:C44	3:D:620:PCW:H483	0.43	2.33	2	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:244:SER:HA	1:A:248:GLU:HG2	0.43	1.90	3	1
2:B:161:ARG:HB3	2:C:135:ARG:HG3	0.43	1.90	3	1
3:B:206:PCW:H272	3:C:209:PCW:C19	0.43	2.44	3	1
3:A:408:PCW:C3	3:A:413:PCW:H121	0.43	2.43	4	1
3:C:203:PCW:H181	3:C:203:PCW:H211	0.43	1.56	4	1
3:A:403:PCW:C28	3:A:414:PCW:H20	0.43	2.44	5	1
3:C:206:PCW:C4	4:C:214:17F:H42	0.43	2.44	5	1
3:A:401:PCW:C34	3:B:207:PCW:H382	0.43	2.41	8	1
3:A:410:PCW:H462	3:A:412:PCW:C43	0.43	2.29	8	1
3:D:613:PCW:H322	3:D:619:PCW:O11	0.43	2.14	8	1
3:D:622:PCW:H362	4:D:631:17F:C32	0.43	2.44	10	2
4:A:416:17F:C42	4:B:209:17F:H74	0.43	2.44	9	1
3:D:622:PCW:C19	4:D:631:17F:H20	0.43	2.44	9	1
4:B:210:17F:C1X	4:C:215:17F:H10A	0.43	2.43	9	1
3:C:216:PCW:H481	3:C:217:PCW:C43	0.43	2.36	9	1
4:A:416:17F:P1	4:B:209:17F:H18A	0.43	2.54	10	1
3:B:205:PCW:C23	3:C:210:PCW:H283	0.43	2.41	10	1
3:D:614:PCW:O4P	3:D:614:PCW:C8	0.43	2.66	11	1
1:D:572:GLY:O	1:D:576:VAL:HB	0.43	2.14	13	1
3:A:403:PCW:O11	3:A:403:PCW:H73	0.43	2.13	14	1
3:D:621:PCW:H41	3:D:621:PCW:O31	0.43	2.13	14	1
3:A:405:PCW:H283	3:A:418:PCW:C48	0.43	2.44	15	1
3:A:406:PCW:H461	3:D:619:PCW:C48	0.43	2.43	16	1
3:A:412:PCW:C45	3:C:210:PCW:H19	0.43	2.43	16	1
2:C:79:LEU:HB2	2:C:159:LEU:HD22	0.43	1.88	16	1
3:A:417:PCW:H152	3:A:420:PCW:H361	0.43	1.91	17	1
3:D:605:PCW:C46	3:D:624:PCW:H471	0.43	2.43	19	1
4:D:632:17F:O8	4:D:632:17F:H5	0.43	2.11	19	1
4:C:215:17F:H30	4:C:215:17F:C35	0.43	2.43	19	1
3:A:403:PCW:H452	3:D:618:PCW:H281	0.43	1.89	20	1
3:A:408:PCW:H182	3:A:413:PCW:C26	0.43	2.44	4	1
3:A:408:PCW:H372	3:A:408:PCW:H411	0.43	1.89	4	1
3:C:204:PCW:H221	3:C:217:PCW:H472	0.43	1.91	4	1
3:C:216:PCW:H382	3:C:216:PCW:H411	0.43	1.55	4	4
3:A:409:PCW:C46	3:A:419:PCW:H221	0.43	2.44	5	2
1:D:444:ASP:O	1:D:448:VAL:HG23	0.43	2.13	5	1
3:A:414:PCW:C32	4:A:415:17F:H19A	0.43	2.35	6	1
3:D:608:PCW:C20	4:D:629:17F:H50	0.43	2.44	6	1
3:D:612:PCW:O31	3:D:612:PCW:C11	0.43	2.67	6	1
3:D:613:PCW:C5	3:D:619:PCW:O11	0.43	2.66	7	1
4:D:628:17F:C22	4:D:629:17F:H74	0.43	2.44	7	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
3:B:207:PCW:H381	3:B:207:PCW:H412	0.43	1.53	10	4
3:C:216:PCW:H481	3:C:217:PCW:H442	0.43	1.90	8	1
3:A:408:PCW:C4	3:A:413:PCW:C1	0.43	2.93	9	1
3:D:606:PCW:O31	3:D:606:PCW:O3P	0.43	2.37	9	1
3:D:614:PCW:H212	4:B:209:17F:C29	0.43	2.40	9	1
3:D:624:PCW:C31	3:D:624:PCW:H61	0.43	2.44	10	1
3:B:208:PCW:C34	3:C:203:PCW:H172	0.43	2.40	11	2
3:A:401:PCW:H411	3:B:204:PCW:C28	0.43	2.32	11	1
3:D:622:PCW:C19	3:C:217:PCW:H82	0.43	2.44	12	2
2:C:131:GLN:HG3	2:C:141:PHE:CD2	0.43	2.48	15	1
1:A:250:VAL:HG11	3:A:412:PCW:H252	0.43	1.90	16	1
3:C:204:PCW:H40	3:C:216:PCW:H232	0.43	1.90	16	1
3:C:211:PCW:C24	4:C:215:17F:H52	0.43	2.43	18	1
4:C:213:17F:H77	4:C:219:17F:C30	0.43	2.43	18	1
3:B:203:PCW:C45	4:C:215:17F:H47	0.43	2.44	19	1
2:C:5:LYS:HB2	2:C:76:GLU:HG3	0.43	1.91	20	2
3:A:408:PCW:C3	3:A:408:PCW:P	0.43	3.06	1	1
3:A:421:PCW:H41	3:A:421:PCW:C1	0.43	2.44	1	1
3:D:605:PCW:H411	3:D:605:PCW:H372	0.43	1.90	16	4
4:C:215:17F:O9	4:C:215:17F:C7	0.43	2.66	15	4
1:A:380:GLU:O	1:A:384:VAL:HG23	0.43	2.12	2	1
3:A:402:PCW:H483	3:C:206:PCW:C40	0.43	2.44	2	1
4:A:422:17F:H67	3:D:622:PCW:C45	0.43	2.39	2	1
3:C:212:PCW:O4P	3:C:212:PCW:C8	0.43	2.67	2	2
1:A:264:LYS:O	1:A:268:GLU:HG3	0.43	2.14	3	1
3:D:615:PCW:H42	3:D:625:PCW:H62	0.43	1.90	3	1
4:C:215:17F:H48	4:C:215:17F:H77	0.43	1.90	5	2
3:D:606:PCW:O11	3:D:606:PCW:H82	0.43	2.14	6	1
3:A:421:PCW:H422	3:D:618:PCW:C20	0.43	2.43	7	1
4:C:219:17F:C17	4:C:219:17F:O7	0.43	2.66	7	1
3:A:413:PCW:H412	3:C:210:PCW:H441	0.43	1.90	8	1
3:D:608:PCW:C26	4:D:629:17F:H58	0.43	2.39	8	1
3:D:623:PCW:H39	3:D:623:PCW:H151	0.43	1.90	8	1
3:B:204:PCW:H2	3:B:204:PCW:C4	0.43	2.43	8	1
3:D:622:PCW:C19	4:D:631:17F:C17	0.43	2.96	9	1
3:A:420:PCW:H32	3:A:420:PCW:O4P	0.43	2.14	10	1
1:D:565:ALA:O	1:D:569:LEU:HG	0.43	2.14	10	1
3:B:206:PCW:C8	4:B:210:17F:O1	0.43	2.67	11	1
3:D:602:PCW:H371	4:C:214:17F:H77	0.43	1.91	12	1
3:A:403:PCW:H142	3:A:403:PCW:C38	0.43	2.43	13	1
3:D:610:PCW:C8	4:D:631:17F:O8	0.43	2.66	13	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
3:B:203:PCW:C48	4:C:215:17F:H47	0.43	2.44	14	2
1:D:563:LYS:HB2	1:D:564:PRO:CD	0.43	2.44	16	1
3:D:607:PCW:H411	3:D:607:PCW:H382	0.43	1.57	16	1
4:A:416:17F:O7	4:A:416:17F:C17	0.43	2.67	17	1
3:B:205:PCW:H51	3:C:204:PCW:C6	0.43	2.44	18	1
3:A:414:PCW:H132	4:A:415:17F:H20	0.43	1.90	20	1
1:D:563:LYS:O	1:D:567:GLU:HG2	0.43	2.14	1	2
3:C:212:PCW:C35	4:C:213:17F:H11	0.43	2.43	3	1
3:D:612:PCW:H432	3:D:620:PCW:C48	0.43	2.40	4	1
3:C:212:PCW:C35	4:C:213:17F:C9	0.43	2.84	4	1
3:D:604:PCW:C48	3:D:606:PCW:H61	0.43	2.44	5	1
3:D:625:PCW:H82	3:D:625:PCW:H132	0.43	1.88	6	2
3:B:208:PCW:C45	3:C:203:PCW:H161	0.43	2.43	6	1
3:B:205:PCW:O2P	4:B:211:17F:N1	0.43	2.52	7	1
3:A:408:PCW:C3	3:A:413:PCW:O3	0.43	2.67	8	1
3:A:403:PCW:O2	3:A:403:PCW:C11	0.43	2.67	9	1
3:A:414:PCW:C33	4:B:209:17F:H9A	0.43	2.44	10	1
3:A:408:PCW:H162	3:A:411:PCW:C23	0.43	2.44	11	1
3:A:411:PCW:H181	3:A:411:PCW:H212	0.43	1.54	11	2
3:A:411:PCW:C5	4:B:211:17F:O4	0.43	2.66	13	1
3:C:212:PCW:H181	3:C:212:PCW:H211	0.43	1.58	14	2
3:D:617:PCW:H40	3:D:627:PCW:H182	0.43	1.89	14	1
3:D:625:PCW:H12	3:D:626:PCW:C2	0.43	2.44	14	1
4:B:211:17F:H49	3:C:204:PCW:C39	0.43	2.44	15	1
3:A:403:PCW:C33	3:A:406:PCW:H12	0.43	2.43	16	1
3:C:206:PCW:C6	3:C:212:PCW:O2P	0.43	2.67	16	1
3:D:605:PCW:H322	3:D:612:PCW:H12	0.43	1.91	18	1
3:D:614:PCW:H462	3:D:620:PCW:H411	0.43	1.90	18	1
3:D:621:PCW:H271	4:D:632:17F:H35	0.43	1.89	18	1
3:D:622:PCW:H281	4:D:631:17F:H35	0.43	1.90	18	1
4:A:422:17F:H39	4:C:219:17F:C39	0.43	2.32	19	1
3:B:204:PCW:C12	3:B:207:PCW:H411	0.43	2.44	19	1
3:A:406:PCW:H382	3:C:204:PCW:C34	0.43	2.44	20	1
3:D:614:PCW:H251	4:B:209:17F:H51	0.43	1.90	20	1
3:D:617:PCW:H421	3:D:627:PCW:C22	0.43	2.43	20	1
3:C:207:PCW:H321	3:C:207:PCW:H63	0.43	1.91	1	2
4:C:215:17F:H18	4:C:215:17F:H5	0.43	1.47	15	7
4:B:210:17F:O1	3:C:205:PCW:H371	0.43	2.14	2	1
3:A:407:PCW:C8	3:A:410:PCW:O31	0.43	2.67	3	1
3:D:619:PCW:H482	3:B:205:PCW:H242	0.43	1.91	4	1
3:C:216:PCW:H141	3:C:216:PCW:C37	0.43	2.43	4	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
3:A:410:PCW:C22	4:A:422:17F:C41	0.43	2.97	20	2
3:D:626:PCW:H211	3:D:626:PCW:H181	0.43	1.58	13	3
4:D:628:17F:H69	4:D:629:17F:H48	0.43	1.90	5	1
3:B:208:PCW:C48	3:C:203:PCW:H181	0.43	2.44	6	1
3:D:618:PCW:O31	3:D:618:PCW:N	0.43	2.52	7	2
4:D:632:17F:O8	4:D:632:17F:C5	0.43	2.53	8	1
3:B:208:PCW:C39	3:C:204:PCW:H131	0.43	2.44	8	1
3:A:403:PCW:C25	3:D:618:PCW:H282	0.43	2.44	9	2
3:A:409:PCW:H432	3:A:419:PCW:C24	0.43	2.39	9	1
4:B:210:17F:H35	4:C:215:17F:C8	0.43	2.44	9	1
1:A:268:GLU:OE1	1:D:506:ARG:HD3	0.43	2.13	11	5
3:D:603:PCW:O31	3:D:603:PCW:H12	0.43	2.13	13	1
3:B:204:PCW:C11	3:B:207:PCW:H372	0.43	2.44	13	1
3:C:206:PCW:C15	3:C:208:PCW:C17	0.43	2.96	13	1
2:B:126:ASP:OD2	2:B:128:LYS:HG2	0.43	2.13	14	1
3:C:206:PCW:H152	3:C:207:PCW:C24	0.43	2.44	14	1
3:C:206:PCW:H142	3:C:208:PCW:H342	0.43	1.89	14	1
3:A:401:PCW:C40	3:B:204:PCW:H281	0.43	2.43	15	1
4:A:422:17F:H50	4:C:218:17F:H10	0.43	1.91	15	1
3:B:208:PCW:H331	3:C:203:PCW:C20	0.43	2.36	15	1
3:C:203:PCW:C23	3:C:204:PCW:H352	0.43	2.43	15	1
3:A:414:PCW:H141	4:A:415:17F:H66	0.43	1.91	19	1
3:B:206:PCW:H283	4:C:214:17F:H33	0.43	1.90	19	1
2:C:16:LYS:HB2	5:C:201:GSP:O2G	0.43	2.13	19	1
3:C:205:PCW:C33	3:C:209:PCW:H332	0.42	2.43	1	1
3:A:411:PCW:C31	3:A:411:PCW:O3	0.42	2.67	2	2
3:D:621:PCW:C7	3:D:621:PCW:H32	0.42	2.44	2	1
3:C:211:PCW:H172	4:C:215:17F:H61	0.42	1.91	17	2
4:A:422:17F:H12A	4:C:218:17F:H78	0.42	1.89	4	1
3:D:606:PCW:H63	3:D:606:PCW:C11	0.42	2.43	4	3
3:B:204:PCW:C48	3:C:205:PCW:H481	0.42	2.41	4	1
1:A:337:ALA:O	1:A:341:ASN:HB2	0.42	2.13	5	1
3:A:406:PCW:C35	4:B:211:17F:H6	0.42	2.36	5	1
2:C:15:GLY:HA3	2:C:116:ASN:ND2	0.42	2.29	5	3
3:C:204:PCW:H122	3:C:207:PCW:H82	0.42	1.90	5	1
4:C:219:17F:H65	4:C:219:17F:C2X	0.42	2.37	5	1
3:B:207:PCW:C34	3:B:207:PCW:H162	0.42	2.44	6	1
4:C:215:17F:H5	4:C:215:17F:H18	0.42	1.45	20	4
3:C:216:PCW:H442	3:C:217:PCW:C35	0.42	2.44	6	1
3:C:216:PCW:H411	3:C:216:PCW:H382	0.42	1.56	6	2
3:D:606:PCW:H321	3:D:608:PCW:C7	0.42	2.44	7	2

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
3:D:603:PCW:H32	3:D:604:PCW:C8	0.42	2.44	8	1
3:B:208:PCW:C48	3:C:203:PCW:H161	0.42	2.36	8	1
3:A:411:PCW:O2P	4:B:211:17F:C1	0.42	2.67	11	3
3:A:414:PCW:H73	4:B:209:17F:O2	0.42	2.14	10	1
3:D:616:PCW:H182	3:D:616:PCW:H212	0.42	1.54	19	4
3:A:402:PCW:H321	3:A:410:PCW:H31	0.42	1.91	12	1
1:D:584:PHE:O	1:D:588:LEU:HG	0.42	2.14	12	1
3:D:609:PCW:C45	3:C:206:PCW:H20	0.42	2.41	14	1
3:D:616:PCW:C12	4:D:632:17F:H8	0.42	2.42	16	1
3:D:624:PCW:O31	3:D:624:PCW:O3	0.42	2.36	16	1
3:B:206:PCW:H122	3:C:209:PCW:H372	0.42	1.91	16	1
3:A:421:PCW:C35	3:D:618:PCW:H132	0.42	2.44	17	1
3:D:627:PCW:O31	3:D:627:PCW:H12	0.42	2.14	17	1
1:D:525:LEU:HD23	1:D:528:ARG:HD2	0.42	1.91	18	1
5:B:201:GSP:O2B	5:B:201:GSP:O1A	0.42	2.36	18	2
3:C:210:PCW:H121	3:C:210:PCW:C35	0.42	2.44	1	1
3:D:604:PCW:H452	3:D:606:PCW:C19	0.42	2.44	2	1
3:D:615:PCW:C5	3:D:625:PCW:O31	0.42	2.67	2	1
3:B:204:PCW:C17	3:B:204:PCW:H211	0.42	2.37	3	1
3:A:408:PCW:H182	3:A:408:PCW:H232	0.42	1.90	5	1
3:D:605:PCW:H39	3:D:612:PCW:O3	0.42	2.14	5	1
3:A:414:PCW:H411	3:A:414:PCW:H381	0.42	1.55	6	1
3:D:602:PCW:H351	4:C:214:17F:H70	0.42	1.89	7	1
3:D:627:PCW:C28	4:D:631:17F:C29	0.42	2.97	19	2
3:B:207:PCW:H141	4:B:210:17F:O10	0.42	2.14	7	2
4:C:214:17F:H62	4:C:214:17F:H59	0.42	1.62	19	2
3:D:606:PCW:H431	3:D:609:PCW:H31	0.42	1.91	8	1
3:A:418:PCW:H411	3:A:418:PCW:H381	0.42	1.59	9	1
3:D:609:PCW:C38	3:C:208:PCW:C28	0.42	2.94	9	1
3:C:203:PCW:H152	4:C:213:17F:H37	0.42	1.89	9	1
4:A:415:17F:P1	4:A:415:17F:O9	0.42	2.77	10	1
3:D:612:PCW:H131	3:D:620:PCW:H151	0.42	1.89	10	1
3:B:206:PCW:H283	4:C:214:17F:C20	0.42	2.43	10	1
3:A:404:PCW:H352	3:A:404:PCW:C5	0.42	2.42	11	1
4:A:415:17F:H58	4:A:415:17F:H62	0.42	1.57	11	1
3:D:602:PCW:C27	4:D:629:17F:H76	0.42	2.40	11	1
3:D:604:PCW:H411	4:C:218:17F:C21	0.42	2.44	11	1
3:A:405:PCW:O2P	3:A:406:PCW:H151	0.42	2.14	12	1
3:C:206:PCW:H142	3:C:208:PCW:C14	0.42	2.44	12	1
3:A:401:PCW:H342	3:B:207:PCW:C24	0.42	2.44	13	1
3:A:409:PCW:H371	4:B:210:17F:C35	0.42	2.42	13	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
3:A:413:PCW:O31	3:A:413:PCW:H132	0.42	2.14	13	1
3:B:207:PCW:H132	3:B:207:PCW:C32	0.42	2.44	13	3
3:A:418:PCW:C44	3:D:613:PCW:C27	0.42	2.97	14	1
3:D:604:PCW:C31	3:D:606:PCW:H122	0.42	2.43	15	1
3:A:409:PCW:H19	3:A:409:PCW:C12	0.42	2.44	19	1
4:C:218:17F:O9	4:C:218:17F:O1	0.42	2.37	20	1
1:A:261:PHE:O	1:A:265:TRP:HB2	0.42	2.14	1	1
3:C:210:PCW:C12	3:C:210:PCW:H351	0.42	2.45	2	2
3:C:210:PCW:H482	3:C:210:PCW:H212	0.42	1.90	1	1
3:D:607:PCW:H182	3:D:607:PCW:H211	0.42	1.67	4	4
3:D:621:PCW:C37	3:D:621:PCW:C41	0.42	2.90	2	1
3:C:205:PCW:H172	3:C:209:PCW:H361	0.42	1.90	2	1
4:A:416:17F:H64	3:B:204:PCW:C28	0.42	2.45	3	1
4:A:416:17F:H58	3:B:204:PCW:H271	0.42	1.90	3	1
3:B:205:PCW:H12	3:B:208:PCW:H61	0.42	1.91	3	1
3:C:204:PCW:C21	3:C:216:PCW:H281	0.42	2.44	3	1
4:B:210:17F:H5	4:B:210:17F:H18	0.42	1.52	4	2
3:B:207:PCW:H73	3:B:207:PCW:C12	0.42	2.44	5	1
3:A:409:PCW:O31	3:A:409:PCW:C1	0.42	2.61	6	1
3:D:610:PCW:H212	3:D:610:PCW:H182	0.42	1.64	6	1
2:C:86:ASN:OD1	2:C:88:LYS:HB3	0.42	2.14	6	1
3:D:607:PCW:C43	3:D:626:PCW:C47	0.42	2.89	7	1
3:D:609:PCW:H381	3:C:208:PCW:H281	0.42	1.91	7	1
1:A:330:ARG:O	1:A:334:ARG:HG2	0.42	2.14	19	2
3:C:205:PCW:C4	4:C:214:17F:H6A	0.42	2.40	8	1
3:A:402:PCW:H52	3:A:410:PCW:O4P	0.42	2.13	9	1
3:A:414:PCW:H321	4:A:415:17F:H20	0.42	1.90	9	1
3:A:404:PCW:H20	3:D:611:PCW:C27	0.42	2.43	10	1
3:C:206:PCW:C14	3:C:208:PCW:H151	0.42	2.44	10	1
3:D:612:PCW:O1P	3:D:614:PCW:H61	0.42	2.14	11	1
3:A:404:PCW:H471	4:A:415:17F:H54	0.42	1.89	12	1
3:A:411:PCW:O3P	3:B:205:PCW:H32	0.42	2.14	12	1
3:D:603:PCW:H331	3:D:624:PCW:C12	0.42	2.43	12	1
4:A:415:17F:H29	4:A:415:17F:H39	0.42	1.91	13	1
2:C:16:LYS:HG2	2:C:81:VAL:HB	0.42	1.92	13	1
3:A:404:PCW:H172	3:A:404:PCW:C46	0.42	2.44	15	1
3:D:622:PCW:O2	3:D:622:PCW:C11	0.42	2.67	15	1
3:B:205:PCW:H73	3:C:204:PCW:H62	0.42	1.90	15	1
3:C:212:PCW:H381	3:C:212:PCW:H412	0.42	1.57	15	1
3:D:621:PCW:H11	3:D:621:PCW:H73	0.42	1.91	16	1
2:C:6:LEU:HB2	2:C:55:ILE:HG12	0.42	1.90	17	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
3:C:203:PCW:H39	4:C:213:17F:H69	0.42	1.90	18	1
4:A:415:17F:C36	4:B:209:17F:H41	0.42	2.40	20	1
3:A:401:PCW:C1	3:B:207:PCW:H362	0.42	2.45	1	1
3:A:406:PCW:C16	3:A:406:PCW:C21	0.42	2.98	13	2
3:C:211:PCW:O3P	3:C:211:PCW:C31	0.42	2.67	1	1
4:A:415:17F:C24	4:B:209:17F:H33	0.42	2.33	2	1
3:A:403:PCW:C28	3:A:403:PCW:C24	0.42	2.95	3	2
3:C:204:PCW:H382	3:C:204:PCW:H411	0.42	1.57	17	3
3:A:409:PCW:O31	3:B:206:PCW:C6	0.42	2.62	4	1
3:A:420:PCW:C38	3:D:611:PCW:H161	0.42	2.45	8	2
3:A:421:PCW:O3P	3:D:618:PCW:H42	0.42	2.12	4	1
3:C:204:PCW:C23	3:C:210:PCW:H261	0.42	2.43	4	1
3:C:211:PCW:O3P	3:C:211:PCW:C6	0.42	2.54	4	1
3:A:414:PCW:H483	4:B:209:17F:H69	0.42	1.90	6	1
3:D:627:PCW:C21	3:C:217:PCW:H372	0.42	2.41	6	1
2:B:68:ARG:HG3	2:B:71:TYR:OH	0.42	2.15	6	1
4:B:211:17F:C25	3:C:204:PCW:H422	0.42	2.39	6	1
3:A:407:PCW:C8	3:A:410:PCW:H362	0.42	2.38	7	1
3:D:624:PCW:H211	3:D:624:PCW:H182	0.42	1.63	7	3
3:B:207:PCW:H61	4:B:210:17F:O9	0.42	2.14	7	1
3:C:206:PCW:H52	4:C:214:17F:C21	0.42	2.15	8	1
4:A:422:17F:H29	4:C:218:17F:H70	0.42	1.90	9	1
3:D:614:PCW:H211	3:D:614:PCW:H182	0.42	1.60	9	1
4:B:210:17F:O8	4:B:210:17F:O9	0.42	2.38	9	1
3:D:612:PCW:H222	3:D:620:PCW:H452	0.42	1.82	10	1
4:C:213:17F:H58	4:C:213:17F:H62	0.42	1.65	10	1
3:D:603:PCW:H212	3:D:603:PCW:C43	0.42	2.45	11	1
3:B:208:PCW:C34	3:C:203:PCW:C19	0.42	2.97	11	1
3:D:626:PCW:O3	3:D:626:PCW:O31	0.42	2.37	12	1
1:D:459:PHE:CE2	3:D:602:PCW:H281	0.42	2.50	14	1
3:D:619:PCW:O1P	3:D:627:PCW:C8	0.42	2.68	14	1
1:A:386:PHE:HZ	4:A:415:17F:C42	0.42	2.27	15	1
3:A:418:PCW:H39	3:D:613:PCW:H412	0.42	1.91	16	1
3:A:403:PCW:H152	3:A:404:PCW:O2	0.42	2.13	17	2
3:A:409:PCW:H472	3:A:409:PCW:C26	0.42	2.44	18	1
4:A:422:17F:C30	3:D:606:PCW:H411	0.42	2.45	19	1
4:B:210:17F:C2X	4:C:215:17F:C21	0.42	2.98	19	1
3:A:414:PCW:H121	4:A:415:17F:H33	0.42	1.90	20	1
3:A:407:PCW:O31	3:A:407:PCW:C4	0.42	2.66	1	1
3:A:411:PCW:H212	3:A:411:PCW:H181	0.42	1.66	15	5
3:B:204:PCW:H441	4:B:210:17F:C27	0.42	2.41	2	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
3:B:204:PCW:H73	3:B:204:PCW:C31	0.42	2.44	2	1
1:A:268:GLU:HG2	1:D:506:ARG:HD3	0.42	1.91	3	1
3:A:408:PCW:H261	3:D:619:PCW:H451	0.42	1.91	3	1
3:D:605:PCW:C6	4:D:630:17F:C3	0.42	2.97	3	1
3:D:611:PCW:O31	3:D:611:PCW:H11	0.42	2.14	3	1
3:D:617:PCW:H361	3:C:216:PCW:H362	0.42	1.91	3	1
4:D:631:17F:C30	3:C:210:PCW:H252	0.42	2.45	11	2
3:D:616:PCW:H481	3:C:206:PCW:H122	0.42	1.89	5	1
3:A:404:PCW:H472	4:A:415:17F:C30	0.42	2.29	6	1
3:A:421:PCW:H63	4:D:630:17F:H6A	0.42	1.88	6	1
3:D:606:PCW:H462	3:D:609:PCW:O2P	0.42	2.14	6	1
3:D:609:PCW:H52	4:D:632:17F:N1	0.42	2.25	7	1
3:A:414:PCW:H381	3:A:414:PCW:H411	0.42	1.61	13	3
3:D:624:PCW:C46	4:B:209:17F:H75	0.42	2.43	8	1
3:A:417:PCW:C17	3:A:420:PCW:H361	0.42	2.44	10	1
3:B:206:PCW:O4P	3:B:206:PCW:H73	0.42	2.15	10	1
3:D:603:PCW:C36	3:D:611:PCW:H342	0.42	2.44	11	1
3:B:207:PCW:H442	4:B:210:17F:H50	0.42	1.90	11	2
3:C:208:PCW:O31	3:C:208:PCW:C4	0.42	2.63	12	1
3:B:203:PCW:H42	3:C:211:PCW:H341	0.42	1.91	13	1
4:C:214:17F:H39	4:C:214:17F:H36	0.42	1.58	13	1
3:A:405:PCW:C24	3:A:418:PCW:H262	0.42	2.42	14	1
3:A:410:PCW:C22	3:D:622:PCW:C40	0.42	2.94	14	1
3:D:605:PCW:H212	3:D:614:PCW:H382	0.42	1.91	14	1
3:C:205:PCW:O31	3:C:209:PCW:H31	0.42	2.14	14	1
3:D:607:PCW:C3	3:D:626:PCW:C38	0.42	2.87	15	1
3:D:604:PCW:C11	3:D:604:PCW:O31	0.42	2.67	16	1
3:C:217:PCW:O3P	3:C:217:PCW:C31	0.42	2.68	16	1
3:A:413:PCW:H462	3:D:627:PCW:C28	0.42	2.45	17	1
3:D:621:PCW:C12	4:D:632:17F:C4	0.42	2.97	17	1
4:C:215:17F:H18A	4:C:215:17F:H4A	0.42	1.90	17	1
3:C:217:PCW:H19	4:C:219:17F:H19A	0.42	1.91	17	1
3:D:603:PCW:H441	3:D:603:PCW:C22	0.42	2.44	18	1
2:B:6:LEU:HD11	2:B:53:LEU:HD22	0.42	1.91	19	1
4:B:210:17F:H30	4:C:215:17F:C12	0.42	2.44	19	1
4:B:211:17F:H12A	4:B:211:17F:C38	0.42	2.40	19	1
1:A:309:ALA:HA	1:A:312:HIS:HB2	0.42	1.90	1	3
3:A:406:PCW:H141	4:B:211:17F:H10	0.42	1.92	1	1
3:A:417:PCW:C11	3:D:618:PCW:H341	0.42	2.45	1	1
3:A:414:PCW:H122	4:A:415:17F:C36	0.42	2.43	2	1
3:A:421:PCW:H61	4:D:630:17F:H5	0.42	1.90	2	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
3:D:604:PCW:C3	3:D:604:PCW:P	0.42	3.08	2	2
2:B:135:ARG:HH21	2:C:161:ARG:HG2	0.42	1.74	2	1
3:A:408:PCW:H162	3:A:413:PCW:C37	0.42	2.38	3	1
3:D:616:PCW:C5	4:D:632:17F:C3	0.42	2.94	3	1
1:A:216:LYS:HD2	1:D:557:THR:HG22	0.42	1.92	4	1
3:D:615:PCW:H411	3:D:615:PCW:H381	0.42	1.57	12	2
3:C:211:PCW:O31	3:C:211:PCW:H11	0.42	2.14	4	1
3:A:407:PCW:O3P	3:A:412:PCW:O1P	0.42	2.38	5	2
3:A:410:PCW:H381	3:A:410:PCW:H412	0.42	1.63	5	2
3:A:418:PCW:O3	3:A:418:PCW:C31	0.42	2.68	15	2
1:D:413:SER:O	1:D:417:GLU:HG3	0.42	2.15	13	2
3:B:208:PCW:H462	4:C:213:17F:H29	0.42	1.92	5	1
3:C:206:PCW:H172	3:C:208:PCW:H362	0.42	1.90	5	1
3:A:406:PCW:C20	4:B:211:17F:C20	0.42	2.96	6	1
3:D:606:PCW:H62	3:D:626:PCW:H19	0.42	1.92	6	1
3:A:404:PCW:H222	3:A:404:PCW:H182	0.42	1.89	14	2
3:D:616:PCW:H211	4:D:632:17F:C23	0.42	2.44	7	1
3:B:203:PCW:C48	4:C:215:17F:H52	0.42	2.44	7	1
3:D:601:PCW:H412	3:D:601:PCW:H381	0.42	1.56	12	3
3:C:203:PCW:C5	4:C:213:17F:H6A	0.42	2.39	9	1
3:C:205:PCW:C6	4:C:214:17F:C9	0.42	2.92	9	1
3:B:203:PCW:H461	4:C:215:17F:C27	0.42	2.40	10	1
3:B:205:PCW:H2	3:B:205:PCW:O11	0.42	2.14	10	1
3:A:404:PCW:H141	3:A:404:PCW:C39	0.42	2.44	12	2
3:B:206:PCW:H212	3:C:205:PCW:H171	0.42	1.92	12	1
3:A:408:PCW:H12	3:A:411:PCW:H381	0.42	1.90	16	2
1:A:273:ARG:O	1:A:276:VAL:HG12	0.42	2.15	15	1
1:A:334:ARG:HD3	1:D:440:GLU:OE1	0.42	2.14	15	1
3:B:205:PCW:H231	3:C:210:PCW:C24	0.42	2.26	15	1
1:A:262:GLN:O	1:A:266:GLN:HG3	0.42	2.14	16	1
1:A:348:GLU:HB3	1:A:352:LYS:HE2	0.42	1.90	16	3
3:C:209:PCW:C12	4:C:214:17F:C18	0.42	2.97	16	1
2:B:16:LYS:HG3	2:B:57:ASP:OD1	0.42	2.14	17	1
3:C:203:PCW:O2P	3:C:207:PCW:C33	0.42	2.68	17	1
3:C:208:PCW:H63	4:C:213:17F:C1	0.42	2.43	17	1
3:A:406:PCW:C39	3:C:204:PCW:H342	0.42	2.43	18	1
1:A:349:TYR:CE1	3:A:401:PCW:H19	0.42	2.49	1	1
3:B:203:PCW:C16	4:B:209:17F:H18	0.42	2.42	1	1
3:A:408:PCW:H182	3:A:408:PCW:H212	0.42	1.56	3	1
2:C:113:LEU:O	2:C:141:PHE:HA	0.42	2.14	3	2
3:A:409:PCW:H381	3:A:409:PCW:H411	0.42	1.63	4	3

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
3:D:603:PCW:H51	4:C:219:17F:H1A	0.42	1.91	4	1
3:D:603:PCW:C36	3:D:611:PCW:H321	0.42	2.44	4	1
3:B:204:PCW:H411	3:B:207:PCW:C19	0.42	2.45	4	1
3:B:204:PCW:C40	4:B:210:17F:H12A	0.42	2.44	4	1
3:A:417:PCW:H11	3:D:611:PCW:H2	0.42	1.91	7	1
4:D:630:17F:H39	4:D:630:17F:H36	0.42	1.59	7	3
3:B:204:PCW:O31	3:B:204:PCW:C5	0.42	2.67	8	1
3:C:206:PCW:H19	3:C:207:PCW:H241	0.42	1.91	8	1
3:A:414:PCW:C24	4:A:415:17F:H59	0.42	2.45	12	1
3:A:403:PCW:H63	3:A:403:PCW:O11	0.42	2.13	13	1
3:D:607:PCW:H211	3:D:607:PCW:H182	0.42	1.59	13	1
3:C:209:PCW:H51	3:C:209:PCW:C11	0.42	2.40	13	1
3:C:211:PCW:H132	4:C:215:17F:H57	0.42	1.90	13	1
1:A:307:ASP:O	1:A:310:ARG:HB2	0.42	2.15	16	2
3:C:206:PCW:C4	4:C:214:17F:H35	0.42	2.45	14	1
3:C:210:PCW:H372	3:C:210:PCW:H142	0.42	1.91	14	1
3:C:205:PCW:H242	3:C:209:PCW:C28	0.42	2.45	15	1
3:D:615:PCW:O4P	3:D:615:PCW:C3	0.42	2.68	17	1
3:B:206:PCW:H141	3:B:206:PCW:H362	0.42	1.91	17	1
2:C:84:ILE:HD12	2:C:123:ARG:CB	0.42	2.44	17	1
3:D:610:PCW:H42	4:D:631:17F:C6	0.42	2.45	18	1
3:C:205:PCW:C44	3:C:212:PCW:H282	0.42	2.45	18	1
3:A:404:PCW:C11	3:B:205:PCW:H451	0.42	2.44	19	1
3:A:406:PCW:H40	3:B:205:PCW:C17	0.42	2.44	20	1
3:D:625:PCW:O31	3:D:625:PCW:O3	0.42	2.37	20	1
3:C:204:PCW:H63	3:C:204:PCW:O4P	0.42	2.15	20	1
3:A:414:PCW:O3	3:A:414:PCW:C31	0.42	2.68	1	1
3:A:421:PCW:H61	4:D:630:17F:C5	0.42	2.45	2	1
1:A:392:GLU:HB3	1:D:591:TYR:HE1	0.42	1.74	3	1
3:C:203:PCW:H211	3:C:203:PCW:H181	0.42	1.54	16	2
4:A:422:17F:H36	4:C:219:17F:H64	0.42	1.91	4	1
1:D:417:GLU:O	1:D:421:PRO:HD2	0.42	2.13	5	1
3:B:207:PCW:H412	3:B:207:PCW:H381	0.42	1.67	5	1
3:C:209:PCW:H451	3:C:212:PCW:C19	0.42	2.45	5	1
4:A:415:17F:O10	4:A:415:17F:C4	0.42	2.55	6	1
3:B:203:PCW:H231	4:B:209:17F:H18A	0.42	1.90	6	1
3:B:204:PCW:H381	3:B:204:PCW:H412	0.42	1.58	13	4
3:D:614:PCW:H282	4:B:209:17F:C12	0.42	2.40	7	1
3:B:208:PCW:H431	3:C:203:PCW:H151	0.42	1.91	7	1
3:C:212:PCW:H422	4:C:215:17F:H10	0.42	1.92	7	1
3:D:603:PCW:C31	3:D:603:PCW:O3	0.42	2.68	8	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
3:C:206:PCW:C35	3:C:208:PCW:H142	0.42	2.44	8	1
3:C:207:PCW:H212	3:C:207:PCW:H181	0.42	1.57	15	2
4:A:416:17F:O1	4:B:209:17F:H18A	0.42	2.14	10	1
3:D:608:PCW:H51	3:D:608:PCW:O3P	0.42	2.14	10	1
3:C:209:PCW:C38	3:C:209:PCW:C42	0.42	2.79	11	1
3:A:402:PCW:H483	4:D:632:17F:H50	0.42	1.91	12	1
3:A:421:PCW:H19	4:D:630:17F:H56	0.42	1.91	12	1
3:D:616:PCW:C16	4:D:632:17F:H11A	0.42	2.42	12	1
3:B:203:PCW:C39	3:C:211:PCW:H421	0.42	2.44	13	1
3:B:204:PCW:H32	3:B:207:PCW:C37	0.42	2.43	13	1
3:A:406:PCW:H421	3:B:205:PCW:H283	0.42	1.91	14	1
3:B:206:PCW:H211	3:B:206:PCW:H182	0.42	1.59	20	2
3:B:208:PCW:H41	3:B:208:PCW:C31	0.42	2.41	14	1
2:C:7:VAL:HG11	2:C:71:TYR:CD2	0.42	2.50	14	1
3:C:206:PCW:H181	3:C:208:PCW:C15	0.42	2.44	14	1
3:A:404:PCW:O2P	3:A:406:PCW:H41	0.42	2.14	15	1
3:D:618:PCW:O3P	3:D:618:PCW:C5	0.42	2.67	15	1
3:D:610:PCW:H171	4:D:631:17F:C34	0.42	2.44	16	1
3:C:206:PCW:H171	3:C:208:PCW:H342	0.42	1.91	16	1
2:C:39:SER:HB2	2:C:41:ARG:NH1	0.42	2.30	17	1
3:C:209:PCW:H51	3:C:209:PCW:O3P	0.42	2.14	17	1
3:A:406:PCW:C38	3:C:204:PCW:C34	0.42	2.91	18	2
3:D:619:PCW:H483	3:B:205:PCW:H242	0.42	1.91	18	1
3:B:204:PCW:O3P	3:B:204:PCW:O31	0.42	2.38	18	1
4:A:422:17F:H36	4:C:219:17F:C37	0.42	2.43	19	1
3:D:601:PCW:O31	3:D:601:PCW:H341	0.42	2.15	20	1
1:D:473:LYS:O	1:D:477:LEU:HB2	0.42	2.15	1	2
3:D:613:PCW:H52	3:D:613:PCW:H322	0.42	1.90	1	1
3:A:414:PCW:H372	4:A:415:17F:H65	0.42	1.92	2	1
1:D:422:VAL:O	1:D:426:PHE:HB2	0.42	2.15	4	1
3:A:410:PCW:H40	3:A:412:PCW:C35	0.42	2.45	5	1
3:A:403:PCW:O31	3:A:403:PCW:H351	0.42	2.15	13	3
1:A:387:LEU:O	1:A:391:GLU:HG3	0.42	2.15	15	3
3:C:203:PCW:H231	3:C:216:PCW:C25	0.42	2.44	8	1
3:D:605:PCW:H182	3:D:605:PCW:H211	0.42	1.56	11	2
3:D:610:PCW:H41	4:D:631:17F:O8	0.42	2.15	12	1
3:C:205:PCW:H212	3:C:209:PCW:H242	0.42	1.90	12	1
3:C:206:PCW:H62	4:C:213:17F:C6	0.42	2.43	12	1
3:D:609:PCW:N	3:D:621:PCW:O11	0.42	2.53	13	1
1:D:508:ARG:O	1:D:512:ASP:HB2	0.42	2.15	14	1
3:D:614:PCW:H471	3:D:620:PCW:C42	0.42	2.45	15	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
3:B:205:PCW:H151	3:C:204:PCW:H321	0.42	1.90	15	1
3:B:206:PCW:C44	3:C:205:PCW:H282	0.42	2.45	15	1
3:C:203:PCW:C45	3:C:210:PCW:H19	0.42	2.45	15	1
1:A:348:GLU:O	1:A:352:LYS:HG3	0.42	2.15	19	1
3:A:412:PCW:H462	3:C:210:PCW:H19	0.42	1.91	19	1
3:D:612:PCW:H481	3:B:203:PCW:H272	0.42	1.91	19	1
3:C:203:PCW:C11	4:C:213:17F:H37	0.42	2.44	19	1
1:A:323:TYR:OH	1:D:454:PRO:HB2	0.42	2.14	20	1
3:A:421:PCW:C6	4:D:630:17F:C4	0.42	2.91	20	1
1:A:319:HIS:CE1	1:D:458:ASP:HB2	0.42	2.49	1	1
3:A:404:PCW:H62	3:A:404:PCW:C37	0.42	2.45	1	1
3:D:606:PCW:H381	3:D:606:PCW:H412	0.42	1.59	11	2
2:C:116:ASN:ND2	5:C:201:GSP:N7	0.42	2.64	5	3
3:C:205:PCW:C40	4:C:215:17F:H8	0.42	2.45	2	1
3:C:207:PCW:H412	4:C:213:17F:C11	0.42	2.44	20	2
3:A:419:PCW:O3P	3:A:419:PCW:O31	0.42	2.38	3	1
3:A:403:PCW:H51	3:A:404:PCW:O3P	0.42	2.15	4	1
4:A:415:17F:O10	4:A:415:17F:H4	0.42	2.15	4	1
4:A:415:17F:C25	3:B:205:PCW:H462	0.42	2.43	4	1
3:A:421:PCW:O31	3:D:618:PCW:C8	0.42	2.66	4	1
3:D:613:PCW:H52	3:D:619:PCW:H31	0.42	1.91	4	2
4:C:213:17F:O10	4:C:213:17F:H4	0.42	2.14	4	1
3:A:420:PCW:H371	3:D:611:PCW:H161	0.42	1.90	5	1
1:D:522:SER:O	1:D:526:ARG:HG3	0.42	2.15	10	4
3:D:602:PCW:H52	4:C:214:17F:C19	0.42	2.40	5	1
3:B:203:PCW:C8	4:C:215:17F:O5	0.42	2.67	5	1
2:B:15:GLY:HA2	5:B:201:GSP:O1A	0.42	2.15	6	1
3:A:407:PCW:C1	3:A:412:PCW:C7	0.42	2.98	7	1
2:C:6:LEU:HD12	2:C:55:ILE:HG12	0.42	1.90	8	1
3:C:207:PCW:H422	4:C:213:17F:C1Y	0.42	2.45	8	1
3:C:212:PCW:H441	4:C:215:17F:C2X	0.42	2.45	9	1
3:D:615:PCW:H381	3:D:615:PCW:H411	0.42	1.52	10	2
3:D:626:PCW:O2	3:D:626:PCW:O2P	0.42	2.38	10	1
3:C:205:PCW:H181	3:C:205:PCW:H212	0.42	1.64	15	2
3:D:605:PCW:H252	3:D:614:PCW:H412	0.42	1.91	11	1
3:C:210:PCW:C35	3:C:210:PCW:C31	0.42	2.98	11	1
1:A:235:GLU:HG3	1:D:539:ASN:ND2	0.42	2.30	13	1
1:D:427:TRP:O	1:D:431:GLU:HG3	0.42	2.15	13	1
3:A:406:PCW:P	3:B:205:PCW:H372	0.42	2.54	14	1
3:A:407:PCW:H332	3:A:410:PCW:C37	0.42	2.43	14	1
1:D:521:TYR:HA	1:D:524:GLU:OE1	0.42	2.14	14	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
3:D:612:PCW:C1	3:D:620:PCW:H63	0.42	2.43	14	1
3:B:204:PCW:H2	3:B:204:PCW:H73	0.42	1.92	14	1
3:A:418:PCW:H411	3:D:613:PCW:H172	0.42	1.92	17	1
3:D:619:PCW:C41	4:D:631:17F:H45	0.42	2.15	17	1
2:B:46:ILE:HB	2:B:51:CYS:SG	0.42	2.55	17	1
3:C:211:PCW:H283	4:C:215:17F:H51	0.42	1.92	17	1
3:C:212:PCW:H351	4:C:215:17F:H32	0.42	1.91	17	1
3:B:205:PCW:O2P	3:B:205:PCW:H51	0.42	2.15	19	1
3:C:204:PCW:H411	3:C:204:PCW:H382	0.42	1.56	19	1
3:A:403:PCW:H351	3:A:403:PCW:O31	0.42	2.14	20	1
3:A:403:PCW:H211	3:A:403:PCW:H181	0.42	1.72	20	1
3:A:409:PCW:O31	3:A:409:PCW:O3	0.42	2.37	20	1
4:A:422:17F:H54	3:D:606:PCW:C21	0.41	2.41	1	1
1:A:233:GLU:O	1:A:237:GLU:HB2	0.41	2.15	20	3
4:C:219:17F:H20	4:C:219:17F:H11	0.41	1.91	2	1
1:D:588:LEU:HD22	4:D:630:17F:H50	0.41	1.91	20	2
3:D:602:PCW:H461	3:D:608:PCW:C47	0.41	2.40	3	1
2:C:149:ARG:O	2:C:149:ARG:HG3	0.41	2.14	3	1
3:A:411:PCW:O3P	4:B:211:17F:H4A	0.41	2.14	4	1
1:A:214:PHE:CE1	3:A:405:PCW:H162	0.41	2.50	6	1
3:B:208:PCW:O1P	3:B:208:PCW:H51	0.41	2.13	6	1
3:A:401:PCW:H422	3:B:207:PCW:C47	0.41	2.38	8	1
3:A:414:PCW:H262	4:B:209:17F:H37	0.41	1.91	8	1
3:A:418:PCW:H141	3:D:618:PCW:C48	0.41	2.45	8	1
1:D:589:GLU:O	1:D:593:LYS:HG3	0.41	2.14	8	1
2:C:41:ARG:HD2	2:C:54:ASP:OD2	0.41	2.15	8	1
3:C:207:PCW:C6	3:C:207:PCW:C13	0.41	2.98	8	1
2:C:97:ARG:NH1	2:C:101:LYS:HE2	0.41	2.30	9	1
3:A:405:PCW:H51	3:A:406:PCW:H132	0.41	1.91	11	1
3:D:608:PCW:H421	3:C:205:PCW:C28	0.41	2.45	12	1
3:C:205:PCW:C31	3:C:205:PCW:O2P	0.41	2.68	12	1
4:A:422:17F:H48	4:C:218:17F:C12	0.41	2.45	13	1
2:B:117:LYS:HE2	5:B:201:GSP:C5	0.41	2.50	13	1
2:C:62:GLU:O	2:C:63:GLU:HB3	0.41	2.15	13	1
3:D:612:PCW:O1P	3:D:624:PCW:C7	0.41	2.68	14	1
3:C:205:PCW:H452	4:C:215:17F:H10A	0.41	1.92	15	1
3:D:601:PCW:C39	4:D:628:17F:C30	0.41	2.97	16	1
3:D:604:PCW:C47	3:D:626:PCW:H282	0.41	2.44	16	1
3:D:619:PCW:H361	3:D:627:PCW:H161	0.41	1.92	16	1
3:B:207:PCW:C44	4:B:210:17F:H55	0.41	2.44	16	1
3:D:609:PCW:H381	3:C:208:PCW:C28	0.41	2.45	17	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
3:D:601:PCW:O31	3:D:601:PCW:O3	0.41	2.38	18	1
3:D:610:PCW:C15	4:D:631:17F:C33	0.41	2.98	19	1
3:B:203:PCW:C46	4:C:215:17F:H47	0.41	2.45	19	1
3:A:405:PCW:C6	3:A:406:PCW:O11	0.41	2.66	20	1
3:A:406:PCW:H11	3:A:406:PCW:C4	0.41	2.35	20	1
3:C:206:PCW:C13	3:C:207:PCW:C19	0.41	2.96	20	1
3:A:413:PCW:O3P	3:C:210:PCW:H11	0.41	2.15	2	1
4:B:210:17F:C3	4:C:215:17F:H6	0.41	2.45	2	1
3:C:205:PCW:C38	3:C:212:PCW:C22	0.41	2.96	2	1
2:B:99:GLN:O	2:B:103:VAL:HG23	0.41	2.15	3	3
2:B:127:THR:HG23	2:B:141:PHE:HE2	0.41	1.76	3	2
1:A:324:SER:HA	1:A:327:LEU:HD12	0.41	1.91	4	1
3:A:404:PCW:C35	4:A:415:17F:H9A	0.41	2.46	4	1
3:D:609:PCW:O1P	4:D:632:17F:H18A	0.41	2.15	4	1
3:C:208:PCW:C23	4:C:214:17F:H55	0.41	2.35	4	1
1:A:351:ALA:O	1:A:355:GLU:HG2	0.41	2.15	6	1
3:D:614:PCW:H241	4:B:209:17F:C39	0.41	2.43	6	1
3:B:203:PCW:H51	3:C:211:PCW:O31	0.41	2.14	6	1
3:D:601:PCW:H51	3:C:209:PCW:C7	0.41	2.44	7	1
3:D:617:PCW:H482	3:C:210:PCW:H281	0.41	1.92	7	1
1:A:396:LYS:HE2	1:D:587:ALA:CA	0.41	2.45	9	1
3:D:615:PCW:O1P	3:D:615:PCW:C5	0.41	2.64	9	1
3:B:206:PCW:O4P	3:B:206:PCW:C7	0.41	2.67	10	1
1:A:240:ARG:O	1:A:243:MET:HB3	0.41	2.15	11	1
3:A:406:PCW:H142	4:B:211:17F:O10	0.41	2.15	11	1
1:D:453:GLN:HB2	1:D:454:PRO:HD3	0.41	1.91	12	2
3:D:617:PCW:H371	3:D:619:PCW:H122	0.41	1.92	13	1
3:B:204:PCW:H32	3:B:207:PCW:C35	0.41	2.43	13	1
3:D:609:PCW:H62	4:D:632:17F:O2	0.41	2.15	14	1
2:B:15:GLY:HA3	2:B:116:ASN:ND2	0.41	2.30	14	1
2:C:79:LEU:HD12	2:C:112:VAL:HB	0.41	1.93	14	1
3:C:209:PCW:C42	3:C:212:PCW:H283	0.41	2.45	15	1
4:A:422:17F:O1	4:A:422:17F:H5	0.41	2.15	16	1
2:C:68:ARG:HA	2:C:71:TYR:CD2	0.41	2.50	16	1
3:C:207:PCW:H421	4:C:213:17F:H63	0.41	1.92	16	1
3:A:414:PCW:C34	4:A:415:17F:C32	0.41	2.98	17	1
3:D:605:PCW:H121	3:D:614:PCW:O11	0.41	2.15	17	1
3:D:612:PCW:O3	3:D:612:PCW:C31	0.41	2.68	17	1
4:B:211:17F:H30	4:B:211:17F:C36	0.41	2.37	17	1
2:B:41:ARG:HD2	2:B:54:ASP:OD2	0.41	2.15	18	1
2:B:25:GLN:HB3	2:B:27:HIS:HD2	0.41	1.75	19	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
3:D:602:PCW:C26	4:D:629:17F:H76	0.41	2.43	20	1
3:A:420:PCW:C36	3:D:618:PCW:H431	0.41	2.45	1	1
4:D:628:17F:H35	4:D:628:17F:H39	0.41	1.62	1	1
3:A:410:PCW:H171	3:A:410:PCW:H212	0.41	1.93	2	1
4:D:631:17F:H53	3:C:210:PCW:H272	0.41	1.92	2	1
4:B:209:17F:H58	4:B:209:17F:H64	0.41	1.91	2	1
3:C:205:PCW:C38	3:C:212:PCW:H221	0.41	2.45	2	1
3:C:204:PCW:H211	3:C:216:PCW:H281	0.41	1.91	3	1
3:C:206:PCW:C5	4:C:213:17F:O1	0.41	2.69	20	2
3:C:209:PCW:H162	4:C:214:17F:H8A	0.41	1.89	3	1
3:A:419:PCW:H412	3:A:419:PCW:H382	0.41	1.56	4	1
3:B:204:PCW:O3	3:B:207:PCW:H371	0.41	2.16	4	1
4:B:211:17F:H59	4:B:211:17F:H62	0.41	1.56	8	2
3:C:211:PCW:H73	3:C:211:PCW:O1P	0.41	2.15	4	1
3:A:411:PCW:O2P	4:B:211:17F:N1	0.41	2.39	5	2
3:B:206:PCW:H182	3:B:206:PCW:H211	0.41	1.59	7	1
4:B:210:17F:H35	4:C:215:17F:H8	0.41	1.93	9	1
3:C:207:PCW:H422	4:C:213:17F:H12	0.41	1.91	9	1
3:A:410:PCW:H283	4:A:422:17F:C42	0.41	2.45	10	1
1:D:565:ALA:O	1:D:569:LEU:HB2	0.41	2.16	11	1
3:D:614:PCW:H2	3:D:614:PCW:O11	0.41	2.15	11	1
3:B:205:PCW:H221	3:C:210:PCW:H283	0.41	1.92	11	1
2:C:79:LEU:HG	2:C:81:VAL:HG23	0.41	1.92	12	1
3:C:212:PCW:O3P	3:C:212:PCW:C8	0.41	2.65	12	1
4:A:416:17F:C42	4:B:209:17F:H78	0.41	2.42	13	1
3:B:208:PCW:H12	3:C:211:PCW:H351	0.41	1.92	13	1
3:C:211:PCW:C15	4:C:215:17F:H58	0.41	2.44	13	1
3:A:408:PCW:H472	3:A:413:PCW:H251	0.41	1.91	14	1
3:A:414:PCW:C6	4:B:209:17F:O5	0.41	2.68	14	1
3:A:421:PCW:H442	3:D:618:PCW:H211	0.41	1.91	14	1
4:D:632:17F:H52	3:C:208:PCW:H152	0.41	1.92	14	1
3:C:206:PCW:H172	3:C:208:PCW:C34	0.41	2.44	14	1
3:A:406:PCW:H271	4:B:211:17F:C33	0.41	2.45	15	1
3:B:204:PCW:H432	4:B:210:17F:H19A	0.41	1.91	15	1
2:C:28:PHE:HZ	5:C:201:GSP:C2	0.41	2.34	15	1
3:D:624:PCW:H412	3:D:624:PCW:H382	0.41	1.69	17	2
3:C:217:PCW:H181	4:C:219:17F:C1X	0.41	2.44	16	1
1:A:323:TYR:O	1:A:327:LEU:HG	0.41	2.16	17	1
3:D:601:PCW:H451	3:D:601:PCW:H152	0.41	1.91	17	1
3:A:414:PCW:O31	3:A:414:PCW:O3P	0.41	2.37	18	1
3:D:608:PCW:H431	4:D:628:17F:H33	0.41	1.90	18	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
3:C:209:PCW:C13	4:C:214:17F:O7	0.41	2.68	18	1
3:D:613:PCW:H61	3:D:627:PCW:H32	0.41	1.92	19	1
3:A:411:PCW:H121	3:A:411:PCW:H341	0.41	1.92	20	1
4:A:416:17F:H35	4:A:416:17F:H39	0.41	1.60	20	1
1:D:488:LYS:O	1:D:492:LEU:HG	0.41	2.15	1	1
3:B:207:PCW:H162	3:B:207:PCW:C34	0.41	2.44	1	1
3:D:617:PCW:C47	3:C:216:PCW:H242	0.41	2.44	4	1
3:B:206:PCW:O3	3:B:206:PCW:C31	0.41	2.69	4	2
3:A:409:PCW:O4P	3:A:409:PCW:C8	0.41	2.68	5	2
3:D:610:PCW:H342	3:D:610:PCW:O31	0.41	2.14	11	2
3:C:206:PCW:C21	3:C:208:PCW:H411	0.41	2.46	5	1
3:A:405:PCW:H212	3:A:405:PCW:H181	0.41	1.71	6	1
3:D:611:PCW:O2	3:D:611:PCW:C11	0.41	2.68	12	3
3:B:208:PCW:H452	3:C:203:PCW:C16	0.41	2.44	6	1
3:C:205:PCW:C8	3:C:212:PCW:O2P	0.41	2.69	6	1
3:A:409:PCW:H372	3:B:206:PCW:H411	0.41	1.93	7	1
4:A:416:17F:C28	3:D:605:PCW:H281	0.41	2.45	7	1
3:C:206:PCW:H152	3:C:207:PCW:H162	0.41	1.92	7	1
3:C:211:PCW:H212	3:C:211:PCW:H181	0.41	1.72	7	1
3:A:411:PCW:H262	3:C:210:PCW:H222	0.41	1.92	8	1
3:D:624:PCW:H272	3:C:217:PCW:H262	0.41	1.92	8	1
3:A:406:PCW:H252	4:B:211:17F:C34	0.41	2.46	9	1
1:A:217:LEU:CD1	3:A:405:PCW:H251	0.41	2.46	10	1
1:A:237:GLU:HG2	1:A:241:GLN:NE2	0.41	2.30	10	1
3:A:421:PCW:O31	3:A:421:PCW:H341	0.41	2.15	10	1
3:A:421:PCW:O31	3:A:421:PCW:P	0.41	2.78	10	1
3:D:622:PCW:O3P	3:D:622:PCW:C31	0.41	2.68	11	1
3:D:617:PCW:O1P	3:C:216:PCW:H73	0.41	2.16	12	1
3:B:204:PCW:O31	3:B:204:PCW:H52	0.41	2.14	14	1
3:C:209:PCW:H162	4:C:214:17F:C11	0.41	2.32	14	1
3:A:404:PCW:C22	3:A:404:PCW:C18	0.41	2.62	17	2
3:A:410:PCW:H252	4:A:422:17F:H76	0.41	1.91	15	1
3:C:209:PCW:H211	3:C:209:PCW:C17	0.41	2.40	15	1
3:D:622:PCW:O11	3:D:622:PCW:H2	0.41	2.14	16	1
3:A:401:PCW:C47	3:D:612:PCW:H262	0.41	2.39	17	1
3:A:411:PCW:H122	3:A:411:PCW:H362	0.41	1.93	17	1
3:D:604:PCW:C25	4:C:215:17F:H75	0.41	2.44	17	1
1:D:525:LEU:O	1:D:529:LEU:HG	0.41	2.15	18	1
2:C:64:TYR:O	2:C:68:ARG:HB2	0.41	2.16	18	1
3:C:211:PCW:H232	4:C:215:17F:C29	0.41	2.42	18	1
3:D:603:PCW:C8	3:D:603:PCW:H132	0.41	2.45	19	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
3:A:406:PCW:H342	4:B:211:17F:H8A	0.41	1.92	20	1
3:D:612:PCW:H41	3:D:623:PCW:C33	0.41	2.46	20	1
3:A:402:PCW:H441	3:C:208:PCW:H172	0.41	1.90	1	1
3:C:206:PCW:O4P	4:C:214:17F:H10A	0.41	2.16	1	1
1:A:214:PHE:HE1	3:A:405:PCW:H162	0.41	1.75	2	1
3:A:406:PCW:H331	4:B:211:17F:C9	0.41	2.44	2	1
3:D:606:PCW:H261	4:C:219:17F:H78	0.41	1.93	2	1
3:B:204:PCW:H62	3:B:204:PCW:O31	0.41	2.14	2	1
3:A:406:PCW:C34	3:B:205:PCW:H342	0.41	2.43	4	2
3:A:420:PCW:C12	3:D:618:PCW:H451	0.41	2.37	3	1
3:D:602:PCW:C26	4:D:629:17F:C42	0.41	2.98	3	1
3:B:208:PCW:O4P	3:B:208:PCW:C2	0.41	2.68	3	1
3:D:623:PCW:C11	3:D:623:PCW:O2	0.41	2.69	4	1
3:D:623:PCW:O11	3:D:623:PCW:O2	0.41	2.38	4	1
4:C:215:17F:O8	4:C:215:17F:O9	0.41	2.39	4	1
3:A:417:PCW:H452	3:A:421:PCW:H422	0.41	1.91	5	1
3:A:407:PCW:C40	3:A:407:PCW:C18	0.41	2.98	6	1
4:A:422:17F:C36	4:D:632:17F:H68	0.41	2.45	6	1
4:A:422:17F:H65	4:D:632:17F:H72	0.41	1.93	8	1
3:B:208:PCW:H212	3:C:211:PCW:C48	0.41	2.46	8	1
3:C:216:PCW:O4P	3:C:216:PCW:C8	0.41	2.68	9	3
3:A:419:PCW:H483	3:C:212:PCW:H283	0.41	1.93	9	1
3:A:410:PCW:H212	3:A:410:PCW:H181	0.41	1.65	10	1
3:D:610:PCW:H283	4:D:631:17F:C40	0.41	2.45	10	1
3:D:612:PCW:H39	3:D:623:PCW:H452	0.41	1.91	10	1
3:B:205:PCW:H31	4:B:211:17F:O3	0.41	2.15	10	1
3:A:409:PCW:C2	4:B:210:17F:H31	0.41	2.44	11	1
3:D:610:PCW:H381	3:D:610:PCW:H412	0.41	1.72	11	1
3:D:623:PCW:H212	3:D:623:PCW:H182	0.41	1.64	12	2
1:A:323:TYR:O	1:A:327:LEU:HB2	0.41	2.15	13	1
4:B:209:17F:O10	4:B:209:17F:C20	0.41	2.68	13	1
4:B:210:17F:H40	4:B:210:17F:H36	0.41	1.65	14	1
3:A:403:PCW:H321	3:A:406:PCW:C4	0.41	2.45	15	1
4:C:215:17F:H65	4:C:215:17F:C2X	0.41	2.45	15	1
3:A:414:PCW:H161	4:A:415:17F:H33	0.41	1.92	16	1
3:D:601:PCW:O3	3:D:601:PCW:C31	0.41	2.68	16	1
3:D:622:PCW:H221	4:D:631:17F:H31	0.41	1.93	16	1
3:D:627:PCW:C18	3:D:627:PCW:C22	0.41	2.99	16	1
3:C:207:PCW:H122	4:C:213:17F:C18	0.41	2.44	16	1
3:A:410:PCW:C39	3:A:412:PCW:H351	0.41	2.44	18	1
3:A:411:PCW:C4	4:B:211:17F:H1A	0.41	2.46	18	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
4:A:416:17F:O5	3:B:204:PCW:N	0.41	2.53	18	1
3:B:208:PCW:H421	3:C:216:PCW:H283	0.41	1.91	18	1
3:C:205:PCW:C11	3:C:212:PCW:H19	0.41	2.45	19	1
3:A:403:PCW:H362	3:A:403:PCW:O2	0.41	2.12	1	2
3:A:406:PCW:C14	4:B:211:17F:C35	0.41	2.97	1	1
3:A:406:PCW:C28	3:D:619:PCW:H211	0.41	2.46	1	1
3:D:604:PCW:C28	4:C:213:17F:H51	0.41	2.42	1	1
3:D:617:PCW:H211	3:D:617:PCW:H181	0.41	1.67	1	1
3:D:617:PCW:O3	3:D:617:PCW:O31	0.41	2.37	7	4
4:C:218:17F:H11	4:C:219:17F:H8	0.41	1.93	2	1
3:A:403:PCW:C3	3:A:403:PCW:P	0.41	3.08	4	2
3:A:414:PCW:C3	3:A:414:PCW:H351	0.41	2.46	5	1
3:D:624:PCW:C7	3:D:624:PCW:O31	0.41	2.69	6	1
3:B:203:PCW:O4P	3:B:203:PCW:C8	0.41	2.68	6	2
3:D:606:PCW:H412	3:D:606:PCW:H381	0.41	1.54	17	3
3:B:207:PCW:H61	4:B:210:17F:O7	0.41	2.16	7	1
2:C:15:GLY:CA	5:C:201:GSP:H8	0.41	2.29	7	1
3:A:408:PCW:C17	3:A:408:PCW:C23	0.41	2.98	8	1
3:D:604:PCW:H251	4:C:215:17F:C30	0.41	2.46	8	1
3:D:617:PCW:H341	3:C:216:PCW:H351	0.41	1.93	9	1
3:D:618:PCW:C2	3:D:618:PCW:O11	0.41	2.56	9	1
3:D:620:PCW:H131	3:D:620:PCW:H162	0.41	1.72	9	1
3:D:612:PCW:C39	3:D:623:PCW:H461	0.41	2.43	10	1
2:B:118:CYS:SG	2:B:143:GLU:HB3	0.41	2.55	10	1
3:B:205:PCW:H31	4:B:211:17F:C4	0.41	2.46	10	1
3:C:203:PCW:O1P	3:C:211:PCW:H41	0.41	2.16	10	1
3:A:406:PCW:C33	4:B:211:17F:O7	0.41	2.67	11	1
3:C:206:PCW:H82	4:C:214:17F:H10	0.41	1.93	11	1
3:D:609:PCW:H411	3:D:609:PCW:H382	0.41	1.68	12	1
3:D:617:PCW:O1P	3:C:216:PCW:C4	0.41	2.64	12	1
3:D:621:PCW:C7	3:D:621:PCW:C3	0.41	2.99	12	1
3:A:411:PCW:H241	3:A:413:PCW:C40	0.41	2.45	13	1
4:D:632:17F:H63	4:D:632:17F:H58	0.41	1.63	20	2
3:B:205:PCW:H31	4:B:211:17F:C6	0.41	2.45	13	1
2:B:15:GLY:HA3	2:B:116:ASN:HD22	0.41	1.75	14	1
3:D:606:PCW:H232	4:C:218:17F:C21	0.41	2.46	15	1
2:B:15:GLY:CA	5:B:201:GSP:H8	0.41	2.29	15	1
3:A:409:PCW:H412	3:A:419:PCW:H222	0.41	1.91	16	1
4:B:210:17F:C1X	4:C:215:17F:H37	0.41	2.46	19	1
3:A:403:PCW:H181	3:A:403:PCW:H211	0.41	1.62	2	1
3:A:404:PCW:H62	3:B:205:PCW:C39	0.41	2.45	2	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
4:B:210:17F:HN1	3:C:212:PCW:C11	0.41	2.27	2	1
3:C:205:PCW:C13	3:C:209:PCW:H151	0.41	2.46	4	1
3:C:208:PCW:H51	3:C:208:PCW:C32	0.41	2.43	4	1
3:D:609:PCW:C41	3:D:616:PCW:H441	0.41	2.45	5	1
3:D:627:PCW:O1P	3:D:627:PCW:H2	0.41	2.16	5	1
3:C:204:PCW:H272	3:C:217:PCW:C43	0.41	2.45	7	1
3:C:211:PCW:H51	3:C:211:PCW:O1P	0.41	2.16	7	1
3:A:403:PCW:H182	3:A:403:PCW:H211	0.41	1.61	8	1
3:A:405:PCW:O3	3:A:405:PCW:C31	0.41	2.67	8	1
3:D:603:PCW:H162	3:D:624:PCW:H221	0.41	1.92	8	1
3:D:617:PCW:O2P	3:C:216:PCW:H73	0.41	2.15	8	1
3:D:625:PCW:O31	3:D:625:PCW:C4	0.41	2.62	9	1
2:C:16:LYS:HG3	5:C:201:GSP:O1B	0.41	2.16	9	1
3:C:205:PCW:H63	4:C:214:17F:C9	0.41	2.45	9	1
3:A:409:PCW:H472	3:A:409:PCW:C28	0.41	2.46	10	1
3:D:623:PCW:H412	3:D:625:PCW:H212	0.41	1.91	10	1
2:B:41:ARG:HA	2:B:53:LEU:O	0.41	2.15	10	1
3:C:211:PCW:C15	4:C:215:17F:C33	0.41	2.93	12	1
3:D:614:PCW:H251	4:B:209:17F:H50	0.41	1.93	13	1
3:A:420:PCW:H451	3:D:611:PCW:C23	0.41	2.46	14	1
1:D:460:GLN:O	1:D:464:GLN:HB2	0.41	2.15	14	1
3:B:204:PCW:H381	3:B:204:PCW:H422	0.41	1.93	15	1
3:C:206:PCW:H142	3:C:208:PCW:H131	0.41	1.93	15	1
3:A:403:PCW:H411	3:A:403:PCW:H381	0.41	1.57	16	1
4:A:422:17F:H43	4:C:219:17F:H66	0.41	1.90	16	1
3:D:619:PCW:H342	3:D:627:PCW:H342	0.41	1.93	16	1
3:D:618:PCW:O31	3:D:618:PCW:C6	0.41	2.68	19	2
3:D:616:PCW:H431	4:C:214:17F:H54	0.41	1.93	19	1
4:C:215:17F:H62	4:C:215:17F:H59	0.41	1.71	19	1
3:D:611:PCW:O3	3:D:611:PCW:C31	0.41	2.68	20	1
3:C:207:PCW:H281	4:C:214:17F:C24	0.41	2.44	20	1
4:A:415:17F:H36	4:A:415:17F:H39	0.41	1.72	1	1
3:C:206:PCW:H241	3:C:208:PCW:C43	0.41	2.45	1	1
3:D:612:PCW:C3	3:D:620:PCW:C11	0.41	2.96	2	1
3:C:209:PCW:H31	4:C:214:17F:HN1	0.41	1.73	2	1
3:A:414:PCW:C14	4:A:415:17F:H59	0.41	2.43	3	1
3:D:609:PCW:H442	3:D:616:PCW:C48	0.41	2.46	3	1
3:A:420:PCW:H461	3:D:617:PCW:H271	0.41	1.91	5	1
3:D:608:PCW:H20	4:D:629:17F:C27	0.41	2.45	5	1
3:C:203:PCW:C33	3:C:204:PCW:O2P	0.41	2.69	5	1
4:A:416:17F:H62	4:A:416:17F:H59	0.41	1.73	6	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
4:B:210:17F:H78	3:C:209:PCW:C44	0.41	2.34	6	1
3:C:209:PCW:H451	3:C:212:PCW:C43	0.41	2.40	6	1
3:D:605:PCW:C31	3:D:614:PCW:H51	0.41	2.42	7	1
1:A:371:LEU:O	1:A:375:LEU:HG	0.41	2.15	8	1
3:A:402:PCW:H441	3:C:208:PCW:H141	0.41	1.92	8	1
3:C:207:PCW:O11	3:C:207:PCW:C6	0.41	2.69	8	1
3:B:208:PCW:C42	3:C:216:PCW:H271	0.41	2.38	9	1
4:B:211:17F:H10	4:B:211:17F:H59	0.41	1.92	9	1
3:A:418:PCW:H381	3:A:418:PCW:H411	0.41	1.57	10	1
3:D:609:PCW:H431	3:C:208:PCW:C23	0.41	2.46	10	1
3:D:623:PCW:H381	3:D:623:PCW:H411	0.41	1.56	10	1
3:A:403:PCW:H412	3:A:403:PCW:C21	0.41	2.42	11	1
3:B:207:PCW:C11	3:B:207:PCW:O2	0.41	2.68	11	1
2:B:152:VAL:HG12	2:B:156:PHE:CE2	0.41	2.50	13	1
3:B:207:PCW:C3	3:B:207:PCW:P	0.41	3.09	13	1
3:B:206:PCW:C12	3:C:209:PCW:H331	0.41	2.46	14	1
3:B:204:PCW:H452	4:B:210:17F:H32	0.41	1.93	15	1
4:B:210:17F:H62	4:B:210:17F:H59	0.41	1.57	15	2
3:C:212:PCW:H451	4:C:215:17F:H68	0.41	1.93	15	1
3:D:620:PCW:O31	3:D:620:PCW:H11	0.41	2.15	17	1
3:C:212:PCW:C42	4:C:215:17F:H10	0.41	2.43	17	1
2:B:32:TYR:CD1	5:B:201:GSP:C5'	0.41	3.03	18	1
3:B:203:PCW:C5	3:C:211:PCW:H352	0.41	2.46	18	1
3:B:208:PCW:O4P	3:B:208:PCW:C8	0.41	2.69	18	1
4:B:209:17F:O7	4:B:209:17F:C17	0.41	2.69	19	1
4:C:214:17F:H36	4:C:214:17F:H39	0.41	1.60	19	1
4:A:416:17F:C31	3:B:204:PCW:H141	0.41	2.43	20	1
3:A:407:PCW:O31	3:A:407:PCW:H41	0.41	2.15	1	1
3:A:408:PCW:H222	3:A:413:PCW:H432	0.41	1.91	1	1
3:D:627:PCW:C20	3:C:217:PCW:H321	0.41	2.39	1	1
3:C:211:PCW:H262	4:C:215:17F:C30	0.41	2.46	1	1
4:C:213:17F:H39	4:C:213:17F:H36	0.41	1.69	1	1
3:C:216:PCW:H331	3:C:216:PCW:H131	0.41	1.90	1	1
3:A:404:PCW:H121	3:B:205:PCW:C44	0.41	2.37	2	1
3:D:617:PCW:O1P	3:D:617:PCW:C5	0.41	2.66	2	1
3:B:204:PCW:H412	3:B:204:PCW:H381	0.41	1.71	2	1
3:C:203:PCW:H51	4:C:213:17F:O8	0.41	2.15	2	1
3:A:406:PCW:C47	4:B:211:17F:H57	0.41	2.46	3	1
2:C:17:SER:N	5:C:201:GSP:O2B	0.41	2.53	3	1
3:A:418:PCW:C35	3:D:613:PCW:C15	0.41	2.93	4	1
3:D:605:PCW:H472	3:D:620:PCW:C43	0.41	2.44	4	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
3:C:203:PCW:C8	3:C:211:PCW:O2P	0.41	2.68	4	1
3:A:414:PCW:H483	4:B:209:17F:H12A	0.41	1.91	5	1
3:A:401:PCW:C45	3:D:615:PCW:H262	0.41	2.40	6	1
3:D:614:PCW:H31	3:D:620:PCW:C2	0.41	2.43	6	1
3:B:208:PCW:C48	3:C:203:PCW:H232	0.41	2.46	6	1
3:C:209:PCW:O2P	3:C:209:PCW:H31	0.41	2.16	6	1
3:A:408:PCW:C6	3:A:408:PCW:P	0.41	3.09	7	1
3:D:606:PCW:H331	3:D:608:PCW:C6	0.41	2.43	7	1
3:C:206:PCW:H251	3:C:208:PCW:H381	0.41	1.93	7	1
3:A:411:PCW:H211	3:A:411:PCW:H181	0.41	1.58	8	1
3:D:622:PCW:H371	4:D:631:17F:C35	0.41	2.39	20	2
3:A:401:PCW:O2	3:B:207:PCW:C23	0.41	2.67	9	1
3:A:409:PCW:C14	3:A:409:PCW:C18	0.41	2.97	15	2
3:A:413:PCW:H212	3:A:413:PCW:H181	0.41	1.62	11	2
3:A:420:PCW:H482	3:D:619:PCW:C28	0.41	2.46	9	1
3:C:212:PCW:H321	4:C:215:17F:O2	0.41	2.16	9	1
1:A:297:LYS:HB3	1:A:301:LEU:HD12	0.41	1.92	10	1
3:A:408:PCW:H41	3:A:413:PCW:C1	0.41	2.26	10	1
3:A:421:PCW:H221	4:D:630:17F:H19A	0.41	1.92	10	1
2:C:17:SER:HB2	5:C:201:GSP:O2A	0.41	2.16	10	1
3:D:627:PCW:H241	3:C:216:PCW:C43	0.41	2.42	11	1
4:D:628:17F:H39	4:D:628:17F:H35	0.41	1.75	11	1
3:C:211:PCW:H152	4:C:215:17F:C34	0.41	2.45	12	1
4:C:215:17F:H52	4:C:215:17F:H77	0.41	1.91	12	1
3:D:610:PCW:C6	4:D:631:17F:O8	0.41	2.69	13	1
3:B:204:PCW:C7	3:B:204:PCW:C11	0.41	2.98	13	1
3:C:206:PCW:O4P	3:C:206:PCW:C8	0.41	2.68	13	2
1:D:463:TRP:HE1	4:D:629:17F:H77	0.41	1.76	14	1
1:D:555:LEU:HA	1:D:558:LEU:HD12	0.41	1.92	14	1
3:D:601:PCW:H381	3:D:601:PCW:H412	0.41	1.69	14	2
3:C:204:PCW:C25	3:C:217:PCW:H441	0.41	2.42	14	1
1:D:517:HIS:O	1:D:521:TYR:HB2	0.41	2.15	15	2
3:D:601:PCW:H451	3:D:601:PCW:C15	0.41	2.46	15	1
3:D:609:PCW:O31	3:D:616:PCW:C6	0.41	2.69	15	1
3:B:208:PCW:H82	3:C:204:PCW:H12	0.41	1.92	15	1
2:C:137:TYR:HB2	2:C:139:ILE:HG12	0.41	1.92	15	1
3:A:402:PCW:C43	3:C:206:PCW:H262	0.41	2.45	16	1
3:A:406:PCW:H19	4:B:211:17F:H18	0.41	1.93	17	1
3:D:601:PCW:H471	3:D:601:PCW:H132	0.41	1.93	17	1
3:D:602:PCW:H412	4:C:214:17F:H68	0.41	1.91	17	1
3:D:603:PCW:C44	3:D:611:PCW:H351	0.41	2.41	17	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
3:D:604:PCW:H232	4:C:215:17F:H76	0.41	1.91	17	1
3:B:206:PCW:H411	3:C:209:PCW:H40	0.41	1.92	17	1
3:C:206:PCW:C8	3:C:212:PCW:O2	0.41	2.69	17	1
3:D:606:PCW:O31	3:D:606:PCW:P	0.41	2.79	18	1
3:D:610:PCW:H52	3:D:610:PCW:O1P	0.41	2.16	18	1
3:B:206:PCW:H82	3:C:205:PCW:C34	0.41	2.40	18	1
3:A:402:PCW:C37	3:C:208:PCW:H12	0.41	2.46	19	1
3:A:403:PCW:C20	3:A:404:PCW:C25	0.41	2.98	19	1
3:D:603:PCW:O2P	4:C:219:17F:H1A	0.41	2.16	19	1
3:D:604:PCW:H431	3:D:606:PCW:H181	0.41	1.92	19	1
4:D:630:17F:O10	4:D:630:17F:C20	0.41	2.68	19	1
3:B:204:PCW:O31	3:B:204:PCW:C4	0.41	2.69	19	1
3:B:204:PCW:H121	3:B:207:PCW:H411	0.41	1.92	19	1
3:C:205:PCW:H472	4:C:215:17F:C22	0.41	2.46	19	1
3:A:408:PCW:H171	3:A:411:PCW:C21	0.41	2.46	20	1
3:A:414:PCW:H352	4:A:415:17F:C35	0.41	2.46	20	1
3:C:203:PCW:C18	3:C:203:PCW:C22	0.41	2.93	20	1
3:A:418:PCW:H161	3:D:618:PCW:H483	0.41	1.93	1	1
3:D:611:PCW:O31	3:D:611:PCW:H341	0.41	2.15	1	1
4:A:415:17F:H12	4:B:209:17F:C4	0.41	2.46	2	1
2:C:6:LEU:HD13	2:C:159:LEU:HD23	0.41	1.91	2	1
3:C:210:PCW:H121	3:C:210:PCW:C36	0.41	2.45	2	1
3:D:616:PCW:H271	4:C:214:17F:H75	0.41	1.93	3	1
3:D:607:PCW:H40	3:D:626:PCW:C25	0.41	2.46	4	1
3:D:623:PCW:C12	3:D:624:PCW:C35	0.41	2.98	4	1
4:A:422:17F:C1X	4:C:218:17F:H68	0.41	2.34	5	1
3:D:601:PCW:O3P	3:D:601:PCW:C31	0.41	2.69	5	1
3:B:203:PCW:C28	4:B:209:17F:H73	0.41	2.46	5	1
3:B:208:PCW:H461	3:C:216:PCW:H20	0.41	1.91	6	1
4:C:215:17F:N1	4:C:215:17F:P1	0.41	2.93	17	2
3:A:403:PCW:H171	3:A:403:PCW:H211	0.41	1.93	9	1
1:A:364:ALA:HA	1:A:368:LEU:HD12	0.41	1.93	10	1
3:B:207:PCW:C17	4:B:210:17F:C19	0.41	2.99	10	1
3:A:403:PCW:H132	3:A:404:PCW:C32	0.41	2.46	13	1
3:A:408:PCW:C48	3:A:413:PCW:H251	0.41	2.45	14	1
3:A:417:PCW:O3	3:A:417:PCW:C31	0.41	2.68	15	1
2:B:114:VAL:HG12	2:B:142:ILE:HB	0.41	1.92	15	1
3:B:206:PCW:P	3:B:206:PCW:H63	0.41	2.56	15	1
3:A:401:PCW:H472	3:D:612:PCW:H482	0.41	1.92	16	1
3:A:419:PCW:H322	3:D:625:PCW:C34	0.41	2.40	16	1
2:B:142:ILE:CD1	2:B:155:ALA:HA	0.41	2.45	16	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
3:A:406:PCW:H452	3:B:205:PCW:C27	0.41	2.46	17	1
3:A:411:PCW:H271	3:C:203:PCW:H472	0.41	1.93	17	1
3:A:414:PCW:C16	4:A:415:17F:H31	0.41	2.46	17	1
3:C:211:PCW:O2	3:C:211:PCW:O11	0.41	2.39	17	1
3:C:216:PCW:H461	4:C:218:17F:C42	0.41	2.45	17	1
3:D:609:PCW:H483	3:C:208:PCW:C48	0.41	2.45	18	1
4:C:213:17F:H40	4:C:213:17F:H36	0.41	1.66	18	1
3:B:204:PCW:O31	3:B:204:PCW:P	0.41	2.79	19	1
3:D:605:PCW:H52	3:D:614:PCW:H52	0.41	1.93	20	1
3:A:406:PCW:C19	3:A:411:PCW:H472	0.40	2.46	1	1
3:A:419:PCW:H382	3:A:419:PCW:H412	0.40	1.53	1	1
3:C:217:PCW:H212	3:C:217:PCW:H182	0.40	1.75	8	2
1:A:302:GLY:O	1:A:306:ARG:HG3	0.40	2.16	2	1
3:A:404:PCW:H162	3:A:404:PCW:H421	0.40	1.93	2	1
3:A:419:PCW:H63	3:D:626:PCW:O2	0.40	2.17	2	1
3:D:601:PCW:C39	4:D:628:17F:C29	0.40	2.98	3	1
2:B:53:LEU:HD13	2:B:156:PHE:HE1	0.40	1.76	3	1
3:B:205:PCW:H482	3:B:208:PCW:C20	0.40	2.46	4	1
4:B:209:17F:H62	4:B:209:17F:H58	0.40	1.59	4	1
3:D:614:PCW:H161	3:D:620:PCW:H412	0.40	1.93	5	1
3:B:203:PCW:H62	3:C:211:PCW:O3P	0.40	2.16	6	1
3:C:210:PCW:C16	3:C:210:PCW:H441	0.40	2.45	6	1
3:A:414:PCW:C37	4:A:415:17F:H69	0.40	2.39	8	1
3:A:418:PCW:C34	3:D:613:PCW:C13	0.40	2.82	8	1
3:B:207:PCW:O31	3:B:207:PCW:H11	0.40	2.15	8	1
4:B:211:17F:C27	3:C:204:PCW:H39	0.40	2.28	8	1
3:A:419:PCW:H182	3:A:419:PCW:H211	0.40	1.65	9	1
3:D:626:PCW:O2	3:D:626:PCW:C11	0.40	2.68	9	1
3:D:619:PCW:H411	3:D:619:PCW:H382	0.40	1.64	10	1
2:C:72:MET:SD	2:C:100:ILE:HG12	0.40	2.56	10	1
3:A:406:PCW:H122	4:B:211:17F:O10	0.40	2.16	11	1
3:A:419:PCW:C48	3:C:212:PCW:H471	0.40	2.42	11	1
3:C:208:PCW:H61	4:C:213:17F:C2	0.40	2.46	11	1
3:A:419:PCW:H482	3:C:212:PCW:H472	0.40	1.93	13	1
3:B:208:PCW:H12	3:C:211:PCW:C35	0.40	2.46	13	1
3:A:411:PCW:H252	3:C:210:PCW:H231	0.40	1.92	15	1
3:A:414:PCW:C13	4:A:415:17F:H58	0.40	2.46	15	1
3:B:206:PCW:H152	3:C:205:PCW:C26	0.40	2.30	16	1
4:B:211:17F:H30	4:B:211:17F:C35	0.40	2.45	16	1
3:C:203:PCW:C47	3:C:210:PCW:H222	0.40	2.45	16	1
3:A:405:PCW:H321	3:A:406:PCW:C18	0.40	2.44	17	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
3:A:405:PCW:C32	3:A:406:PCW:C18	0.40	2.98	17	1
3:D:608:PCW:H483	3:C:205:PCW:H271	0.40	1.92	18	1
3:A:412:PCW:H182	3:A:412:PCW:H212	0.40	1.70	19	1
4:A:415:17F:H62	4:A:415:17F:H58	0.40	1.64	19	1
3:C:211:PCW:H272	3:C:217:PCW:H281	0.40	1.93	19	1
2:B:68:ARG:HG3	2:B:71:TYR:CE2	0.40	2.51	20	1
3:D:613:PCW:H212	3:D:613:PCW:H181	0.40	1.69	1	2
1:A:306:ARG:O	1:A:310:ARG:HG3	0.40	2.16	2	1
3:D:625:PCW:H432	3:D:626:PCW:H421	0.40	1.93	2	1
3:B:208:PCW:C42	3:C:216:PCW:H262	0.40	2.42	2	1
3:A:403:PCW:H382	3:A:403:PCW:O3	0.40	2.16	3	1
3:D:610:PCW:O3	3:D:610:PCW:C31	0.40	2.69	20	2
3:C:205:PCW:H441	3:C:212:PCW:H252	0.40	1.92	3	1
3:A:407:PCW:O3	3:A:407:PCW:C31	0.40	2.70	4	1
4:A:422:17F:H53	3:D:606:PCW:H211	0.40	1.92	4	1
3:B:205:PCW:H231	3:C:210:PCW:C26	0.40	2.44	4	1
3:A:402:PCW:H431	3:C:206:PCW:H252	0.40	1.93	6	1
3:A:407:PCW:H181	3:A:407:PCW:H40	0.40	1.92	6	1
5:B:201:GSP:S1G	5:B:201:GSP:PA	0.40	3.19	15	2
3:A:403:PCW:H381	3:A:403:PCW:H411	0.40	1.60	7	1
3:A:404:PCW:H411	3:A:414:PCW:C25	0.40	2.46	8	1
3:D:603:PCW:C31	3:D:603:PCW:H42	0.40	2.46	9	1
3:D:608:PCW:H251	4:D:629:17F:H62	0.40	1.93	9	1
4:A:415:17F:C30	3:D:624:PCW:H442	0.40	2.46	10	1
3:D:609:PCW:C28	3:D:616:PCW:H411	0.40	2.41	12	1
3:C:212:PCW:H211	3:C:212:PCW:H181	0.40	1.64	12	1
1:A:375:LEU:O	1:A:379:LEU:HG	0.40	2.16	13	1
1:A:359:THR:HG21	1:D:418:GLN:HG3	0.40	1.93	14	1
3:D:614:PCW:H142	3:D:620:PCW:H39	0.40	1.91	14	1
3:D:621:PCW:C14	4:D:632:17F:O9	0.40	2.69	16	1
4:C:215:17F:H59	4:C:215:17F:H62	0.40	1.66	16	1
3:A:410:PCW:H39	3:A:412:PCW:C35	0.40	2.45	18	1
3:D:614:PCW:H63	3:D:614:PCW:O4P	0.40	2.15	19	1
3:B:207:PCW:H181	3:B:207:PCW:H212	0.40	1.65	19	1
3:D:616:PCW:H132	3:D:616:PCW:C17	0.40	2.43	20	1
3:D:608:PCW:C5	3:D:626:PCW:H222	0.40	2.46	1	1
3:C:204:PCW:H272	3:C:217:PCW:C47	0.40	2.43	1	1
3:C:206:PCW:H171	3:C:207:PCW:C20	0.40	2.46	1	1
3:A:411:PCW:H242	3:B:205:PCW:H283	0.40	1.91	2	1
3:A:417:PCW:O2P	3:A:417:PCW:H2	0.40	2.16	3	1
3:D:604:PCW:C41	3:D:606:PCW:H252	0.40	2.46	3	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
3:D:623:PCW:C12	3:D:624:PCW:H352	0.40	2.47	4	1
1:A:228:PHE:CE1	3:A:405:PCW:H483	0.40	2.51	7	1
3:C:209:PCW:H442	3:C:212:PCW:H481	0.40	1.93	7	1
3:A:411:PCW:O2	3:A:411:PCW:P	0.40	2.79	8	1
3:A:418:PCW:C34	3:D:613:PCW:H152	0.40	2.46	8	1
3:D:604:PCW:O11	3:D:604:PCW:C5	0.40	2.69	8	1
2:B:59:ALA:HA	5:B:201:GSP:O2G	0.40	2.15	9	1
3:A:413:PCW:H412	3:A:413:PCW:H381	0.40	1.56	10	1
3:D:608:PCW:C20	4:D:629:17F:H39	0.40	2.46	11	1
3:A:404:PCW:H63	3:B:205:PCW:H39	0.40	1.93	12	1
3:D:611:PCW:H212	3:D:611:PCW:H182	0.40	1.70	12	1
3:A:409:PCW:H332	3:B:206:PCW:C34	0.40	2.45	13	1
3:A:410:PCW:H412	3:A:410:PCW:H381	0.40	1.62	14	1
3:A:411:PCW:H51	4:B:211:17F:O5	0.40	2.16	14	1
3:A:421:PCW:H161	4:D:630:17F:H57	0.40	1.91	14	1
3:D:601:PCW:O31	3:D:601:PCW:C34	0.40	2.70	15	1
3:A:421:PCW:H382	3:A:421:PCW:H411	0.40	1.58	16	1
3:A:401:PCW:H52	3:B:204:PCW:O2P	0.40	2.17	17	1
3:D:615:PCW:C37	3:D:615:PCW:H411	0.40	2.47	17	1
4:D:632:17F:H39	4:D:632:17F:H36	0.40	1.66	17	1
3:C:212:PCW:O2	3:C:212:PCW:P	0.40	2.80	18	1
3:A:404:PCW:H342	4:A:415:17F:H18A	0.40	1.92	19	1
3:A:411:PCW:H182	3:B:205:PCW:H281	0.40	1.92	19	1
3:D:603:PCW:C22	3:D:611:PCW:C35	0.40	2.97	19	1
3:D:623:PCW:H182	3:D:623:PCW:H212	0.40	1.62	19	1
4:B:210:17F:H30	4:C:215:17F:H37	0.40	1.92	19	1
2:B:41:ARG:HD2	2:B:54:ASP:OD1	0.40	2.16	20	1
1:A:342:GLY:O	1:A:346:LEU:HG	0.40	2.17	1	1
3:A:405:PCW:C8	4:B:211:17F:C3	0.40	2.97	1	1
1:A:309:ALA:O	1:A:313:VAL:HG23	0.40	2.17	2	1
3:A:406:PCW:H331	4:B:211:17F:H9	0.40	1.93	2	1
3:A:407:PCW:O31	3:A:410:PCW:H331	0.40	2.16	2	1
3:A:406:PCW:C25	4:B:211:17F:H56	0.40	2.47	3	1
3:B:203:PCW:C39	3:C:211:PCW:H182	0.40	2.44	3	1
3:C:209:PCW:C27	3:C:209:PCW:H431	0.40	2.45	3	1
3:D:621:PCW:C27	4:D:632:17F:H37	0.40	2.44	5	1
3:B:203:PCW:H61	4:C:215:17F:O5	0.40	2.16	5	1
2:B:84:ILE:HD12	2:B:123:ARG:HB3	0.40	1.93	6	1
3:A:410:PCW:H442	3:A:412:PCW:H432	0.40	1.93	8	1
3:D:606:PCW:C25	4:C:218:17F:H42	0.40	2.47	8	1
3:B:208:PCW:C3	3:B:208:PCW:P	0.40	3.06	8	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
3:C:206:PCW:H152	3:C:208:PCW:H162	0.40	1.94	9	1
3:D:627:PCW:H252	3:C:216:PCW:H451	0.40	1.93	11	1
3:B:203:PCW:H261	4:B:209:17F:H32	0.40	1.93	11	1
3:A:406:PCW:H412	4:B:211:17F:H10A	0.40	1.93	13	1
1:D:449:LYS:O	1:D:453:GLN:HG3	0.40	2.16	13	1
3:D:618:PCW:O31	3:D:618:PCW:C11	0.40	2.69	13	1
2:B:165:LYS:HD3	2:C:135:ARG:HG2	0.40	1.92	13	1
3:C:210:PCW:H142	3:C:210:PCW:C37	0.40	2.46	14	1
3:A:419:PCW:C43	3:D:625:PCW:H462	0.40	2.39	15	1
3:B:206:PCW:O11	3:C:209:PCW:H341	0.40	2.16	15	1
1:A:363:LYS:O	1:A:368:LEU:HG	0.40	2.15	17	1
3:D:603:PCW:H442	3:D:611:PCW:C35	0.40	2.43	17	1
3:A:410:PCW:H181	3:A:410:PCW:H212	0.40	1.74	18	1
3:C:206:PCW:O1P	3:C:208:PCW:C6	0.40	2.69	18	1
3:A:402:PCW:H211	3:A:407:PCW:C20	0.40	2.46	19	1
3:D:602:PCW:H252	4:D:629:17F:C42	0.40	2.47	19	1
3:C:217:PCW:O11	4:C:218:17F:H62	0.40	2.17	19	1
3:A:409:PCW:H11	3:B:206:PCW:H61	0.40	1.93	20	1
3:C:206:PCW:C7	3:C:212:PCW:O2P	0.40	2.69	20	1
3:C:209:PCW:H52	4:C:214:17F:H4A	0.40	1.92	20	1
2:B:158:THR:O	2:B:162:GLU:HG2	0.40	2.16	1	1
3:C:212:PCW:H182	3:C:212:PCW:C45	0.40	2.16	2	1
1:A:268:GLU:HG2	1:D:506:ARG:CD	0.40	2.46	3	1
3:D:601:PCW:H382	4:D:628:17F:C30	0.40	2.47	3	1
3:C:212:PCW:H442	4:C:215:17F:C21	0.40	2.46	3	1
3:D:623:PCW:H122	3:D:624:PCW:H351	0.40	1.94	4	1
3:C:205:PCW:H2	4:C:214:17F:H6	0.40	1.84	4	1
3:D:612:PCW:C4	3:D:623:PCW:C34	0.40	2.99	5	1
2:B:135:ARG:HG3	2:C:161:ARG:HG2	0.40	1.94	6	1
3:B:204:PCW:C1	3:B:207:PCW:H351	0.40	2.45	7	1
1:A:386:PHE:CZ	4:A:415:17F:H76	0.40	2.51	8	1
3:B:203:PCW:H73	4:C:215:17F:C6	0.40	2.47	9	1
4:B:210:17F:C23	4:B:210:17F:H12A	0.40	2.47	9	1
4:B:211:17F:H40	4:B:211:17F:H36	0.40	1.68	9	1
2:C:17:SER:HB2	5:C:201:GSP:PA	0.40	2.57	10	1
3:A:410:PCW:O1P	3:A:410:PCW:C5	0.40	2.65	11	1
4:B:210:17F:H36	4:B:210:17F:H40	0.40	1.66	11	1
3:A:404:PCW:C47	4:A:415:17F:H54	0.40	2.47	12	1
4:A:416:17F:H65	3:B:204:PCW:C25	0.40	2.47	12	1
3:B:206:PCW:C24	3:C:209:PCW:H142	0.40	2.47	12	1
3:C:203:PCW:C7	3:C:212:PCW:O1P	0.40	2.70	12	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
3:C:208:PCW:H411	3:C:208:PCW:H382	0.40	1.70	14	1
1:D:515:ARG:O	1:D:520:PRO:HD3	0.40	2.16	15	2
3:B:206:PCW:H162	3:C:209:PCW:H352	0.40	1.94	15	1
3:C:207:PCW:H411	3:C:207:PCW:H381	0.40	1.56	17	1
3:D:609:PCW:H382	3:C:208:PCW:H283	0.40	1.93	18	1
2:B:47:ASP:HA	2:C:128:LYS:HD2	0.40	1.93	18	1
3:A:408:PCW:H32	3:A:408:PCW:O2P	0.40	2.15	19	1
3:D:617:PCW:H421	3:D:619:PCW:C42	0.40	2.47	19	1
3:A:402:PCW:C6	3:A:410:PCW:O2P	0.40	2.70	20	1

6.3 Torsion angles (i)

6.3.1 Protein backbone (i)

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all PDB entries followed by that with respect to all NMR entries. The Analysed column shows the number of residues for which the backbone conformation was analysed and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	196/200 (98%)	191±1 (97±1%)	4±1 (2±1%)	1±0 (1±0%)	32	76
1	D	196/200 (98%)	190±1 (97±1%)	5±1 (3±1%)	0±0 (0±0%)	54	85
2	B	164/185 (89%)	154±2 (94±1%)	10±2 (6±1%)	0±1 (0±0%)	50	82
2	C	166/185 (90%)	158±2 (95±1%)	8±2 (5±1%)	0±0 (0±0%)	54	85
All	All	14440/15400 (94%)	13864 (96%)	542 (4%)	34 (0%)	50	82

All 9 unique Ramachandran outliers are listed below. They are sorted by the frequency of occurrence in the ensemble.

Mol	Chain	Res	Type	Models (Total)
1	A	365	LYS	20
2	B	37	GLU	3
1	D	420	GLY	3
2	C	37	GLU	2
1	D	498	PRO	2
2	C	47	ASP	1
2	C	64	TYR	1
2	B	24	ILE	1
2	B	64	TYR	1

6.3.2 Protein sidechains (i)

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all PDB entries followed by that with respect to all NMR entries. The Analysed column shows the number of residues for which the sidechain conformation was analysed and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	173/175 (99%)	162±2 (93±1%)	12±2 (7±1%)	20	69
1	D	174/175 (99%)	161±2 (93±1%)	13±2 (7±1%)	18	66
2	B	146/165 (88%)	131±3 (90±2%)	15±3 (10±2%)	11	56
2	C	148/165 (90%)	135±3 (91±2%)	13±3 (9±2%)	13	59
All	All	12820/13600 (94%)	11771 (92%)	1049 (8%)	15	62

All 232 unique residues with a non-rotameric sidechain are listed below. They are sorted by the frequency of occurrence in the ensemble.

Mol	Chain	Res	Type	Models (Total)
1	D	550	LYS	18
1	A	272	TYR	17
2	B	2	THR	16
2	B	87	THR	16
1	D	516	THR	15
1	A	254	VAL	15
1	D	480	GLU	14
2	B	65	SER	14
2	C	35	THR	14
2	C	87	THR	14
2	C	124	THR	14
2	C	2	THR	14
1	D	561	LYS	13
2	B	92	ASP	13
2	C	65	SER	13
2	C	92	ASP	13
1	A	312	HIS	12
1	D	459	PHE	12
1	D	576	VAL	12
2	B	41	ARG	12
2	C	12	ASP	12
1	A	293	GLU	12
1	A	235	GLU	11
2	C	74	THR	11
2	B	124	THR	10

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Mol	Chain	Res	Type	Models (Total)
2	C	38	ASP	10
2	C	50	THR	10
2	B	35	THR	10
2	B	50	THR	10
1	D	552	THR	9
1	D	568	ASP	9
2	B	63	GLU	9
1	D	405	TRP	9
1	D	411	THR	9
1	D	466	GLU	9
2	B	12	ASP	9
2	B	17	SER	9
2	B	58	THR	9
2	B	69	ASP	9
2	C	39	SER	9
2	B	148	THR	9
2	B	127	THR	9
1	A	209	SER	9
1	D	407	SER	8
2	B	38	ASP	8
2	B	74	THR	8
2	C	148	THR	8
1	A	229	TRP	8
1	D	557	THR	8
1	A	250	VAL	8
1	D	448	VAL	8
2	C	41	ARG	8
1	D	483	GLU	8
1	A	319	HIS	7
1	A	359	THR	7
2	C	69	ASP	7
1	A	246	ASP	7
1	D	400	LYS	7
2	C	149	ARG	7
2	C	161	ARG	7
1	A	382	PHE	7
2	B	108	ASP	7
1	A	265	TRP	6
2	B	153	ASP	6
1	A	292	HIS	6
2	C	127	THR	6
1	D	583	SER	6

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Mol	Chain	Res	Type	Models (Total)
2	B	89	SER	6
2	C	153	ASP	6
1	A	206	ASN	5
1	A	212	SER	5
2	B	51	CYS	5
2	B	126	ASP	5
2	C	62	GLU	5
1	A	358	SER	5
1	A	214	PHE	5
1	A	304	GLU	5
2	C	89	SER	5
1	A	381	SER	5
2	C	51	CYS	5
1	A	236	THR	4
1	A	396	LYS	4
2	B	119	ASP	4
2	B	144	THR	4
2	B	161	ARG	4
1	D	547	TYR	4
2	B	29	VAL	4
2	B	136	SER	4
2	C	58	THR	4
1	D	523	ASP	4
1	D	556	SER	4
1	D	559	SER	4
2	B	1	SER	4
2	C	6	LEU	4
2	B	62	GLU	4
2	B	149	ARG	4
2	C	126	ASP	4
1	D	548	HIS	4
2	C	1	SER	4
2	B	39	SER	4
2	B	68	ARG	4
2	B	145	SER	4
1	A	244	SER	4
1	D	462	LYS	3
2	B	128	LYS	3
2	C	108	ASP	3
1	D	505	ASP	3
1	D	584	PHE	3
2	B	30	ASP	3

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Mol	Chain	Res	Type	Models (Total)
2	C	68	ARG	3
2	C	128	LYS	3
1	A	228	PHE	3
1	A	350	HIS	3
1	D	487	GLN	3
1	A	263	LYS	3
1	A	370	ASP	3
2	C	63	GLU	3
1	A	386	PHE	3
1	D	440	GLU	3
1	A	327	LEU	3
1	D	455	TYR	3
1	A	325	ASP	3
2	C	17	SER	3
1	D	429	ASN	3
2	B	6	LEU	3
2	B	44	VAL	3
2	C	20	THR	3
1	A	274	GLN	2
1	A	299	SER	2
1	D	442	SER	2
1	D	415	LEU	2
2	C	26	ASN	2
2	C	143	GLU	2
1	A	394	THR	2
2	B	131	GLN	2
2	C	43	GLN	2
1	D	410	SER	2
1	D	434	THR	2
1	D	524	GLU	2
1	D	594	LYS	2
1	A	262	GLN	2
2	B	80	CYS	2
2	B	135	ARG	2
2	C	144	THR	2
1	D	441	MET	2
1	D	522	SER	2
1	D	538	GLU	2
2	B	71	TYR	2
2	C	45	VAL	2
1	A	369	GLU	2
1	D	482	GLN	2

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Mol	Chain	Res	Type	Models (Total)
1	A	368	LEU	2
2	B	20	THR	2
2	B	55	ILE	2
1	A	211	THR	2
2	C	136	SER	2
1	A	314	ASP	2
2	B	67	MET	2
2	C	29	VAL	2
2	B	22	GLN	2
2	B	109	VAL	2
2	B	150	GLN	2
1	A	289	GLN	2
2	C	123	ARG	2
1	A	225	THR	1
1	A	298	LEU	1
1	A	307	ASP	1
1	D	473	LYS	1
1	A	202	LYS	1
1	D	399	LEU	1
2	B	9	VAL	1
2	C	27	HIS	1
2	B	27	HIS	1
2	B	156	PHE	1
2	C	22	GLN	1
2	C	64	TYR	1
2	C	156	PHE	1
1	A	349	TYR	1
1	D	592	THR	1
2	B	31	GLU	1
1	A	258	LEU	1
1	A	318	THR	1
1	D	472	GLN	1
2	B	129	GLN	1
2	C	19	LEU	1
1	D	580	PHE	1
2	B	94	HIS	1
2	C	119	ASP	1
1	A	205	ASP	1
1	A	249	GLU	1
2	B	105	ASP	1
2	C	37	GLU	1
2	C	55	ILE	1

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Mol	Chain	Res	Type	Models (Total)
2	C	109	VAL	1
1	A	230	ASP	1
1	D	447	GLU	1
1	D	525	LEU	1
1	A	385	SER	1
2	C	135	ARG	1
1	A	275	LYS	1
2	B	26	ASN	1
2	C	71	TYR	1
1	A	326	GLU	1
1	D	412	PHE	1
1	D	443	LYS	1
1	D	586	SER	1
2	C	113	LEU	1
2	C	118	CYS	1
1	D	478	ARG	1
2	C	165	LYS	1
1	D	560	GLU	1
2	B	49	GLU	1
2	C	31	GLU	1
1	D	432	LYS	1
1	D	567	GLU	1
2	C	61	GLN	1
2	C	154	ASP	1
1	A	247	LEU	1
1	D	489	LEU	1
2	B	154	ASP	1
1	A	356	HIS	1
2	B	23	LEU	1
2	B	43	GLN	1
2	C	72	MET	1
2	C	80	CYS	1
2	C	145	SER	1
1	A	276	VAL	1
1	D	465	GLU	1
1	D	403	ASP	1
1	D	554	HIS	1
2	C	107	GLU	1
1	A	237	GLU	1

6.3.3 RNA (i)

There are no RNA molecules in this entry.

6.4 Non-standard residues in protein, DNA, RNA chains (i)

There are no non-standard protein/DNA/RNA residues in this entry.

6.5 Carbohydrates (i)

There are no monosaccharides in this entry.

6.6 Ligand geometry (i)

Of 84 ligands modelled in this entry, 2 are monoatomic - leaving 82 for Mogul analysis.

In the following table, the Counts columns list the number of bonds for which Mogul statistics could be retrieved, the number of bonds that are observed in the model and the number of bonds that are defined in the chemical component dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length is the number of standard deviations the observed value is removed from the expected value. A bond length with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the average root-mean-square of all Z scores of the bond lengths.

Mol	Type	Chain	Res	Link	Bond lengths		
					Counts	RMSZ	#Z>2
3	PCW	C	216	-	53,53,53	0.82±0.00	0±0 (0±0%)
3	PCW	D	612	-	53,53,53	0.82±0.00	0±0 (0±0%)
3	PCW	D	602	-	53,53,53	0.82±0.00	0±0 (0±0%)
4	17F	C	214	-	52,53,53	0.83±0.00	0±0 (0±0%)
3	PCW	D	605	-	53,53,53	0.82±0.00	0±0 (0±0%)
3	PCW	B	207	-	53,53,53	0.82±0.00	0±0 (0±0%)
3	PCW	C	210	-	53,53,53	0.82±0.00	0±0 (0±0%)
3	PCW	D	611	-	53,53,53	0.82±0.00	0±0 (0±0%)
3	PCW	B	203	-	53,53,53	0.82±0.00	0±0 (0±0%)
3	PCW	B	205	-	53,53,53	0.82±0.00	0±0 (0±0%)
3	PCW	A	401	-	53,53,53	0.82±0.00	0±0 (0±0%)
4	17F	D	629	-	52,53,53	0.83±0.00	0±0 (0±0%)
3	PCW	C	211	-	53,53,53	0.82±0.00	0±0 (0±0%)
4	17F	D	632	-	52,53,53	0.83±0.00	0±0 (0±0%)
4	17F	B	210	-	52,53,53	0.83±0.00	0±0 (0±0%)
4	17F	C	213	-	52,53,53	0.82±0.00	0±0 (0±0%)
3	PCW	D	610	-	53,53,53	0.82±0.00	0±0 (0±0%)
3	PCW	D	609	-	53,53,53	0.82±0.00	0±0 (0±0%)

Mol	Type	Chain	Res	Link	Bond lengths		
					Counts	RMSZ	#Z>2
3	PCW	B	208	-	53,53,53	0.82±0.00	0±0 (0±0%)
4	17F	C	219	-	52,53,53	0.82±0.00	0±0 (0±0%)
3	PCW	A	420	-	53,53,53	0.82±0.00	0±0 (0±0%)
3	PCW	B	204	-	53,53,53	0.82±0.00	0±0 (0±0%)
4	17F	B	211	-	52,53,53	0.83±0.00	0±0 (0±0%)
3	PCW	D	627	-	53,53,53	0.82±0.00	0±0 (0±0%)
3	PCW	D	601	-	53,53,53	0.82±0.00	0±0 (0±0%)
3	PCW	D	607	-	53,53,53	0.82±0.00	0±0 (0±0%)
3	PCW	C	205	-	53,53,53	0.82±0.00	0±0 (0±0%)
3	PCW	C	204	-	53,53,53	0.82±0.00	0±0 (0±0%)
4	17F	B	209	-	52,53,53	0.82±0.00	0±0 (0±0%)
3	PCW	D	619	-	53,53,53	0.82±0.00	0±0 (0±0%)
4	17F	A	416	-	52,53,53	0.83±0.00	0±0 (0±0%)
3	PCW	D	608	-	53,53,53	0.82±0.00	0±0 (0±0%)
3	PCW	D	617	-	53,53,53	0.82±0.00	0±0 (0±0%)
3	PCW	A	413	-	53,53,53	0.82±0.00	0±0 (0±0%)
3	PCW	C	206	-	53,53,53	0.82±0.00	0±0 (0±0%)
3	PCW	A	407	-	53,53,53	0.82±0.00	0±0 (0±0%)
3	PCW	A	421	-	53,53,53	0.82±0.00	0±0 (0±0%)
3	PCW	D	616	-	53,53,53	0.82±0.00	0±0 (0±0%)
3	PCW	D	603	-	53,53,53	0.82±0.00	0±0 (0±0%)
4	17F	A	415	-	52,53,53	0.83±0.00	0±0 (0±0%)
3	PCW	A	402	-	53,53,53	0.82±0.00	0±0 (0±0%)
3	PCW	D	623	-	53,53,53	0.82±0.00	0±0 (0±0%)
3	PCW	D	626	-	53,53,53	0.82±0.00	0±0 (0±0%)
3	PCW	C	209	-	53,53,53	0.82±0.00	0±0 (0±0%)
3	PCW	A	408	-	53,53,53	0.82±0.00	0±0 (0±0%)
3	PCW	A	412	-	53,53,53	0.82±0.00	0±0 (0±0%)
3	PCW	A	405	-	53,53,53	0.82±0.00	0±0 (0±0%)
3	PCW	D	620	-	53,53,53	0.82±0.00	0±0 (0±0%)
4	17F	A	422	-	52,53,53	0.82±0.00	0±0 (0±0%)
3	PCW	D	614	-	53,53,53	0.82±0.00	0±0 (0±0%)
3	PCW	C	217	-	53,53,53	0.82±0.00	0±0 (0±0%)
3	PCW	A	404	-	53,53,53	0.82±0.00	0±0 (0±0%)
3	PCW	D	613	-	53,53,53	0.82±0.00	0±0 (0±0%)
3	PCW	D	604	-	53,53,53	0.82±0.00	0±0 (0±0%)
3	PCW	D	625	-	53,53,53	0.82±0.00	0±0 (0±0%)
3	PCW	A	414	-	53,53,53	0.82±0.00	0±0 (0±0%)
3	PCW	A	418	-	53,53,53	0.82±0.00	0±0 (0±0%)
3	PCW	A	419	-	53,53,53	0.82±0.00	0±0 (0±0%)
3	PCW	A	403	-	53,53,53	0.82±0.00	0±0 (0±0%)
3	PCW	B	206	-	53,53,53	0.82±0.00	0±0 (0±0%)
3	PCW	C	203	-	53,53,53	0.82±0.00	0±0 (0±0%)

Mol	Type	Chain	Res	Link	Bond lengths		
					Counts	RMSZ	#Z>2
3	PCW	D	624	-	53,53,53	0.82±0.00	0±0 (0±0%)
3	PCW	D	606	-	53,53,53	0.82±0.00	0±0 (0±0%)
4	17F	D	630	-	52,53,53	0.83±0.00	0±0 (0±0%)
3	PCW	C	208	-	53,53,53	0.82±0.00	0±0 (0±0%)
4	17F	D	628	-	52,53,53	0.83±0.00	0±0 (0±0%)
4	17F	C	218	-	52,53,53	0.83±0.00	0±0 (0±0%)
3	PCW	D	622	-	53,53,53	0.82±0.00	0±0 (0±0%)
3	PCW	A	411	-	53,53,53	0.82±0.00	0±0 (0±0%)
3	PCW	A	410	-	53,53,53	0.82±0.00	0±0 (0±0%)
3	PCW	D	621	-	53,53,53	0.82±0.00	0±0 (0±0%)
3	PCW	D	618	-	53,53,53	0.82±0.00	0±0 (0±0%)
4	17F	C	215	-	52,53,53	0.83±0.00	0±0 (0±0%)
3	PCW	D	615	-	53,53,53	0.82±0.00	0±0 (0±0%)
3	PCW	C	212	-	53,53,53	0.82±0.00	0±0 (0±0%)
3	PCW	A	417	-	53,53,53	0.82±0.00	0±0 (0±0%)
5	GSP	C	201	6	29,34,34	1.41±0.02	2±1 (8±2%)
4	17F	D	631	-	52,53,53	0.82±0.00	0±0 (0±0%)
5	GSP	B	201	-	29,34,34	1.41±0.02	2±1 (8±2%)
3	PCW	C	207	-	53,53,53	0.82±0.00	0±0 (0±0%)
3	PCW	A	409	-	53,53,53	0.82±0.00	0±0 (0±0%)
3	PCW	A	406	-	53,53,53	0.82±0.00	0±0 (0±0%)

In the following table, the Counts columns list the number of angles for which Mogul statistics could be retrieved, the number of angles that are observed in the model and the number of angles that are defined in the chemical component dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond angle is the number of standard deviations the observed value is removed from the expected value. A bond angle with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the average root-mean-square of all Z scores of the bond angles.

Mol	Type	Chain	Res	Link	Bond angles		
					Counts	RMSZ	#Z>2
3	PCW	C	216	-	59,61,61	2.67±0.00	10±0 (17±0%)
3	PCW	D	612	-	59,61,61	2.59±0.01	7±1 (11±1%)
3	PCW	D	602	-	59,61,61	2.58±0.01	6±0 (10±0%)
4	17F	C	214	-	54,60,60	1.12±0.03	4±0 (7±0%)
3	PCW	D	605	-	59,61,61	2.63±0.01	7±0 (12±0%)
3	PCW	B	207	-	59,61,61	2.60±0.01	6±0 (10±0%)
3	PCW	C	210	-	59,61,61	2.60±0.01	7±0 (11±0%)
3	PCW	D	611	-	59,61,61	2.61±0.01	7±1 (11±0%)
3	PCW	B	203	-	59,61,61	2.59±0.01	7±1 (11±1%)

Mol	Type	Chain	Res	Link	Bond angles		
					Counts	RMSZ	#Z>2
3	PCW	B	205	-	59,61,61	2.68±0.01	10±1 (17±0%)
3	PCW	A	401	-	59,61,61	2.60±0.01	6±0 (10±0%)
4	17F	D	629	-	54,60,60	1.12±0.02	4±0 (6±0%)
3	PCW	C	211	-	59,61,61	2.60±0.02	6±0 (10±0%)
4	17F	D	632	-	54,60,60	1.09±0.05	4±0 (8±0%)
4	17F	B	210	-	54,60,60	1.13±0.02	4±1 (8±1%)
4	17F	C	213	-	54,60,60	1.10±0.03	4±0 (7±0%)
3	PCW	D	610	-	59,61,61	2.59±0.01	6±1 (10±0%)
3	PCW	D	609	-	59,61,61	2.59±0.00	7±1 (11±0%)
3	PCW	B	208	-	59,61,61	2.58±0.01	6±1 (10±1%)
4	17F	C	219	-	54,60,60	1.09±0.04	4±0 (8±0%)
3	PCW	A	420	-	59,61,61	2.61±0.01	6±0 (10±0%)
3	PCW	B	204	-	59,61,61	2.59±0.01	6±0 (10±0%)
4	17F	B	211	-	54,60,60	1.16±0.03	4±0 (7±0%)
3	PCW	D	627	-	59,61,61	2.60±0.02	7±1 (12±1%)
3	PCW	D	601	-	59,61,61	2.60±0.01	7±1 (11±1%)
3	PCW	D	607	-	59,61,61	2.59±0.01	7±0 (11±0%)
3	PCW	C	205	-	59,61,61	2.60±0.01	6±0 (10±0%)
3	PCW	C	204	-	59,61,61	2.60±0.01	6±1 (10±0%)
4	17F	B	209	-	54,60,60	1.12±0.03	5±0 (9±0%)
3	PCW	D	619	-	59,61,61	2.61±0.01	7±0 (12±0%)
4	17F	A	416	-	54,60,60	1.13±0.04	4±0 (8±0%)
3	PCW	D	608	-	59,61,61	2.60±0.01	7±1 (11±1%)
3	PCW	D	617	-	59,61,61	2.58±0.01	6±0 (10±0%)
3	PCW	A	413	-	59,61,61	2.59±0.00	6±0 (10±0%)
3	PCW	C	206	-	59,61,61	2.60±0.01	7±0 (11±0%)
3	PCW	A	407	-	59,61,61	2.59±0.02	6±1 (10±0%)
3	PCW	A	421	-	59,61,61	2.59±0.01	7±1 (11±1%)
3	PCW	D	616	-	59,61,61	2.61±0.01	6±0 (10±0%)
3	PCW	D	603	-	59,61,61	2.61±0.02	7±1 (11±1%)
4	17F	A	415	-	54,60,60	1.34±0.04	8±0 (15±0%)
3	PCW	A	402	-	59,61,61	2.59±0.01	6±0 (10±0%)
3	PCW	D	623	-	59,61,61	2.58±0.02	6±0 (10±0%)
3	PCW	D	626	-	59,61,61	2.62±0.01	7±1 (11±0%)
3	PCW	C	209	-	59,61,61	2.58±0.01	6±0 (10±0%)

Mol	Type	Chain	Res	Link	Bond angles		
					Counts	RMSZ	#Z>2
3	PCW	A	408	-	59,61,61	2.59±0.01	6±0 (10±0%)
3	PCW	A	412	-	59,61,61	2.60±0.01	6±0 (10±0%)
3	PCW	A	405	-	59,61,61	2.60±0.01	6±1 (10±0%)
3	PCW	D	620	-	59,61,61	2.58±0.01	6±0 (10±0%)
4	17F	A	422	-	54,60,60	1.12±0.03	4±0 (7±0%)
3	PCW	D	614	-	59,61,61	2.59±0.01	6±0 (10±0%)
3	PCW	C	217	-	59,61,61	2.61±0.01	8±0 (12±0%)
3	PCW	A	404	-	59,61,61	2.58±0.02	7±1 (11±1%)
3	PCW	D	613	-	59,61,61	2.60±0.01	6±0 (10±0%)
3	PCW	D	604	-	59,61,61	2.59±0.01	6±0 (10±0%)
3	PCW	D	625	-	59,61,61	2.57±0.01	6±1 (10±1%)
3	PCW	A	414	-	59,61,61	2.62±0.02	7±1 (11±0%)
3	PCW	A	418	-	59,61,61	2.61±0.02	7±1 (11±0%)
3	PCW	A	419	-	59,61,61	2.60±0.01	7±0 (12±0%)
3	PCW	A	403	-	59,61,61	2.59±0.01	6±0 (10±0%)
3	PCW	B	206	-	59,61,61	2.59±0.01	6±0 (10±0%)
3	PCW	C	203	-	59,61,61	2.60±0.01	6±0 (10±0%)
3	PCW	D	624	-	59,61,61	2.58±0.02	6±0 (10±0%)
3	PCW	D	606	-	59,61,61	2.59±0.01	6±0 (10±0%)
4	17F	D	630	-	54,60,60	1.33±0.03	8±0 (15±0%)
3	PCW	C	208	-	59,61,61	2.60±0.01	7±1 (11±0%)
4	17F	D	628	-	54,60,60	1.10±0.02	4±0 (7±0%)
4	17F	C	218	-	54,60,60	1.12±0.02	5±1 (9±1%)
3	PCW	D	622	-	59,61,61	2.57±0.01	6±0 (10±0%)
3	PCW	A	411	-	59,61,61	2.62±0.01	6±0 (10±0%)
3	PCW	A	410	-	59,61,61	2.59±0.01	6±0 (10±0%)
3	PCW	D	621	-	59,61,61	2.59±0.01	7±1 (11±1%)
3	PCW	D	618	-	59,61,61	2.61±0.01	7±0 (11±0%)
4	17F	C	215	-	54,60,60	1.23±0.03	4±0 (7±0%)
3	PCW	D	615	-	59,61,61	2.61±0.01	6±0 (10±0%)
3	PCW	C	212	-	59,61,61	2.60±0.01	7±0 (11±0%)
3	PCW	A	417	-	59,61,61	2.59±0.02	6±1 (11±1%)
5	GSP	C	201	6	32,54,54	1.58±0.04	6±0 (18±0%)
4	17F	D	631	-	54,60,60	1.15±0.03	4±0 (7±0%)
5	GSP	B	201	-	32,54,54	1.67±0.24	6±0 (18±0%)

Mol	Type	Chain	Res	Link	Bond angles		
					Counts	RMSZ	#Z>2
3	PCW	C	207	-	59,61,61	2.59±0.01	6±0 (10±0%)
3	PCW	A	409	-	59,61,61	2.59±0.01	6±0 (10±0%)
3	PCW	A	406	-	59,61,61	2.60±0.01	6±0 (10±0%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the chemical component dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	PCW	D	608	-	-	0±0,57,57,57	-
3	PCW	C	216	-	-	0±0,57,57,57	-
4	17F	B	211	-	-	0±0,59,59,59	-
3	PCW	D	613	-	-	0±0,57,57,57	-
3	PCW	D	605	-	-	0±0,57,57,57	-
3	PCW	B	206	-	-	0±0,57,57,57	-
3	PCW	D	617	-	-	0±0,57,57,57	-
3	PCW	D	603	-	-	0±0,57,57,57	-
3	PCW	D	614	-	-	0±0,57,57,57	-
4	17F	B	210	-	-	1±0,59,59,59	-
3	PCW	D	625	-	-	0±0,57,57,57	-
3	PCW	A	411	-	-	0±0,57,57,57	-
3	PCW	D	601	-	-	0±0,57,57,57	-
4	17F	C	215	-	-	1±0,59,59,59	-
3	PCW	D	622	-	-	0±0,57,57,57	-
3	PCW	C	203	-	-	0±0,57,57,57	-
3	PCW	D	610	-	-	0±0,57,57,57	-
3	PCW	C	217	-	-	0±0,57,57,57	-
3	PCW	D	606	-	-	0±0,57,57,57	-
3	PCW	D	615	-	-	0±0,57,57,57	-
3	PCW	A	404	-	-	0±0,57,57,57	-
3	PCW	B	208	-	-	0±0,57,57,57	-
3	PCW	B	205	-	-	0±0,57,57,57	-
3	PCW	D	621	-	-	0±0,57,57,57	-
3	PCW	C	208	-	-	0±0,57,57,57	-
3	PCW	C	212	-	-	0±0,57,57,57	-
4	17F	D	629	-	-	0±0,59,59,59	-
3	PCW	C	209	-	-	0±0,57,57,57	-
3	PCW	A	421	-	-	0±0,57,57,57	-
3	PCW	C	204	-	-	0±0,57,57,57	-
3	PCW	D	619	-	-	0±0,57,57,57	-
3	PCW	D	604	-	-	0±0,57,57,57	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	PCW	A	418	-	-	0±0,57,57,57	-
3	PCW	D	624	-	-	0±0,57,57,57	-
3	PCW	A	402	-	-	0±0,57,57,57	-
4	17F	C	213	-	-	0±0,59,59,59	-
3	PCW	A	420	-	-	0±0,57,57,57	-
3	PCW	A	403	-	-	0±0,57,57,57	-
3	PCW	A	419	-	-	0±0,57,57,57	-
3	PCW	B	203	-	-	0±0,57,57,57	-
5	GSP	B	201	-	-	0±0,17,38,38	0±0,3,3,3
4	17F	D	632	-	-	0±0,59,59,59	-
3	PCW	A	409	-	-	0±0,57,57,57	-
3	PCW	A	417	-	-	0±0,57,57,57	-
4	17F	C	214	-	-	0±0,59,59,59	-
4	17F	A	422	-	-	0±0,59,59,59	-
3	PCW	A	413	-	-	0±0,57,57,57	-
3	PCW	D	609	-	-	0±0,57,57,57	-
3	PCW	C	207	-	-	0±0,57,57,57	-
3	PCW	A	412	-	-	0±0,57,57,57	-
3	PCW	D	626	-	-	0±0,57,57,57	-
3	PCW	C	211	-	-	0±0,57,57,57	-
3	PCW	A	405	-	-	0±0,57,57,57	-
3	PCW	D	602	-	-	0±0,57,57,57	-
4	17F	B	209	-	-	0±0,59,59,59	-
3	PCW	D	623	-	-	0±0,57,57,57	-
4	17F	D	628	-	-	0±0,59,59,59	-
3	PCW	D	627	-	-	0±0,57,57,57	-
5	GSP	C	201	6	-	0±0,17,38,38	0±0,3,3,3
3	PCW	A	407	-	-	0±0,57,57,57	-
3	PCW	D	618	-	-	0±0,57,57,57	-
3	PCW	D	616	-	-	0±0,57,57,57	-
3	PCW	D	612	-	-	0±0,57,57,57	-
3	PCW	B	204	-	-	0±0,57,57,57	-
3	PCW	C	205	-	-	0±0,57,57,57	-
4	17F	A	415	-	-	0±0,59,59,59	-
4	17F	C	219	-	-	0±0,59,59,59	-
3	PCW	D	620	-	-	0±0,57,57,57	-
3	PCW	B	207	-	-	0±0,57,57,57	-
3	PCW	A	414	-	-	0±0,57,57,57	-
3	PCW	C	206	-	-	0±0,57,57,57	-
3	PCW	A	410	-	-	0±0,57,57,57	-
4	17F	A	416	-	-	0±0,59,59,59	-
3	PCW	A	401	-	-	0±0,57,57,57	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	PCW	C	210	-	-	0±0,57,57,57	-
3	PCW	D	607	-	-	0±0,57,57,57	-
4	17F	D	631	-	-	0±0,59,59,59	-
3	PCW	D	611	-	-	0±0,57,57,57	-
4	17F	D	630	-	-	0±0,59,59,59	-
3	PCW	A	408	-	-	0±0,57,57,57	-
4	17F	C	218	-	-	1±0,59,59,59	-
3	PCW	A	406	-	-	0±0,57,57,57	-

All unique bond outliers are listed below. They are sorted according to the Z-score of the worst occurrence in the ensemble.

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)	Models	
								Worst	Total
5	C	201	GSP	C5-C6	4.25	1.39	1.47	14	20
5	B	201	GSP	C5-C6	4.25	1.39	1.47	19	20
5	C	201	GSP	O4'-C1'	2.71	1.44	1.40	10	20
5	B	201	GSP	O4'-C1'	2.64	1.44	1.40	17	20
5	C	201	GSP	PA-O3A	2.17	1.61	1.59	18	2
5	B	201	GSP	PB-O3B	2.12	1.61	1.59	3	2
5	C	201	GSP	PB-O3B	2.11	1.61	1.59	19	2
5	B	201	GSP	PA-O3A	2.10	1.61	1.59	15	3
5	C	201	GSP	PB-O3A	2.09	1.61	1.59	18	3
5	B	201	GSP	PB-O3A	2.03	1.61	1.59	7	3

All unique angle outliers are listed below. They are sorted according to the Z-score of the worst occurrence in the ensemble.

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})	Models	
								Worst	Total
3	D	621	PCW	C8-N-C7	17.71	62.46	108.98	15	20
3	D	616	PCW	C8-N-C7	17.70	62.48	108.98	19	20
3	C	212	PCW	C8-N-C7	17.69	62.50	108.98	10	20
3	D	615	PCW	C8-N-C7	17.69	62.51	108.98	18	20
3	D	622	PCW	C8-N-C7	17.69	62.51	108.98	11	20
3	A	414	PCW	C8-N-C7	17.69	62.51	108.98	13	20
3	A	413	PCW	C8-N-C7	17.69	62.52	108.98	15	20
3	C	206	PCW	C8-N-C7	17.69	62.52	108.98	15	20
3	D	603	PCW	C8-N-C7	17.68	62.53	108.98	5	20
3	A	409	PCW	C8-N-C7	17.68	62.53	108.98	10	20
3	A	411	PCW	C8-N-C7	17.68	62.53	108.98	7	20
3	A	405	PCW	C8-N-C7	17.68	62.53	108.98	20	20
3	A	412	PCW	C8-N-C7	17.68	62.53	108.98	5	20

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})	Models	
								Worst	Total
3	A	410	PCW	C8-N-C7	17.68	62.54	108.98	3	20
3	D	618	PCW	C8-N-C7	17.68	62.54	108.98	14	20
3	C	217	PCW	C8-N-C7	17.68	62.54	108.98	5	20
3	D	623	PCW	C8-N-C7	17.68	62.54	108.98	7	20
3	C	204	PCW	C8-N-C7	17.68	62.54	108.98	19	20
3	C	203	PCW	C8-N-C7	17.68	62.54	108.98	7	20
3	C	208	PCW	C8-N-C7	17.68	62.54	108.98	10	20
3	C	216	PCW	C8-N-C7	17.68	62.54	108.98	13	20
3	A	407	PCW	C8-N-C7	17.67	62.55	108.98	17	20
3	D	608	PCW	C8-N-C7	17.68	62.55	108.98	20	20
3	B	205	PCW	C8-N-C7	17.68	62.55	108.98	8	20
3	A	408	PCW	C8-N-C7	17.67	62.55	108.98	12	20
3	D	626	PCW	C8-N-C7	17.67	62.55	108.98	19	20
3	C	207	PCW	C8-N-C7	17.67	62.55	108.98	5	20
3	A	418	PCW	C8-N-C7	17.67	62.55	108.98	10	20
3	D	601	PCW	C8-N-C7	17.67	62.55	108.98	17	20
3	C	209	PCW	C8-N-C7	17.67	62.55	108.98	20	20
3	D	617	PCW	C8-N-C7	17.67	62.55	108.98	14	20
3	B	203	PCW	C8-N-C7	17.67	62.55	108.98	3	20
3	B	207	PCW	C8-N-C7	17.67	62.55	108.98	17	20
3	B	204	PCW	C8-N-C7	17.67	62.56	108.98	6	20
3	B	208	PCW	C8-N-C7	17.67	62.55	108.98	7	20
3	C	210	PCW	C8-N-C7	17.67	62.55	108.98	13	20
3	D	619	PCW	C8-N-C7	17.67	62.56	108.98	17	20
3	A	403	PCW	C8-N-C7	17.67	62.56	108.98	17	20
3	A	406	PCW	C8-N-C7	17.67	62.56	108.98	6	20
3	A	417	PCW	C8-N-C7	17.67	62.57	108.98	5	20
3	D	602	PCW	C8-N-C7	17.67	62.56	108.98	20	20
3	D	604	PCW	C8-N-C7	17.67	62.56	108.98	8	20
3	D	606	PCW	C8-N-C7	17.67	62.56	108.98	16	20
3	A	404	PCW	C8-N-C7	17.67	62.57	108.98	17	20
3	D	607	PCW	C8-N-C7	17.67	62.57	108.98	8	20
3	D	609	PCW	C8-N-C7	17.67	62.56	108.98	20	20
3	D	613	PCW	C8-N-C7	17.67	62.56	108.98	13	20
3	C	205	PCW	C8-N-C7	17.67	62.56	108.98	18	20
3	D	610	PCW	C8-N-C7	17.67	62.57	108.98	9	20
3	D	612	PCW	C8-N-C7	17.67	62.57	108.98	4	20
3	D	614	PCW	C8-N-C7	17.67	62.57	108.98	8	20
3	D	620	PCW	C8-N-C7	17.67	62.57	108.98	3	20
3	D	624	PCW	C8-N-C7	17.67	62.57	108.98	1	20
3	D	625	PCW	C8-N-C7	17.67	62.57	108.98	3	20

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})	Models	
								Worst	Total
3	C	211	PCW	C8-N-C7	17.67	62.57	108.98	20	20
3	A	420	PCW	C8-N-C7	17.67	62.57	108.98	4	20
3	D	605	PCW	C8-N-C7	17.67	62.57	108.98	9	20
3	D	611	PCW	C8-N-C7	17.67	62.57	108.98	13	20
3	A	401	PCW	C8-N-C7	17.67	62.57	108.98	8	20
3	A	421	PCW	C8-N-C7	17.67	62.57	108.98	11	20
3	B	206	PCW	C8-N-C7	17.66	62.58	108.98	19	20
3	A	402	PCW	C8-N-C7	17.66	62.58	108.98	9	20
3	A	419	PCW	C8-N-C7	17.66	62.58	108.98	16	20
3	D	627	PCW	C8-N-C7	17.66	62.58	108.98	2	20
5	B	201	GSP	C4'-O4'-C1'	9.76	100.99	109.92	18	20
4	C	215	17F	O3-C1-C2	5.50	112.86	108.06	10	20
5	C	201	GSP	C4'-O4'-C1'	4.76	105.56	109.92	14	20
4	C	218	17F	O9-C17-C18	4.58	121.40	111.48	13	20
3	D	627	PCW	C2-O2-C31	4.45	107.15	117.80	14	20
4	A	422	17F	O3-C1-C2	4.39	111.89	108.06	14	20
4	C	214	17F	O3-C1-C2	4.39	111.88	108.06	12	20
3	A	414	PCW	O2-C31-C32	4.36	120.91	111.48	18	20
3	D	626	PCW	O2-C31-C32	4.36	120.91	111.48	15	20
3	A	418	PCW	O2-C31-C32	4.34	120.87	111.48	18	20
4	B	210	17F	O3-C1-C2	4.33	111.83	108.06	4	20
3	D	627	PCW	O2-C31-C32	4.29	120.77	111.48	4	20
3	A	420	PCW	O2-C31-C32	4.28	120.73	111.48	2	20
4	B	210	17F	O9-C17-C18	4.26	120.70	111.48	5	20
4	C	213	17F	O3-C1-C2	4.20	111.72	108.06	6	20
4	D	632	17F	O9-C17-C18	4.19	120.56	111.48	4	20
3	D	626	PCW	C2-O2-C31	4.18	107.79	117.80	15	20
4	A	415	17F	O9-C17-C18	4.17	120.51	111.48	15	20
4	D	630	17F	O3-C1-C2	4.17	111.70	108.06	3	20
4	A	416	17F	O3-C1-C2	4.17	111.70	108.06	11	20
4	A	415	17F	O3-C1-C2	4.17	111.69	108.06	2	20
4	C	215	17F	O9-C17-C18	4.16	120.49	111.48	20	20
4	D	631	17F	O3-C1-C2	4.16	111.69	108.06	11	20
3	D	605	PCW	O2-C31-C32	4.15	120.46	111.48	17	20
4	D	628	17F	O3-C1-C2	4.15	111.68	108.06	7	20
3	A	404	PCW	O2-C31-C32	4.13	120.41	111.48	2	20
3	A	418	PCW	C2-O2-C31	4.13	107.92	117.80	17	20
3	B	206	PCW	O2-C31-C32	4.12	120.40	111.48	8	20
3	D	603	PCW	O2-C31-C32	4.12	120.39	111.48	12	20
4	B	211	17F	C5-O9-C17	4.11	107.97	117.80	4	20
3	C	203	PCW	O2-C31-C32	4.11	120.36	111.48	9	20

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})	Models	
								Worst	Total
3	D	616	PCW	O2-C31-C32	4.10	120.36	111.48	3	20
4	D	629	17F	O9-C17-C18	4.08	120.30	111.48	19	20
4	D	631	17F	O9-C17-C18	4.07	120.29	111.48	7	20
4	D	632	17F	O3-C1-C2	4.07	111.61	108.06	18	20
3	D	618	PCW	O2-C31-C32	4.07	120.28	111.48	19	20
4	C	219	17F	O3-C1-C2	4.06	111.60	108.06	14	20
4	B	211	17F	O3-C1-C2	4.05	111.59	108.06	5	20
3	D	615	PCW	O2-C31-C32	4.04	120.21	111.48	10	20
5	B	201	GSP	PB-O3B-PG	4.03	118.41	133.17	13	20
3	A	407	PCW	O2-C31-C32	4.03	120.19	111.48	6	20
3	A	409	PCW	O2-C31-C32	4.02	120.18	111.48	5	20
4	B	209	17F	O3-C1-C2	4.02	111.56	108.06	2	20
3	C	209	PCW	O2-C31-C32	4.01	120.15	111.48	4	20
4	B	211	17F	O9-C17-C18	4.01	120.15	111.48	4	20
3	D	613	PCW	O2-C31-C32	4.00	120.14	111.48	10	20
3	C	206	PCW	O2-C31-C32	4.00	120.14	111.48	3	20
3	A	401	PCW	O2-C31-C32	4.00	120.14	111.48	14	20
3	D	623	PCW	O2-C31-C32	4.00	120.14	111.48	17	20
4	C	219	17F	O9-C17-C18	4.00	120.14	111.48	13	20
4	D	630	17F	O9-C17-C18	4.00	120.13	111.48	7	20
4	A	416	17F	O9-C17-C18	3.99	120.12	111.48	1	20
3	D	604	PCW	O2-C31-C32	3.99	120.10	111.48	17	20
3	A	411	PCW	O2-C31-C32	3.98	120.09	111.48	10	20
3	C	208	PCW	O2-C31-C32	3.98	120.09	111.48	7	20
3	D	624	PCW	O2-C31-C32	3.97	120.08	111.48	6	20
4	A	422	17F	O9-C17-C18	3.97	120.08	111.48	15	20
3	C	212	PCW	O2-C31-C32	3.97	120.07	111.48	11	20
4	C	213	17F	O9-C17-C18	3.97	120.06	111.48	12	20
3	D	619	PCW	O2-C31-C32	3.96	120.04	111.48	12	20
3	D	614	PCW	O2-C31-C32	3.95	120.04	111.48	6	20
3	D	611	PCW	O2-C31-C32	3.95	120.03	111.48	20	20
5	C	201	GSP	PB-O3B-PG	3.95	118.70	133.17	10	20
3	D	608	PCW	O2-C31-C32	3.95	120.03	111.48	4	20
3	D	610	PCW	O2-C31-C32	3.94	120.01	111.48	20	20
3	D	602	PCW	O2-C31-C32	3.94	120.00	111.48	20	20
3	B	206	PCW	C2-O2-C31	3.93	108.39	117.80	8	20
3	A	412	PCW	O2-C31-C32	3.93	119.98	111.48	13	20
4	C	214	17F	O9-C17-C18	3.92	119.97	111.48	12	20
3	B	205	PCW	O2-C31-C32	3.91	119.93	111.48	14	20
4	C	218	17F	O3-C1-C2	3.90	111.46	108.06	20	20
3	A	405	PCW	O2-C31-C32	3.90	119.91	111.48	12	20

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})	Models	
								Worst	Total
3	C	205	PCW	O2-C31-C32	3.89	119.91	111.48	5	20
3	A	413	PCW	O2-C31-C32	3.88	119.88	111.48	18	20
3	A	419	PCW	O2-C31-C32	3.88	119.88	111.48	11	20
5	C	201	GSP	O4'-C1'-N9	3.88	113.89	108.75	17	20
3	A	403	PCW	O2-C31-C32	3.88	119.88	111.48	19	20
3	A	411	PCW	C2-O2-C31	3.88	108.51	117.80	4	20
3	A	421	PCW	O2-C31-C32	3.88	119.88	111.48	4	20
3	D	606	PCW	O2-C31-C32	3.88	119.86	111.48	6	20
3	B	207	PCW	O2-C31-C32	3.87	119.86	111.48	3	20
3	B	204	PCW	O2-C31-C32	3.87	119.85	111.48	16	20
3	D	607	PCW	O2-C31-C32	3.85	119.82	111.48	16	20
5	B	201	GSP	O4'-C1'-N9	3.85	113.85	108.75	13	20
3	C	207	PCW	O2-C31-C32	3.84	119.80	111.48	13	20
3	D	623	PCW	C2-O2-C31	3.84	108.60	117.80	1	19
3	B	203	PCW	O2-C31-C32	3.84	119.79	111.48	1	20
3	C	204	PCW	O2-C31-C32	3.84	119.78	111.48	4	20
4	D	628	17F	O9-C17-C18	3.83	119.77	111.48	19	20
3	B	207	PCW	C2-O2-C31	3.83	108.64	117.80	3	20
3	C	210	PCW	O2-C31-C32	3.81	119.73	111.48	14	20
4	D	629	17F	O3-C1-C2	3.81	111.38	108.06	18	20
3	D	621	PCW	O2-C31-C32	3.80	119.70	111.48	11	20
3	A	417	PCW	O2-C31-C32	3.80	119.70	111.48	2	20
3	D	616	PCW	C2-O2-C31	3.79	108.72	117.80	13	20
4	D	629	17F	C5-O9-C17	3.79	108.73	117.80	14	20
3	D	620	PCW	O2-C31-C32	3.79	119.67	111.48	20	20
4	B	209	17F	O9-C17-C18	3.79	119.67	111.48	2	20
3	C	211	PCW	O2-C31-C32	3.78	119.66	111.48	10	20
3	A	402	PCW	O2-C31-C32	3.78	119.66	111.48	12	20
3	A	420	PCW	C2-O2-C31	3.77	108.77	117.80	7	20
4	D	632	17F	C5-O9-C17	3.77	108.76	117.80	4	20
3	D	615	PCW	C2-O2-C31	3.77	108.78	117.80	10	20
3	A	406	PCW	O2-C31-C32	3.77	119.63	111.48	19	20
3	A	401	PCW	C2-O2-C31	3.76	108.79	117.80	13	20
3	D	601	PCW	O2-C31-C32	3.77	119.63	111.48	16	20
3	B	208	PCW	O2-C31-C32	3.76	119.62	111.48	11	20
3	A	408	PCW	O2-C31-C32	3.76	119.61	111.48	8	20
3	D	617	PCW	O2-C31-C32	3.76	119.61	111.48	17	20
3	A	410	PCW	O2-C31-C32	3.75	119.59	111.48	8	20
4	A	415	17F	C5-O9-C17	3.74	108.84	117.80	15	20
3	D	612	PCW	O2-C31-C32	3.72	119.53	111.48	14	20
3	A	409	PCW	C2-O2-C31	3.72	108.90	117.80	5	20

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})	Models	
								Worst	Total
3	C	211	PCW	C2-O2-C31	3.71	108.91	117.80	10	20
3	C	217	PCW	O2-C31-C32	3.71	119.51	111.48	3	20
3	A	404	PCW	C2-O2-C31	3.71	108.92	117.80	2	19
3	C	203	PCW	C2-O2-C31	3.71	108.93	117.80	11	20
4	A	416	17F	C5-O9-C17	3.70	108.93	117.80	1	20
3	D	618	PCW	C2-O2-C31	3.70	108.94	117.80	20	20
4	D	630	17F	C5-O9-C17	3.69	108.97	117.80	7	20
3	D	609	PCW	O2-C31-C32	3.68	119.44	111.48	18	20
3	D	603	PCW	C2-O2-C31	3.67	109.02	117.80	19	20
4	C	219	17F	C5-O9-C17	3.64	109.08	117.80	13	20
3	C	205	PCW	C2-O2-C31	3.64	109.10	117.80	12	20
3	C	208	PCW	C2-O2-C31	3.64	109.09	117.80	16	20
3	C	216	PCW	O2-C31-C32	3.63	119.34	111.48	20	20
3	D	611	PCW	C2-O2-C31	3.63	109.11	117.80	19	20
4	C	214	17F	C5-O9-C17	3.61	109.15	117.80	18	20
4	D	631	17F	C5-O9-C17	3.61	109.16	117.80	5	19
3	D	622	PCW	O2-C31-C32	3.61	119.28	111.48	16	20
3	D	604	PCW	C2-O2-C31	3.60	109.18	117.80	17	20
3	C	217	PCW	C2-O2-C31	3.58	109.22	117.80	17	20
3	A	414	PCW	C2-O2-C31	3.58	109.22	117.80	5	20
3	D	625	PCW	O2-C31-C32	3.58	119.23	111.48	20	20
4	C	213	17F	C5-O9-C17	3.58	109.23	117.80	12	20
3	D	614	PCW	C7-N-C6	3.57	118.36	108.98	16	20
3	C	212	PCW	C2-O2-C31	3.56	109.28	117.80	13	20
3	C	206	PCW	C2-O2-C31	3.56	109.28	117.80	1	20
3	D	613	PCW	C2-O2-C31	3.55	109.31	117.80	3	20
3	A	407	PCW	C2-O2-C31	3.54	109.33	117.80	3	19
3	A	402	PCW	C2-O2-C31	3.53	109.34	117.80	12	20
4	A	422	17F	C5-O9-C17	3.53	109.34	117.80	11	20
3	B	205	PCW	C2-O2-C31	3.53	109.35	117.80	14	20
3	B	208	PCW	C2-O2-C31	3.53	109.35	117.80	8	18
3	D	619	PCW	C2-O2-C31	3.49	109.44	117.80	13	20
3	D	608	PCW	C2-O2-C31	3.48	109.47	117.80	17	20
3	A	403	PCW	C2-O2-C31	3.47	109.48	117.80	3	20
3	A	405	PCW	C2-O2-C31	3.47	109.49	117.80	18	20
3	A	417	PCW	C2-O2-C31	3.46	109.52	117.80	9	20
3	D	627	PCW	C7-N-C6	3.45	118.05	108.98	13	20
3	A	410	PCW	C2-O2-C31	3.45	109.55	117.80	8	20
3	D	624	PCW	C2-O2-C31	3.45	109.55	117.80	6	8
4	C	215	17F	C5-O9-C17	3.44	109.56	117.80	13	20
3	A	412	PCW	C2-O2-C31	3.44	109.56	117.80	2	20

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})	Models	
								Worst	Total
3	D	614	PCW	C2-O2-C31	3.43	109.58	117.80	6	20
3	D	605	PCW	C8-N-C6	3.43	117.99	108.98	3	20
3	B	203	PCW	C2-O2-C31	3.43	109.58	117.80	18	20
3	A	408	PCW	C2-O2-C31	3.43	109.59	117.80	6	20
3	C	207	PCW	C2-O2-C31	3.43	109.59	117.80	13	20
3	A	414	PCW	C8-N-C6	3.42	117.97	108.98	9	20
3	A	401	PCW	C7-N-C6	3.42	117.95	108.98	11	20
3	D	627	PCW	C8-N-C6	3.42	117.95	108.98	15	20
3	C	205	PCW	C7-N-C6	3.42	117.95	108.98	5	20
3	D	610	PCW	C2-O2-C31	3.41	109.63	117.80	2	20
3	C	211	PCW	C7-N-C6	3.41	117.94	108.98	4	20
3	D	608	PCW	C8-N-C6	3.41	117.93	108.98	13	20
3	D	615	PCW	C8-N-C6	3.39	117.89	108.98	8	20
3	D	620	PCW	C8-N-C6	3.39	117.89	108.98	19	20
3	D	614	PCW	C8-N-C6	3.38	117.86	108.98	18	20
3	D	621	PCW	C2-O2-C31	3.38	109.70	117.80	17	19
3	D	624	PCW	C7-N-C6	3.38	117.86	108.98	6	20
3	A	405	PCW	C8-N-C6	3.38	117.85	108.98	6	20
3	A	406	PCW	C2-O2-C31	3.38	109.71	117.80	7	20
3	D	608	PCW	C7-N-C6	3.37	117.84	108.98	7	20
3	A	418	PCW	C7-N-C6	3.37	117.83	108.98	7	20
3	D	610	PCW	C7-N-C6	3.37	117.82	108.98	7	20
3	A	407	PCW	C7-N-C6	3.37	117.82	108.98	9	20
3	A	404	PCW	C8-N-C6	3.36	117.81	108.98	14	20
3	A	411	PCW	C7-N-C6	3.36	117.81	108.98	13	20
3	A	414	PCW	C7-N-C6	3.36	117.81	108.98	6	20
3	D	601	PCW	C2-O2-C31	3.36	109.75	117.80	19	20
3	D	618	PCW	C8-N-C6	3.36	117.80	108.98	18	20
4	D	628	17F	C5-O9-C17	3.36	109.76	117.80	12	20
3	A	417	PCW	C8-N-C6	3.35	117.78	108.98	14	20
3	A	419	PCW	C8-N-C6	3.35	117.78	108.98	18	20
3	C	205	PCW	C8-N-C6	3.35	117.78	108.98	7	20
3	D	605	PCW	C2-O2-C31	3.35	109.79	117.80	17	20
3	A	418	PCW	C8-N-C6	3.34	117.76	108.98	14	20
3	A	404	PCW	C7-N-C6	3.34	117.75	108.98	20	20
3	D	603	PCW	C7-N-C6	3.34	117.75	108.98	13	20
3	D	621	PCW	C7-N-C6	3.34	117.76	108.98	18	20
4	B	210	17F	C5-O9-C17	3.34	109.80	117.80	12	20
3	D	617	PCW	C8-N-C6	3.34	117.74	108.98	12	20
3	C	208	PCW	C8-N-C6	3.33	117.73	108.98	6	20
3	D	603	PCW	C8-N-C6	3.33	117.73	108.98	9	20

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})	Models	
								Worst	Total
4	B	209	17F	C5-O9-C17	3.33	109.84	117.80	2	20
5	C	201	GSP	C8-N7-C5	3.33	108.21	102.55	14	20
3	A	403	PCW	C8-N-C6	3.32	117.71	108.98	14	20
3	D	609	PCW	C7-N-C6	3.32	117.70	108.98	13	20
3	D	613	PCW	C7-N-C6	3.32	117.71	108.98	4	20
3	B	205	PCW	C7-N-C6	3.32	117.70	108.98	8	20
3	C	206	PCW	C7-N-C6	3.32	117.71	108.98	17	20
3	D	616	PCW	C7-N-C6	3.32	117.70	108.98	15	20
3	A	413	PCW	C8-N-C6	3.32	117.70	108.98	10	20
3	D	622	PCW	C7-N-C6	3.32	117.70	108.98	17	20
3	A	420	PCW	C7-N-C6	3.32	117.70	108.98	18	20
3	A	406	PCW	C7-N-C6	3.32	117.69	108.98	15	20
3	D	606	PCW	C2-O2-C31	3.32	109.86	117.80	2	20
3	D	611	PCW	C7-N-C6	3.32	117.69	108.98	20	20
3	D	618	PCW	C7-N-C6	3.32	117.69	108.98	8	20
3	D	613	PCW	C8-N-C6	3.31	117.68	108.98	20	20
3	D	625	PCW	C7-N-C6	3.31	117.68	108.98	2	20
3	D	607	PCW	C8-N-C6	3.31	117.68	108.98	20	20
3	D	617	PCW	C7-N-C6	3.31	117.68	108.98	15	20
5	B	201	GSP	C2-N1-C6	3.31	119.05	125.11	3	20
3	D	626	PCW	C8-N-C6	3.31	117.66	108.98	1	20
3	D	616	PCW	C8-N-C6	3.31	117.66	108.98	6	20
3	C	210	PCW	C8-N-C6	3.31	117.66	108.98	2	20
3	C	211	PCW	C8-N-C6	3.31	117.66	108.98	2	20
3	A	412	PCW	C7-N-C6	3.30	117.65	108.98	17	20
3	D	621	PCW	C8-N-C6	3.30	117.65	108.98	15	20
3	C	203	PCW	C8-N-C6	3.30	117.65	108.98	17	20
3	D	604	PCW	C7-N-C6	3.30	117.65	108.98	11	20
3	B	208	PCW	C8-N-C6	3.30	117.65	108.98	3	20
5	B	201	GSP	C8-N7-C5	3.30	108.17	102.55	19	20
3	A	421	PCW	C8-N-C6	3.30	117.64	108.98	13	20
3	B	208	PCW	C7-N-C6	3.30	117.64	108.98	12	20
3	D	601	PCW	C8-N-C6	3.30	117.64	108.98	14	20
3	A	402	PCW	C8-N-C6	3.30	117.63	108.98	18	20
3	C	204	PCW	C2-O2-C31	3.30	109.91	117.80	16	20
3	D	622	PCW	C8-N-C6	3.29	117.63	108.98	18	20
3	D	602	PCW	C7-N-C6	3.29	117.63	108.98	10	20
3	B	204	PCW	C8-N-C6	3.29	117.63	108.98	8	20
3	C	204	PCW	C7-N-C6	3.29	117.63	108.98	5	20
3	D	604	PCW	C8-N-C6	3.29	117.62	108.98	13	20
3	D	607	PCW	C7-N-C6	3.29	117.63	108.98	9	20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)	Models	
								Worst	Total
3	D	602	PCW	C8-N-C6	3.29	117.62	108.98	20	20
3	C	208	PCW	C7-N-C6	3.29	117.62	108.98	11	20
3	D	619	PCW	C8-N-C6	3.29	117.62	108.98	20	20
3	D	625	PCW	C8-N-C6	3.29	117.62	108.98	1	20
3	C	212	PCW	C8-N-C6	3.29	117.62	108.98	20	20
3	A	405	PCW	C7-N-C6	3.29	117.61	108.98	16	20
3	D	610	PCW	C8-N-C6	3.29	117.61	108.98	4	20
3	D	612	PCW	C7-N-C6	3.29	117.61	108.98	20	20
3	B	207	PCW	C7-N-C6	3.29	117.61	108.98	3	20
3	A	420	PCW	C8-N-C6	3.29	117.61	108.98	5	20
3	D	611	PCW	C8-N-C6	3.29	117.61	108.98	8	20
3	B	203	PCW	C7-N-C6	3.29	117.61	108.98	8	20
3	B	204	PCW	C7-N-C6	3.29	117.61	108.98	12	20
3	D	601	PCW	C7-N-C6	3.28	117.60	108.98	6	20
3	D	605	PCW	C7-N-C6	3.28	117.60	108.98	16	20
3	A	419	PCW	C7-N-C6	3.28	117.60	108.98	17	20
3	A	408	PCW	C7-N-C6	3.28	117.59	108.98	10	20
3	D	606	PCW	C8-N-C6	3.28	117.59	108.98	10	20
3	B	207	PCW	C8-N-C6	3.28	117.59	108.98	14	20
3	C	204	PCW	C8-N-C6	3.28	117.59	108.98	15	20
3	C	212	PCW	C7-N-C6	3.28	117.59	108.98	4	20
3	A	409	PCW	C8-N-C6	3.28	117.59	108.98	2	20
3	D	623	PCW	C7-N-C6	3.28	117.58	108.98	17	20
3	B	203	PCW	C8-N-C6	3.28	117.58	108.98	20	20
3	C	207	PCW	C7-N-C6	3.28	117.58	108.98	7	20
3	C	209	PCW	C7-N-C6	3.28	117.58	108.98	6	20
3	C	210	PCW	C2-O2-C31	3.28	109.96	117.80	14	20
3	C	216	PCW	C7-N-C6	3.28	117.58	108.98	15	20
3	A	407	PCW	C8-N-C6	3.27	117.57	108.98	19	20
3	A	412	PCW	C8-N-C6	3.27	117.58	108.98	7	20
3	A	421	PCW	C7-N-C6	3.27	117.57	108.98	18	20
3	D	622	PCW	C2-O2-C31	3.27	109.96	117.80	16	20
3	D	626	PCW	C7-N-C6	3.27	117.57	108.98	9	20
3	C	207	PCW	C8-N-C6	3.27	117.57	108.98	13	20
3	A	410	PCW	C7-N-C6	3.27	117.56	108.98	18	20
3	C	210	PCW	C7-N-C6	3.27	117.56	108.98	9	20
3	D	623	PCW	C8-N-C6	3.27	117.56	108.98	11	20
3	A	403	PCW	C7-N-C6	3.27	117.55	108.98	6	20
3	B	205	PCW	C8-N-C6	3.27	117.55	108.98	1	20
3	C	206	PCW	C8-N-C6	3.26	117.55	108.98	15	20
3	D	615	PCW	C7-N-C6	3.26	117.54	108.98	3	20

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})	Models	
								Worst	Total
3	C	209	PCW	C8-N-C6	3.26	117.55	108.98	18	20
3	A	417	PCW	C7-N-C6	3.26	117.54	108.98	9	20
3	C	203	PCW	C7-N-C6	3.26	117.54	108.98	8	20
3	C	216	PCW	C8-N-C6	3.26	117.54	108.98	6	20
3	A	410	PCW	C8-N-C6	3.26	117.53	108.98	17	20
3	B	206	PCW	C7-N-C6	3.26	117.53	108.98	10	20
3	A	413	PCW	C7-N-C6	3.25	117.52	108.98	13	20
3	A	419	PCW	C2-O2-C31	3.25	110.01	117.80	13	20
3	C	217	PCW	C7-N-C6	3.25	117.53	108.98	14	20
3	D	606	PCW	C7-N-C6	3.25	117.52	108.98	2	20
5	C	201	GSP	C2-N1-C6	3.25	119.16	125.11	6	20
3	D	619	PCW	C7-N-C6	3.25	117.51	108.98	5	20
3	A	406	PCW	C8-N-C6	3.25	117.50	108.98	6	20
3	A	409	PCW	C7-N-C6	3.25	117.50	108.98	14	20
3	C	209	PCW	C2-O2-C31	3.24	110.03	117.80	13	20
3	A	402	PCW	C7-N-C6	3.24	117.49	108.98	8	20
4	D	630	17F	O3-P1-O1	3.24	96.11	108.94	11	20
3	A	411	PCW	C8-N-C6	3.23	117.47	108.98	15	20
3	D	612	PCW	C8-N-C6	3.23	117.47	108.98	13	20
3	D	620	PCW	C7-N-C6	3.23	117.47	108.98	1	20
3	A	401	PCW	C8-N-C6	3.23	117.45	108.98	3	20
3	D	617	PCW	C2-O2-C31	3.22	110.08	117.80	11	20
3	D	609	PCW	C8-N-C6	3.22	117.43	108.98	6	20
3	C	217	PCW	C8-N-C6	3.22	117.43	108.98	3	20
3	D	612	PCW	C2-O2-C31	3.21	110.10	117.80	14	20
3	A	408	PCW	C8-N-C6	3.21	117.41	108.98	19	20
3	B	206	PCW	C8-N-C6	3.19	117.35	108.98	7	20
3	D	620	PCW	C2-O2-C31	3.16	110.24	117.80	6	20
3	B	205	PCW	O4P-P-O2P	3.15	96.46	108.94	6	20
4	A	415	17F	O3-P1-O1	3.12	96.57	108.94	9	20
3	B	204	PCW	C2-O2-C31	3.12	110.33	117.80	16	20
3	C	216	PCW	O4P-P-O2P	3.10	96.67	108.94	1	20
3	D	624	PCW	C8-N-C6	3.09	117.10	108.98	9	20
3	D	602	PCW	C2-O2-C31	3.04	110.51	117.80	9	20
3	D	609	PCW	C2-O2-C31	3.04	110.51	117.80	11	20
3	A	413	PCW	C2-O2-C31	3.02	110.57	117.80	1	20
3	D	625	PCW	C2-O2-C31	2.98	110.66	117.80	3	16
3	A	414	PCW	O3-C11-C12	2.96	120.87	111.83	8	20
3	D	607	PCW	C2-O2-C31	2.94	110.75	117.80	11	20
3	C	216	PCW	C2-O2-C31	2.92	110.81	117.80	20	20
3	D	605	PCW	O3-C11-C12	2.91	120.71	111.83	17	20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)	Models	
								Worst	Total
3	A	418	PCW	O3-C11-C12	2.87	120.59	111.83	5	20
3	D	616	PCW	O3-C11-C12	2.87	120.59	111.83	6	20
3	A	421	PCW	C2-O2-C31	2.86	110.96	117.80	1	20
3	C	204	PCW	O3-C11-C12	2.83	120.47	111.83	5	20
3	D	611	PCW	O3-C11-C12	2.82	120.43	111.83	15	20
3	C	203	PCW	O3-C11-C12	2.81	120.42	111.83	20	20
3	D	618	PCW	O3-C11-C12	2.81	120.41	111.83	16	20
3	D	603	PCW	O3-C11-C12	2.80	120.38	111.83	2	20
3	C	217	PCW	O3-C11-C12	2.77	120.29	111.83	16	20
3	A	419	PCW	O3-C11-C12	2.77	120.27	111.83	12	20
3	C	216	PCW	O1P-P-O2P	2.76	125.31	112.44	2	20
3	C	210	PCW	O3-C11-C12	2.76	120.24	111.83	2	20
4	B	209	17F	O7-C7-C8	2.75	120.22	111.83	13	20
3	C	206	PCW	O3-C11-C12	2.74	120.20	111.83	11	20
4	D	630	17F	O2-P1-O1	2.74	125.20	112.44	9	20
4	C	219	17F	O7-C7-C8	2.74	120.19	111.83	5	20
3	B	205	PCW	O1P-P-O2P	2.74	125.17	112.44	7	20
3	A	417	PCW	O3-C11-C12	2.73	120.17	111.83	11	20
3	A	421	PCW	O3-C11-C12	2.73	120.17	111.83	18	20
4	A	416	17F	O7-C7-C8	2.73	120.17	111.83	14	20
3	A	402	PCW	O3-C11-C12	2.73	120.16	111.83	1	20
3	D	621	PCW	O3-C11-C12	2.73	120.15	111.83	18	20
4	A	415	17F	O2-P1-O1	2.73	125.14	112.44	20	20
3	C	211	PCW	O3-C11-C12	2.72	120.14	111.83	10	20
4	D	630	17F	O7-C7-C8	2.73	120.14	111.83	17	20
4	D	632	17F	O7-C7-C8	2.72	120.13	111.83	4	20
3	C	205	PCW	O3-C11-C12	2.72	120.12	111.83	18	20
3	A	414	PCW	C3-O3-C11	2.71	107.19	117.12	2	16
3	D	612	PCW	O3-C11-C12	2.71	120.11	111.83	11	20
3	D	627	PCW	O3-C11-C12	2.71	120.11	111.83	17	20
3	D	619	PCW	O3-C11-C12	2.71	120.10	111.83	4	20
4	C	218	17F	C5-O9-C17	2.71	111.31	117.80	8	17
3	A	408	PCW	O3-C11-C12	2.71	120.09	111.83	12	20
3	D	624	PCW	O3-C11-C12	2.71	120.08	111.83	3	20
3	C	216	PCW	O3-C11-C12	2.70	120.06	111.83	5	20
3	D	601	PCW	O3-C11-C12	2.70	120.06	111.83	1	20
4	A	422	17F	O7-C7-C8	2.69	120.05	111.83	17	20
4	C	215	17F	O7-C7-C8	2.69	120.05	111.83	1	20
3	C	209	PCW	O3-C11-C12	2.69	120.03	111.83	4	20
4	B	211	17F	O7-C7-C8	2.69	120.03	111.83	10	20
3	D	626	PCW	O3-C11-C12	2.67	119.99	111.83	18	20

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})	Models	
								Worst	Total
3	B	203	PCW	O3-C11-C12	2.67	119.99	111.83	11	20
3	C	212	PCW	O3-C11-C12	2.67	119.99	111.83	18	20
3	B	208	PCW	O3-C11-C12	2.67	119.98	111.83	18	20
3	C	208	PCW	O3-C11-C12	2.67	119.97	111.83	20	20
3	D	609	PCW	O3-C11-C12	2.66	119.96	111.83	5	20
4	A	415	17F	O7-C7-C8	2.66	119.96	111.83	3	20
3	A	409	PCW	O3-C11-C12	2.65	119.92	111.83	12	20
3	D	625	PCW	O3-C11-C12	2.63	119.87	111.83	15	20
3	C	207	PCW	O3-C11-C12	2.63	119.86	111.83	16	20
4	D	631	17F	O7-C7-C8	2.63	119.86	111.83	18	20
4	B	210	17F	O7-C7-C8	2.62	119.83	111.83	16	20
3	A	403	PCW	O3-C11-C12	2.62	119.82	111.83	19	20
3	A	411	PCW	O3-C11-C12	2.62	119.82	111.83	10	20
3	A	405	PCW	O3-C11-C12	2.62	119.82	111.83	19	20
3	D	605	PCW	C3-O3-C11	2.61	107.56	117.12	6	20
3	D	613	PCW	O3-C11-C12	2.61	119.80	111.83	18	20
3	D	622	PCW	O3-C11-C12	2.61	119.79	111.83	11	20
4	D	628	17F	O7-C7-C8	2.61	119.79	111.83	2	20
3	D	607	PCW	O3-C11-C12	2.60	119.76	111.83	6	20
4	C	214	17F	O7-C7-C8	2.60	119.76	111.83	10	20
3	D	608	PCW	O3-C11-C12	2.59	119.74	111.83	2	20
3	A	413	PCW	O3-C11-C12	2.59	119.73	111.83	16	20
3	B	204	PCW	O3-C11-C12	2.59	119.73	111.83	7	20
3	B	207	PCW	O3-C11-C12	2.59	119.73	111.83	8	20
3	B	206	PCW	O3-C11-C12	2.59	119.72	111.83	4	20
4	C	213	17F	O7-C7-C8	2.58	119.69	111.83	4	20
3	D	617	PCW	O3-C11-C12	2.57	119.69	111.83	11	20
3	A	404	PCW	O3-C11-C12	2.57	119.66	111.83	19	20
4	C	218	17F	O7-C7-C8	2.56	119.66	111.83	14	20
3	D	623	PCW	O3-C11-C12	2.55	119.62	111.83	10	20
3	B	205	PCW	O3-C11-C12	2.55	119.60	111.83	17	20
3	A	410	PCW	O3-C11-C12	2.54	119.57	111.83	10	20
3	D	614	PCW	O3-C11-C12	2.53	119.56	111.83	18	20
3	D	615	PCW	O3-C11-C12	2.53	119.56	111.83	12	20
3	A	421	PCW	C3-O3-C11	2.53	107.88	117.12	14	13
3	A	401	PCW	O3-C11-C12	2.52	119.52	111.83	1	20
3	A	407	PCW	O3-C11-C12	2.52	119.52	111.83	2	20
3	C	216	PCW	O1P-P-O4P	2.52	96.16	107.57	9	20
3	A	412	PCW	O3-C11-C12	2.51	119.50	111.83	17	20
3	B	205	PCW	O1P-P-O4P	2.50	96.22	107.57	19	20
3	A	406	PCW	O3-C11-C12	2.50	119.45	111.83	6	20

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})	Models	
								Worst	Total
3	C	217	PCW	C3-O3-C11	2.50	107.99	117.12	19	20
3	D	606	PCW	O3-C11-C12	2.49	119.42	111.83	2	20
3	A	420	PCW	O3-C11-C12	2.48	119.41	111.83	10	20
3	D	602	PCW	O3-C11-C12	2.48	119.40	111.83	17	20
3	D	610	PCW	O3-C11-C12	2.47	119.37	111.83	18	20
4	A	415	17F	O2-P1-O3	2.47	96.36	107.57	8	20
3	D	621	PCW	C3-O3-C11	2.47	108.10	117.12	18	12
5	B	201	GSP	C5-C6-N1	2.46	118.77	114.07	19	20
3	B	205	PCW	O1P-P-O3P	2.46	118.72	107.57	15	20
3	C	203	PCW	C3-O3-C11	2.46	108.13	117.12	20	1
5	C	201	GSP	C5-C6-N1	2.45	118.74	114.07	14	20
3	D	616	PCW	C3-O3-C11	2.42	108.27	117.12	6	6
3	D	604	PCW	O3-C11-C12	2.41	119.19	111.83	13	20
3	D	601	PCW	C3-O3-C11	2.41	108.32	117.12	1	11
3	C	210	PCW	C3-O3-C11	2.40	108.33	117.12	6	18
4	B	209	17F	C6-O7-C7	2.40	108.33	117.12	13	19
3	D	619	PCW	C3-O3-C11	2.40	108.36	117.12	12	20
3	D	603	PCW	C3-O3-C11	2.39	108.37	117.12	2	7
3	D	618	PCW	C3-O3-C11	2.38	108.40	117.12	13	17
4	D	630	17F	O6-P1-O1	2.38	118.39	108.94	11	20
3	D	611	PCW	C3-O3-C11	2.38	108.44	117.12	15	11
3	C	206	PCW	C3-O3-C11	2.36	108.49	117.12	11	13
3	A	419	PCW	C3-O3-C11	2.35	108.51	117.12	12	18
3	C	216	PCW	O1P-P-O3P	2.35	118.21	107.57	17	20
4	A	415	17F	O6-P1-O1	2.35	118.23	108.94	13	20
4	D	630	17F	O2-P1-O3	2.34	96.94	107.57	11	20
3	D	617	PCW	C3-O3-C11	2.33	108.59	117.12	11	7
4	D	631	17F	C6-O7-C7	2.31	108.69	117.12	20	6
3	D	627	PCW	C3-O3-C11	2.29	108.75	117.12	17	12
3	A	418	PCW	C3-O3-C11	2.29	108.75	117.12	5	15
3	D	619	PCW	C3-C2-C1	2.29	106.46	111.78	12	2
3	D	624	PCW	C3-O3-C11	2.28	108.77	117.12	14	18
3	D	625	PCW	C3-O3-C11	2.28	108.77	117.12	20	4
4	A	416	17F	C6-O7-C7	2.28	108.77	117.12	14	7
4	D	629	17F	O7-C7-C8	2.27	118.77	111.83	10	15
4	D	630	17F	C6-O7-C7	2.27	108.84	117.12	16	10
3	D	622	PCW	C3-O3-C11	2.26	108.85	117.12	16	2
4	C	218	17F	O9-C17-O10	2.26	118.42	123.70	13	17
3	D	627	PCW	C4-C5-N	2.24	108.63	115.82	17	5
4	C	219	17F	C6-O7-C7	2.24	108.92	117.12	5	10
3	D	620	PCW	O3-C11-C12	2.24	118.67	111.83	2	18

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)	Models	
								Worst	Total
3	A	417	PCW	C3-O3-C11	2.24	108.94	117.12	11	7
3	A	408	PCW	C3-O3-C11	2.23	108.95	117.12	8	9
3	A	402	PCW	C3-O3-C11	2.23	108.98	117.12	1	8
3	C	209	PCW	C3-O3-C11	2.21	109.03	117.12	4	3
3	D	615	PCW	C3-O3-C11	2.21	109.04	117.12	12	7
3	D	612	PCW	C3-O3-C11	2.21	109.05	117.12	11	14
3	C	205	PCW	C3-O3-C11	2.21	109.06	117.12	18	8
3	D	608	PCW	C4-C5-N	2.20	108.75	115.82	5	6
4	D	632	17F	C6-O7-C7	2.20	109.07	117.12	5	7
3	B	203	PCW	C3-O3-C11	2.20	109.08	117.12	1	10
3	C	212	PCW	C3-O3-C11	2.20	109.09	117.12	19	11
3	A	406	PCW	C3-C2-C1	2.19	106.67	111.78	10	2
3	C	208	PCW	C3-O3-C11	2.19	109.10	117.12	8	13
4	C	218	17F	C6-O7-C7	2.19	109.10	117.12	14	5
4	B	210	17F	C6-O7-C7	2.19	109.11	117.12	16	3
3	D	609	PCW	C3-O3-C11	2.18	109.14	117.12	4	14
3	D	613	PCW	C3-O3-C11	2.18	109.15	117.12	18	2
3	A	412	PCW	C3-O3-C11	2.18	109.16	117.12	17	2
3	A	407	PCW	C4-C5-N	2.17	108.87	115.82	19	5
3	B	204	PCW	C3-O3-C11	2.17	109.20	117.12	20	6
3	A	411	PCW	C3-O3-C11	2.16	109.21	117.12	18	7
3	D	614	PCW	C4-C5-N	2.16	108.88	115.82	6	4
4	B	211	17F	C6-O7-C7	2.16	109.23	117.12	10	5
3	D	622	PCW	C4-C5-N	2.16	108.90	115.82	14	2
3	D	607	PCW	C3-O3-C11	2.15	109.26	117.12	4	12
3	A	409	PCW	C3-O3-C11	2.15	109.27	117.12	12	3
3	C	217	PCW	C4-C5-N	2.15	108.92	115.82	16	11
3	D	626	PCW	C3-O3-C11	2.15	109.27	117.12	13	10
3	C	204	PCW	C3-O3-C11	2.14	109.29	117.12	2	8
3	D	610	PCW	C4-C5-N	2.13	108.97	115.82	9	8
3	A	404	PCW	C4-C5-N	2.13	108.98	115.82	16	9
3	A	419	PCW	C4-C5-N	2.12	109.00	115.82	5	3
3	D	605	PCW	C3-C2-C1	2.13	106.83	111.78	10	4
3	A	413	PCW	C3-O3-C11	2.12	109.36	117.12	16	2
4	A	422	17F	C6-O7-C7	2.12	109.38	117.12	4	5
3	A	413	PCW	C4-C5-N	2.12	109.03	115.82	19	6
3	D	603	PCW	C4-C5-N	2.12	109.03	115.82	13	8
3	D	621	PCW	C4-C5-N	2.12	109.03	115.82	19	2
3	D	610	PCW	C3-O3-C11	2.11	109.39	117.12	5	1
3	A	414	PCW	C4-C5-N	2.11	109.06	115.82	10	4
3	D	621	PCW	C7-N-C5	2.11	118.28	109.91	3	6

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})	Models	
								Worst	Total
4	D	628	17F	C6-O7-C7	2.10	109.44	117.12	17	5
3	C	207	PCW	C3-O3-C11	2.10	109.45	117.12	16	1
3	C	216	PCW	C3-O3-C11	2.10	109.45	117.12	9	2
3	A	421	PCW	C4-C5-N	2.09	109.10	115.82	6	5
3	B	205	PCW	C3-O3-C11	2.09	109.46	117.12	8	4
3	C	211	PCW	C3-O3-C11	2.09	109.48	117.12	10	2
4	A	415	17F	C6-O7-C7	2.09	109.49	117.12	3	5
3	A	404	PCW	C3-O3-C11	2.08	109.50	117.12	3	3
3	B	208	PCW	C4-C5-N	2.07	109.19	115.82	12	2
3	A	419	PCW	C3-C2-C1	2.07	106.97	111.78	6	1
3	D	627	PCW	C8-N-C5	2.07	118.12	109.91	2	4
3	A	406	PCW	C4-C5-N	2.06	109.20	115.82	5	2
4	B	210	17F	O9-C17-O10	2.06	118.88	123.70	17	6
3	A	402	PCW	C4-C5-N	2.06	109.21	115.82	15	1
3	C	208	PCW	C4-C5-N	2.06	109.21	115.82	11	1
3	D	626	PCW	C4-C5-N	2.05	109.23	115.82	8	2
3	B	208	PCW	C3-O3-C11	2.05	109.61	117.12	4	5
4	C	215	17F	C6-O7-C7	2.05	109.61	117.12	11	4
3	D	617	PCW	C4-C5-N	2.05	109.23	115.82	14	1
3	A	405	PCW	C7-N-C5	2.05	118.06	109.91	2	2
3	D	608	PCW	C3-C2-C1	2.05	107.01	111.78	5	2
3	B	206	PCW	C3-O3-C11	2.05	109.64	117.12	20	3
3	A	418	PCW	C7-N-C5	2.04	118.04	109.91	14	1
3	D	611	PCW	C4-C5-N	2.05	109.26	115.82	19	1
3	B	208	PCW	C8-N-C5	2.04	118.03	109.91	11	2
3	A	405	PCW	C3-O3-C11	2.04	109.65	117.12	19	2
3	D	604	PCW	C4-C5-N	2.04	109.29	115.82	8	1
3	D	606	PCW	C4-C5-N	2.04	109.28	115.82	15	3
3	D	608	PCW	C7-N-C5	2.04	118.01	109.91	1	2
3	A	401	PCW	C3-O3-C11	2.03	109.68	117.12	1	2
3	A	418	PCW	C4-C5-N	2.03	109.29	115.82	14	1
3	A	405	PCW	C8-N-C5	2.03	117.99	109.91	19	1
3	A	417	PCW	C4-C5-N	2.03	109.30	115.82	10	2
3	D	601	PCW	C3-C2-C1	2.03	107.04	111.78	20	1
3	B	204	PCW	C4-C5-N	2.03	109.30	115.82	1	1
3	C	210	PCW	C4-C5-N	2.03	109.30	115.82	5	2
3	D	601	PCW	C4-C5-N	2.03	109.31	115.82	13	4
3	D	612	PCW	C4-C5-N	2.03	109.32	115.82	3	2
3	D	619	PCW	C4-C5-N	2.03	109.32	115.82	20	2
3	B	203	PCW	C8-N-C5	2.03	117.97	109.91	2	2
3	C	205	PCW	C8-N-C5	2.03	117.97	109.91	5	1

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})	Models	
								Worst	Total
4	C	213	17F	C6-O7-C7	2.02	109.73	117.12	8	1
4	C	215	17F	O9-C17-O10	2.02	118.97	123.70	15	1
3	D	627	PCW	O2-C31-O31	2.02	118.98	123.70	4	2
3	D	608	PCW	C8-N-C5	2.02	117.94	109.91	15	1
3	A	404	PCW	C8-N-C5	2.02	117.93	109.91	6	1
3	A	418	PCW	C8-N-C5	2.02	117.93	109.91	15	2
3	D	609	PCW	C7-N-C5	2.02	117.93	109.91	2	2
3	D	623	PCW	C3-O3-C11	2.02	109.74	117.12	3	1
3	D	620	PCW	C8-N-C5	2.02	117.92	109.91	2	2
3	B	205	PCW	C4-C5-N	2.02	109.35	115.82	11	1
3	C	209	PCW	C4-C5-N	2.02	109.35	115.82	17	2
3	D	625	PCW	C4-C5-N	2.01	109.38	115.82	20	2
3	D	605	PCW	C8-N-C5	2.01	117.89	109.91	4	1
3	D	605	PCW	C4-C5-N	2.01	109.38	115.82	12	1
3	C	204	PCW	C4-C5-N	2.01	109.38	115.82	8	1
3	C	216	PCW	C8-N-C5	2.01	117.88	109.91	6	1
3	A	420	PCW	C4-C5-N	2.00	109.39	115.82	5	1
3	D	615	PCW	C7-N-C5	2.00	117.88	109.91	3	1
3	A	417	PCW	C8-N-C5	2.00	117.87	109.91	12	1
3	A	401	PCW	C7-N-C5	2.00	117.86	109.91	10	1
3	D	622	PCW	C8-N-C5	2.00	117.86	109.91	13	1
3	C	203	PCW	C8-N-C5	2.00	117.86	109.91	11	1
3	C	203	PCW	C4-C5-N	2.00	109.40	115.82	19	1
3	C	211	PCW	C4-C5-N	2.00	109.40	115.82	10	1

There are no chirality outliers.

All unique torsion outliers are listed below. They are sorted by the frequency of occurrence in the ensemble.

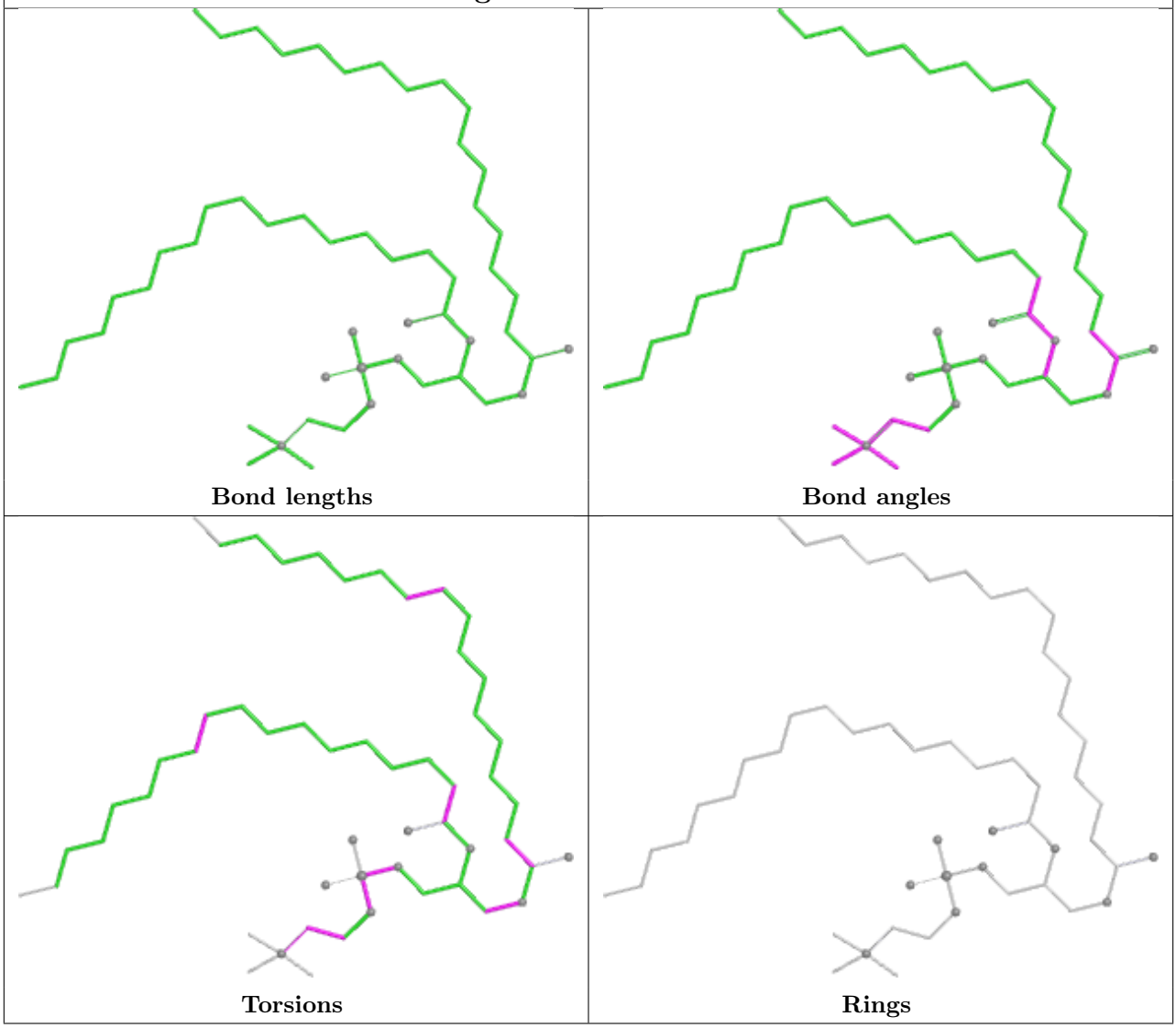
Mol	Chain	Res	Type	Atoms	Models (Total)
4	B	210	17F	O10-C17-O9-C5	20
4	C	215	17F	O10-C17-O9-C5	20
4	C	218	17F	O10-C17-O9-C5	20
4	C	218	17F	C18-C17-O9-C5	8
4	C	215	17F	C18-C17-O9-C5	3
4	B	210	17F	C18-C17-O9-C5	1

There are no ring outliers.

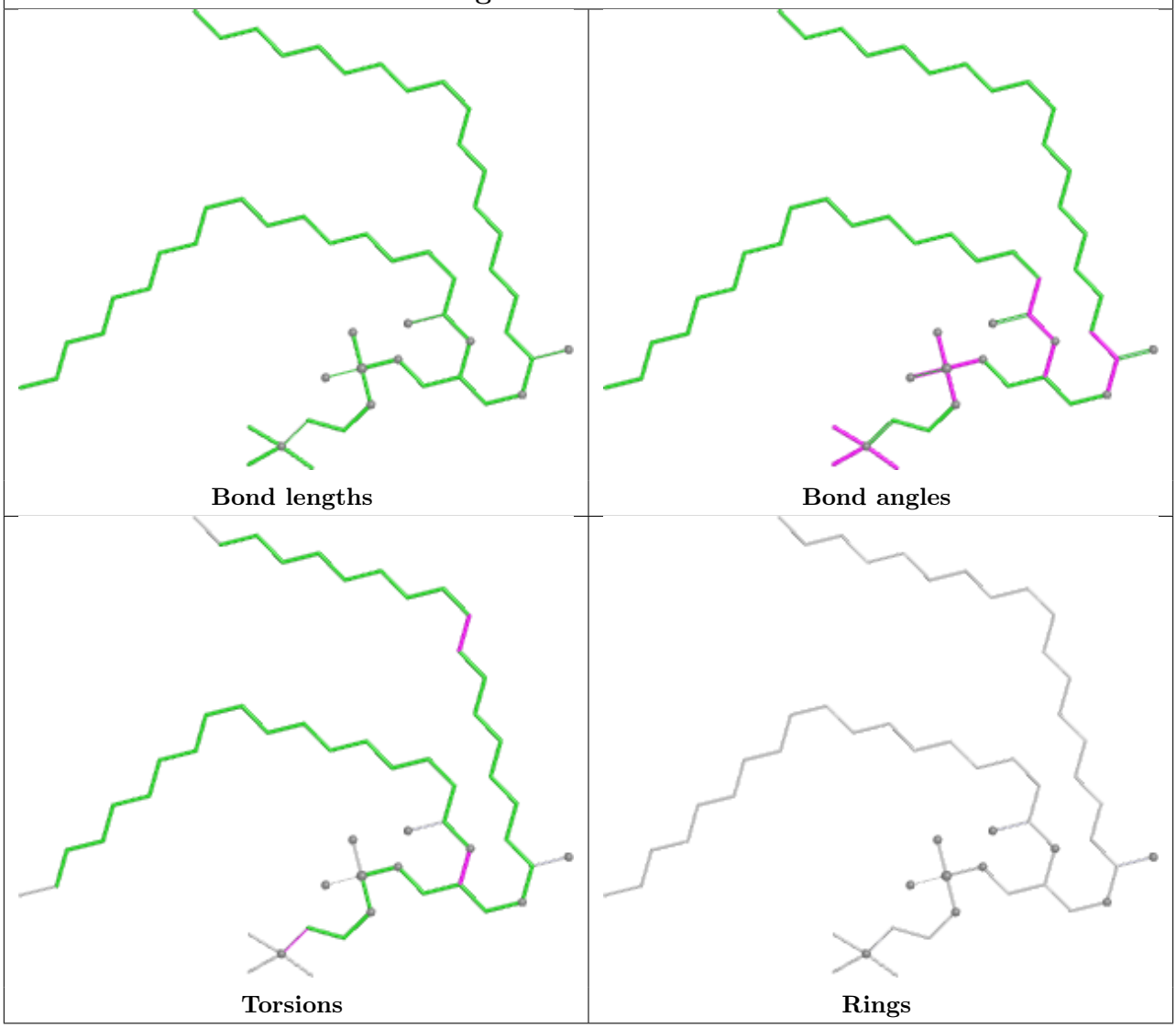
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will

also be included. For torsion angles, if less then 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

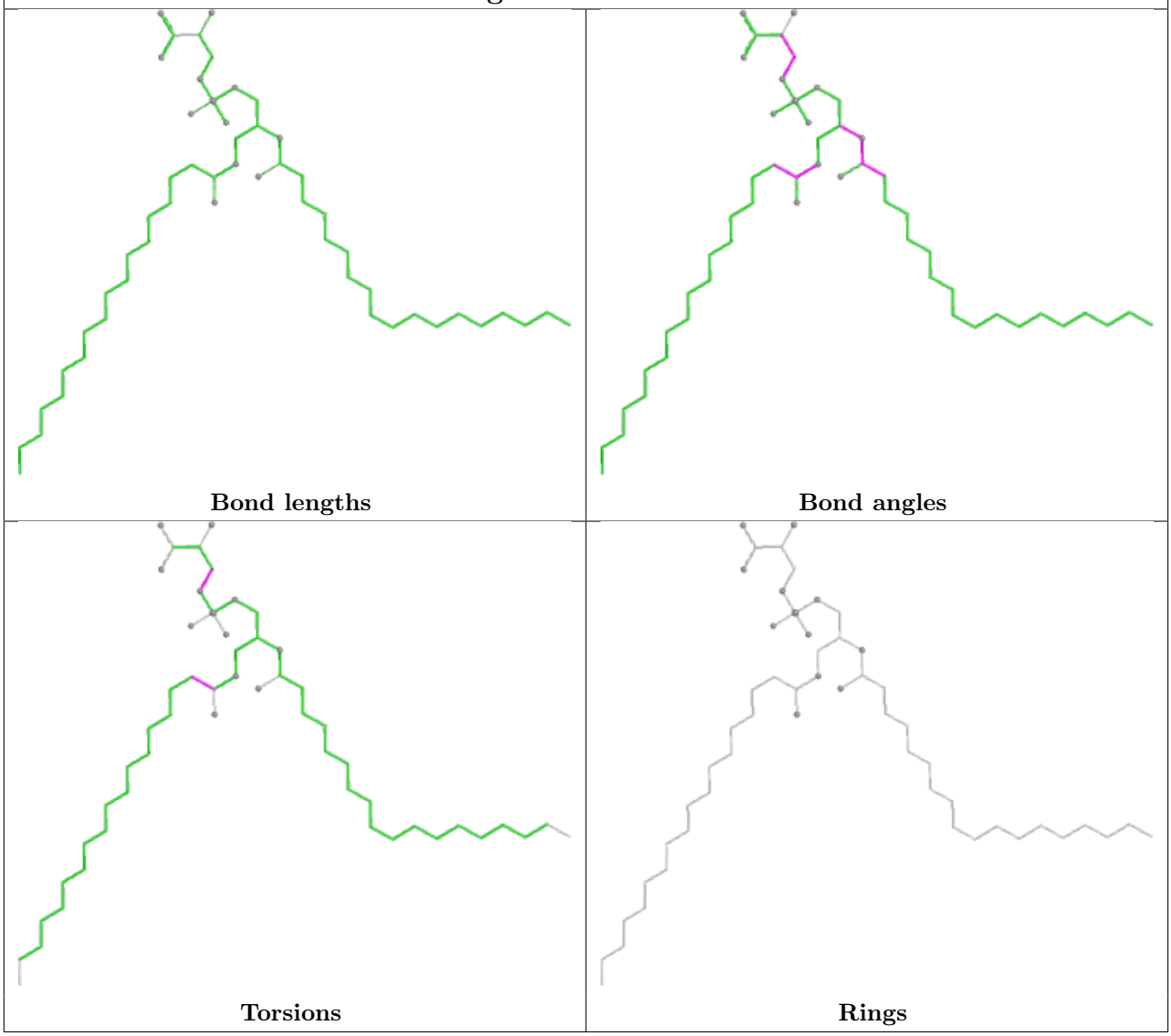
Ligand PCW D 608



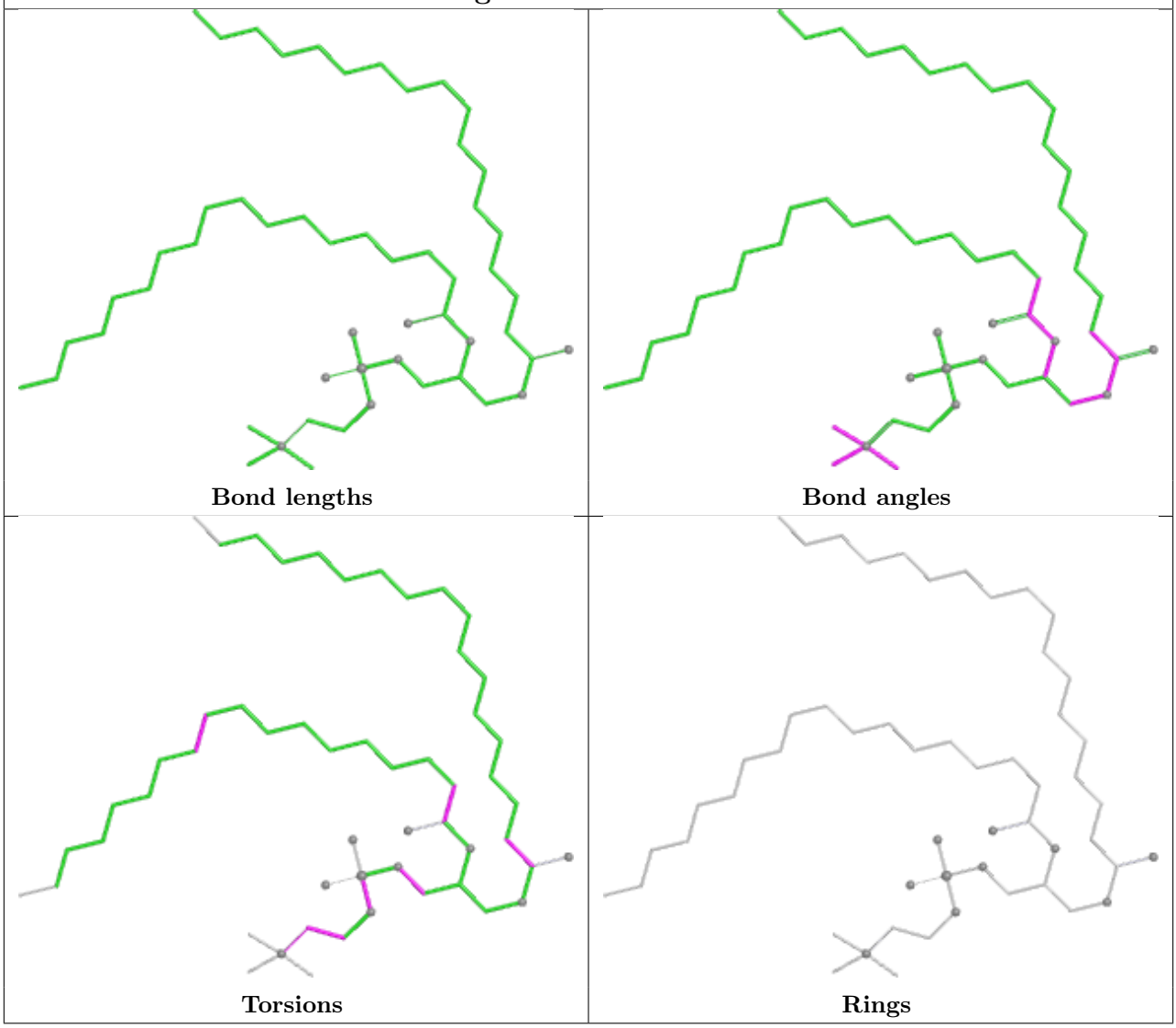
Ligand PCW C 216



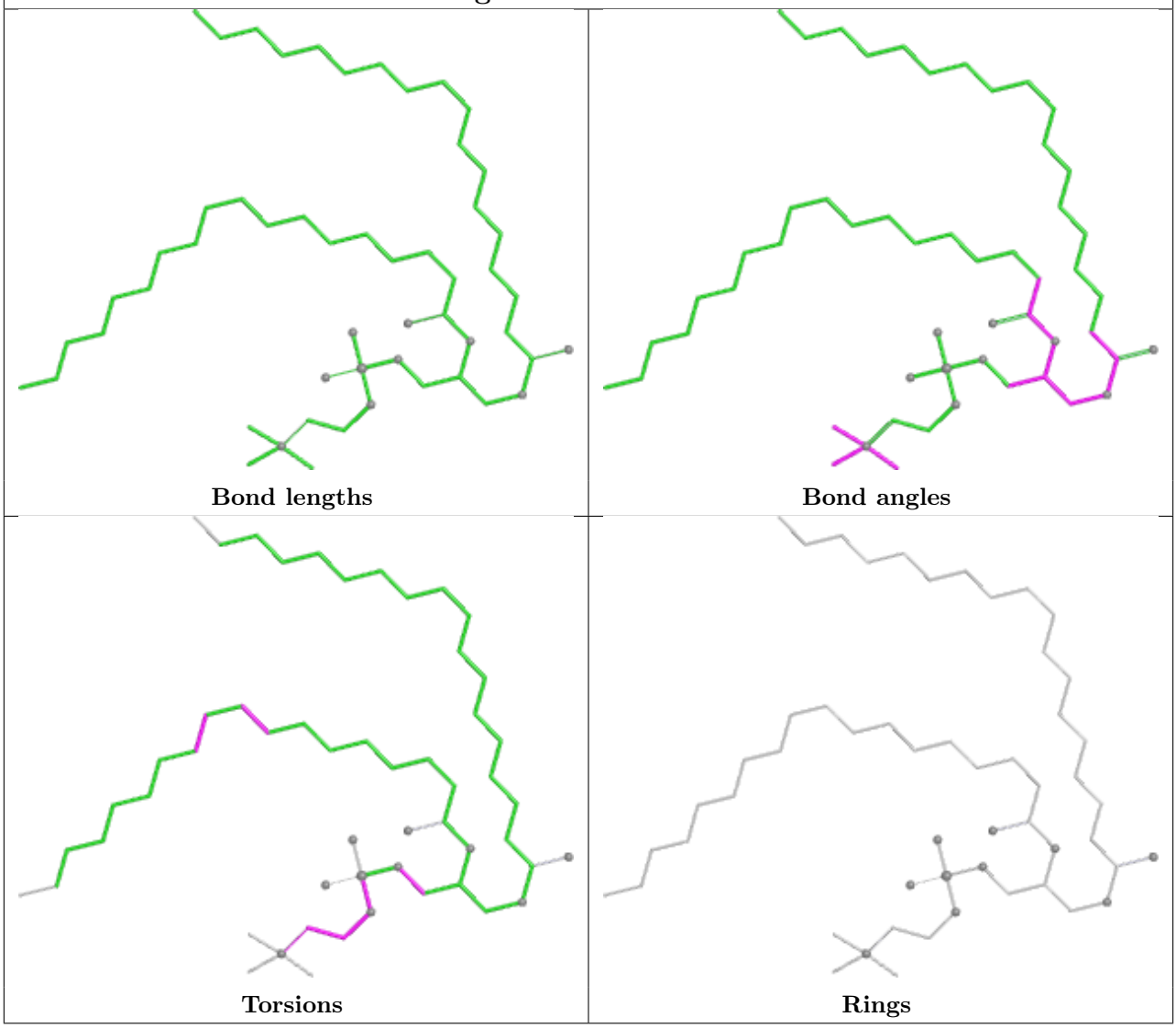
Ligand 17F B 211



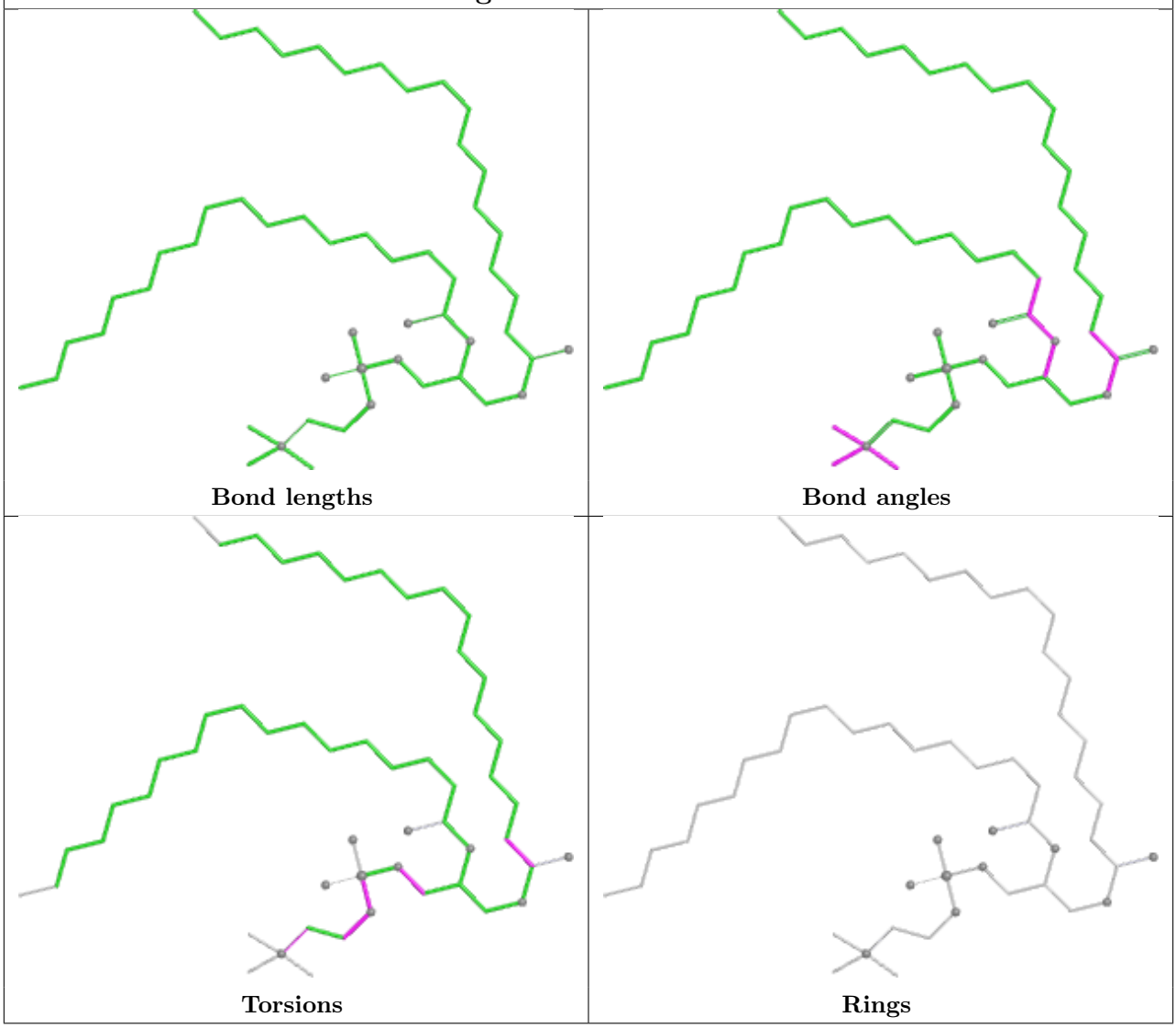
Ligand PCW D 613



Ligand PCW D 605



Ligand PCW B 206



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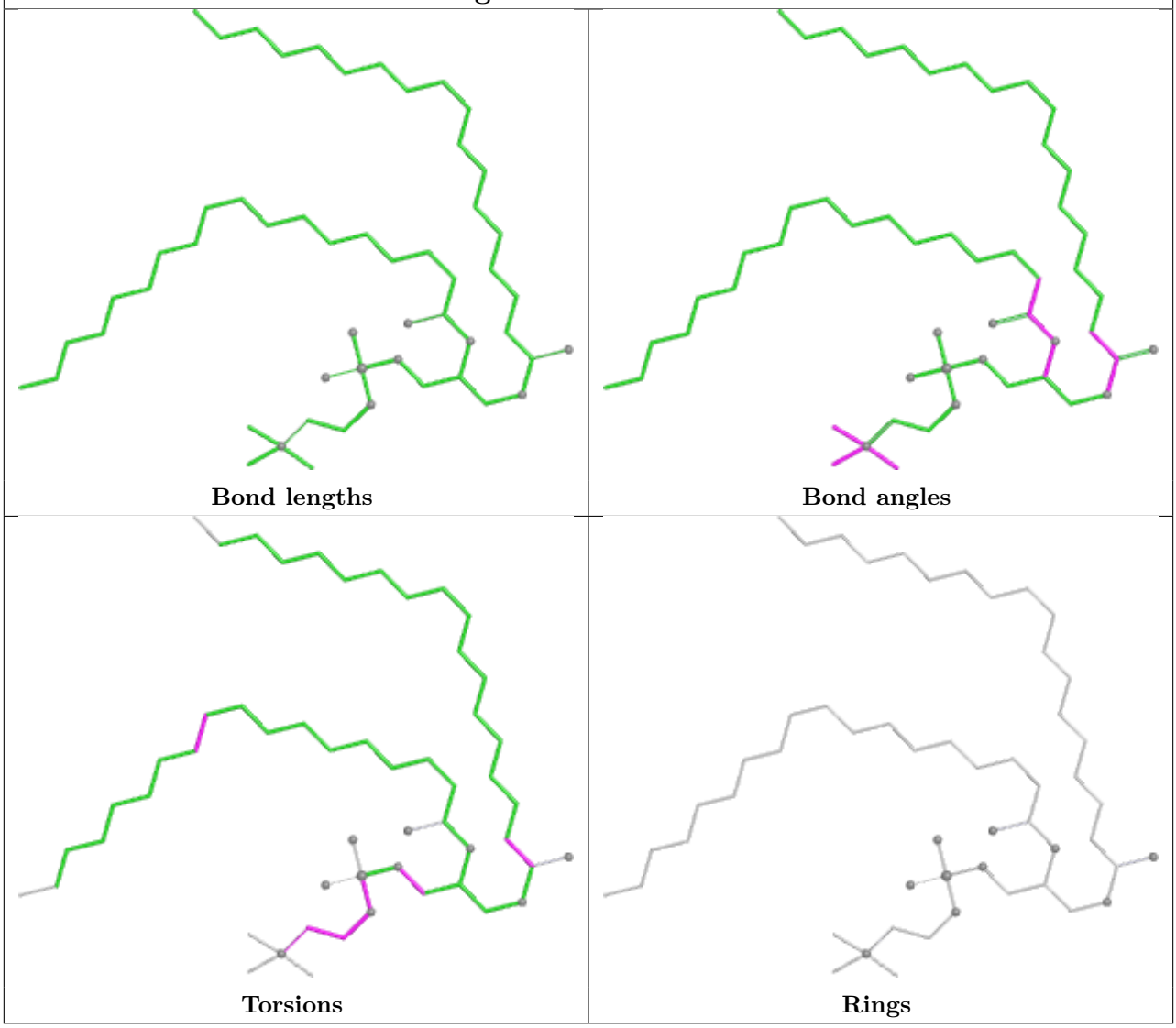

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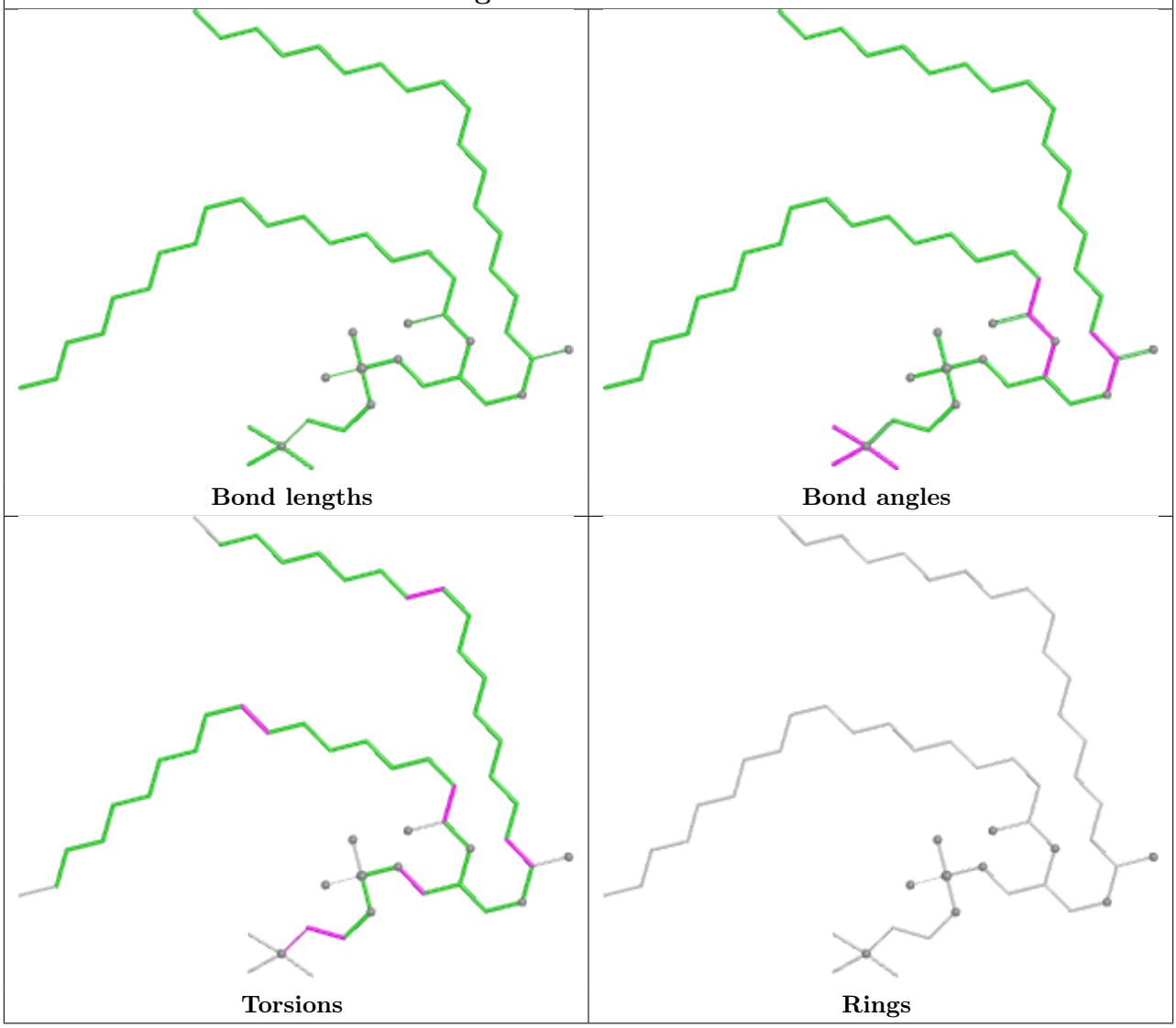
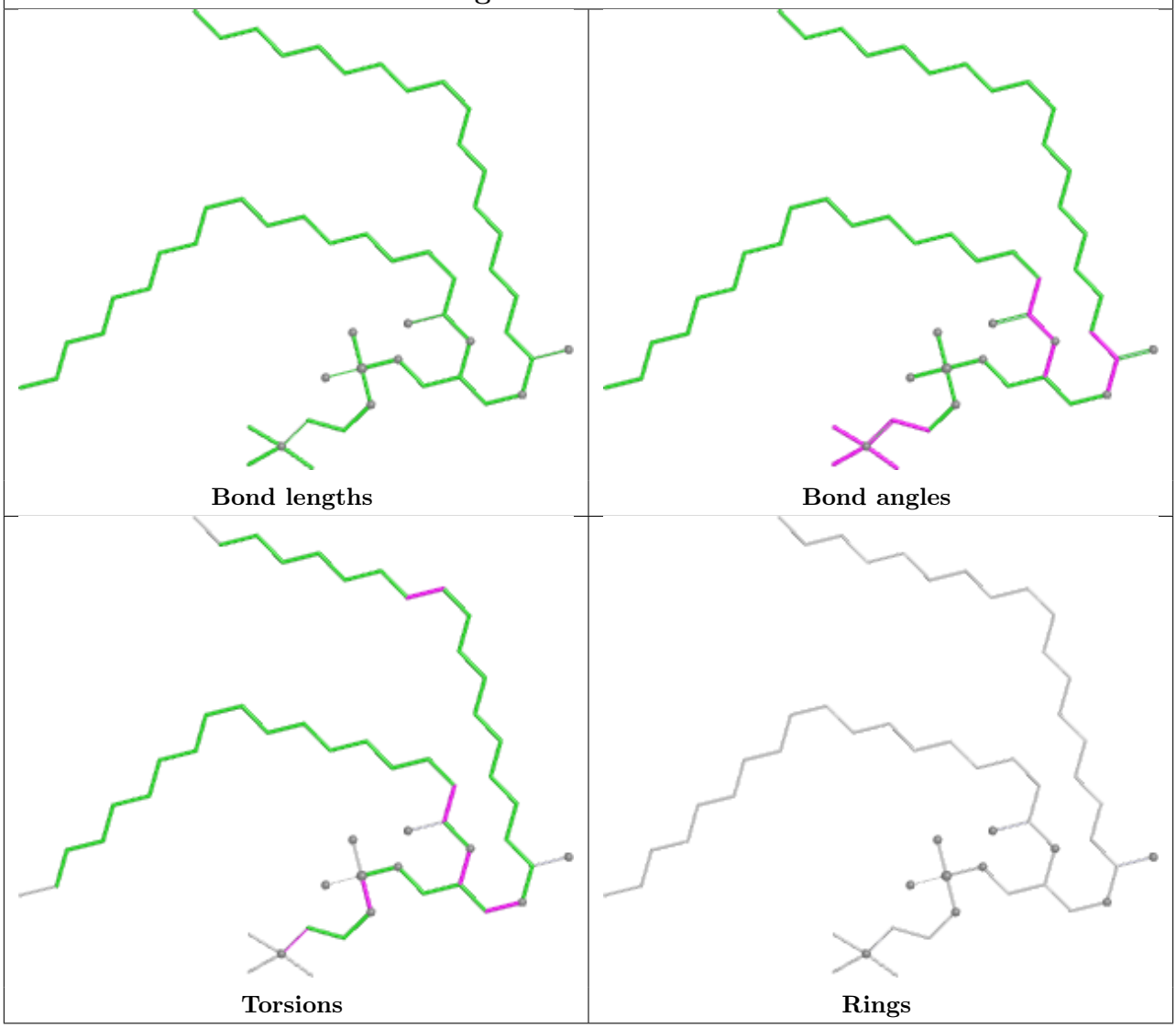
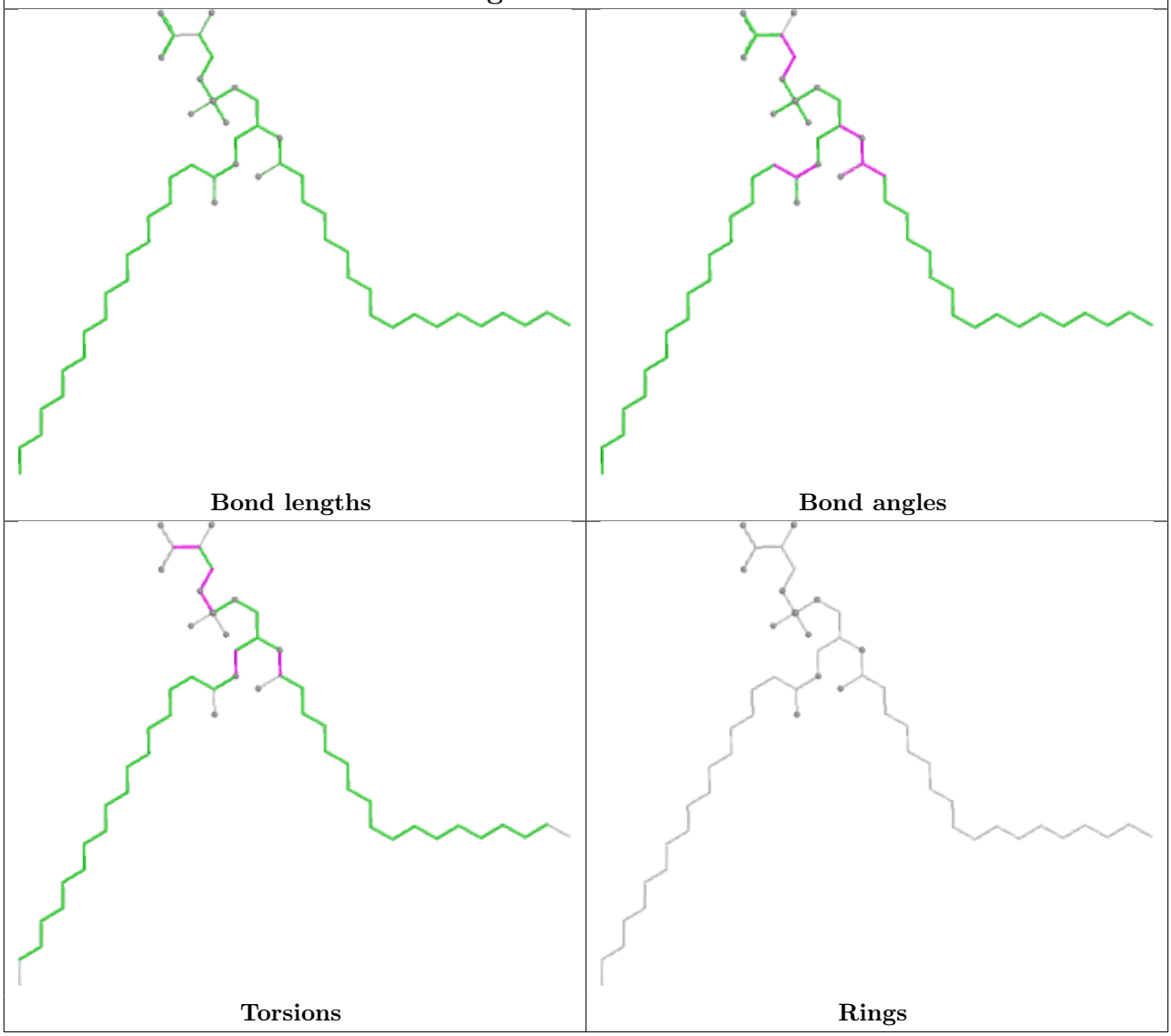


Ligand PCW D 614



Ligand 17F B 210



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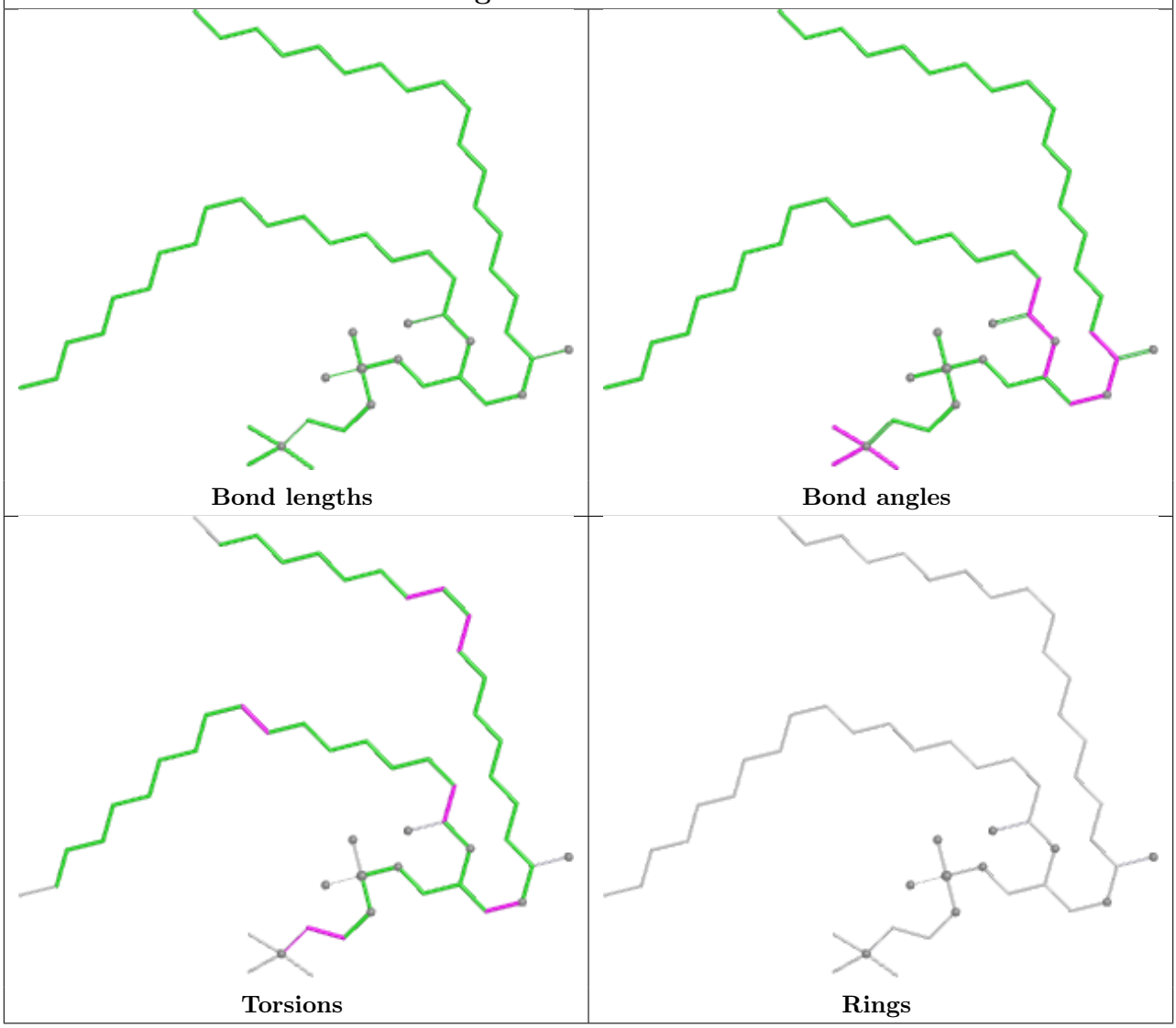
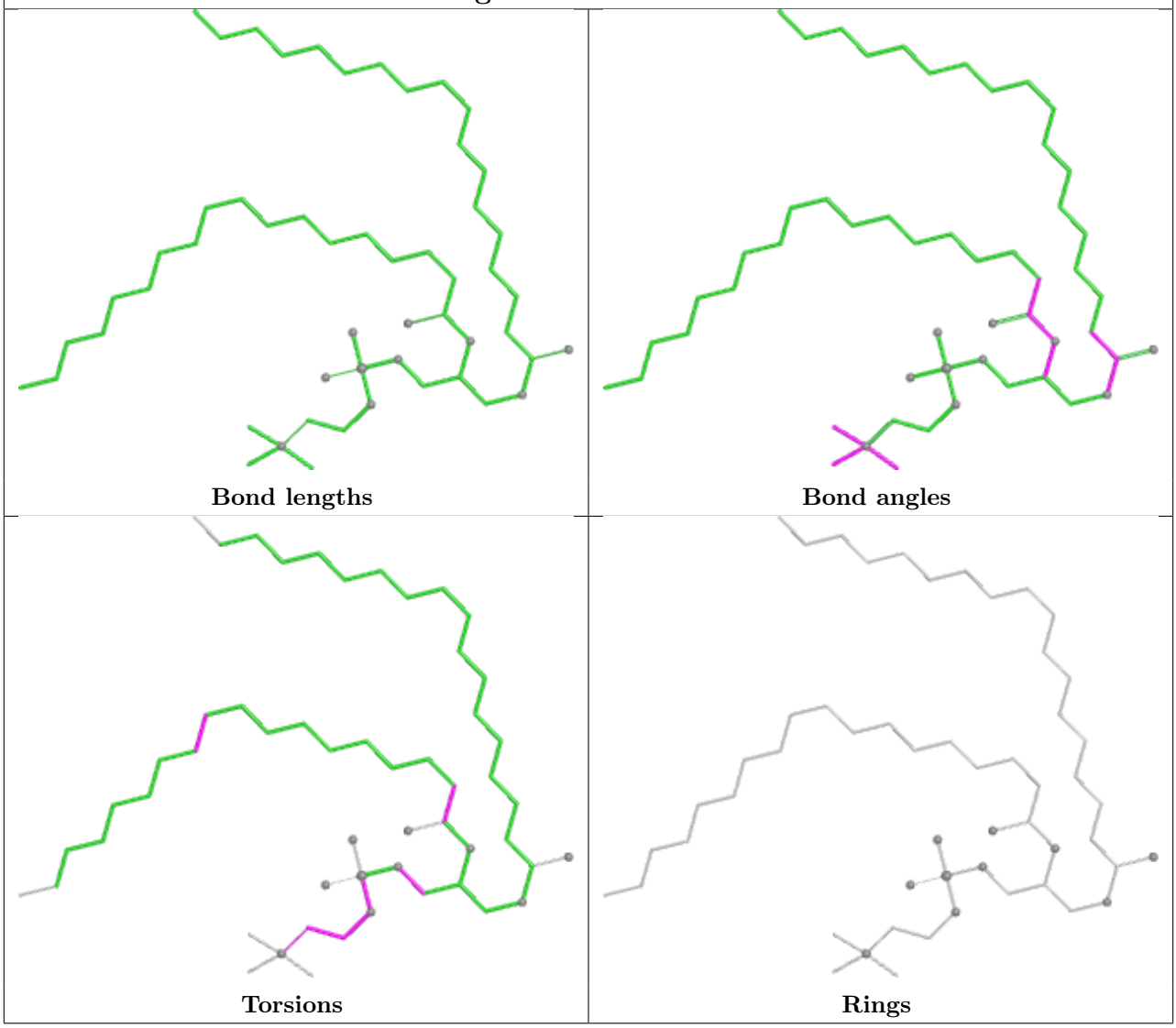


Ligand PCW A 411



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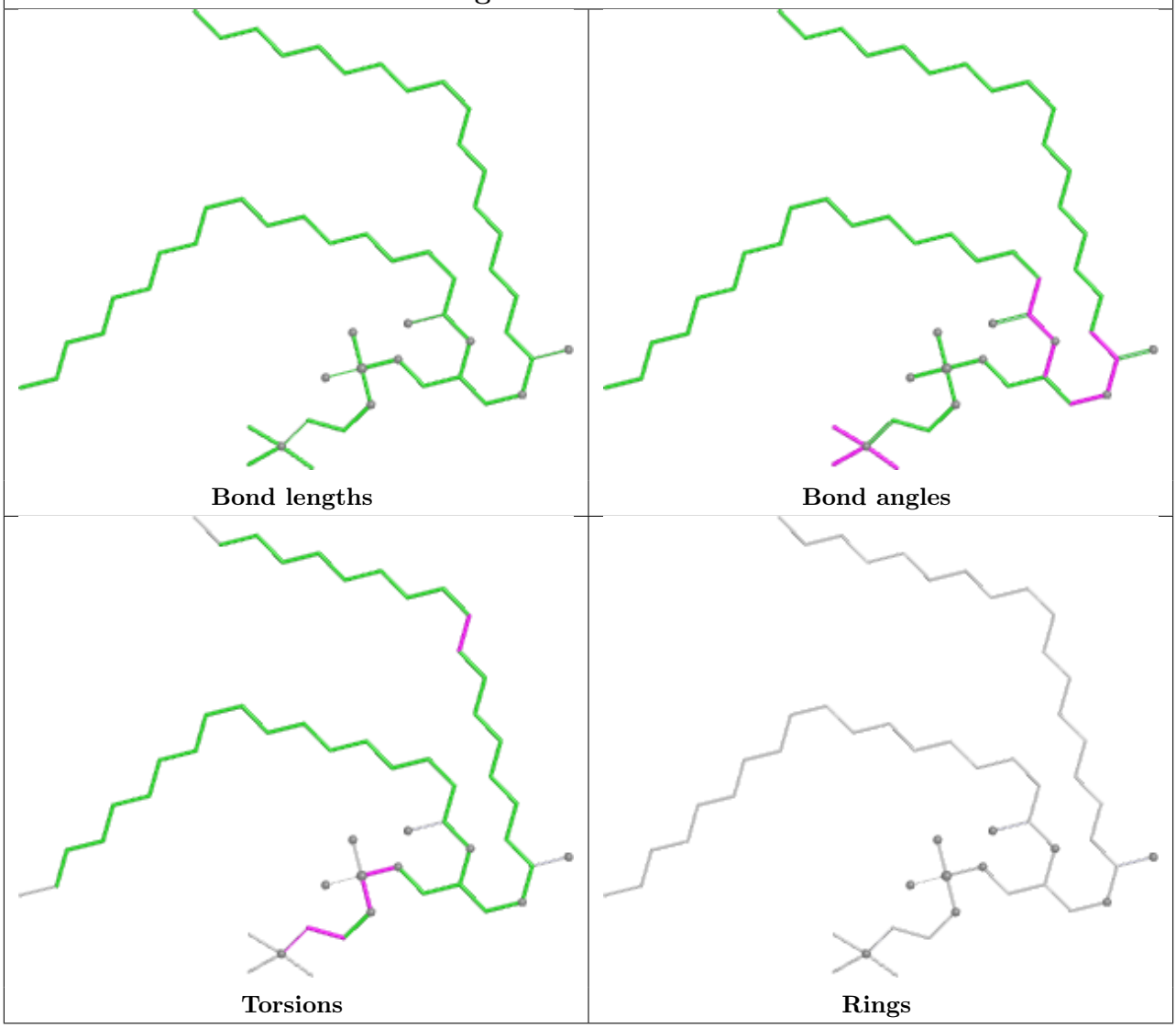
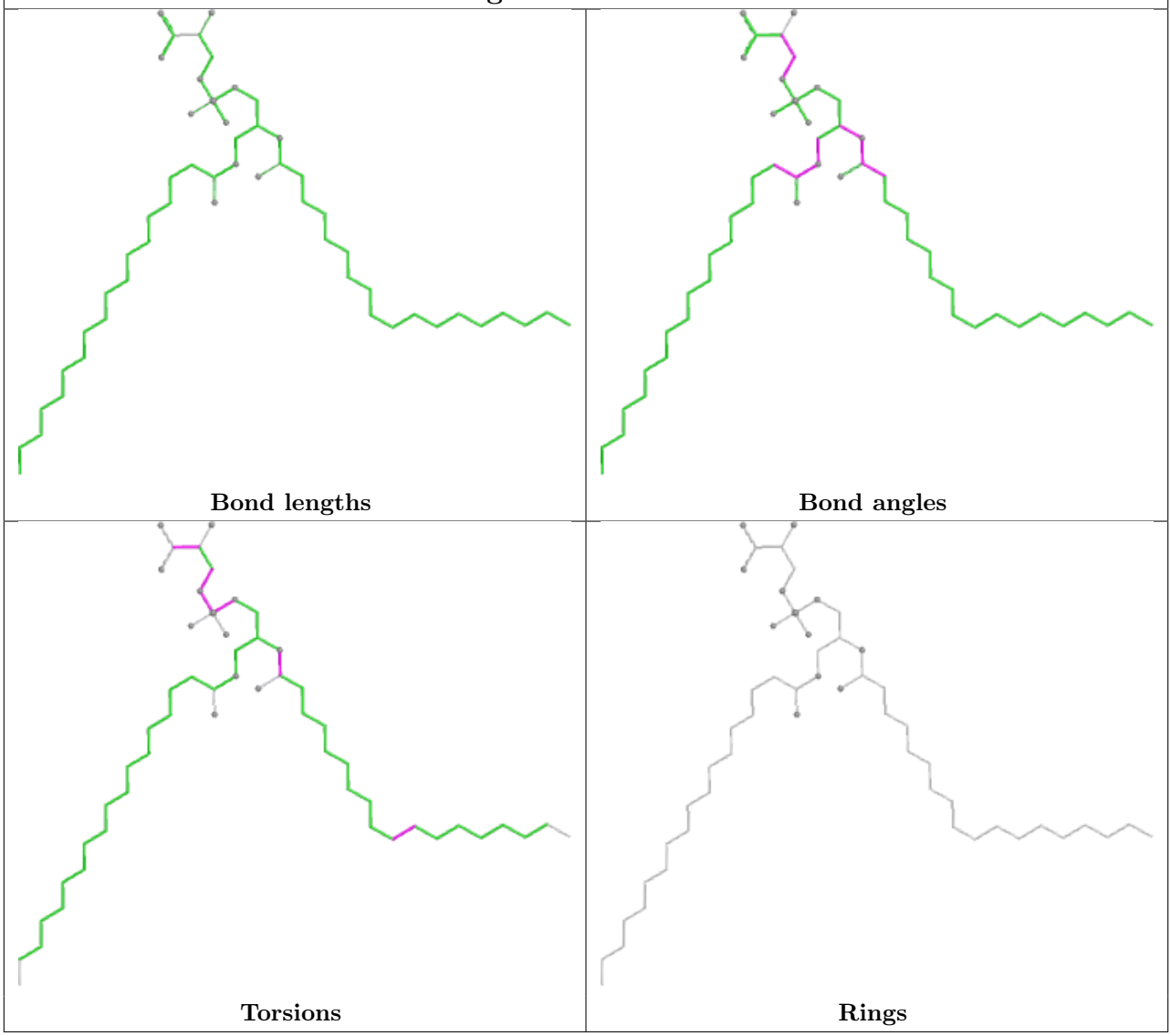


Ligand 17F C 215



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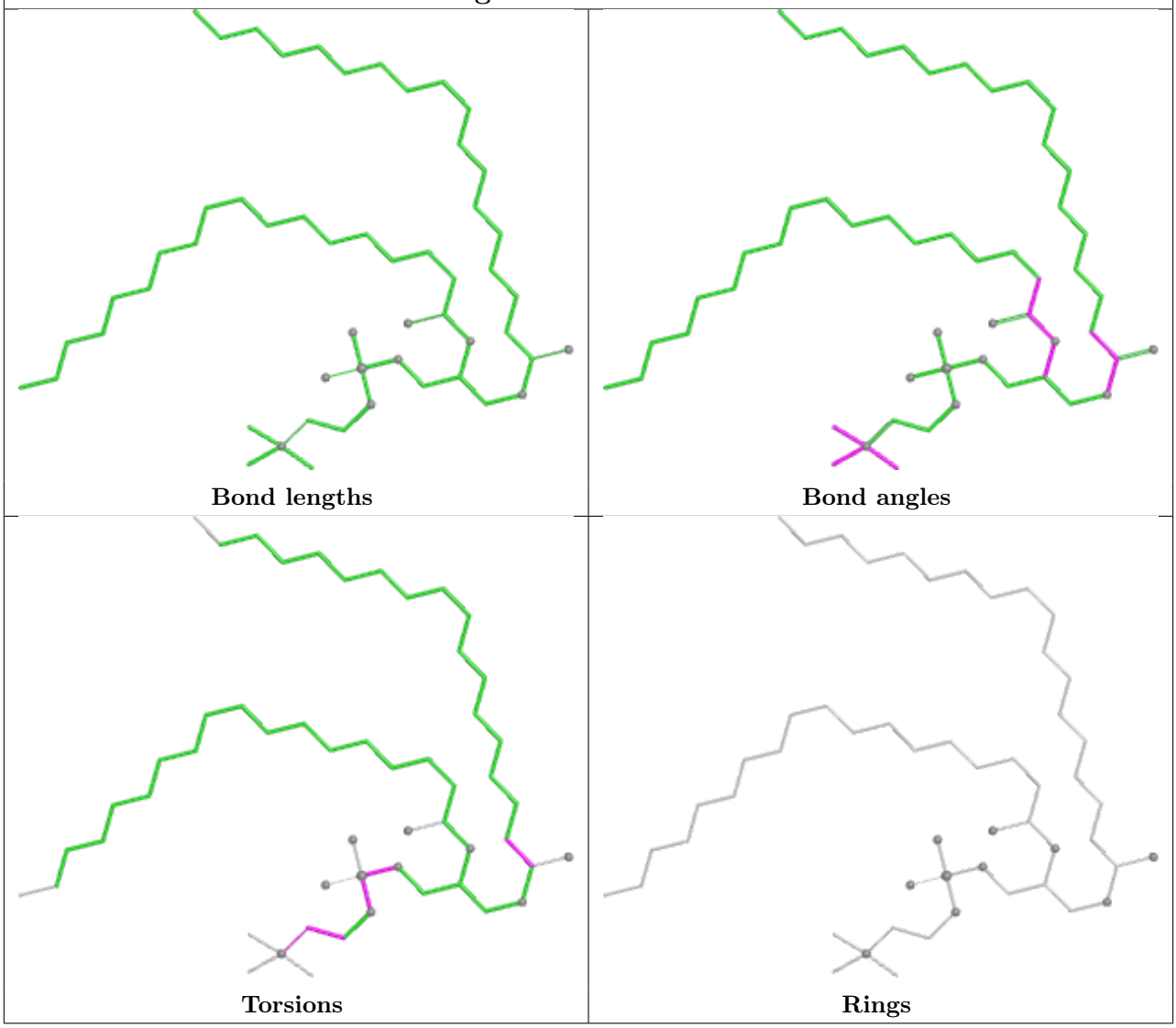

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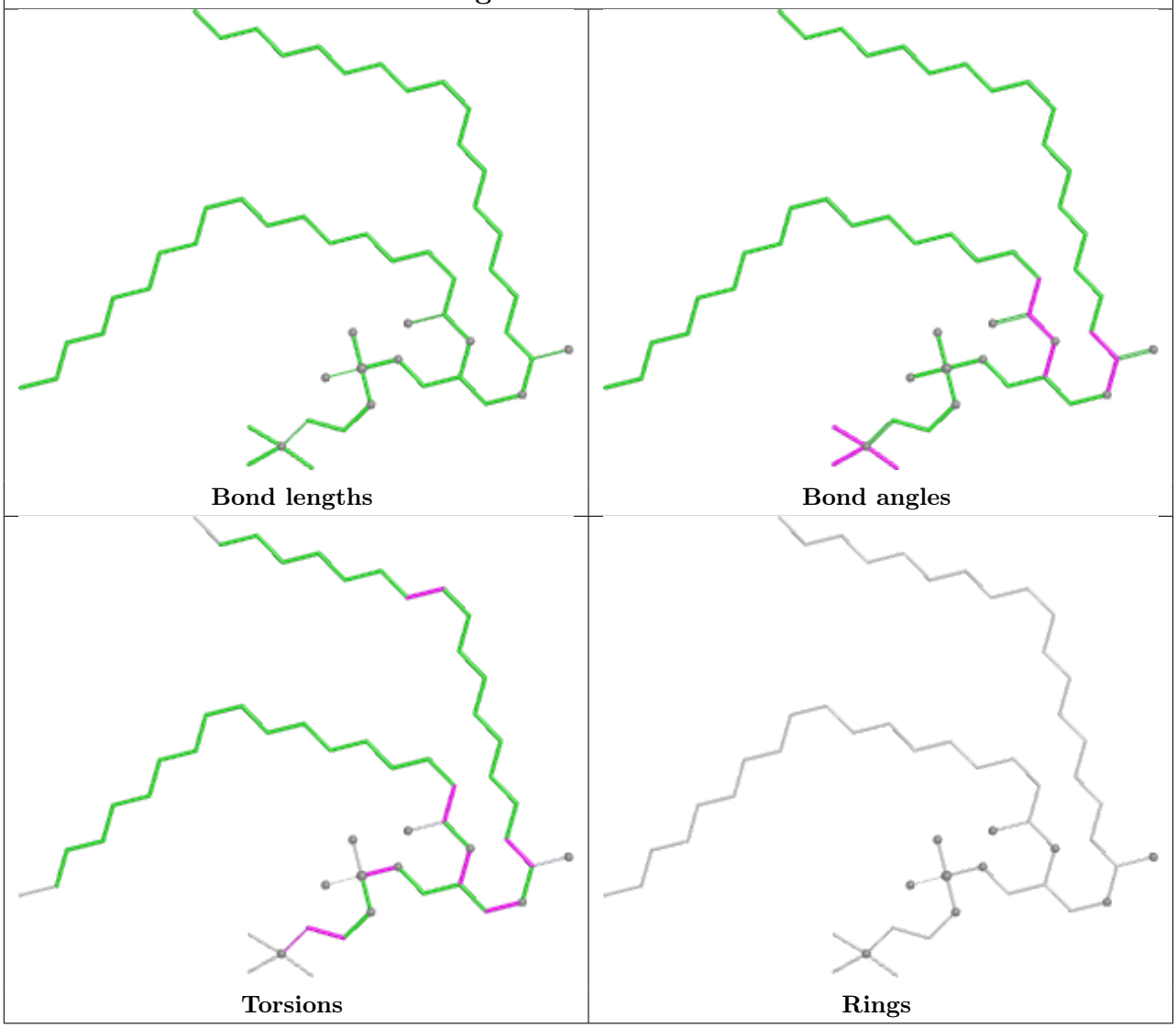

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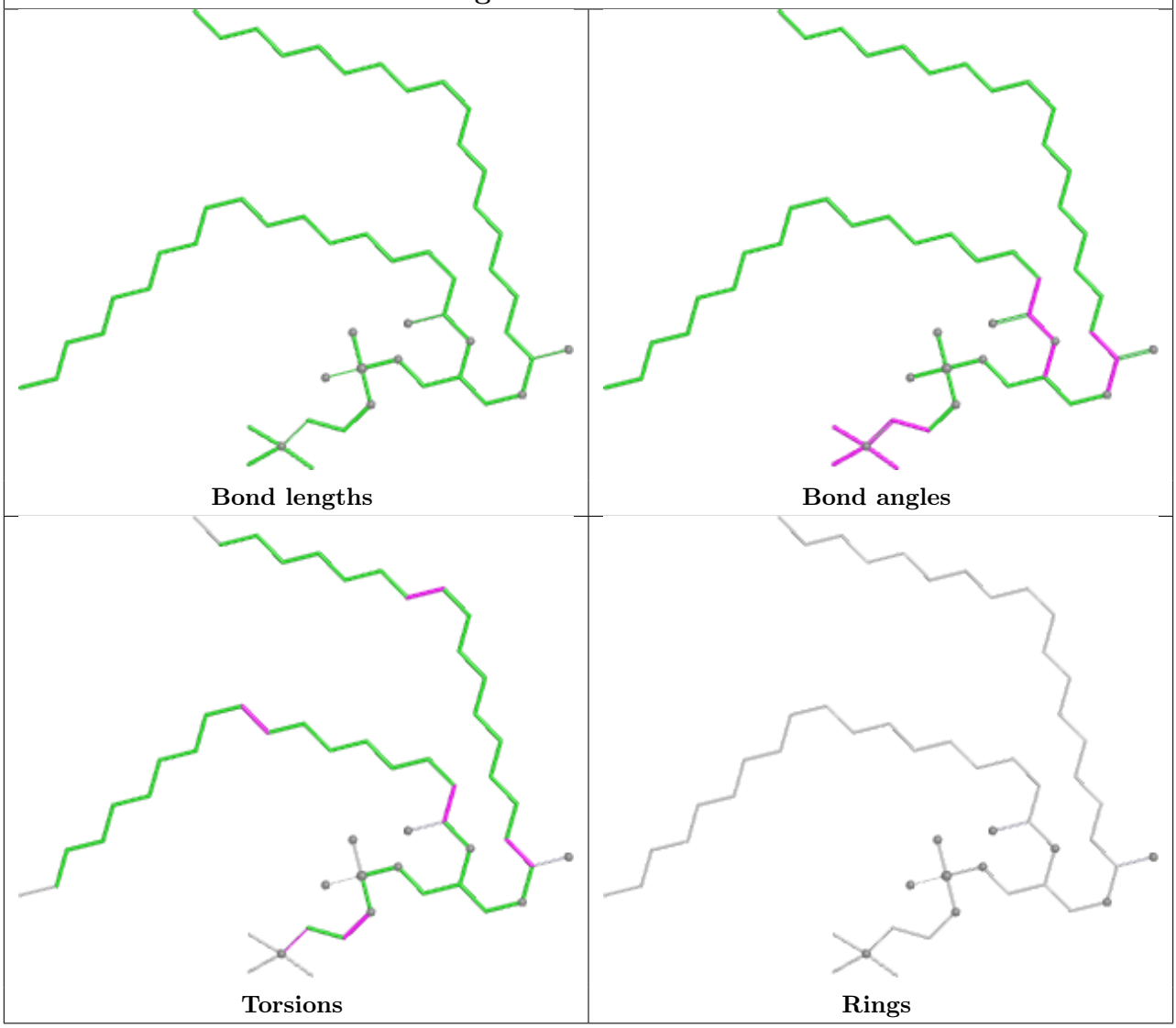

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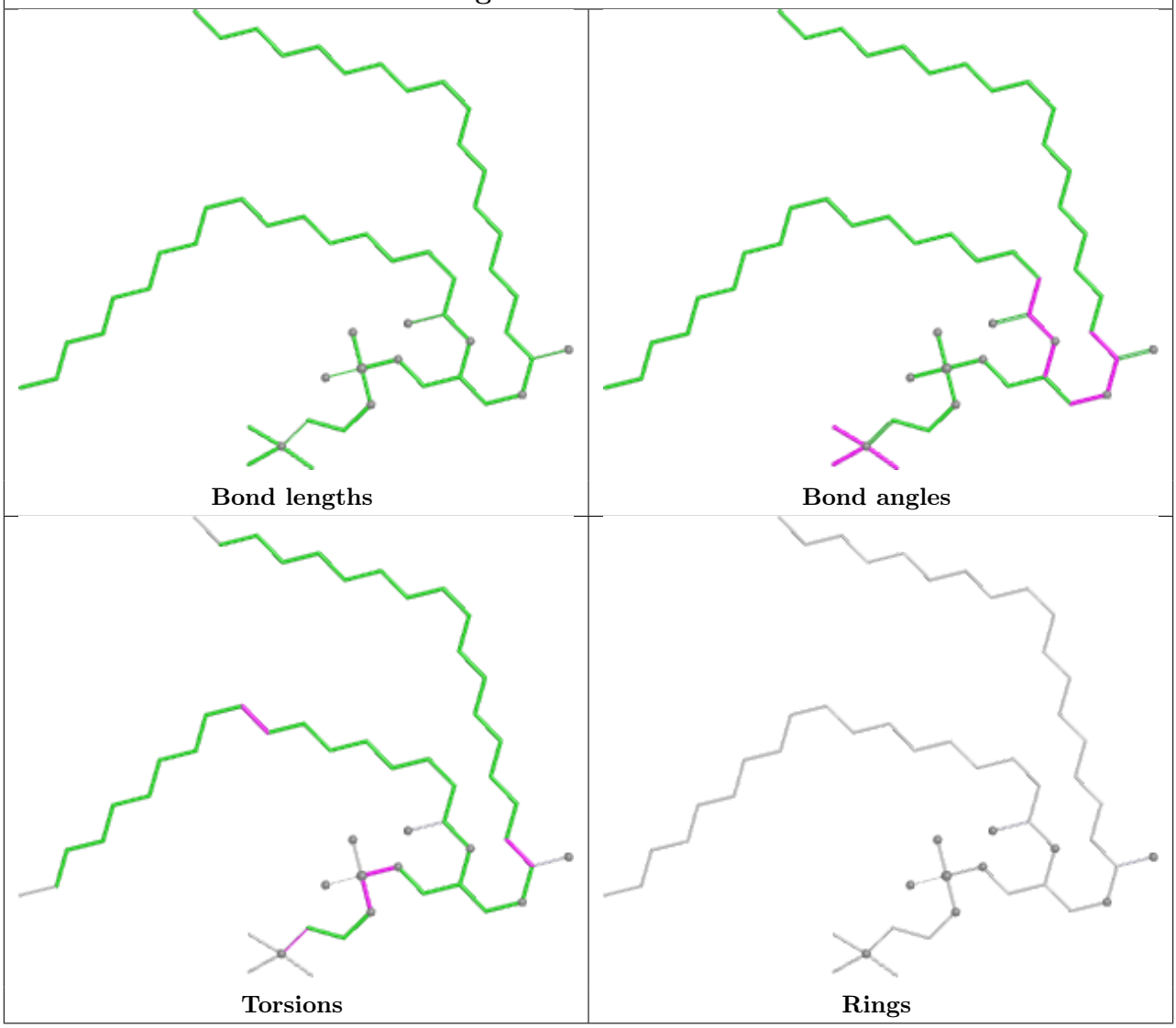

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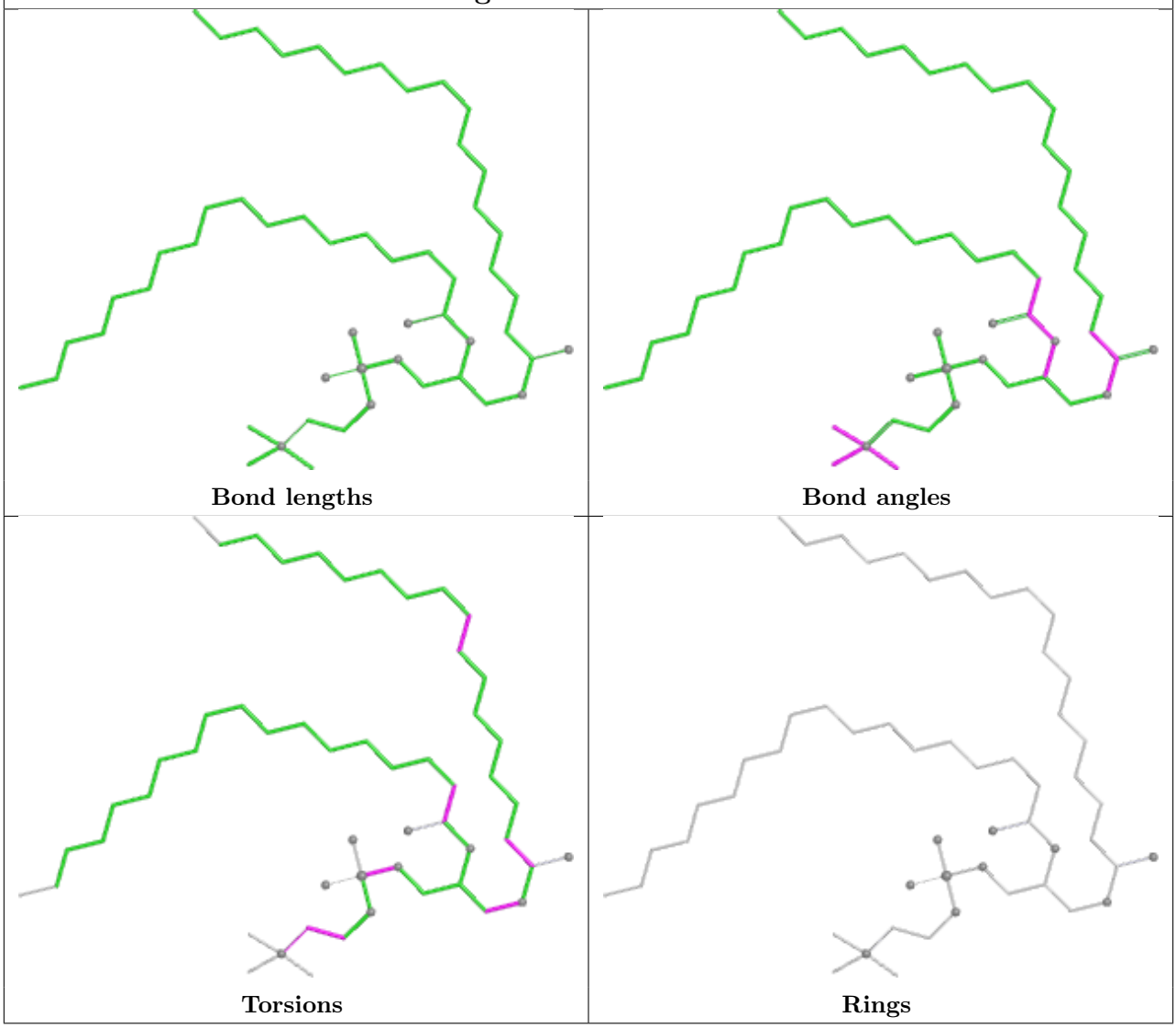

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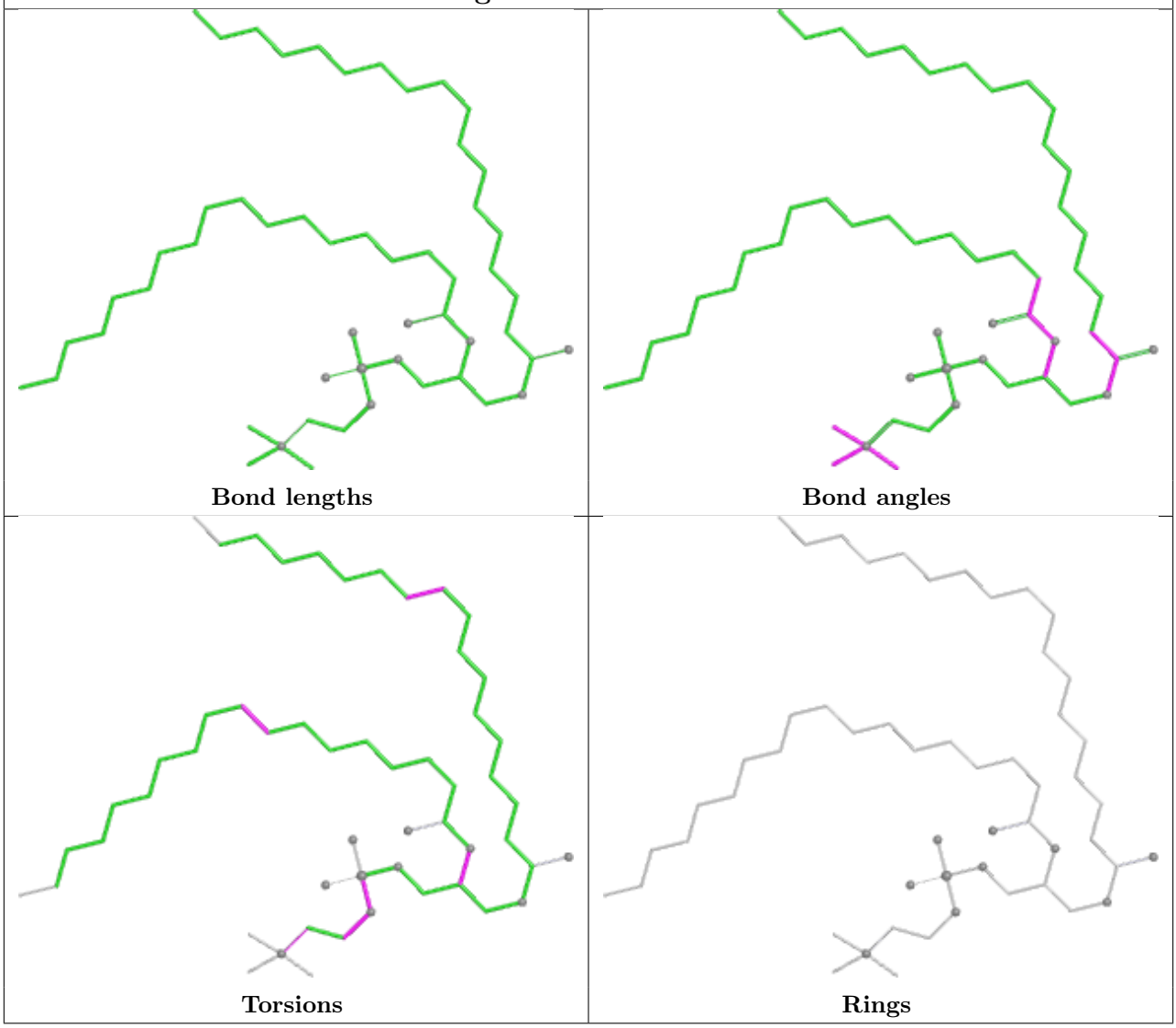
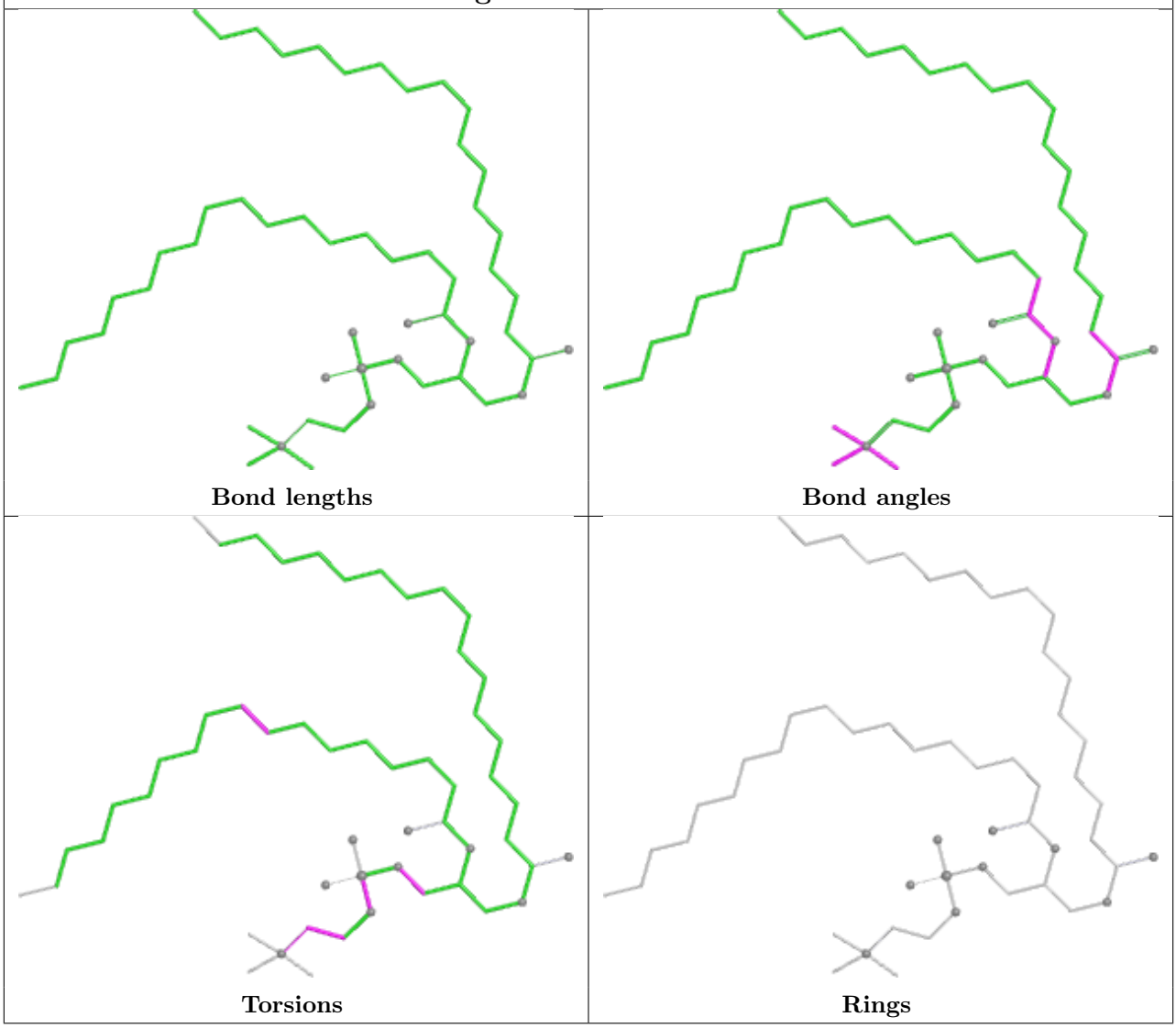
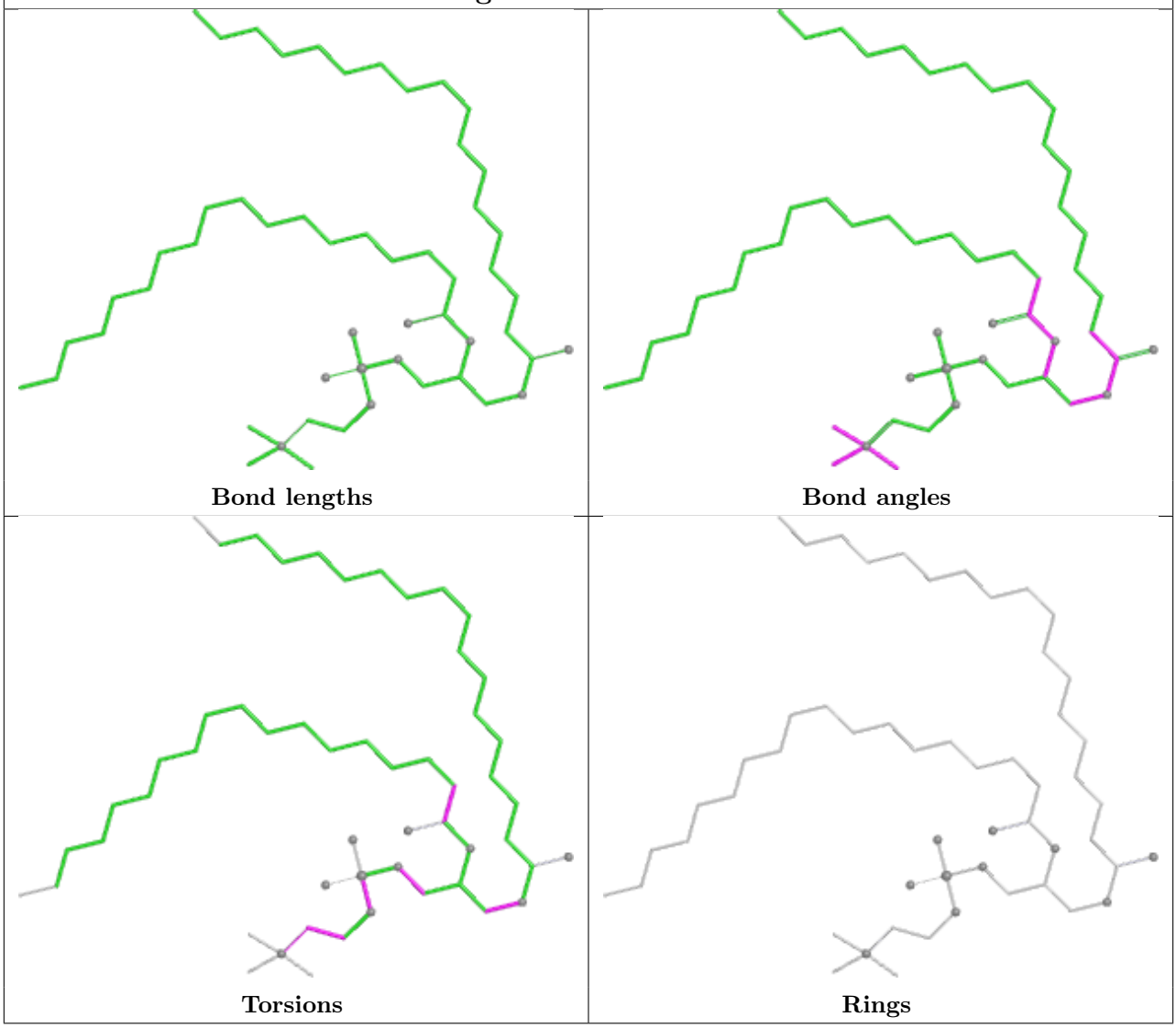


Ligand PCW A 404



Ligand PCW B 208



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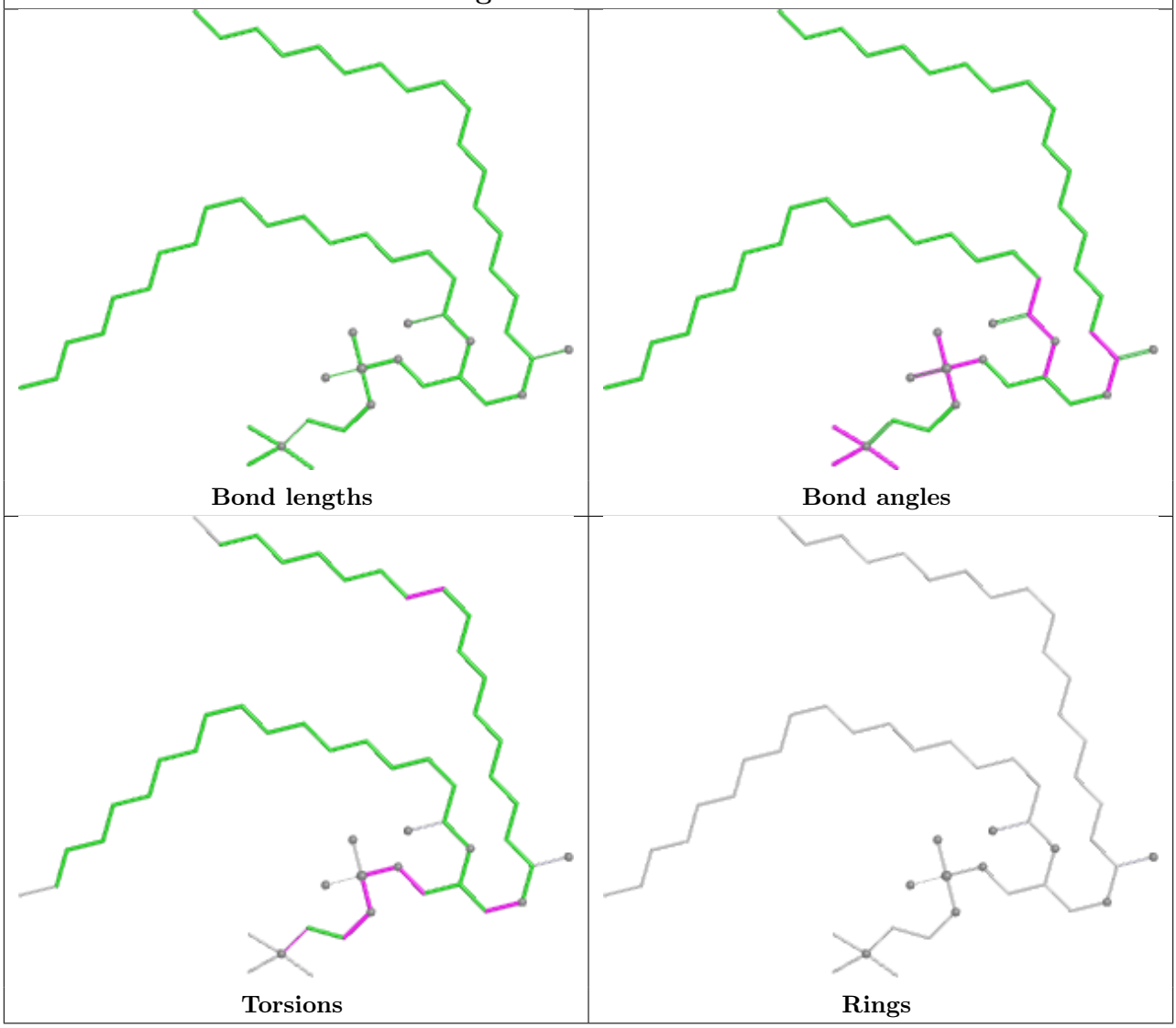

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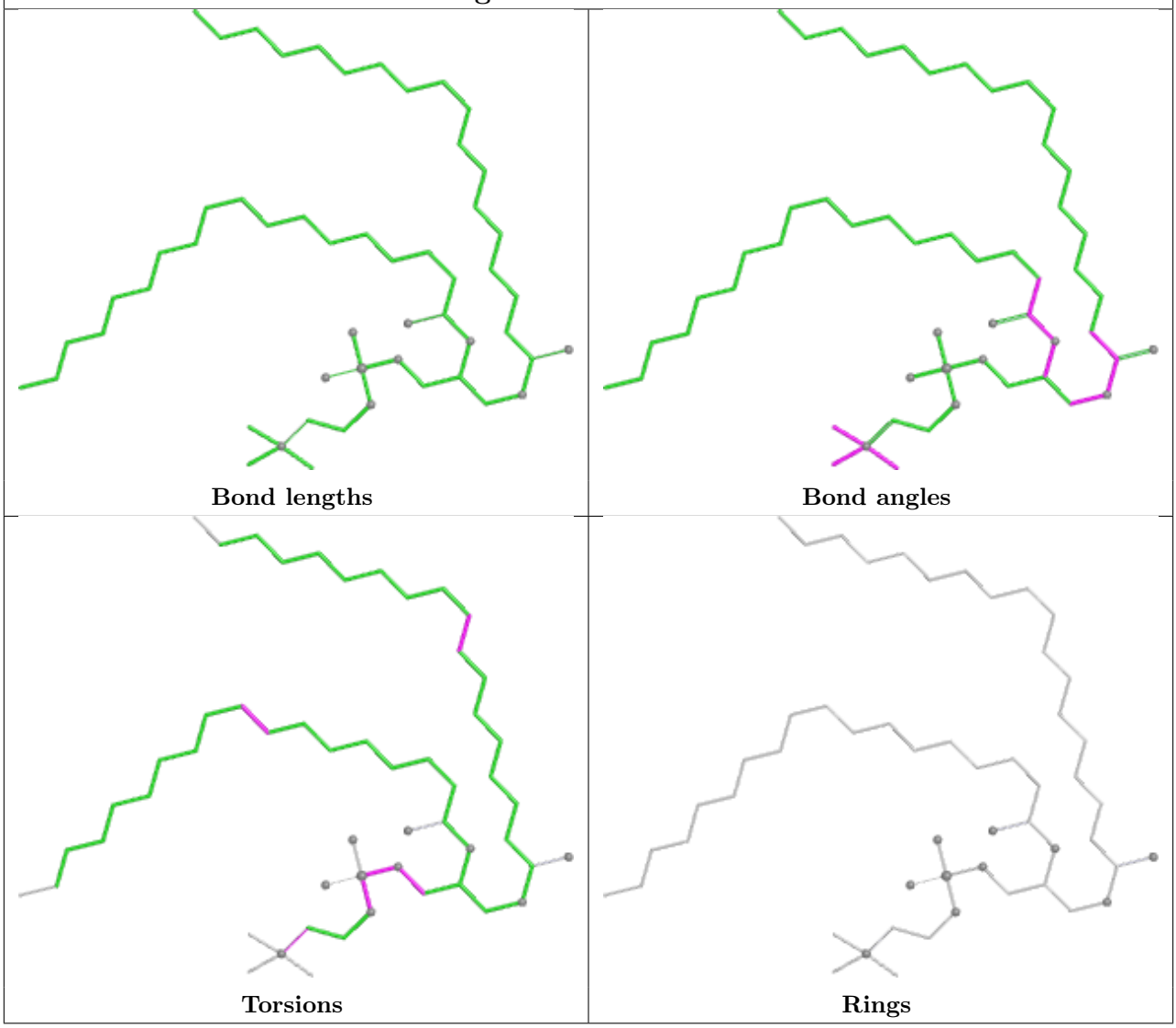
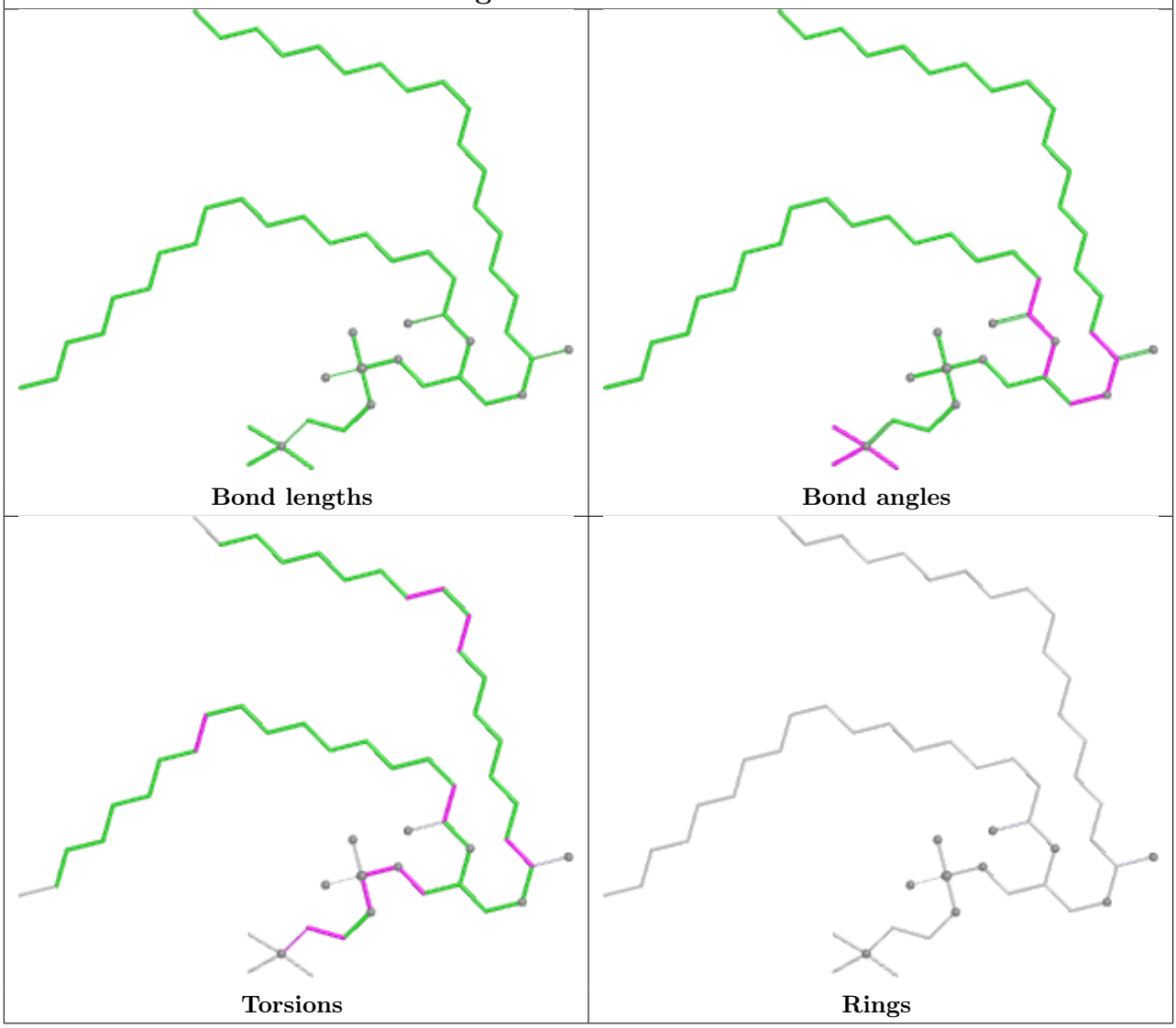
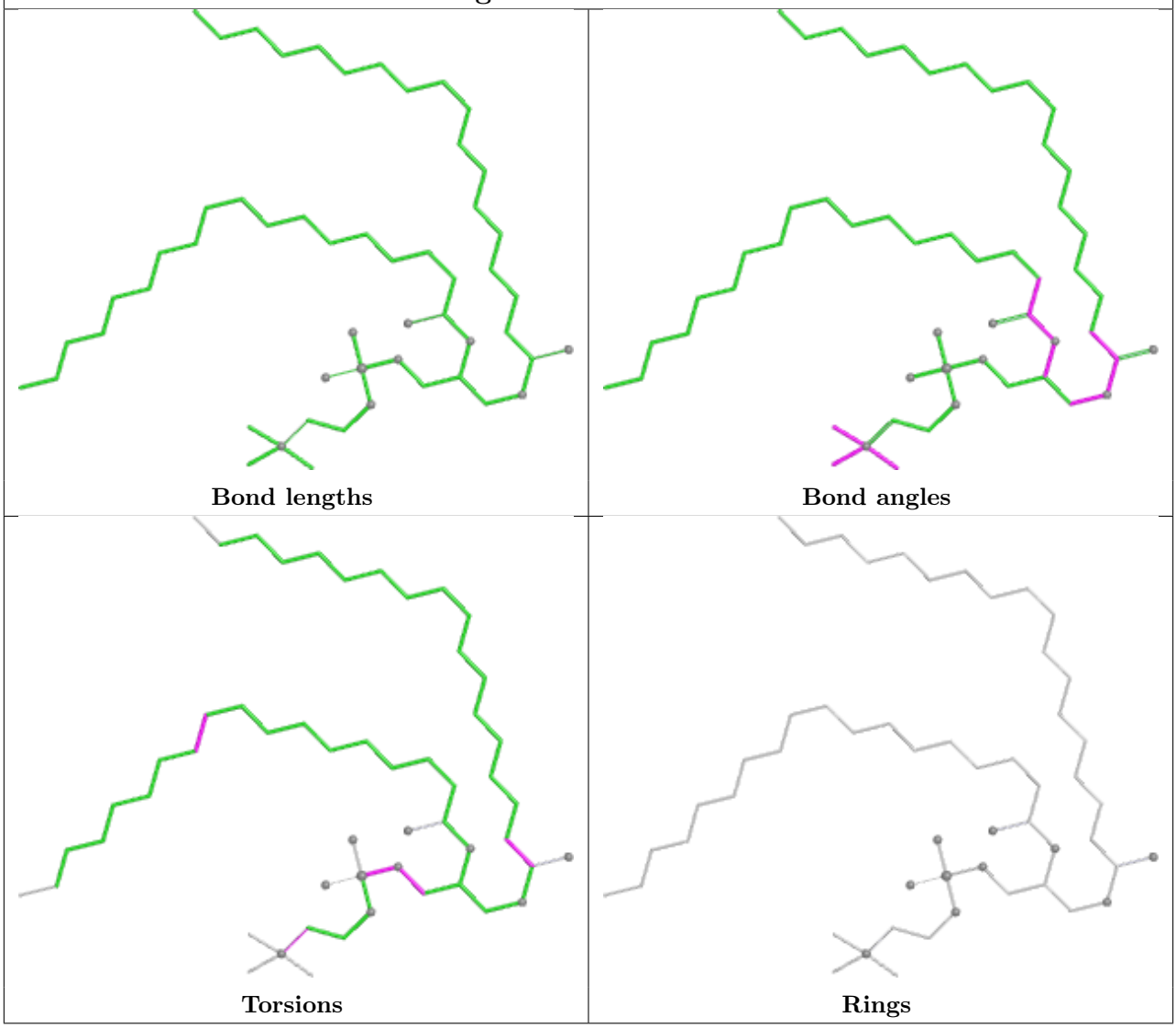


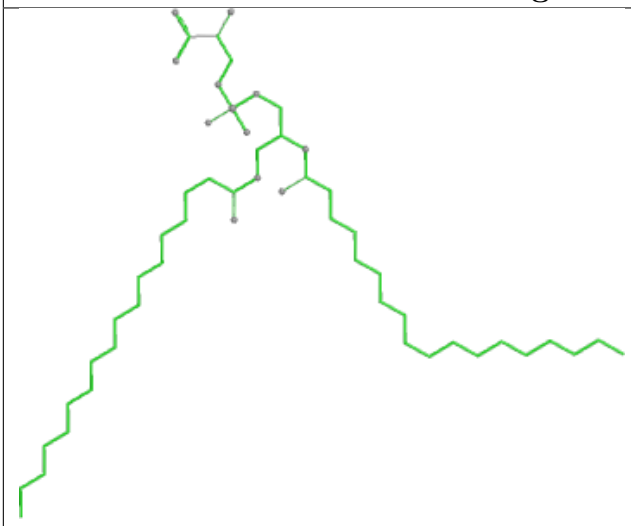
Ligand PCW C 208



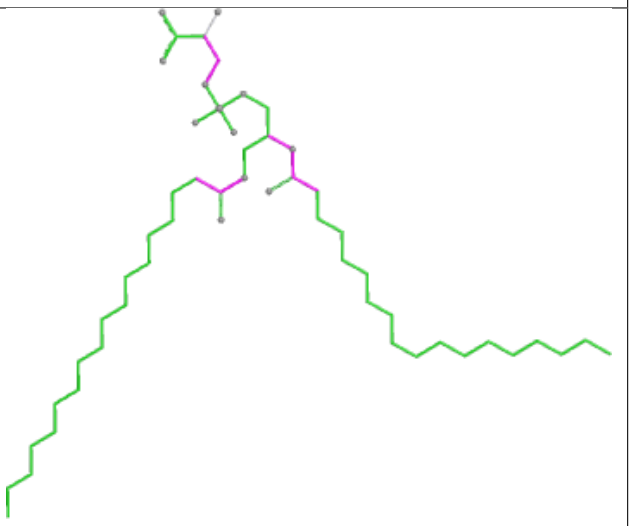
Ligand PCW C 212



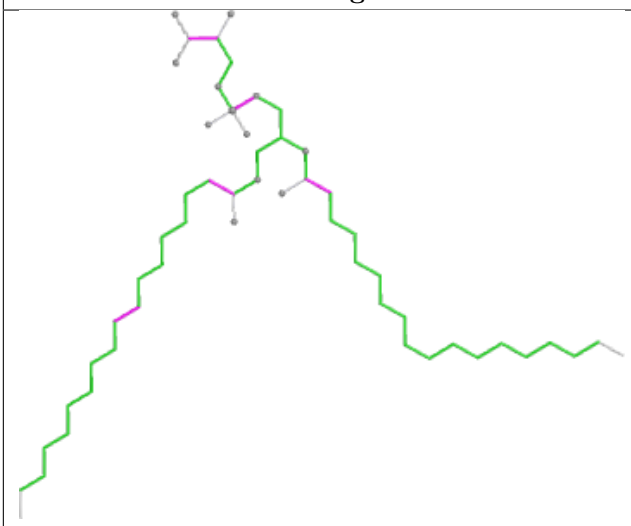
Ligand 17F D 629



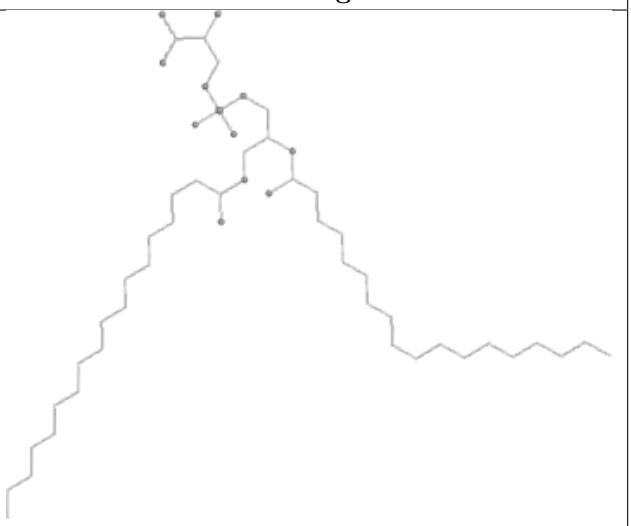
Bond lengths



Bond angles

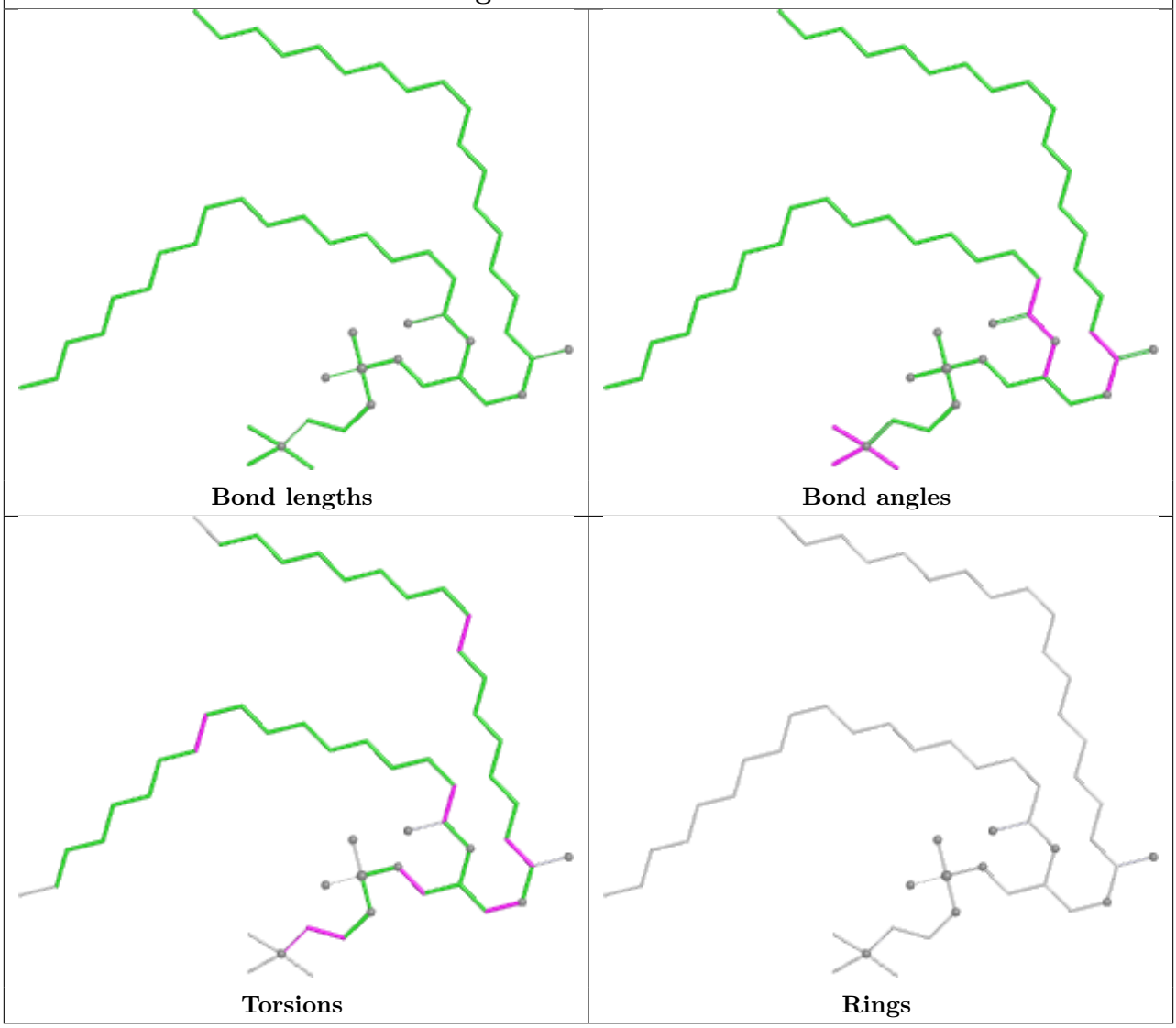


Torsions

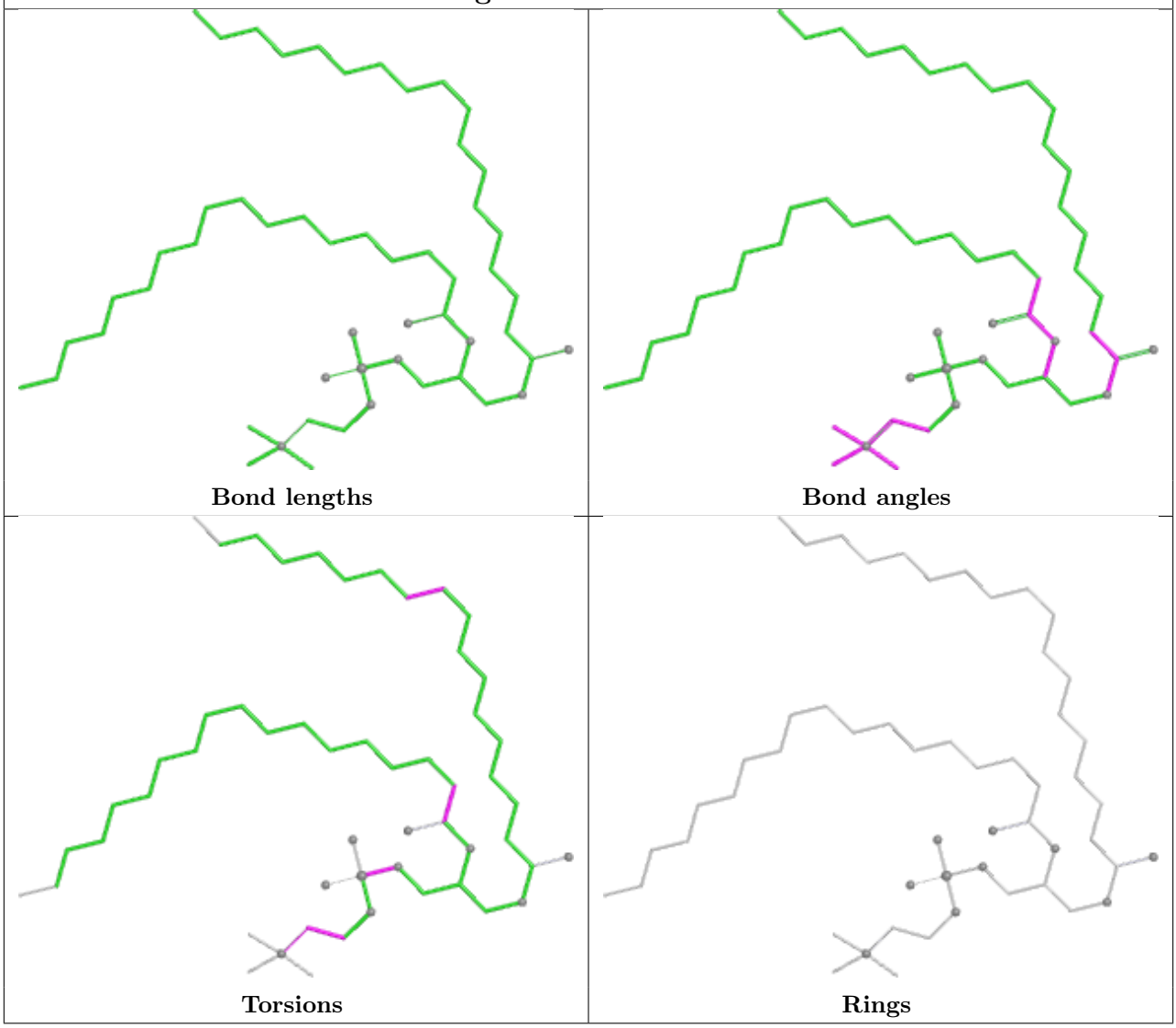


Rings

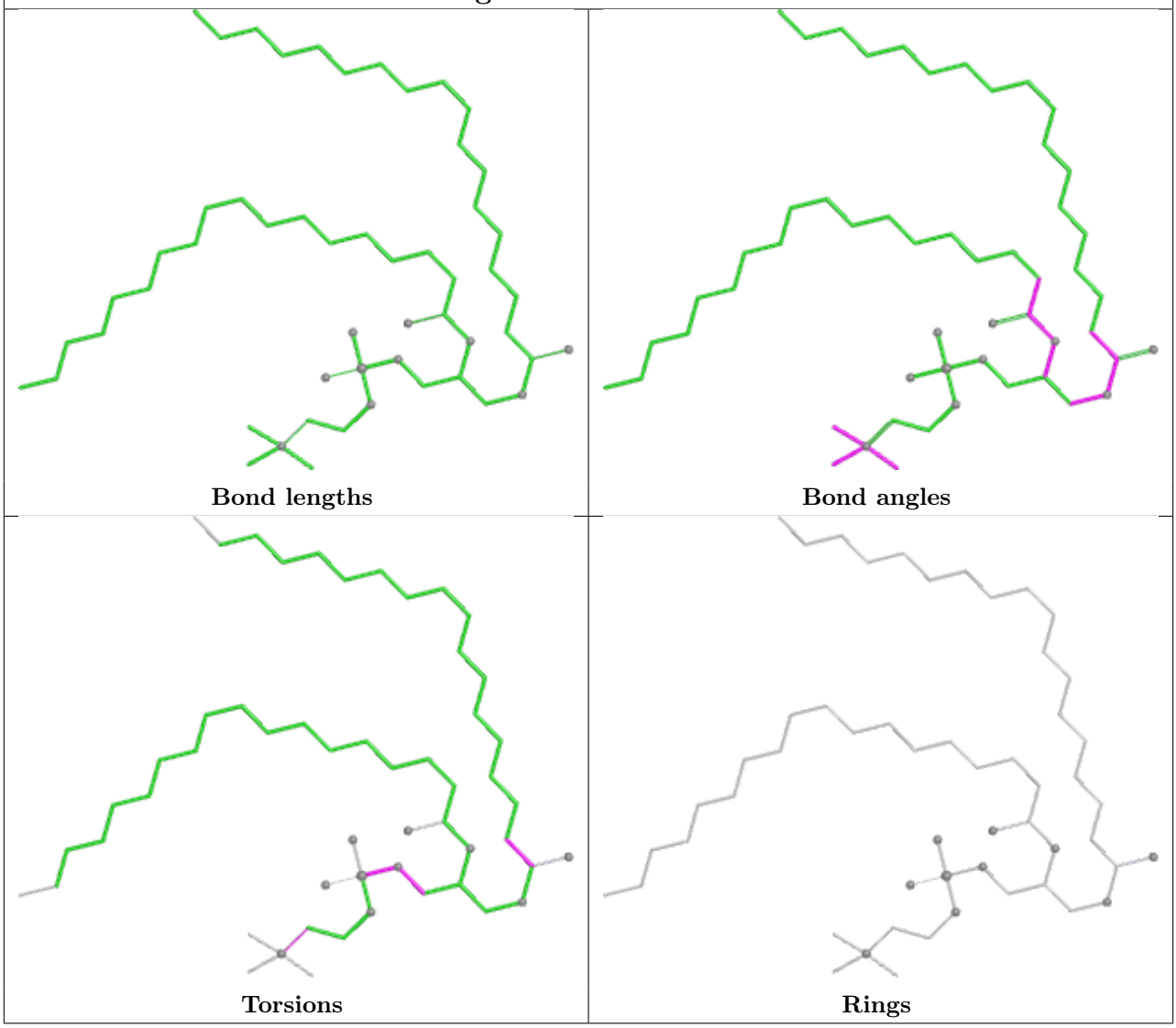
Ligand PCW C 209



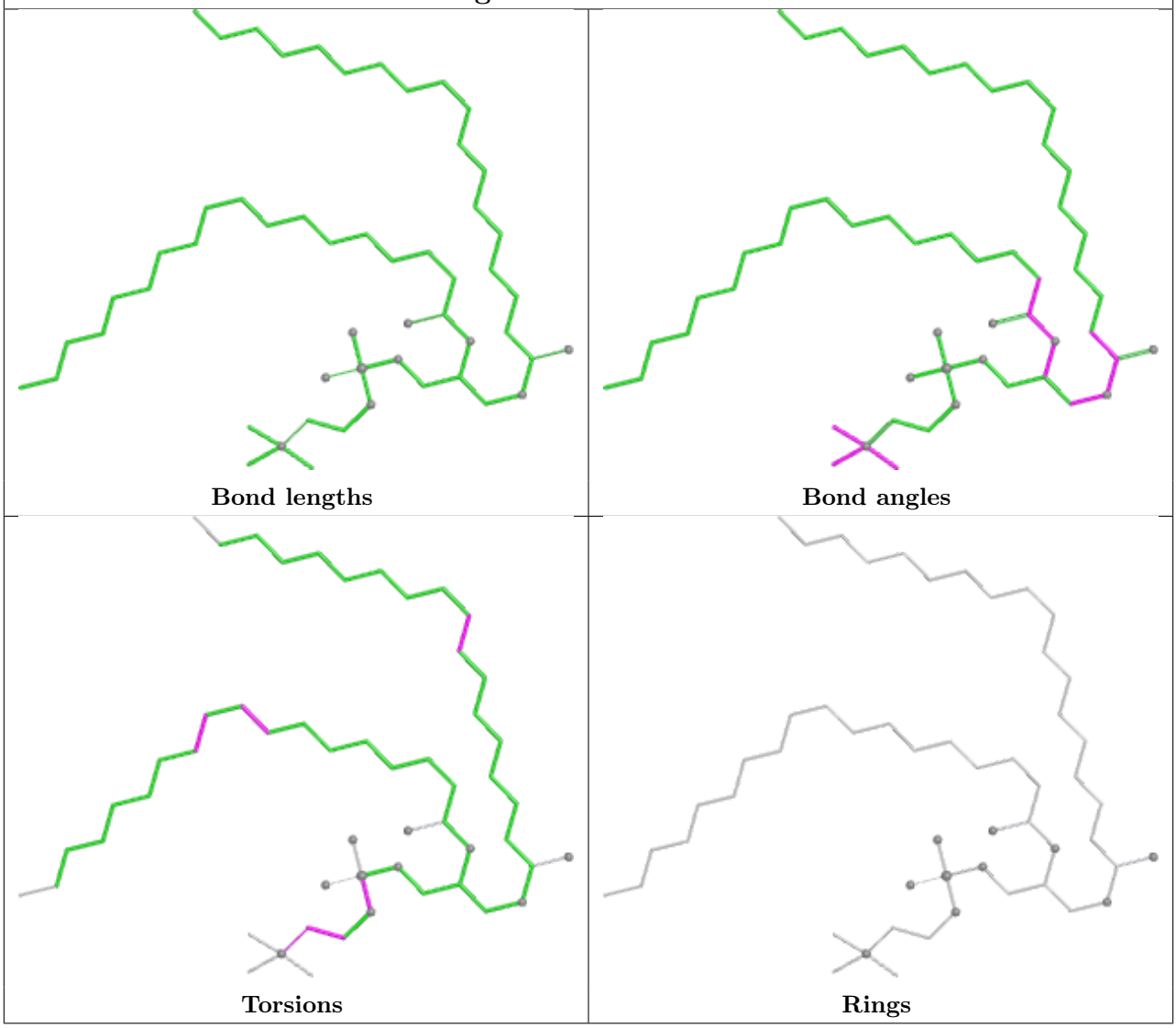
Ligand PCW A 421



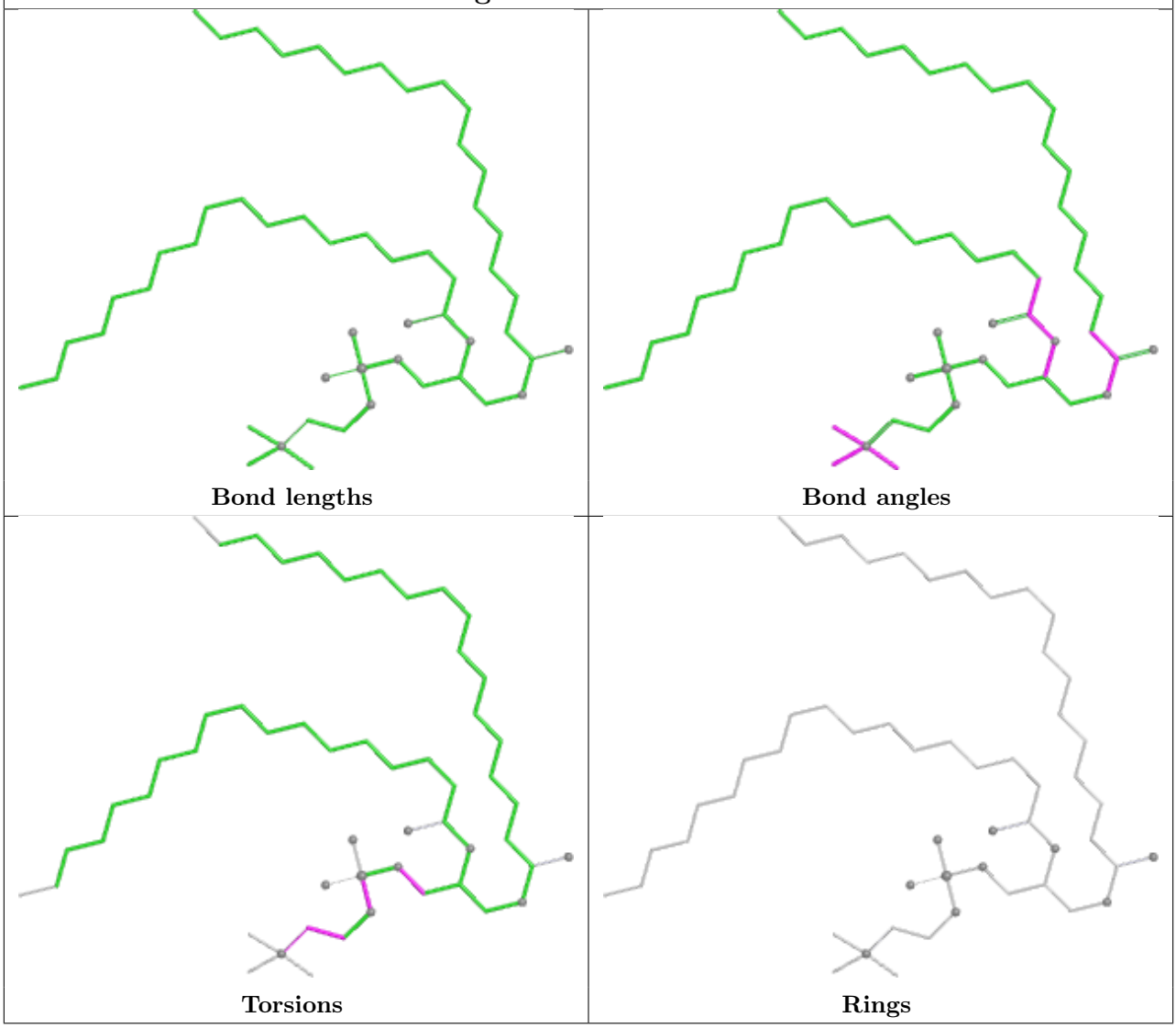
Ligand PCW C 204



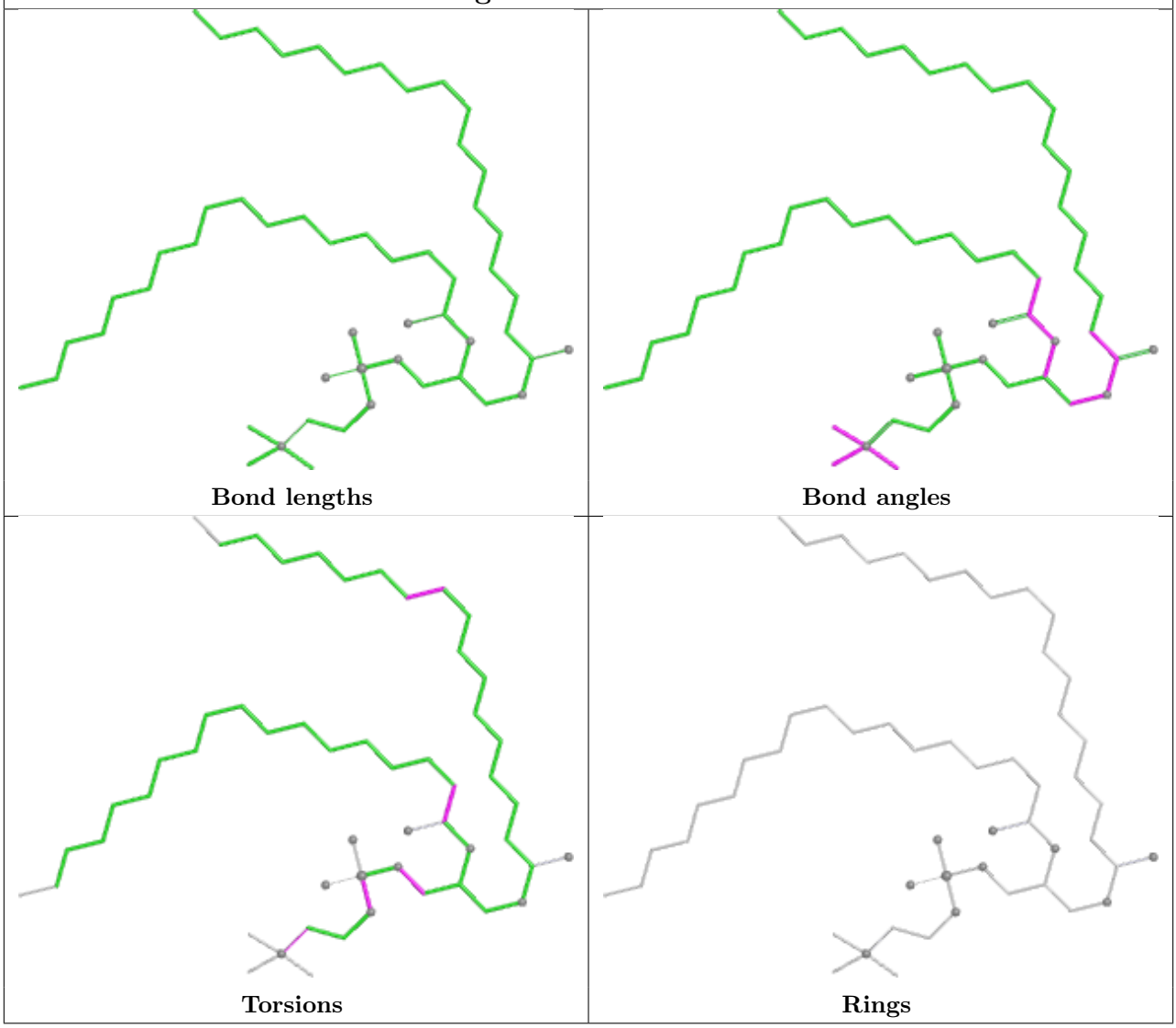
Ligand PCW D 619



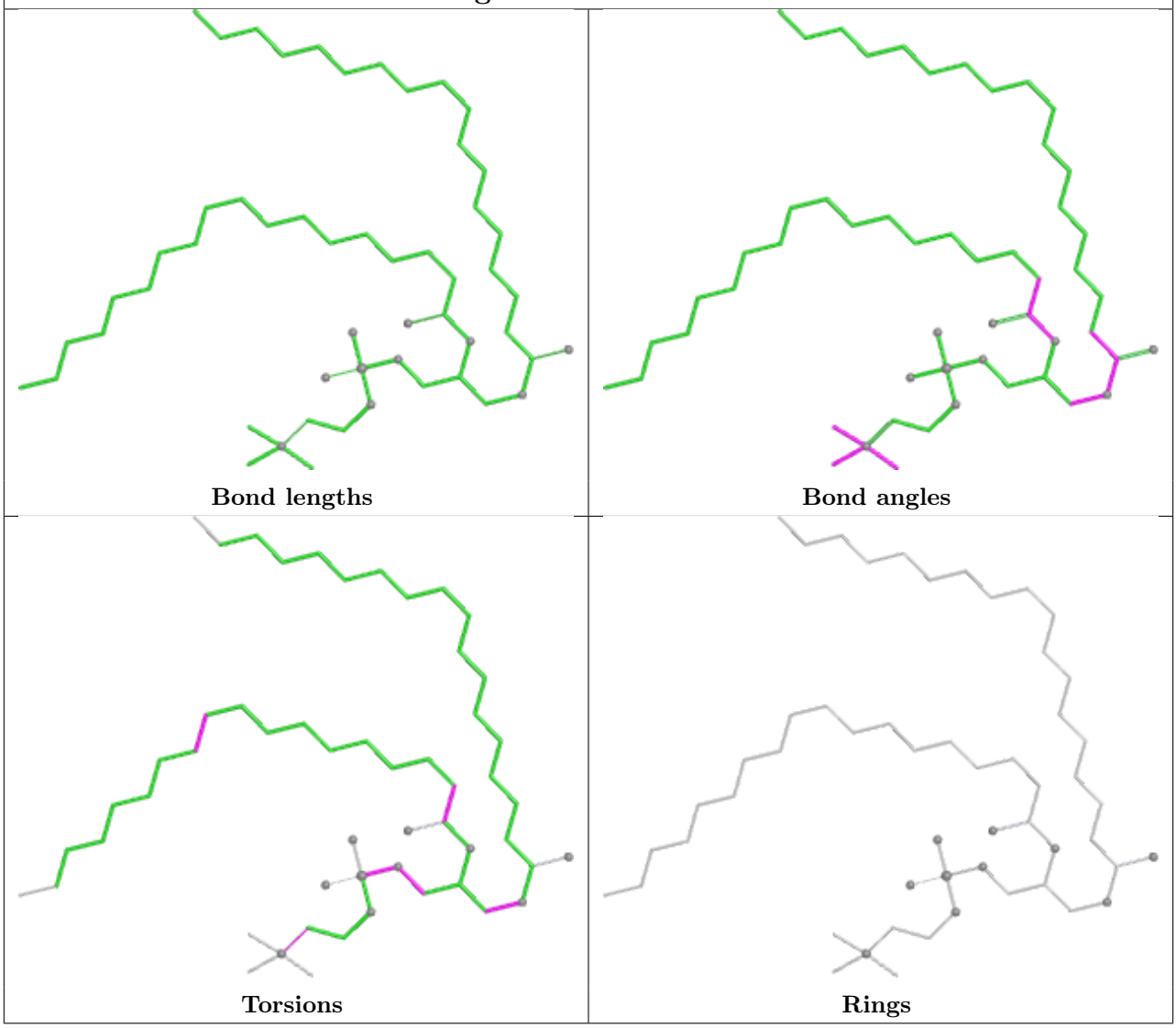
Ligand PCW D 604



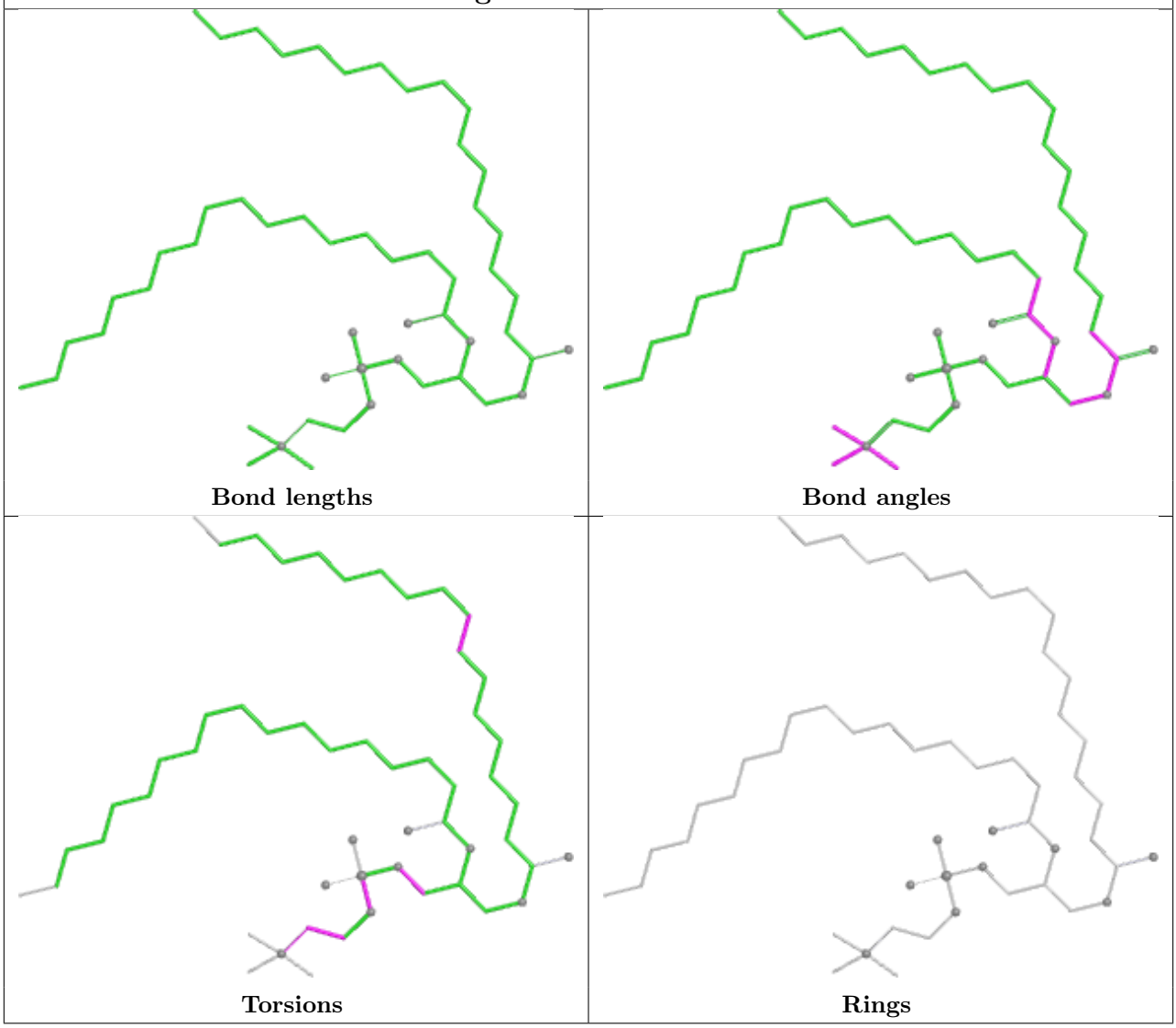
Ligand PCW A 418



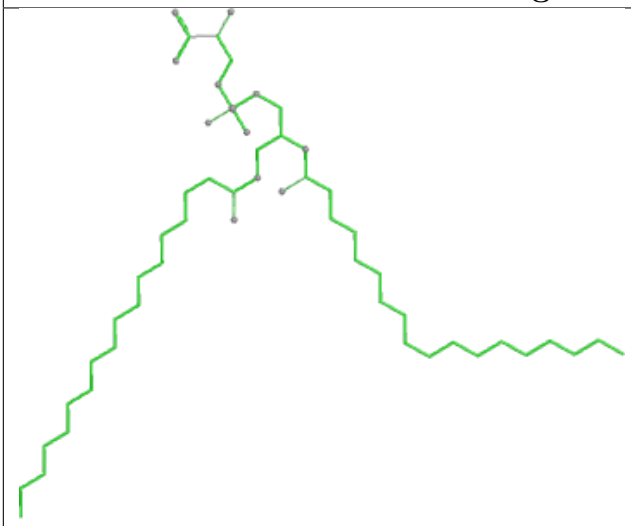
Ligand PCW D 624



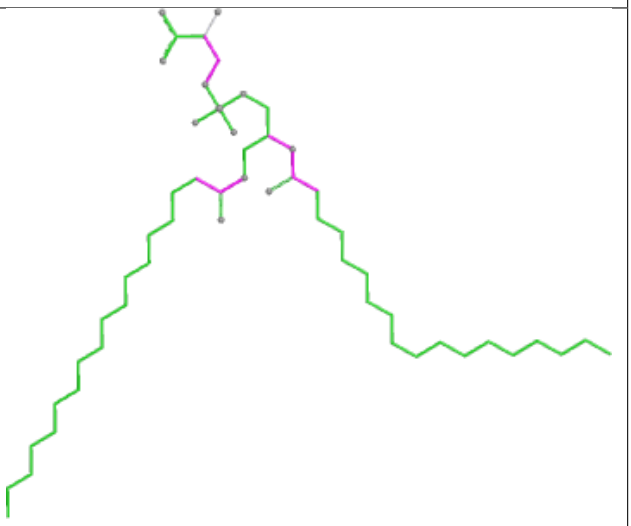
Ligand PCW A 402



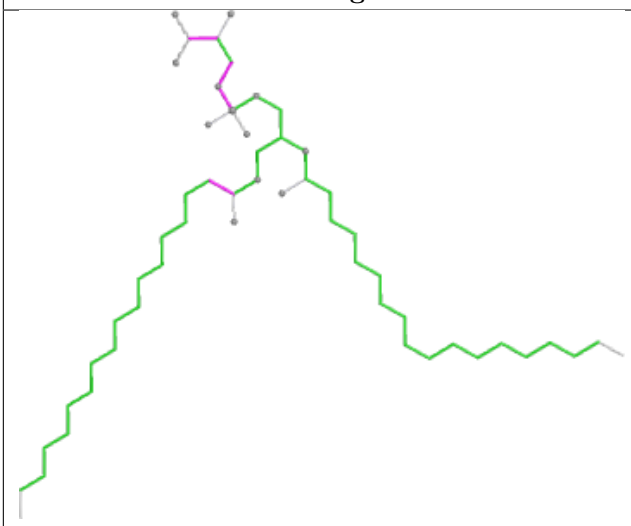
Ligand 17F C 213



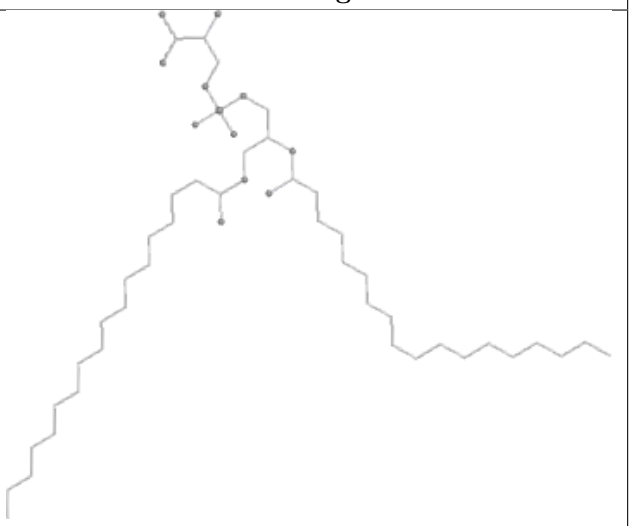
Bond lengths



Bond angles

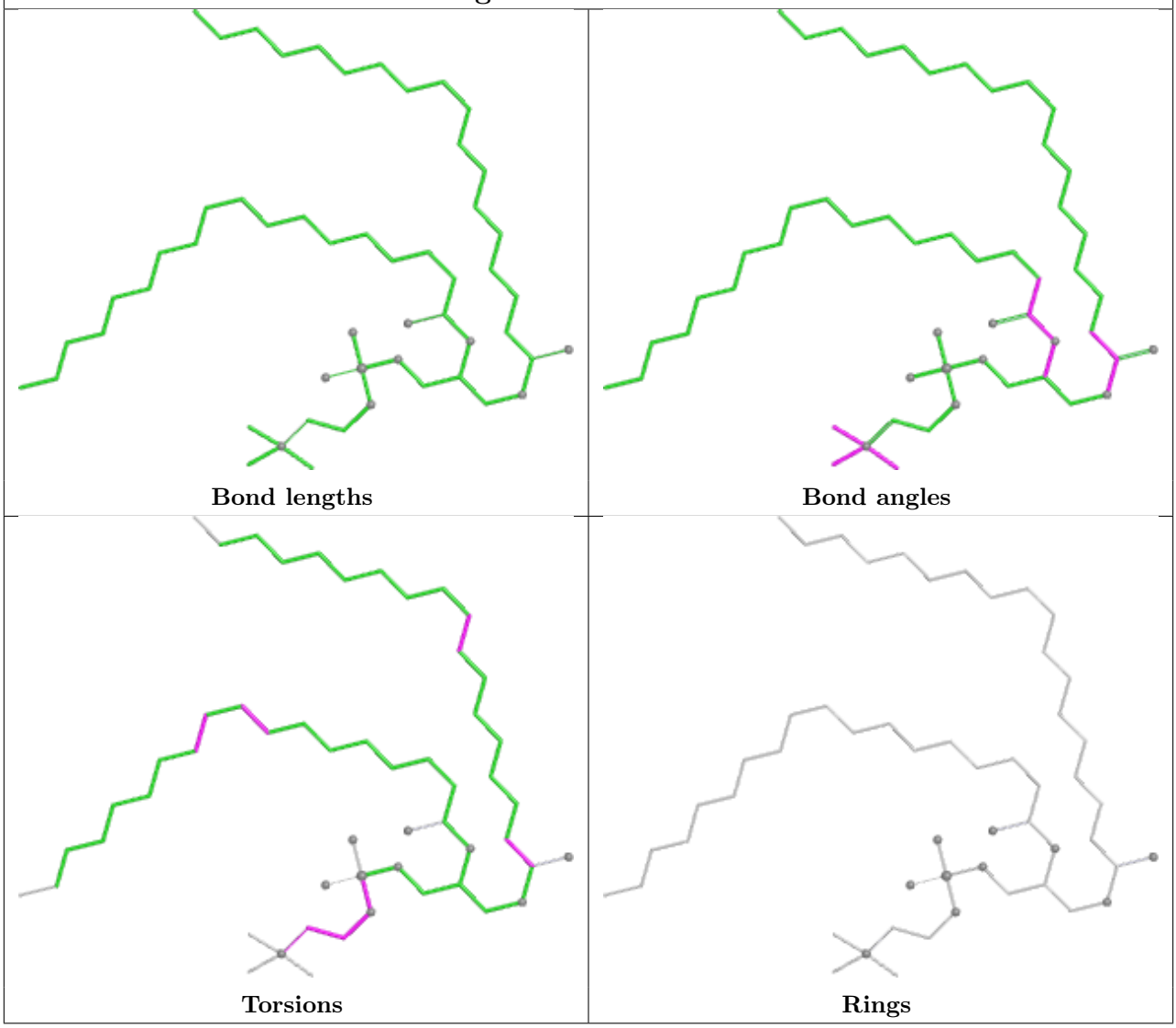


Torsions

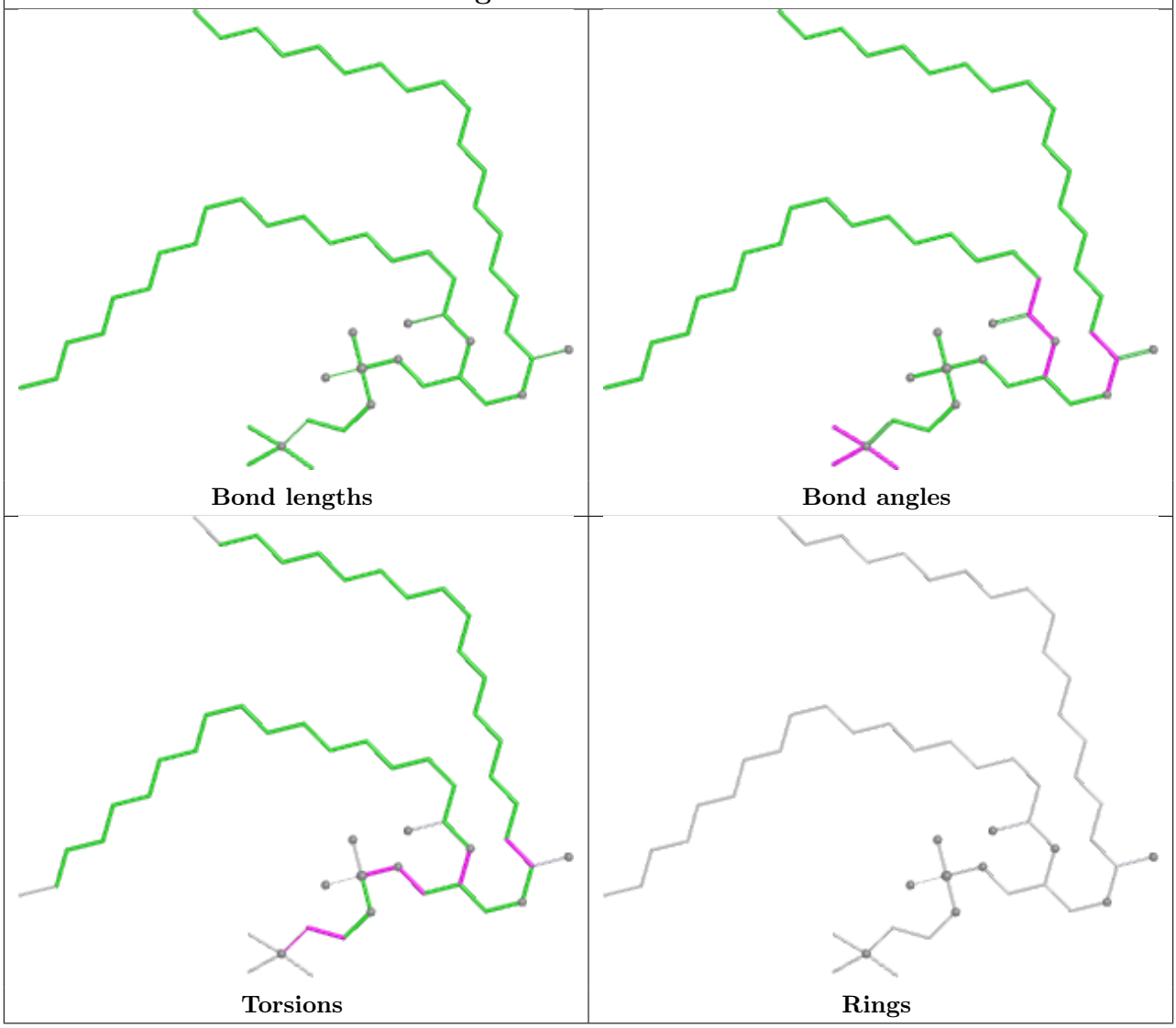


Rings

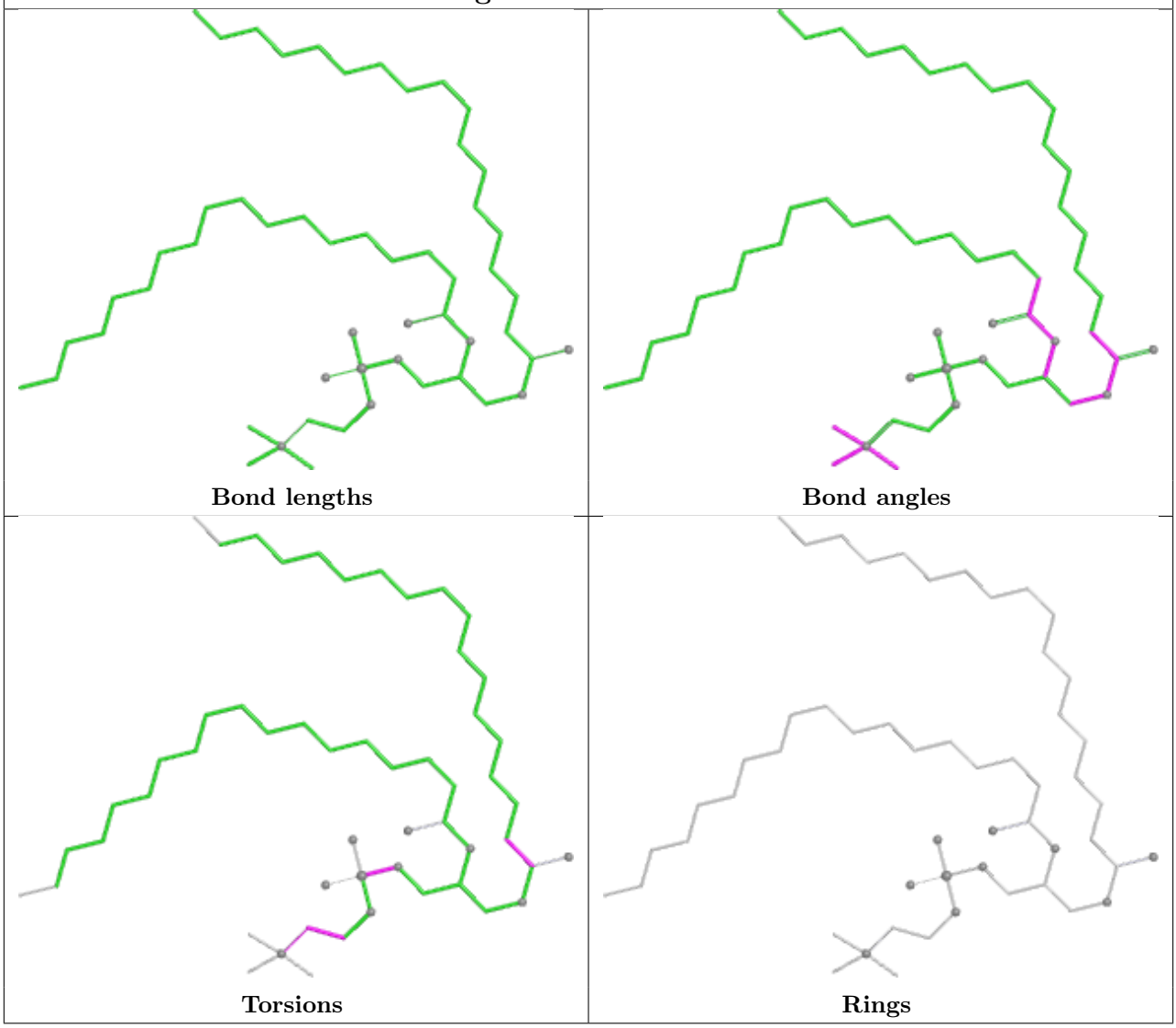
Ligand PCW A 420



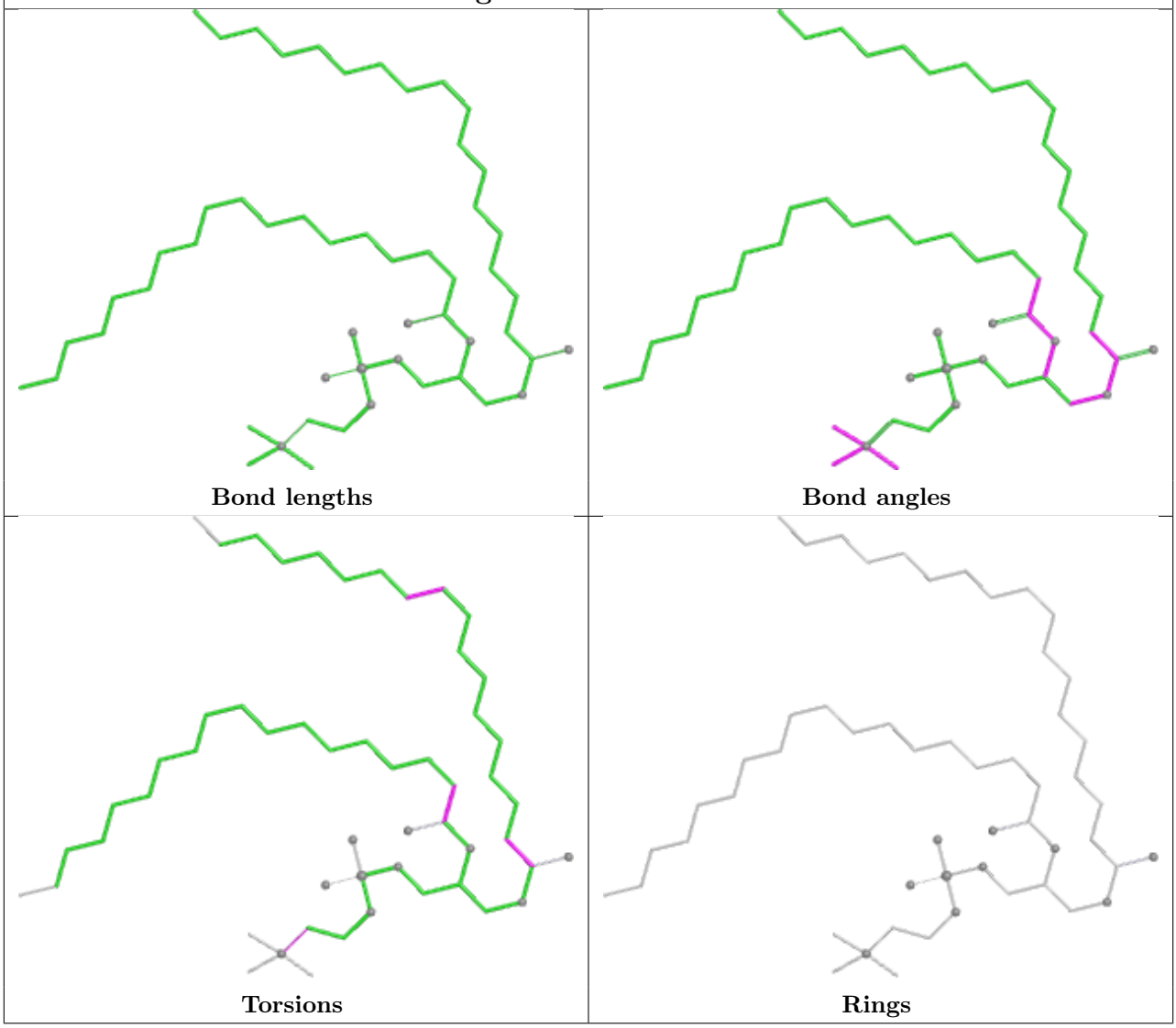
Ligand PCW A 403



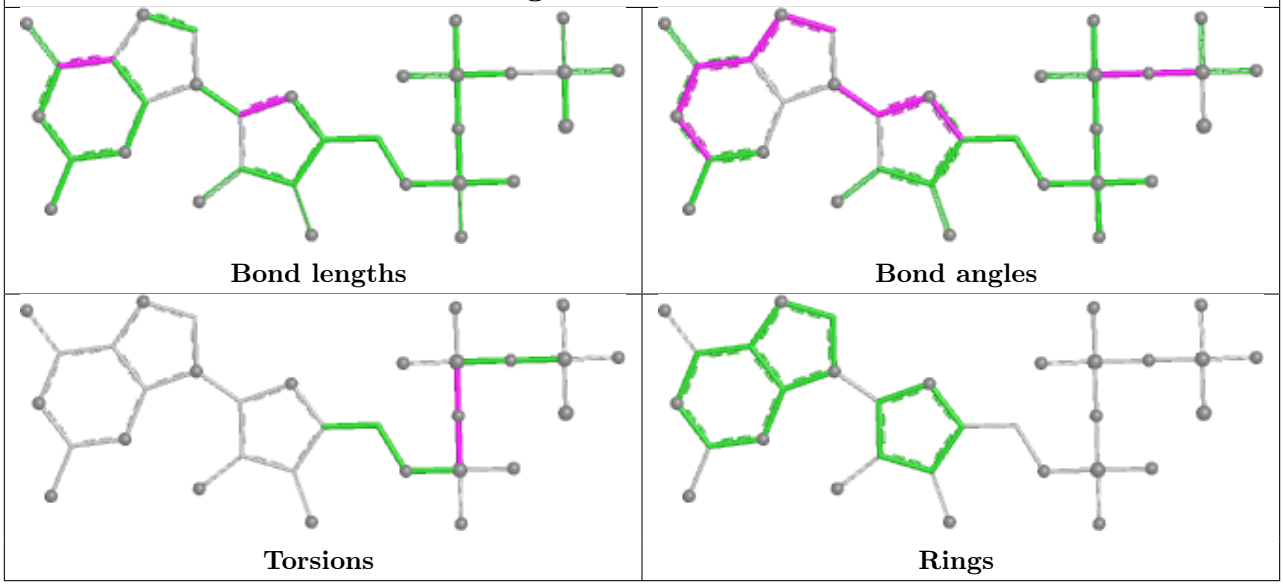
Ligand PCW A 419



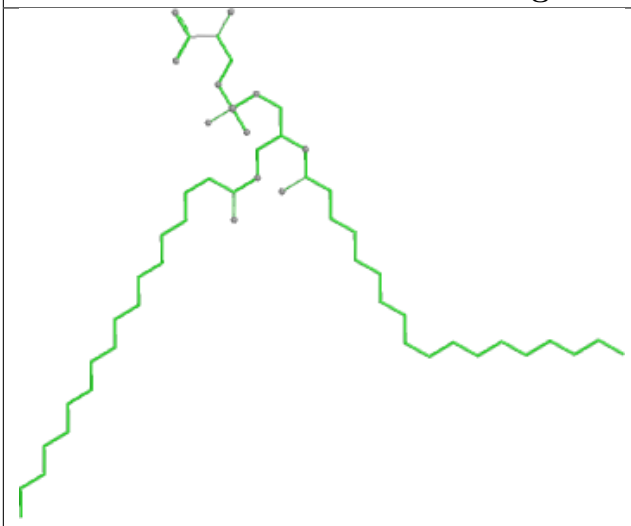
Ligand PCW B 203



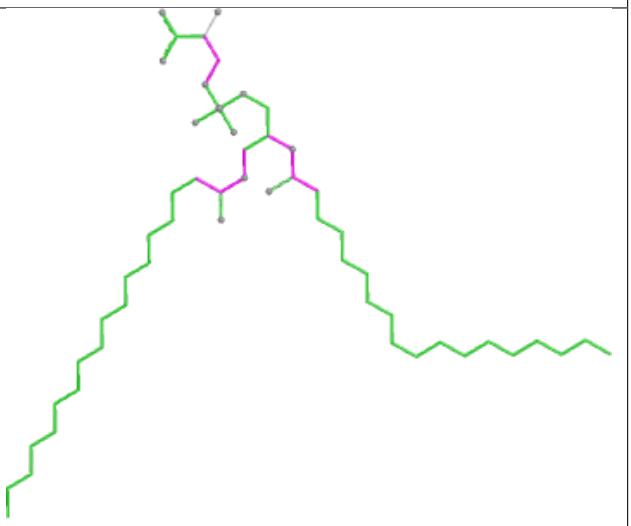
Ligand GSP B 201



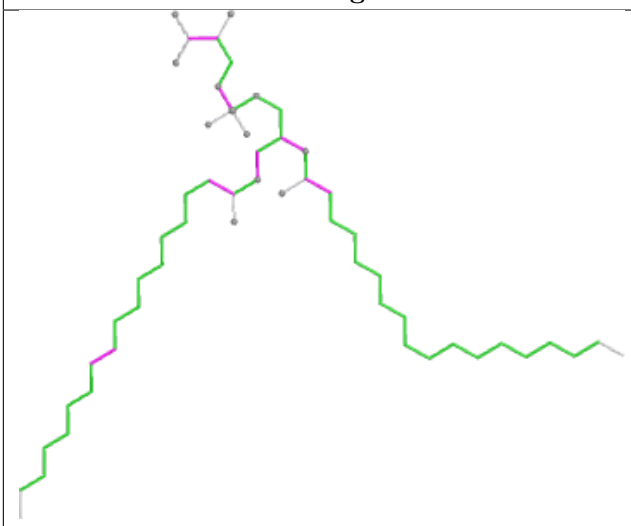
Ligand 17F D 632



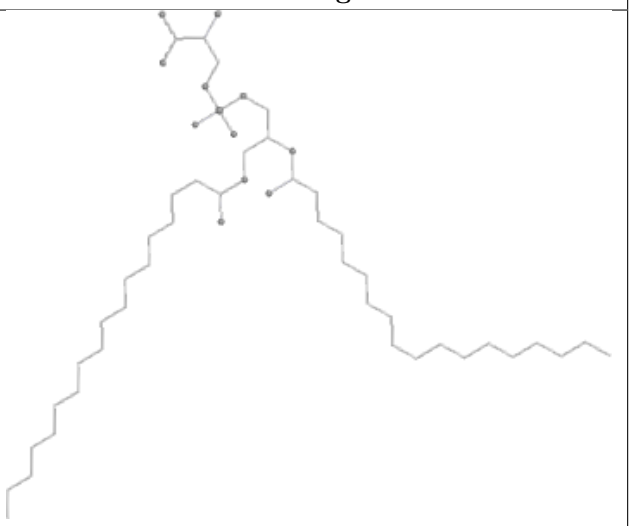
Bond lengths



Bond angles

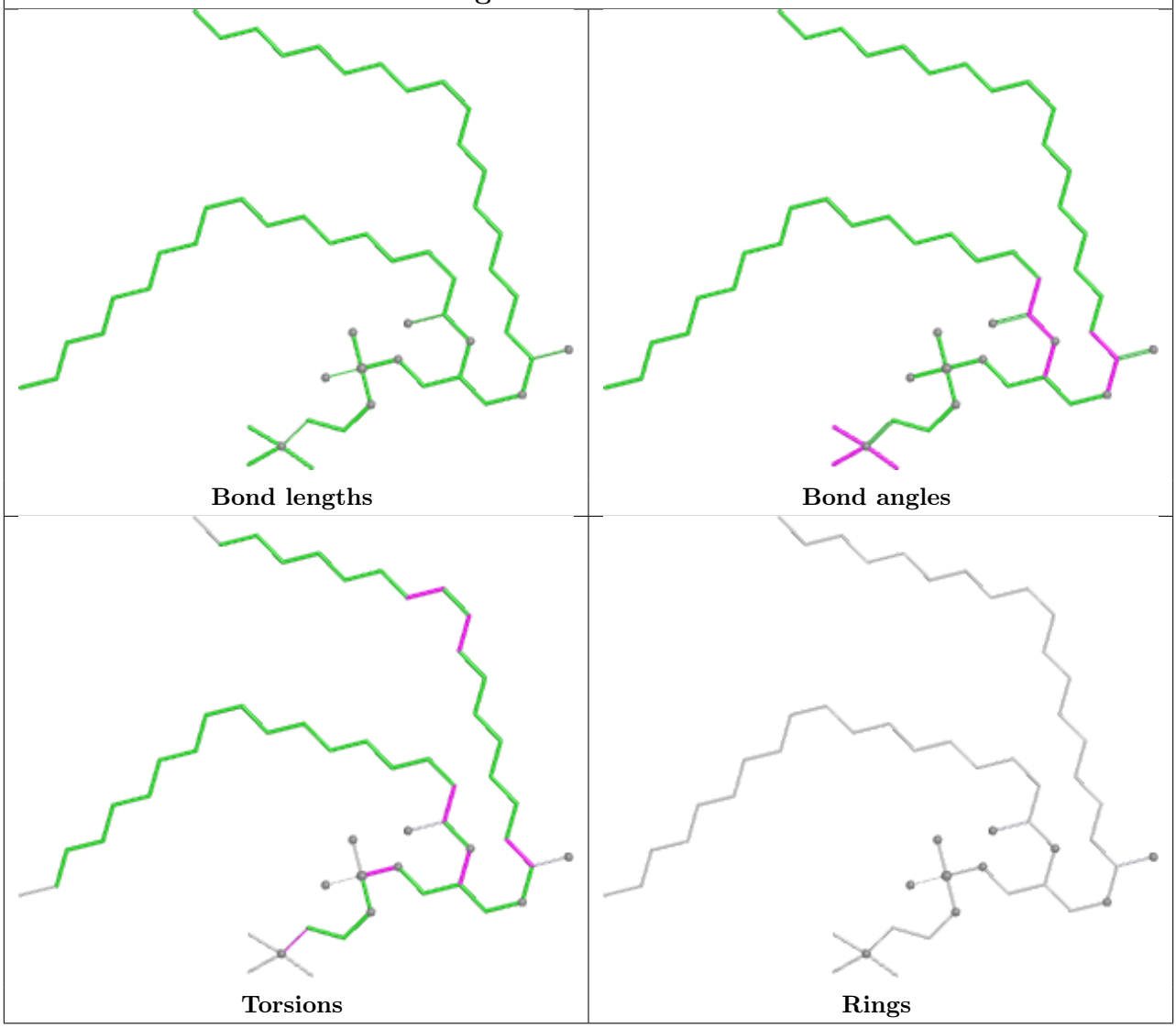


Torsions

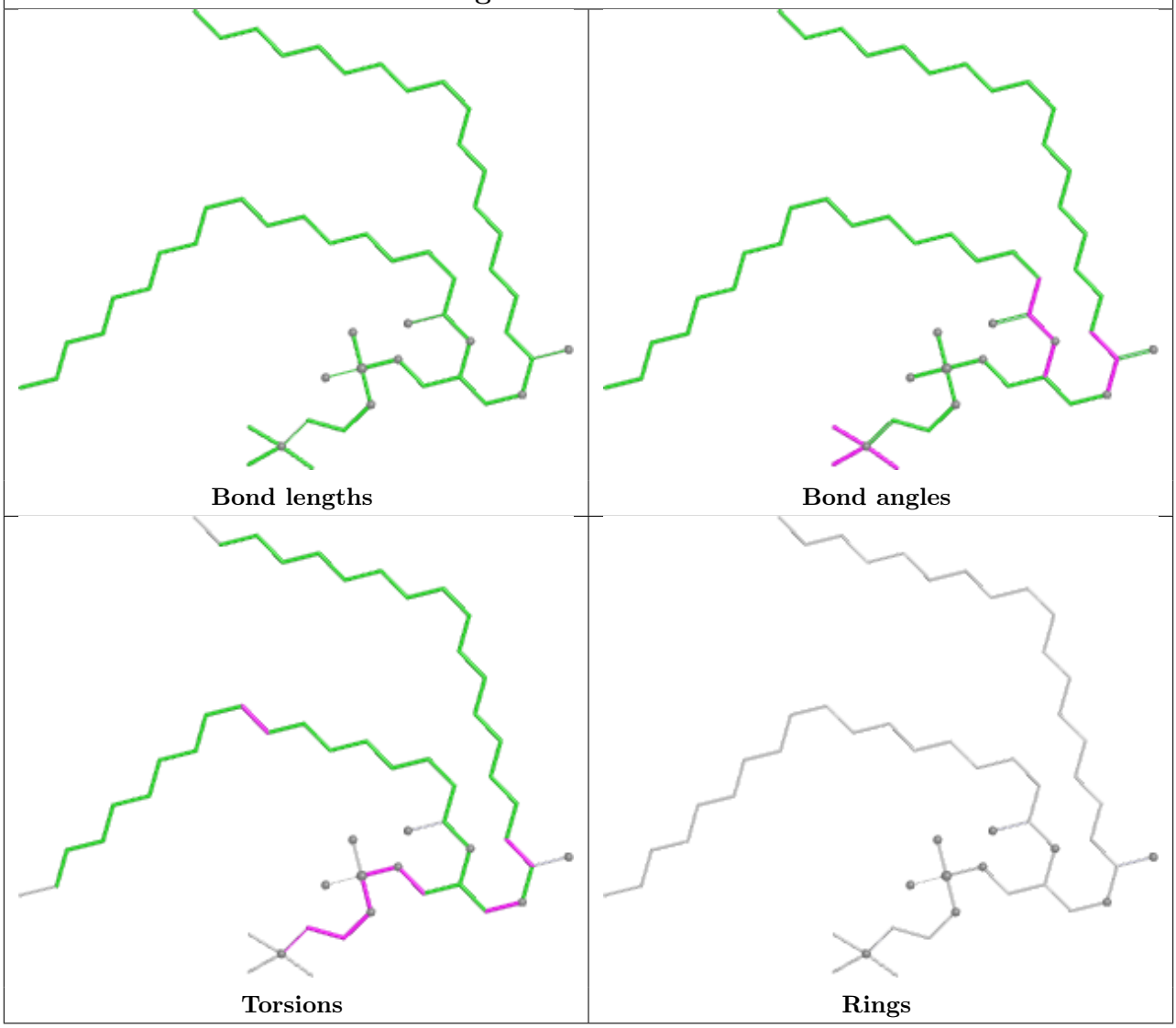


Rings

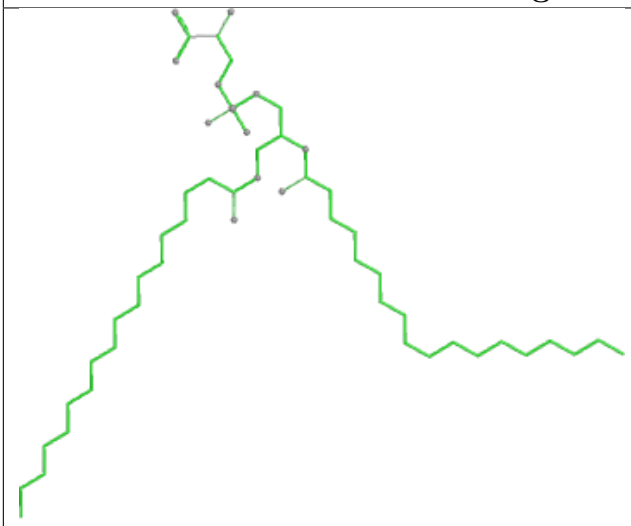
Ligand PCW A 409



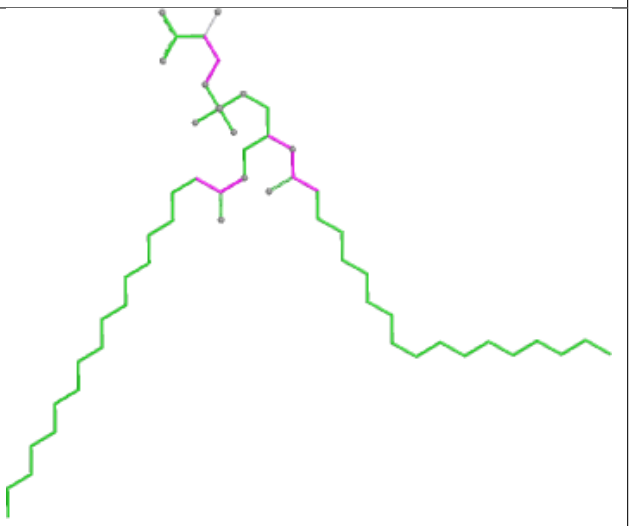
Ligand PCW A 417



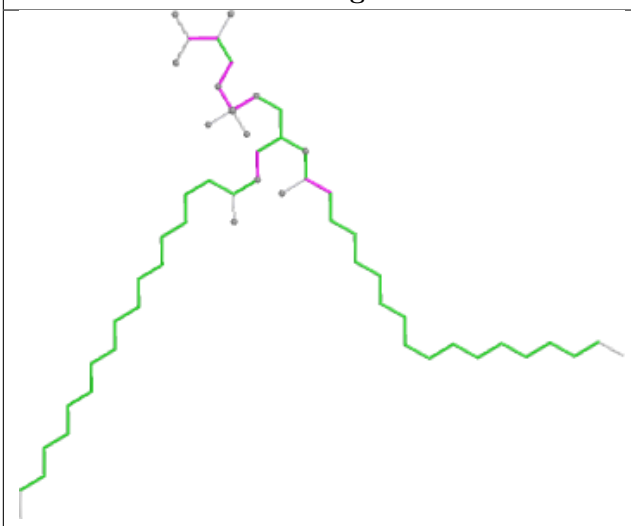
Ligand 17F C 214



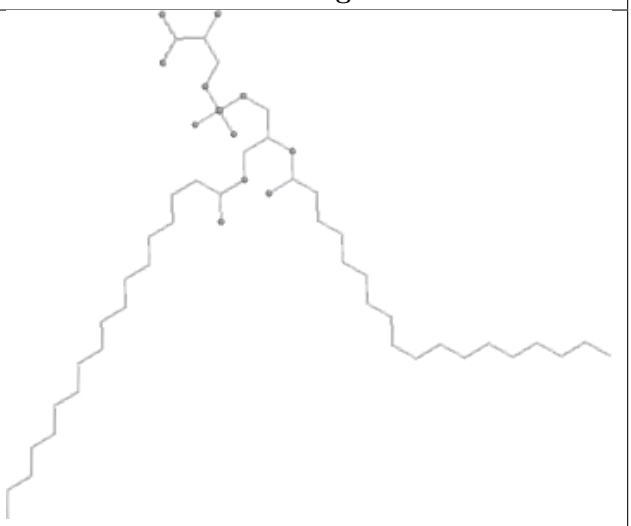
Bond lengths



Bond angles

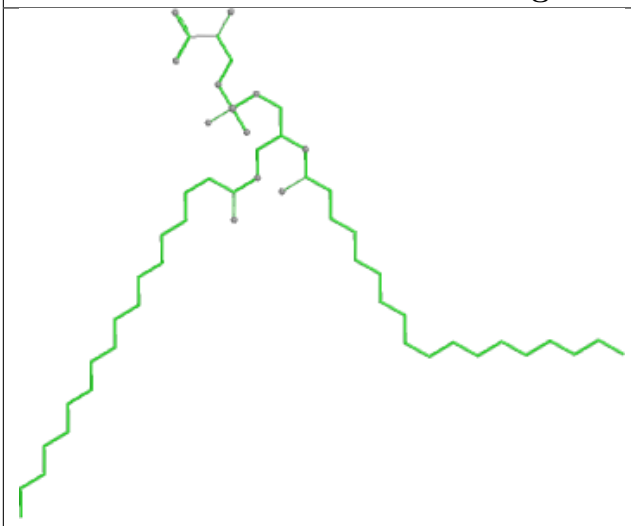


Torsions

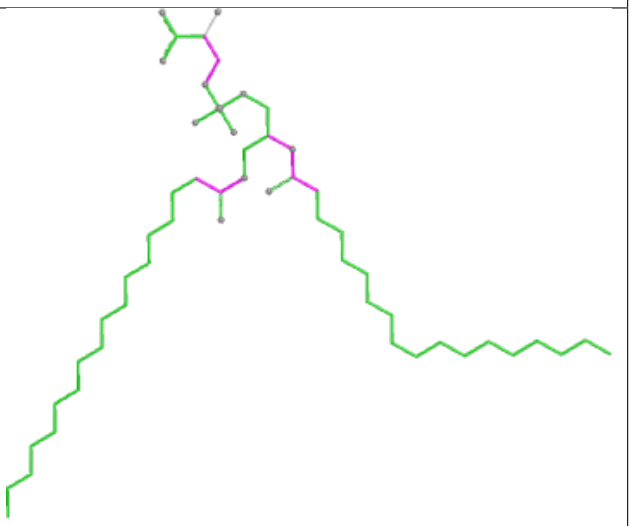


Rings

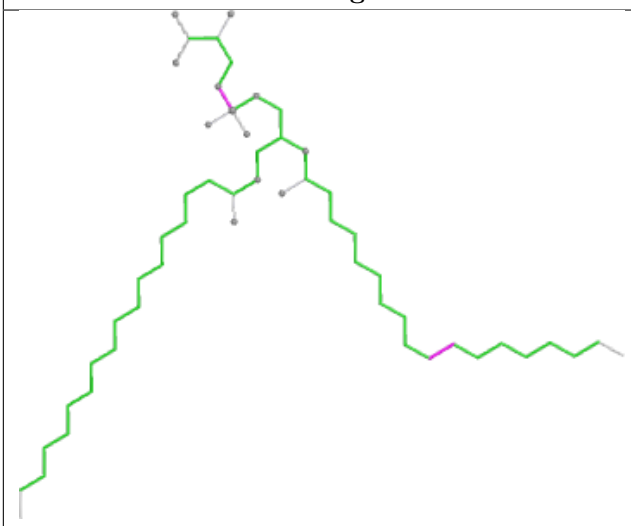
Ligand 17F A 422



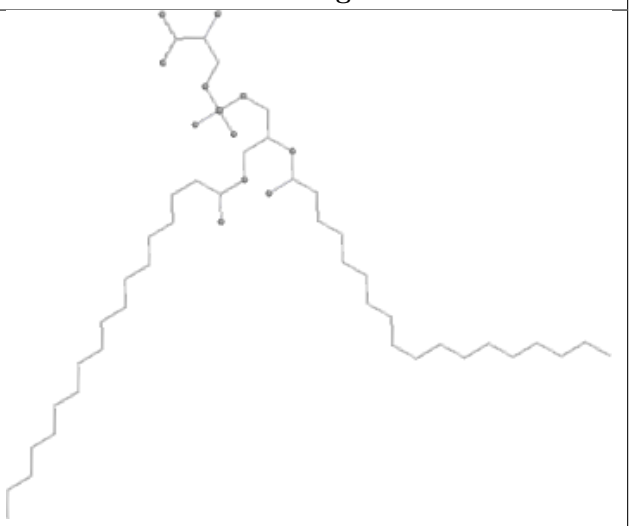
Bond lengths



Bond angles

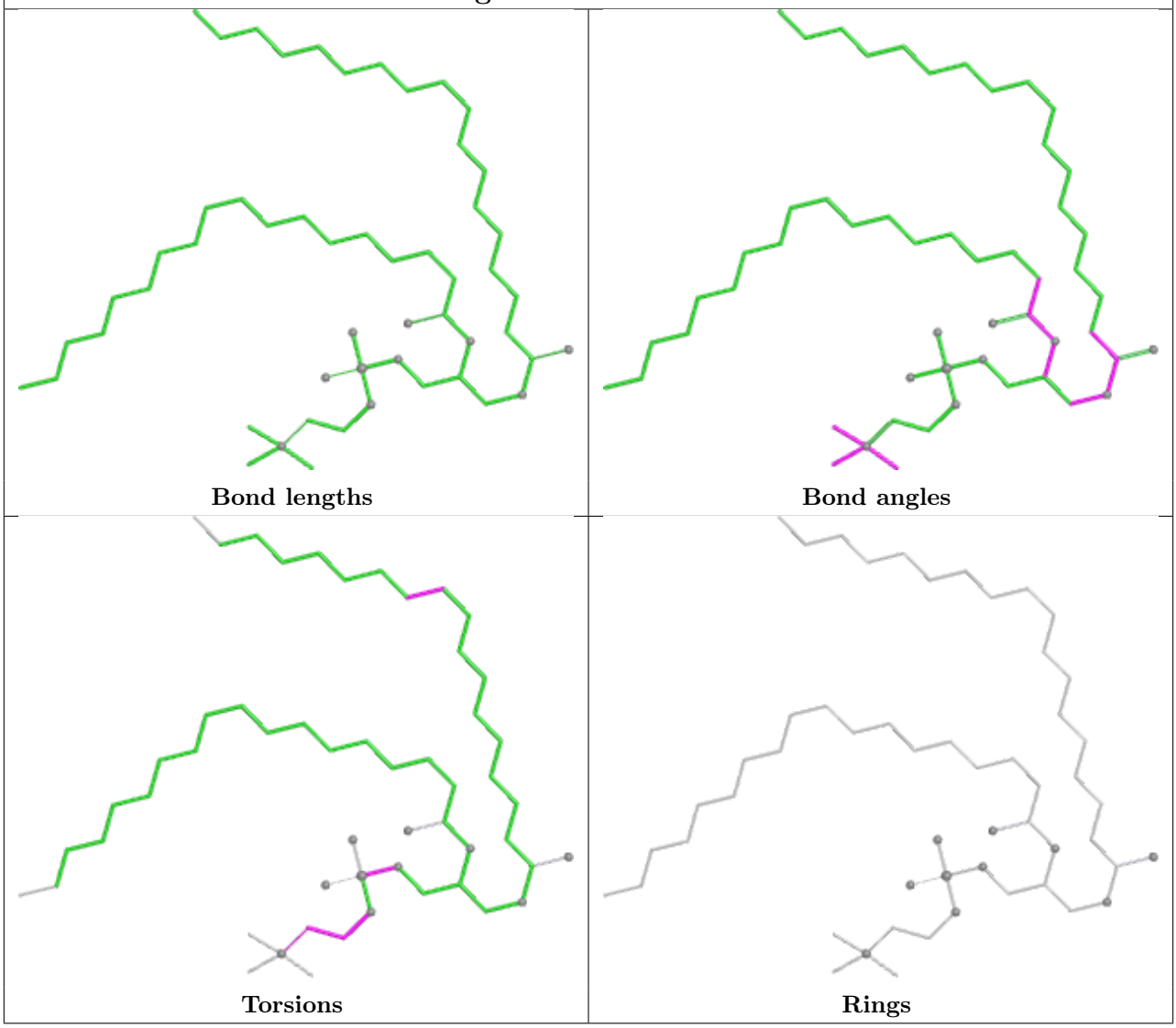


Torsions

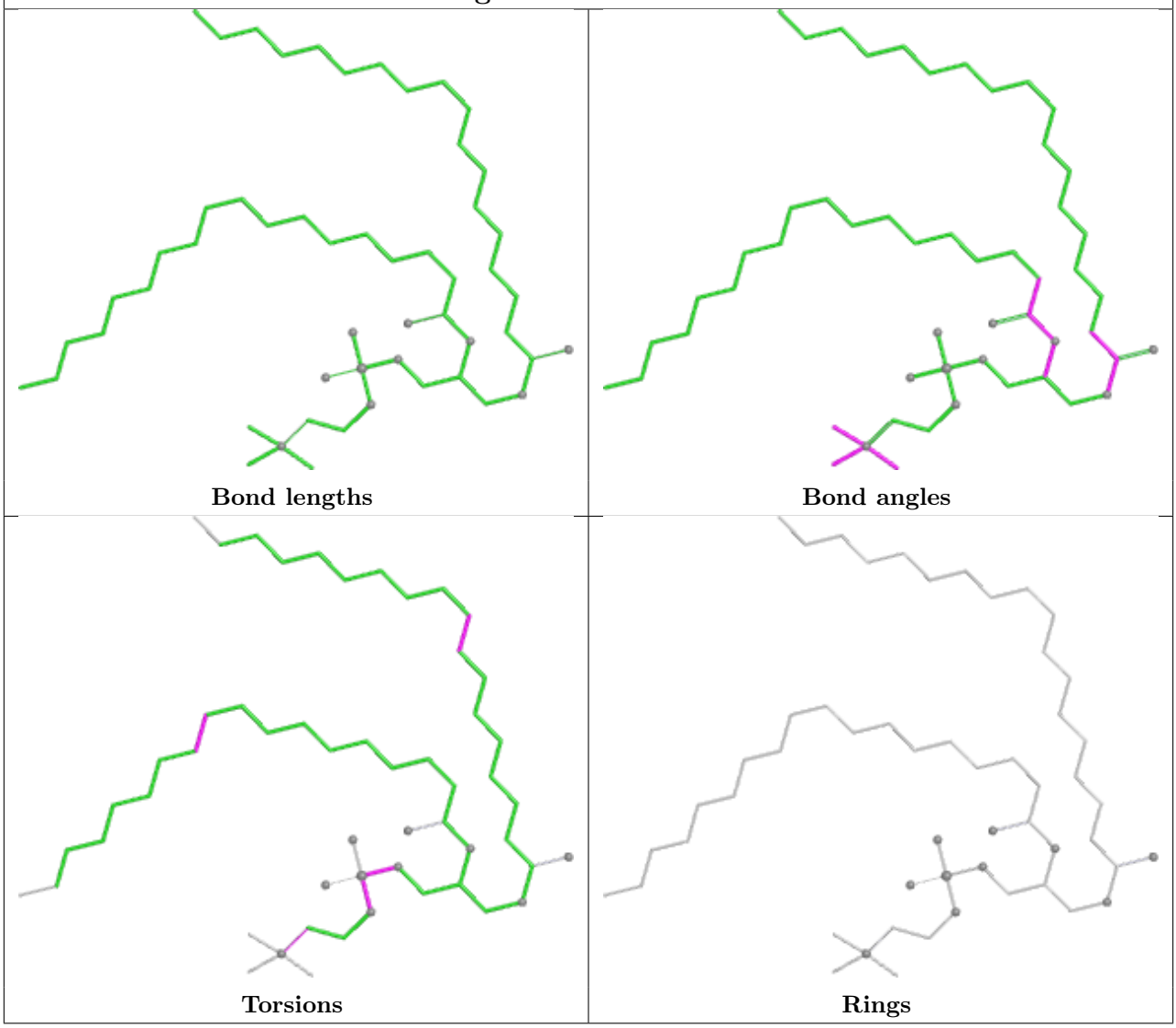


Rings

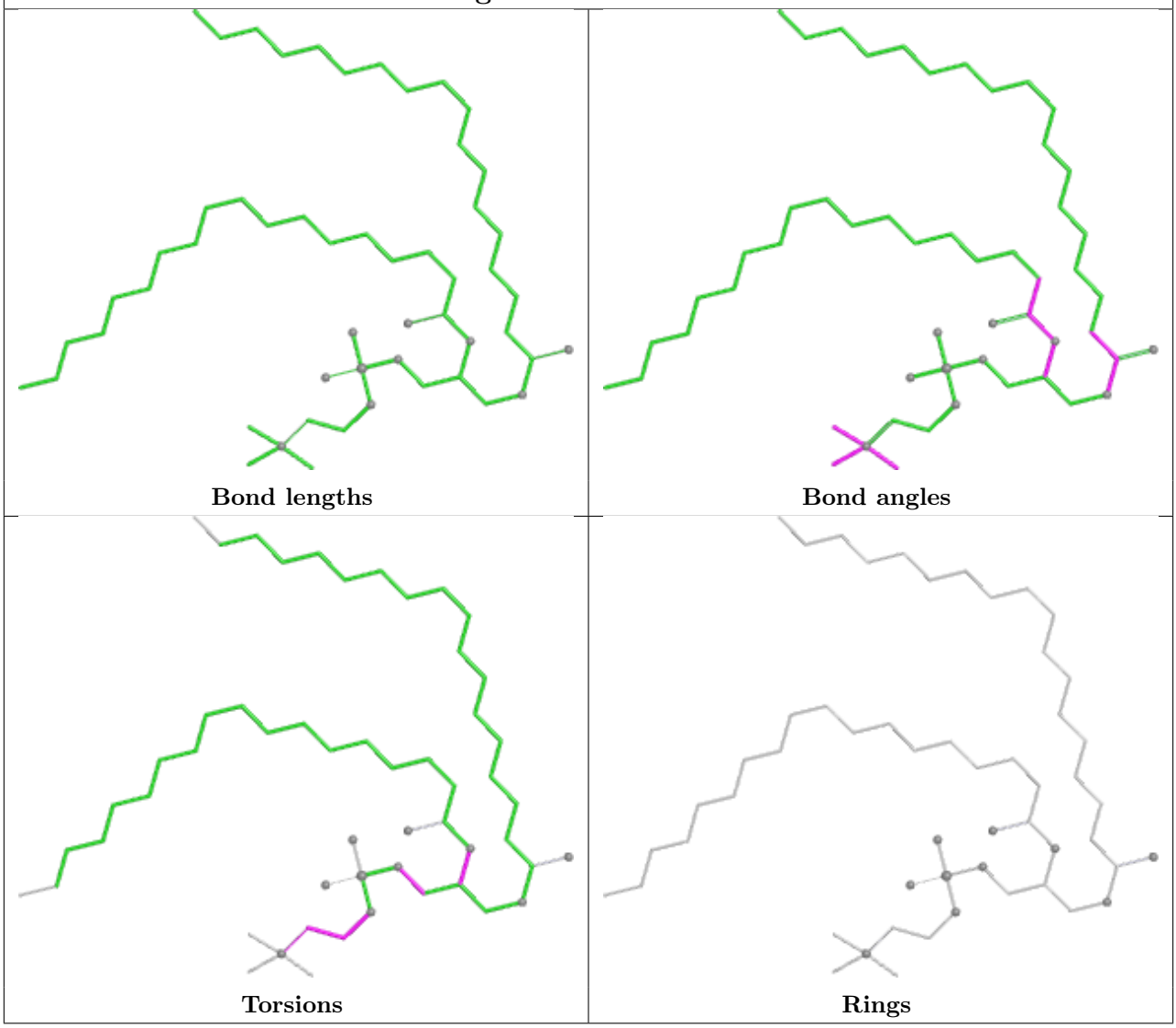
Ligand PCW A 413



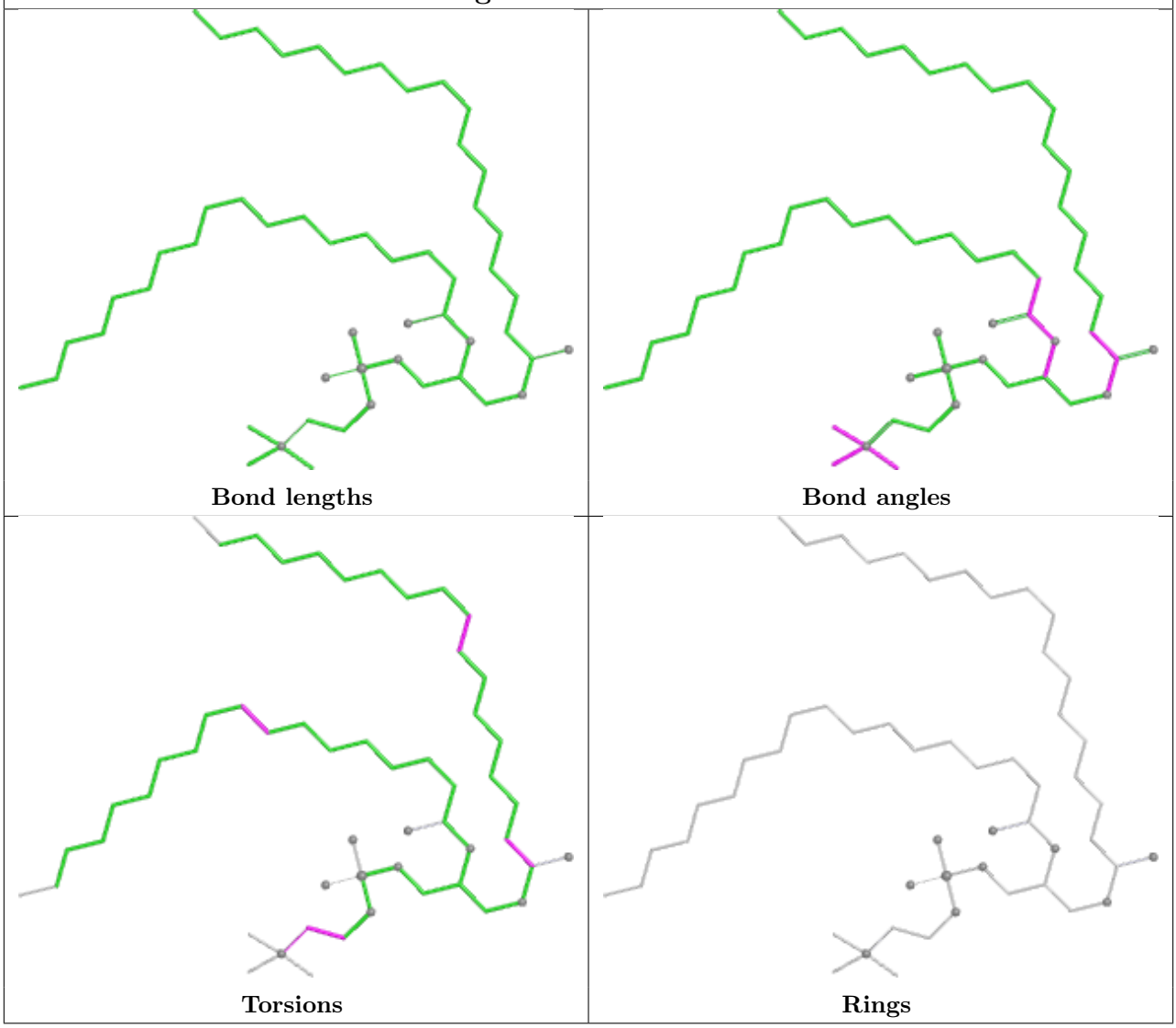
Ligand PCW D 609



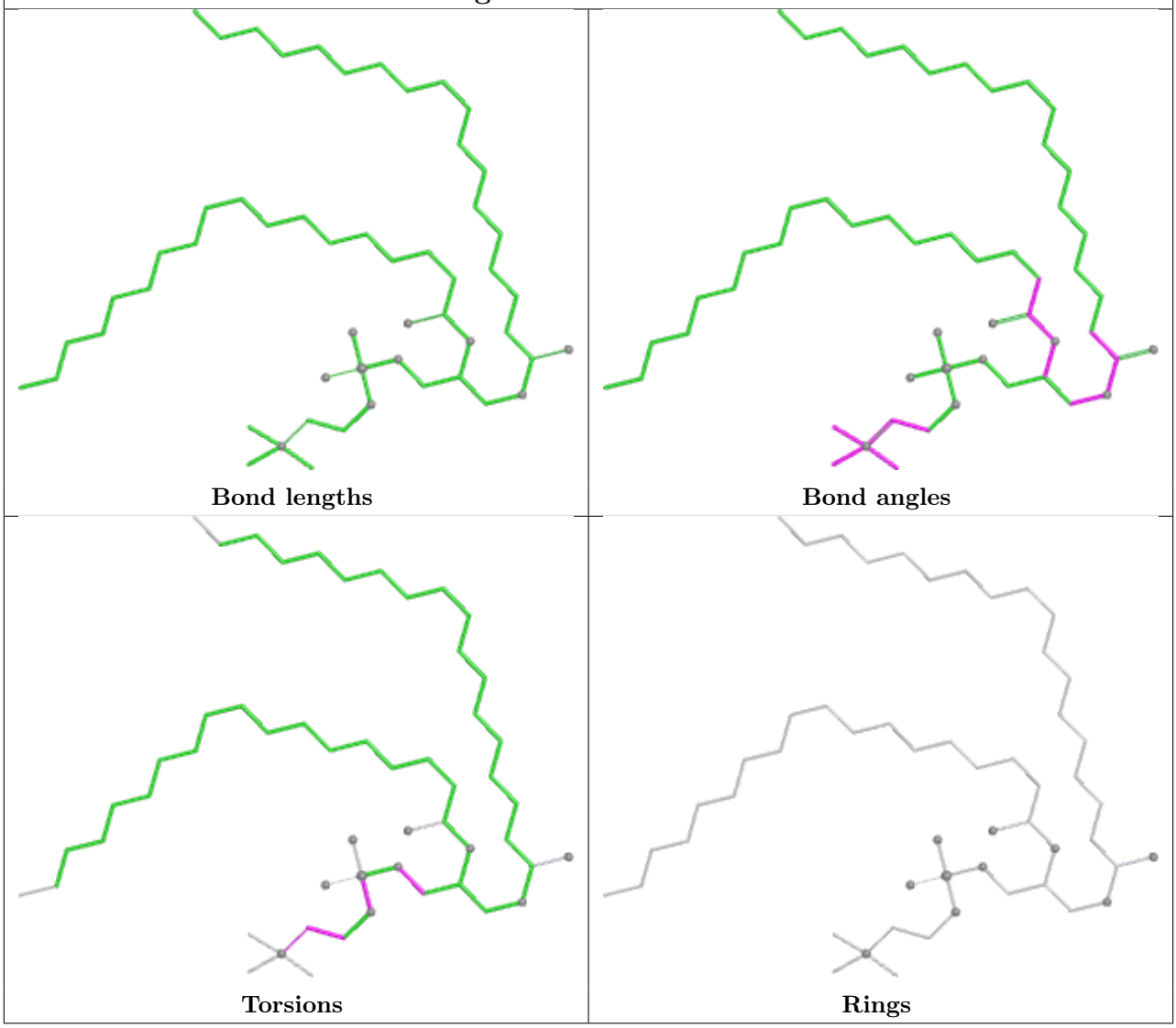
Ligand PCW C 207



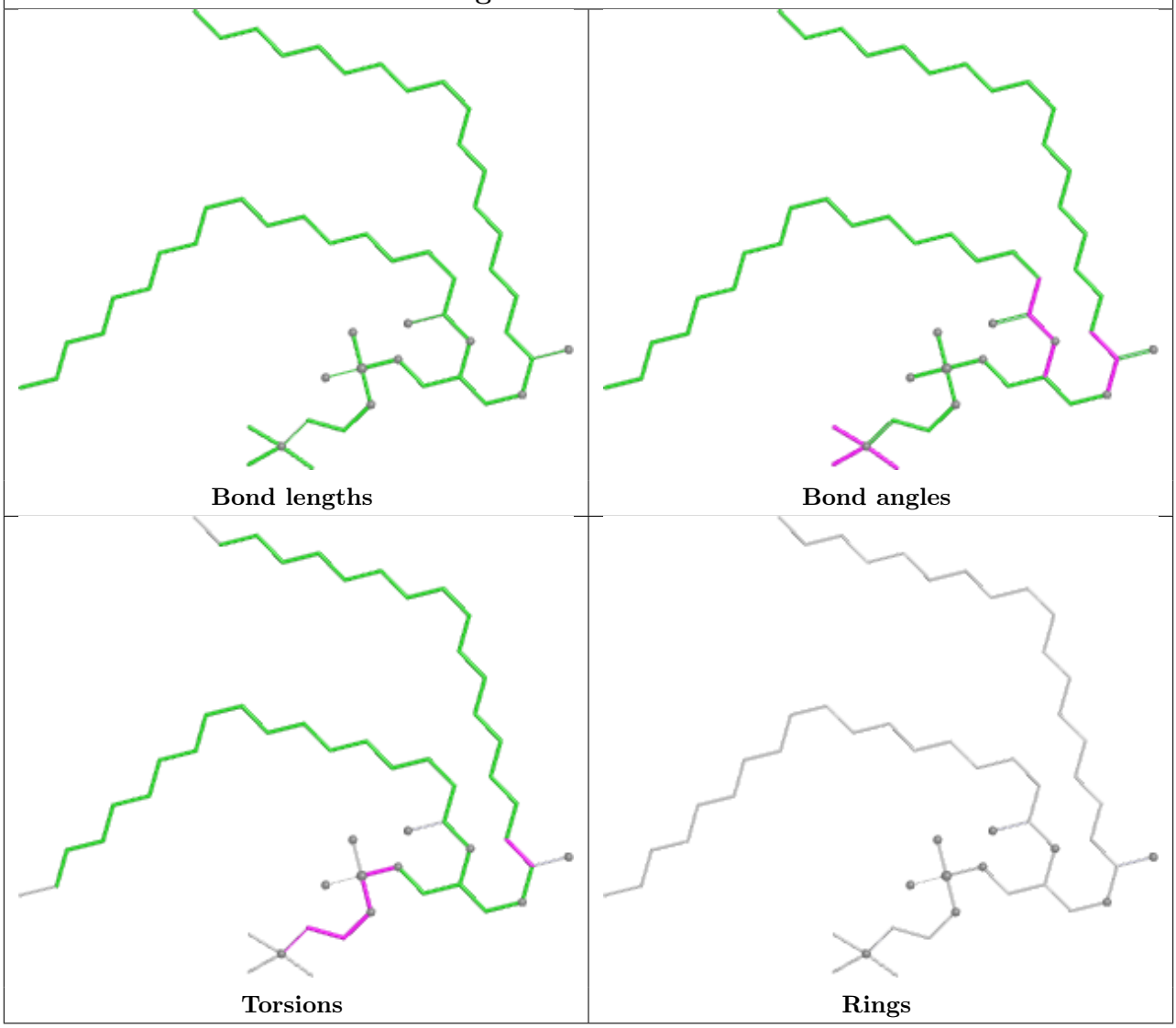
Ligand PCW A 412



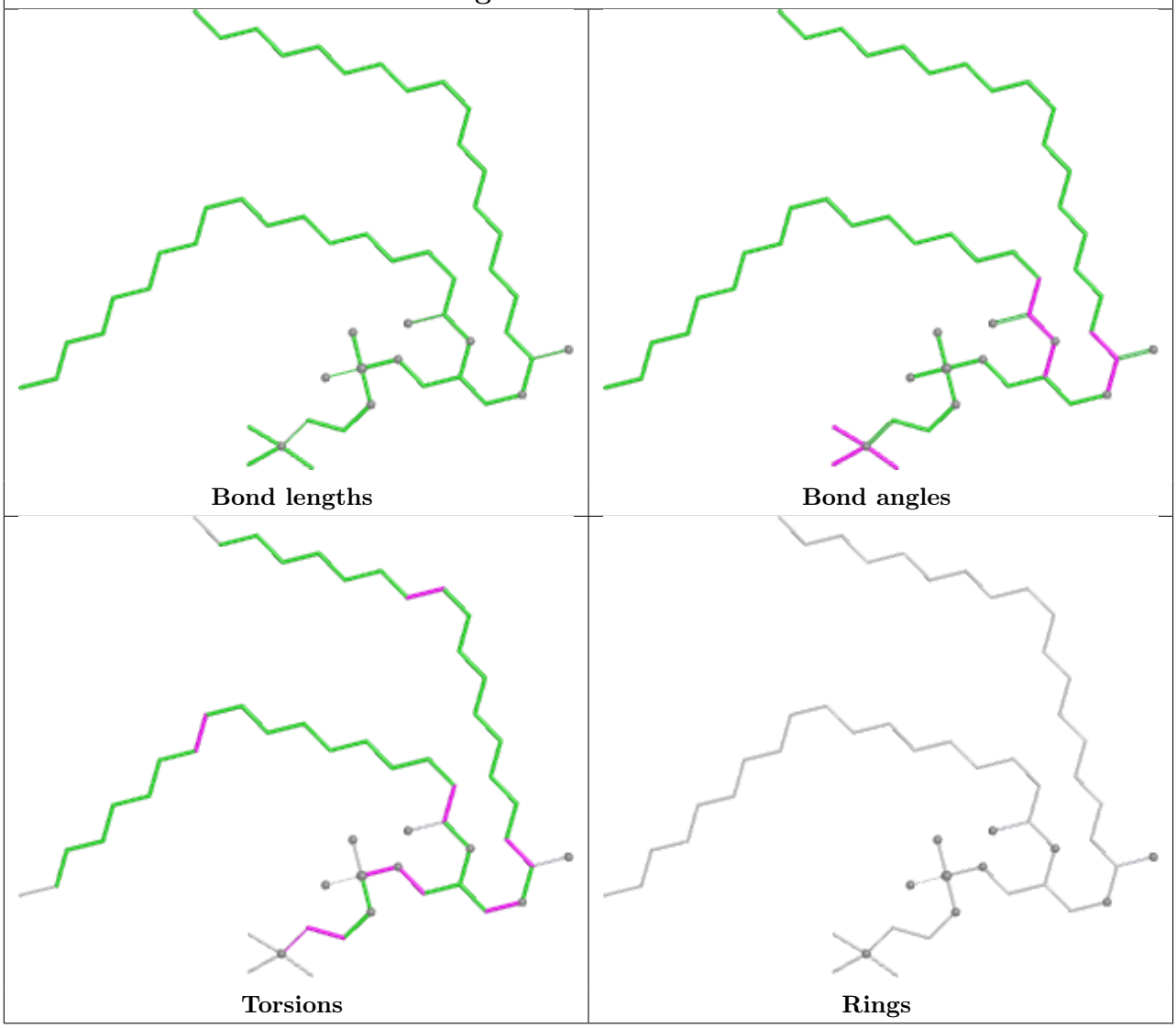
Ligand PCW D 626



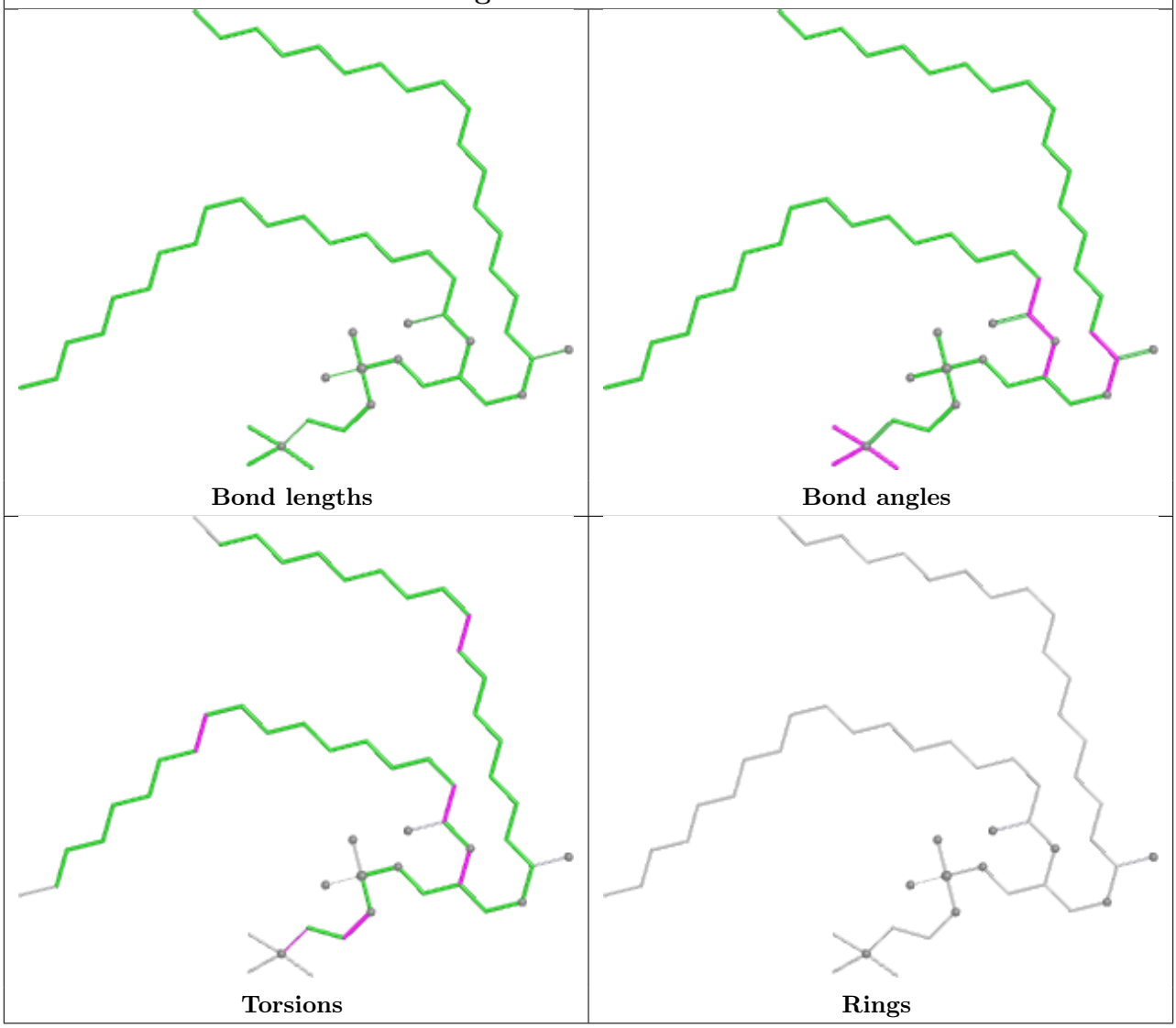
Ligand PCW C 211



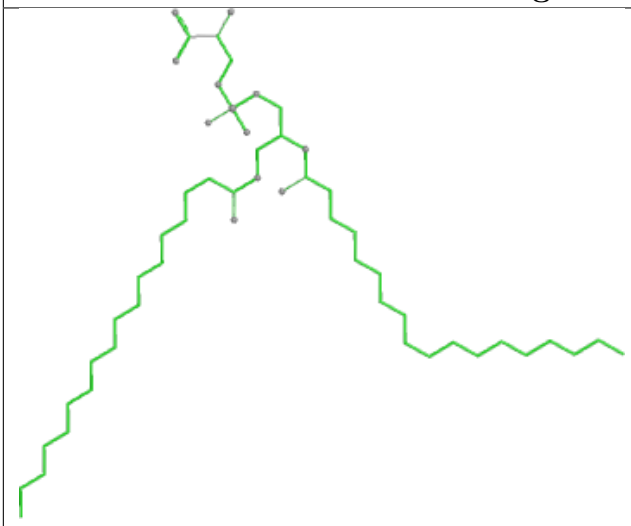
Ligand PCW A 405



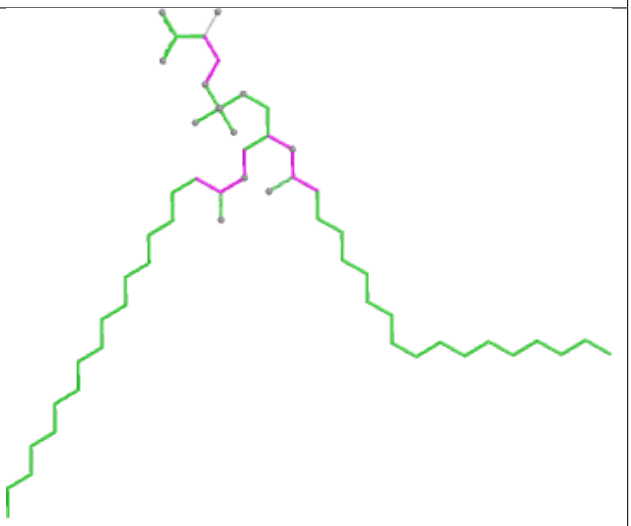
Ligand PCW D 602



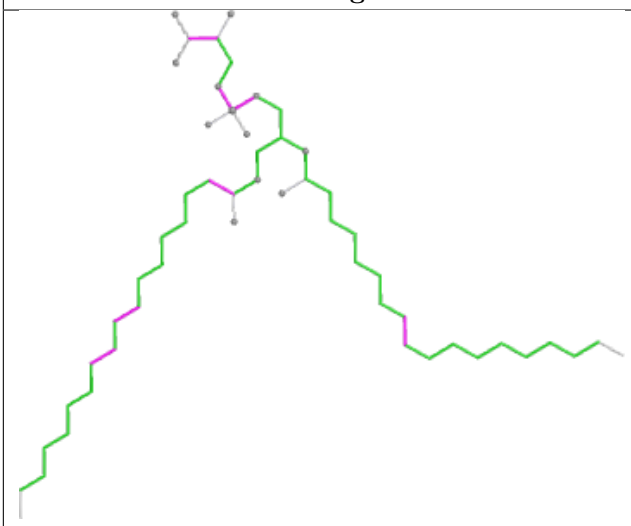
Ligand 17F B 209



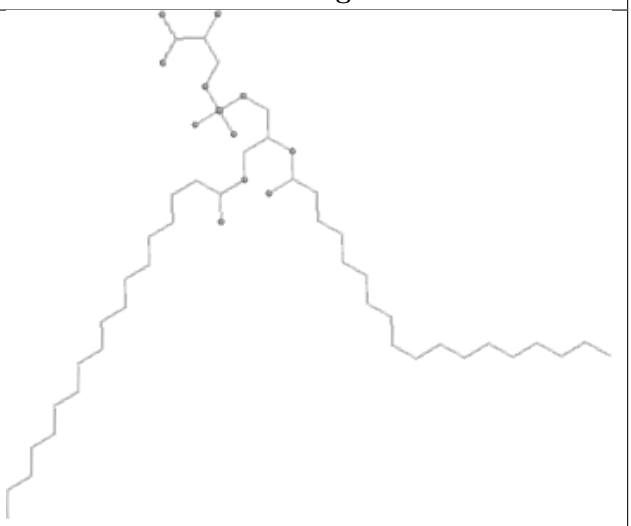
Bond lengths



Bond angles

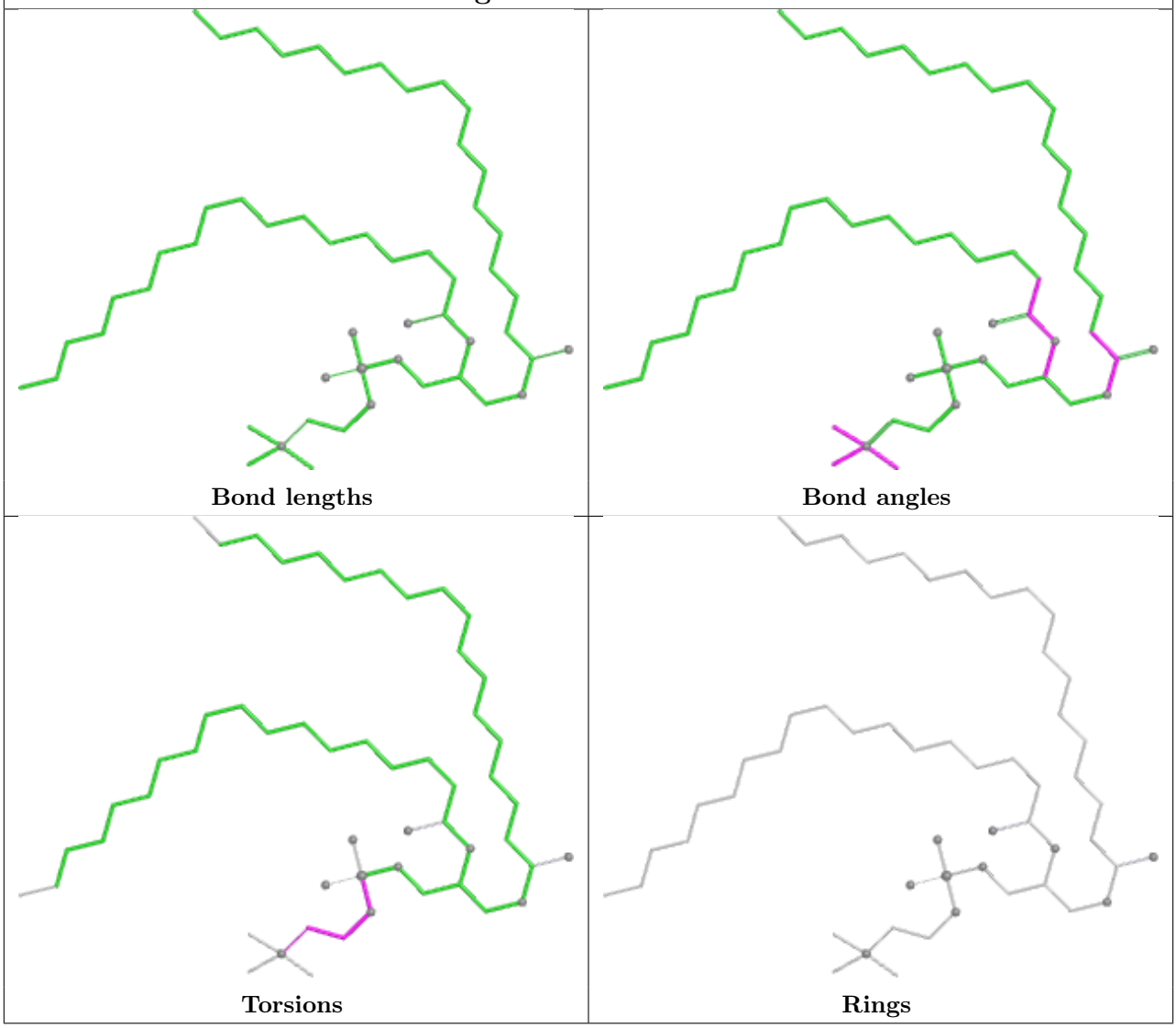


Torsions

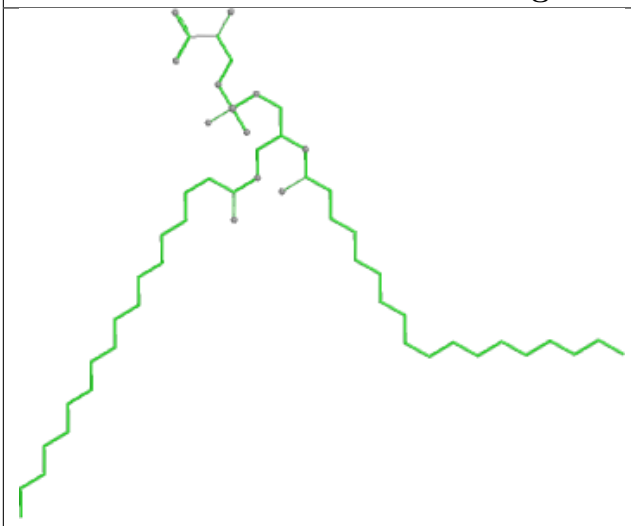


Rings

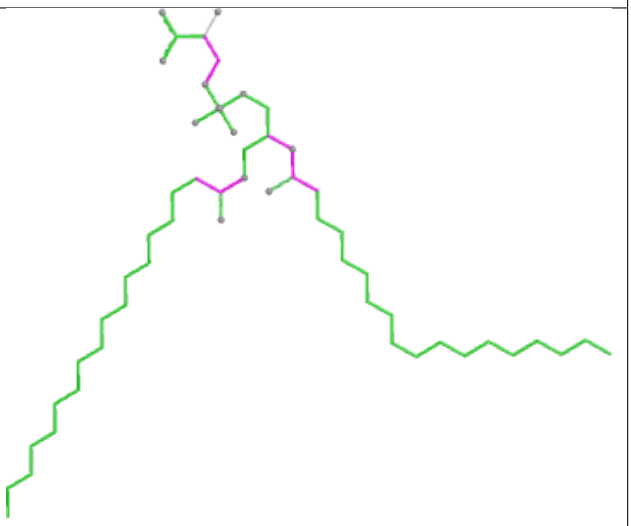
Ligand PCW D 623



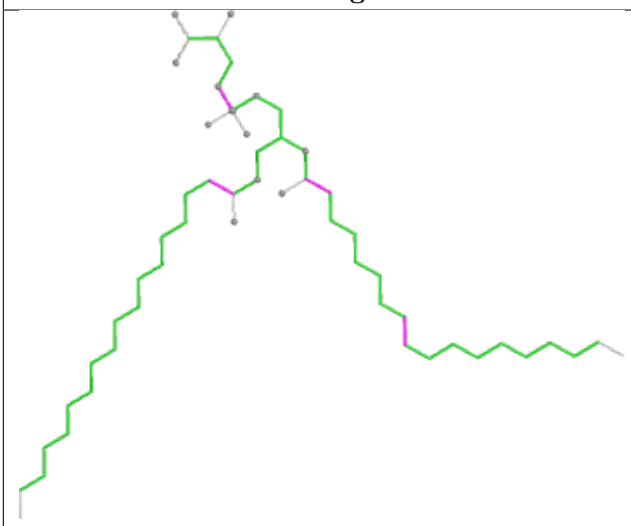
Ligand 17F D 628



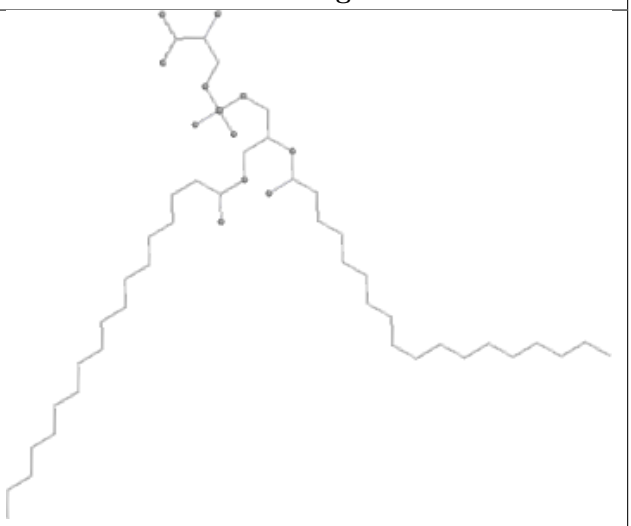
Bond lengths



Bond angles

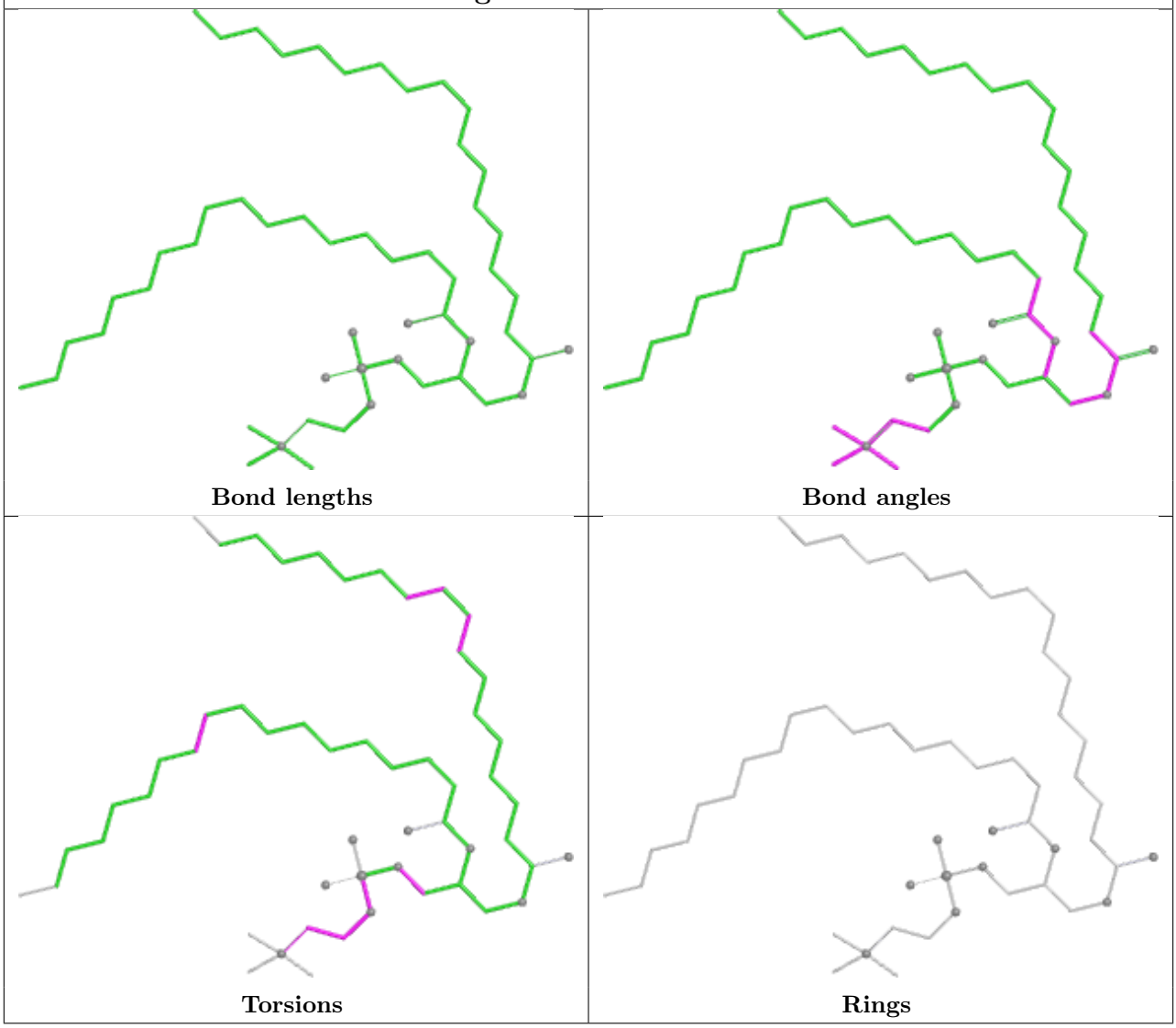


Torsions

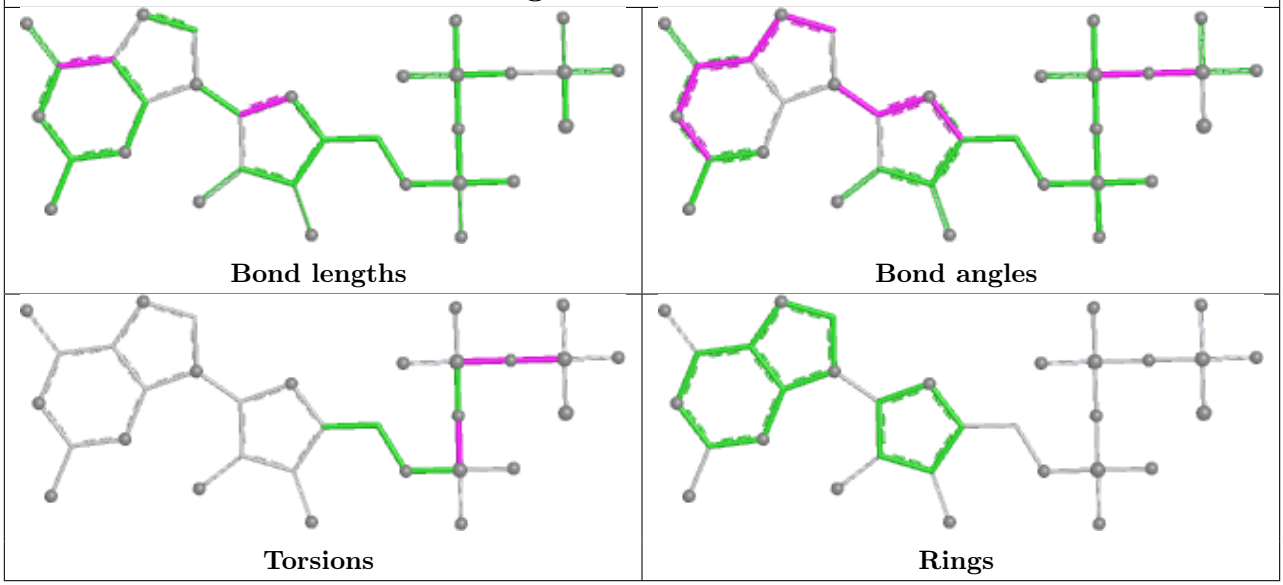


Rings

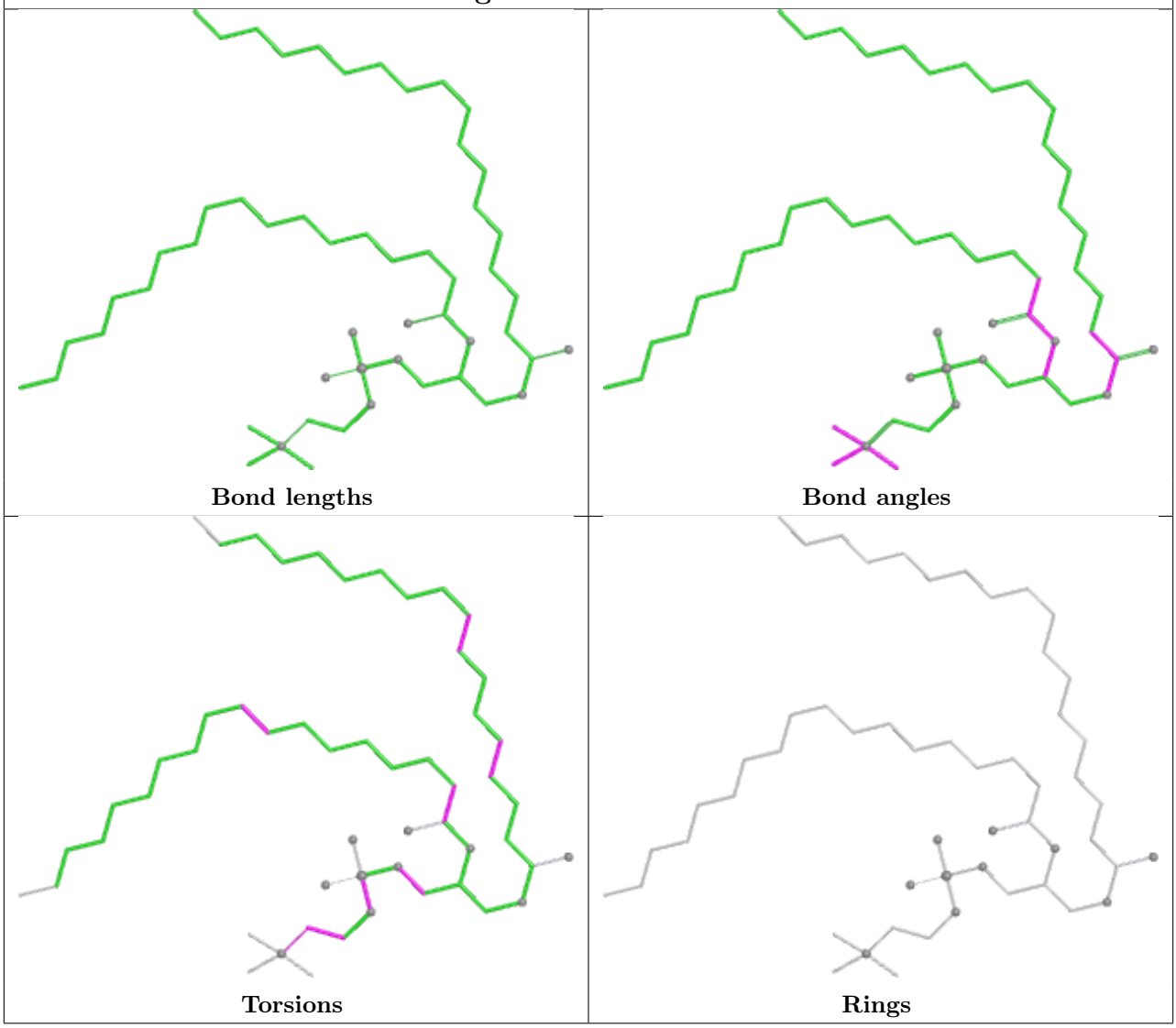
Ligand PCW D 627



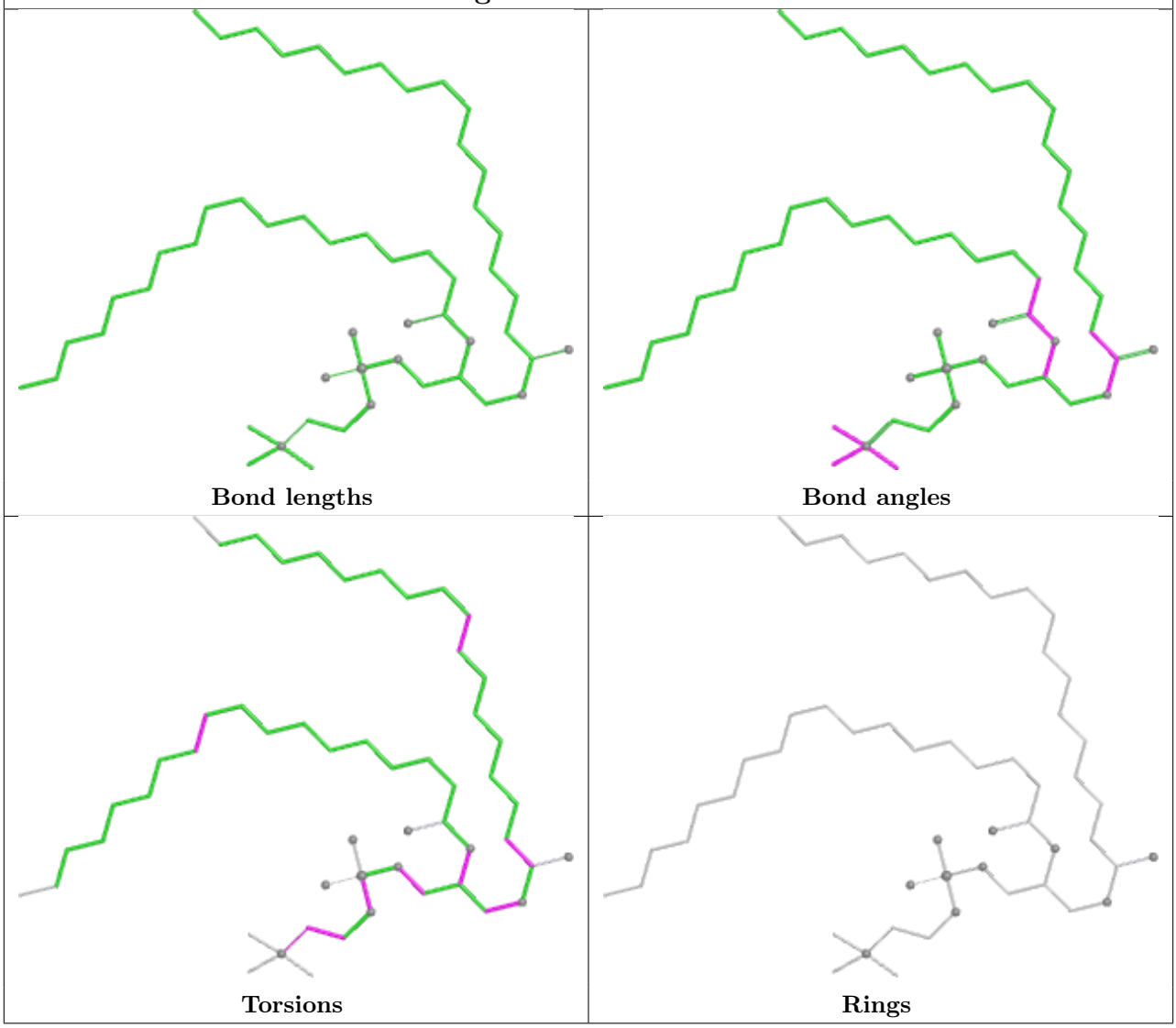
Ligand GSP C 201



Ligand PCW A 407



Ligand PCW D 618



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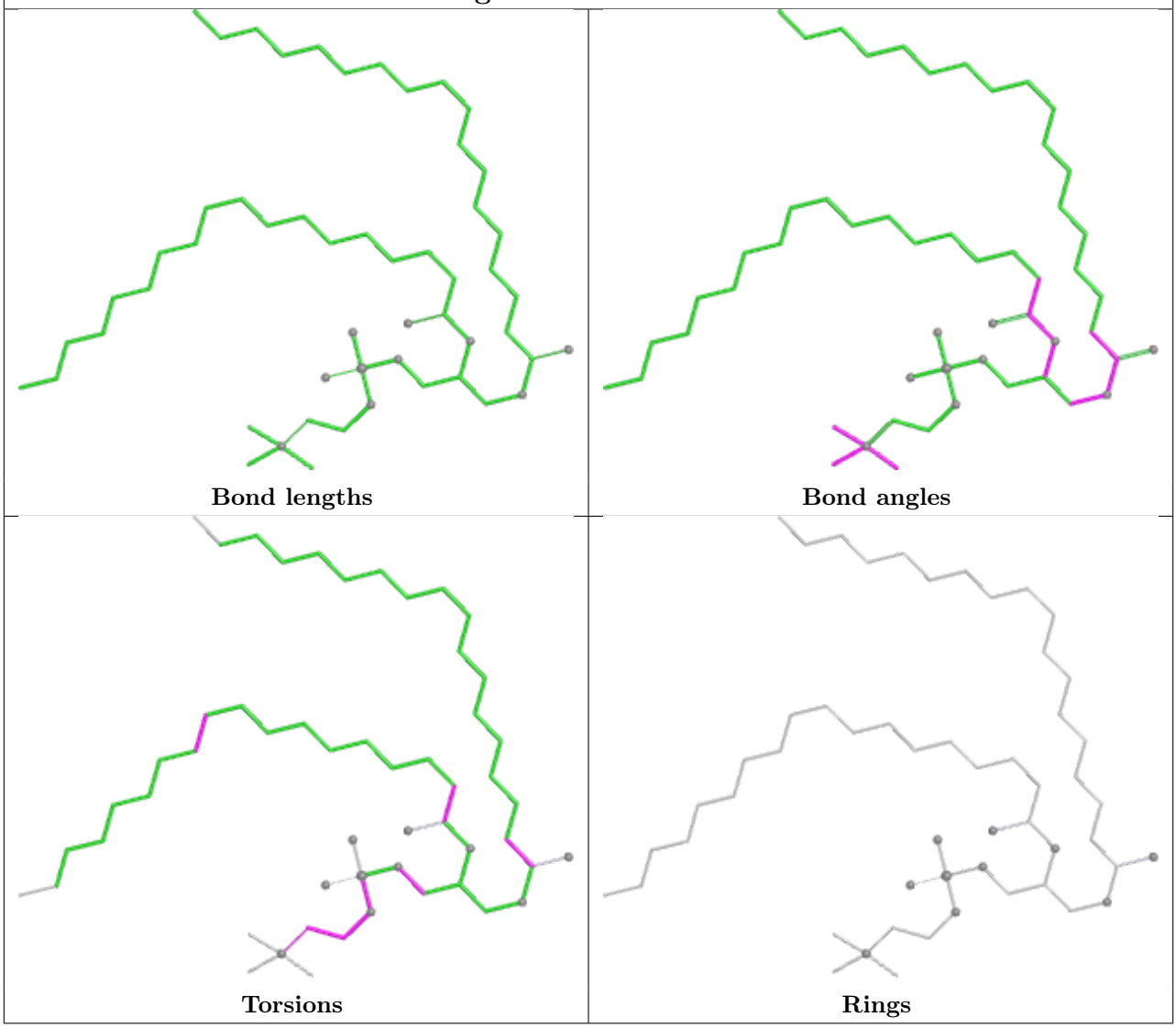
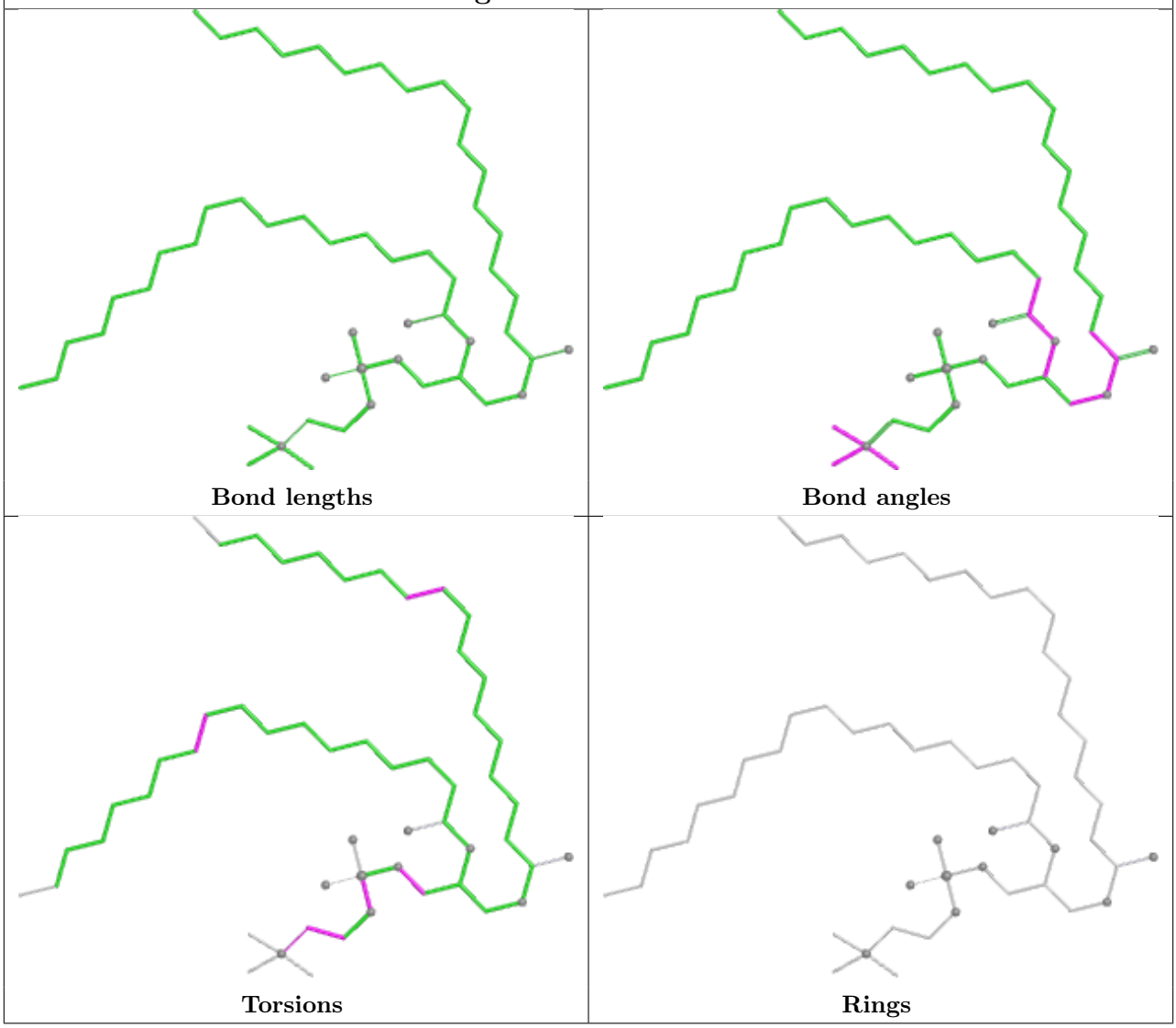
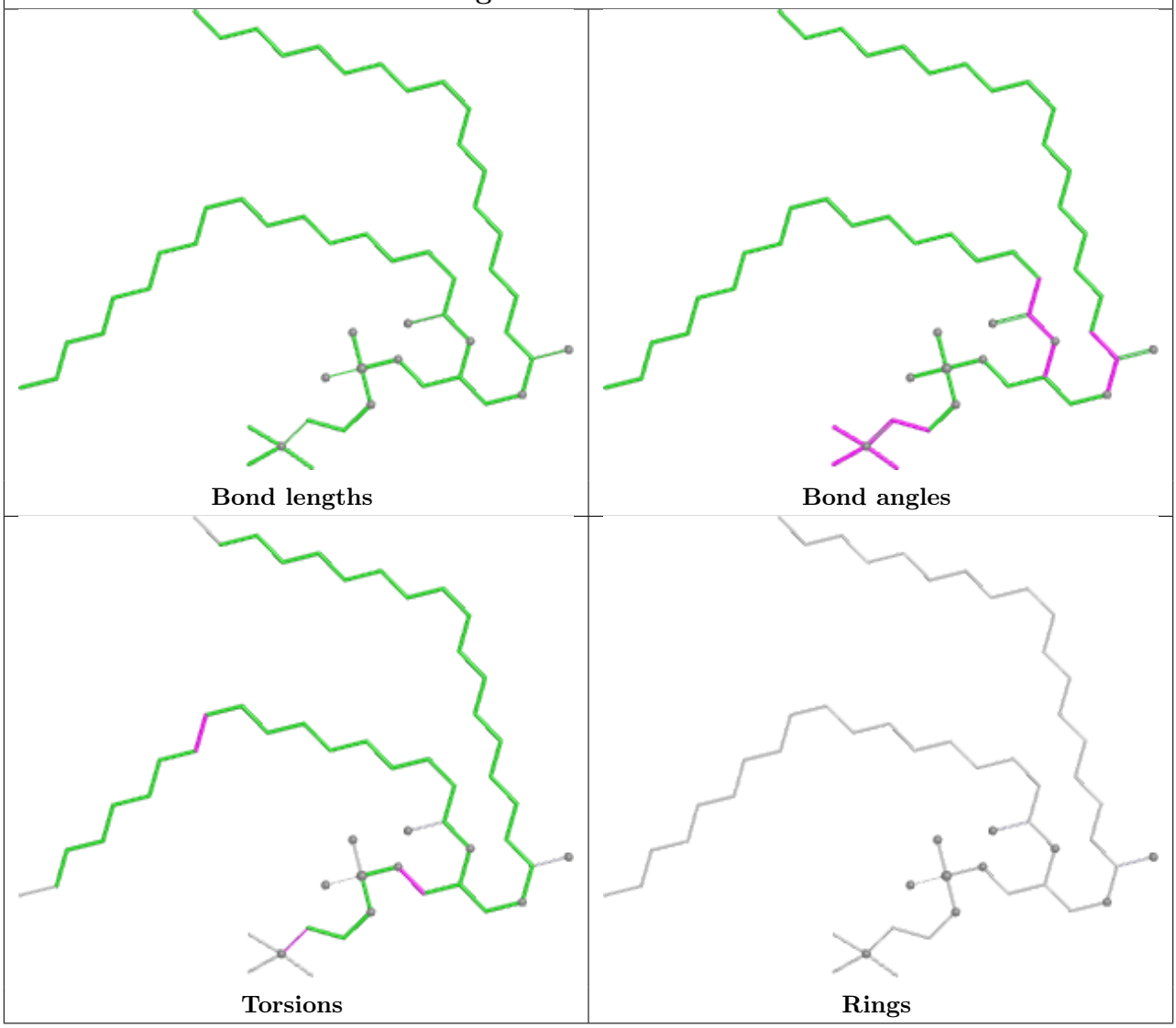


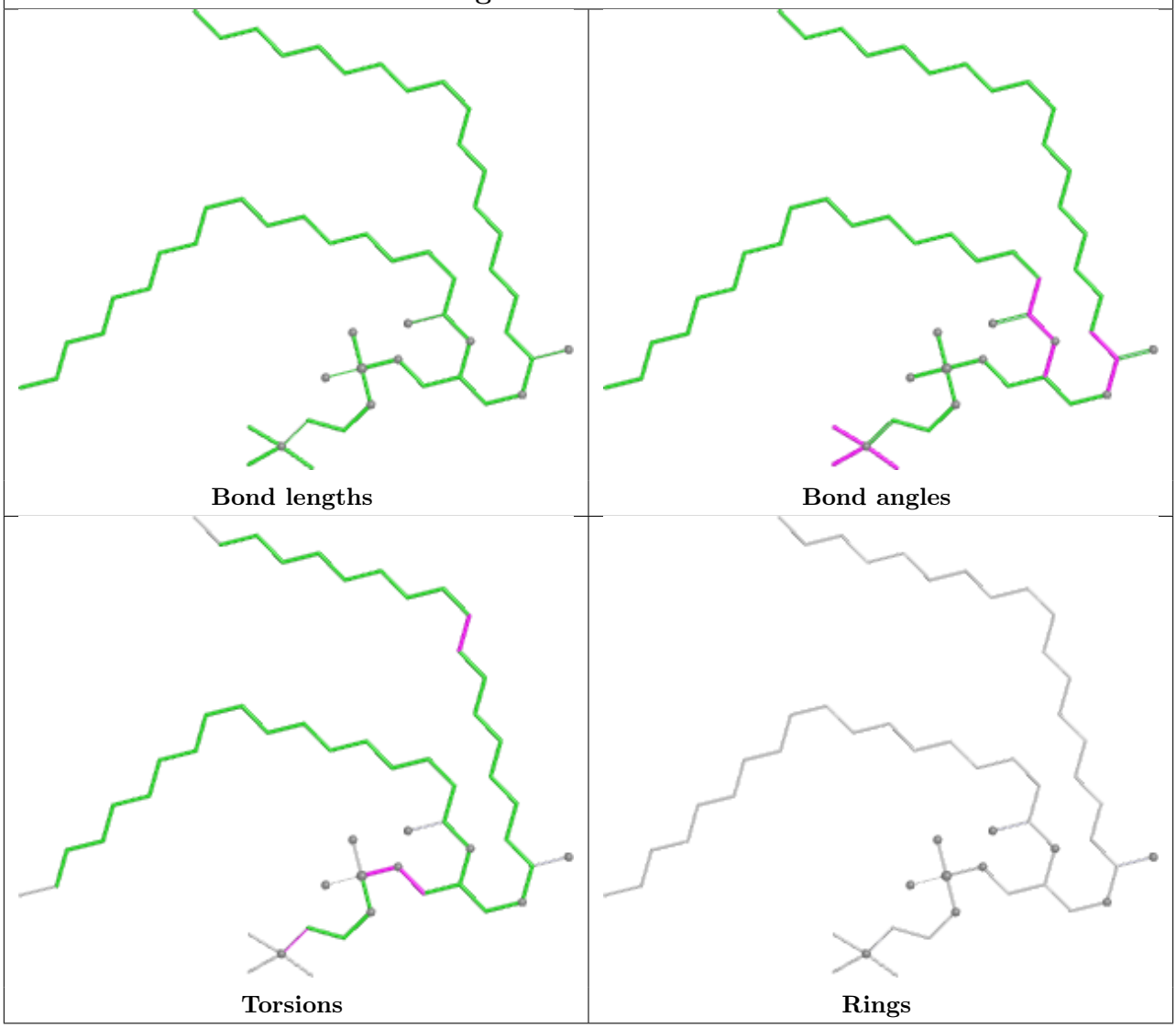
Ligand PCW D 612



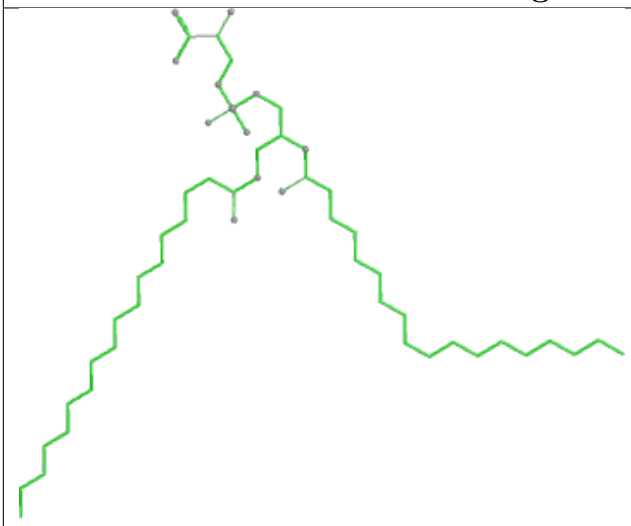
Ligand PCW B 204



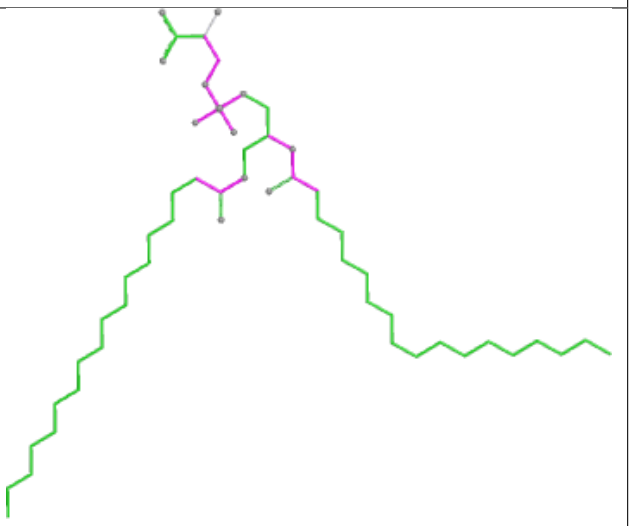
Ligand PCW C 205



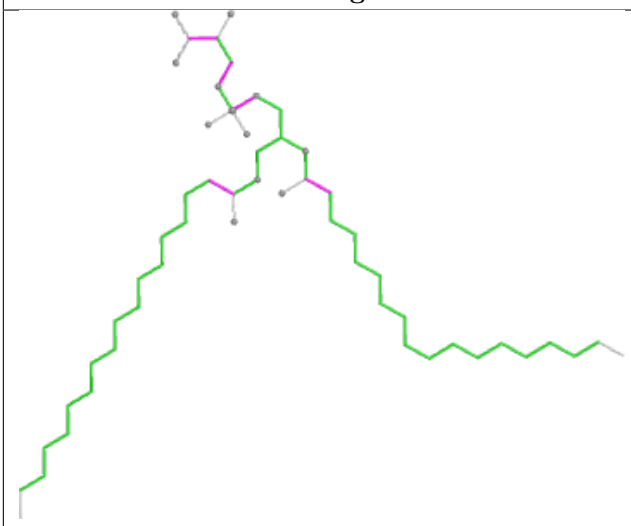
Ligand 17F A 415



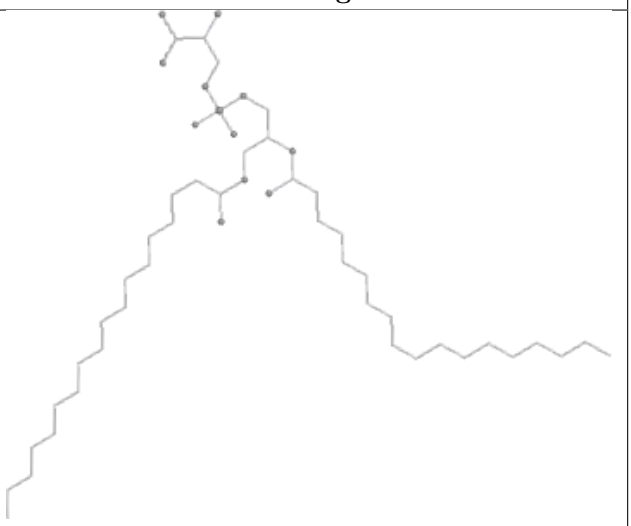
Bond lengths



Bond angles

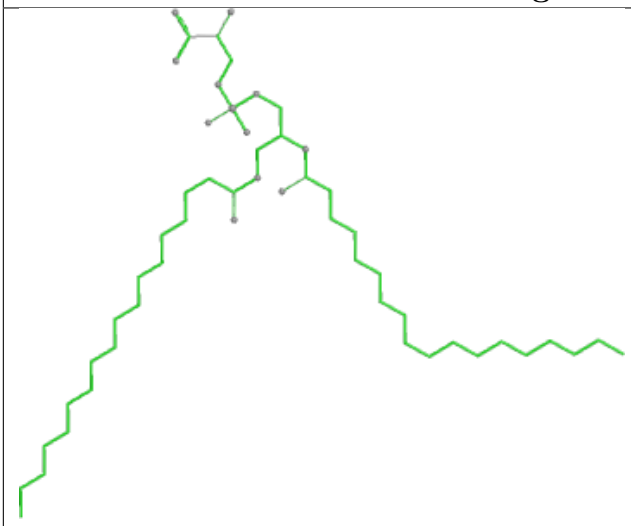


Torsions

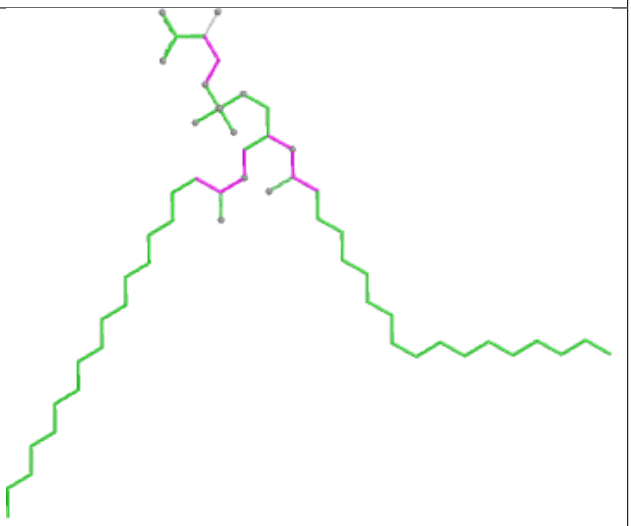


Rings

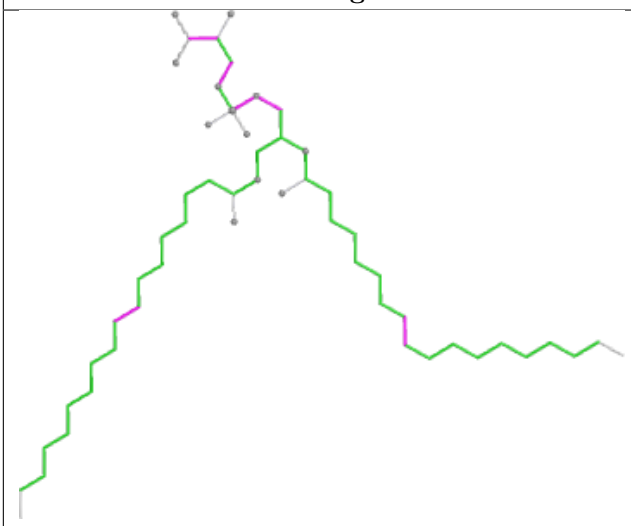
Ligand 17F C 219



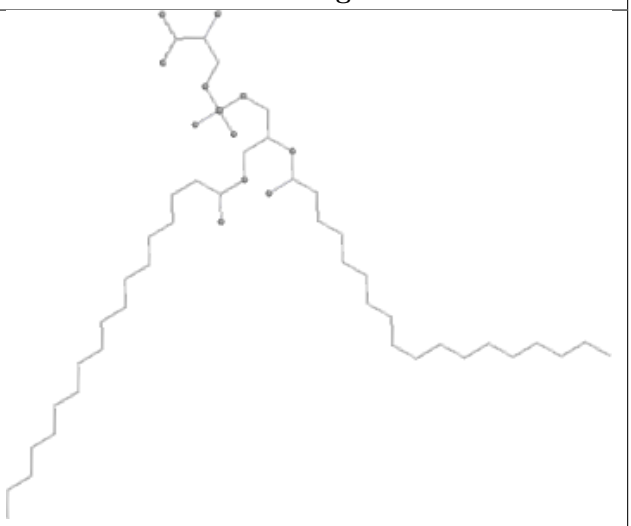
Bond lengths



Bond angles

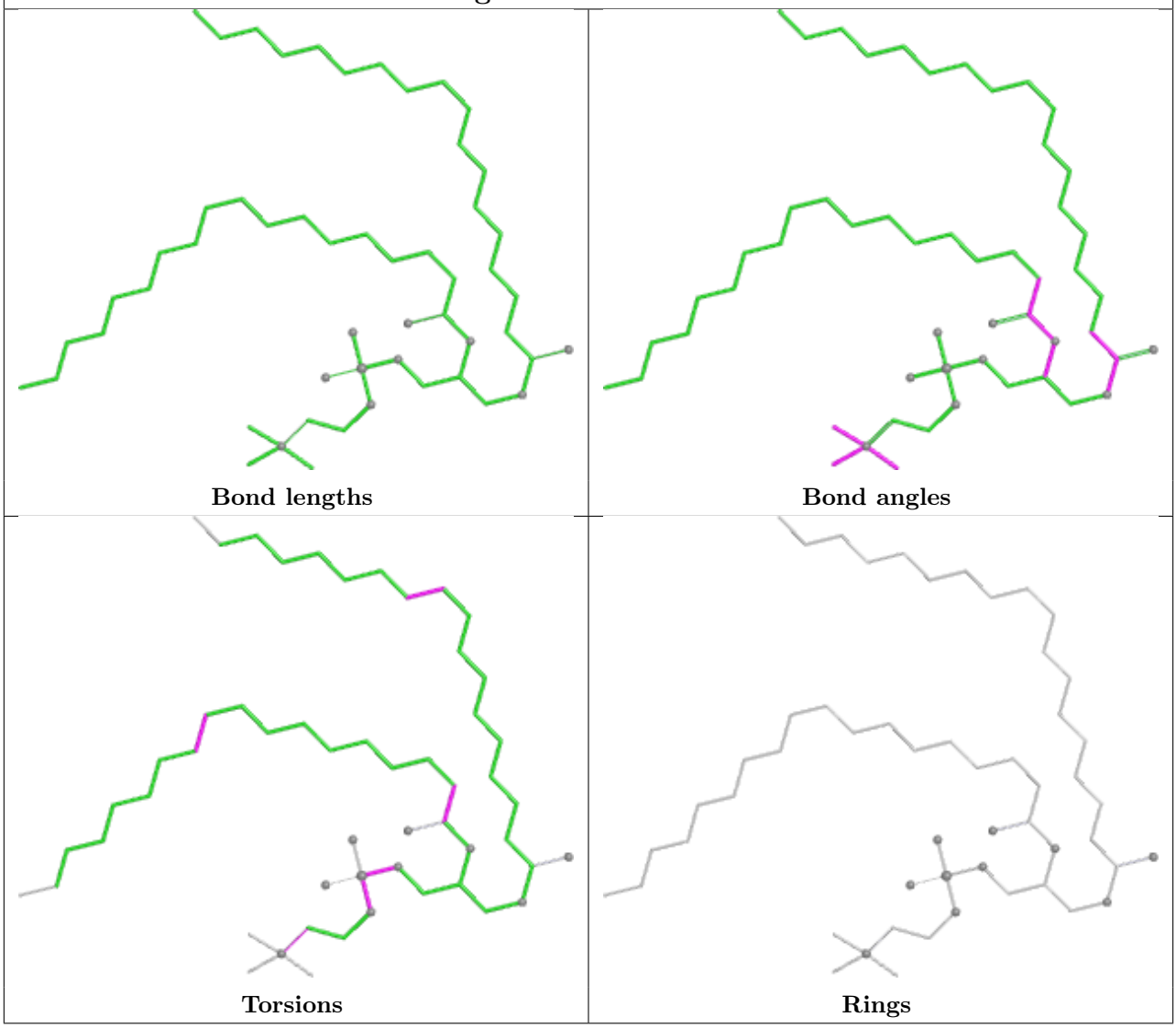


Torsions

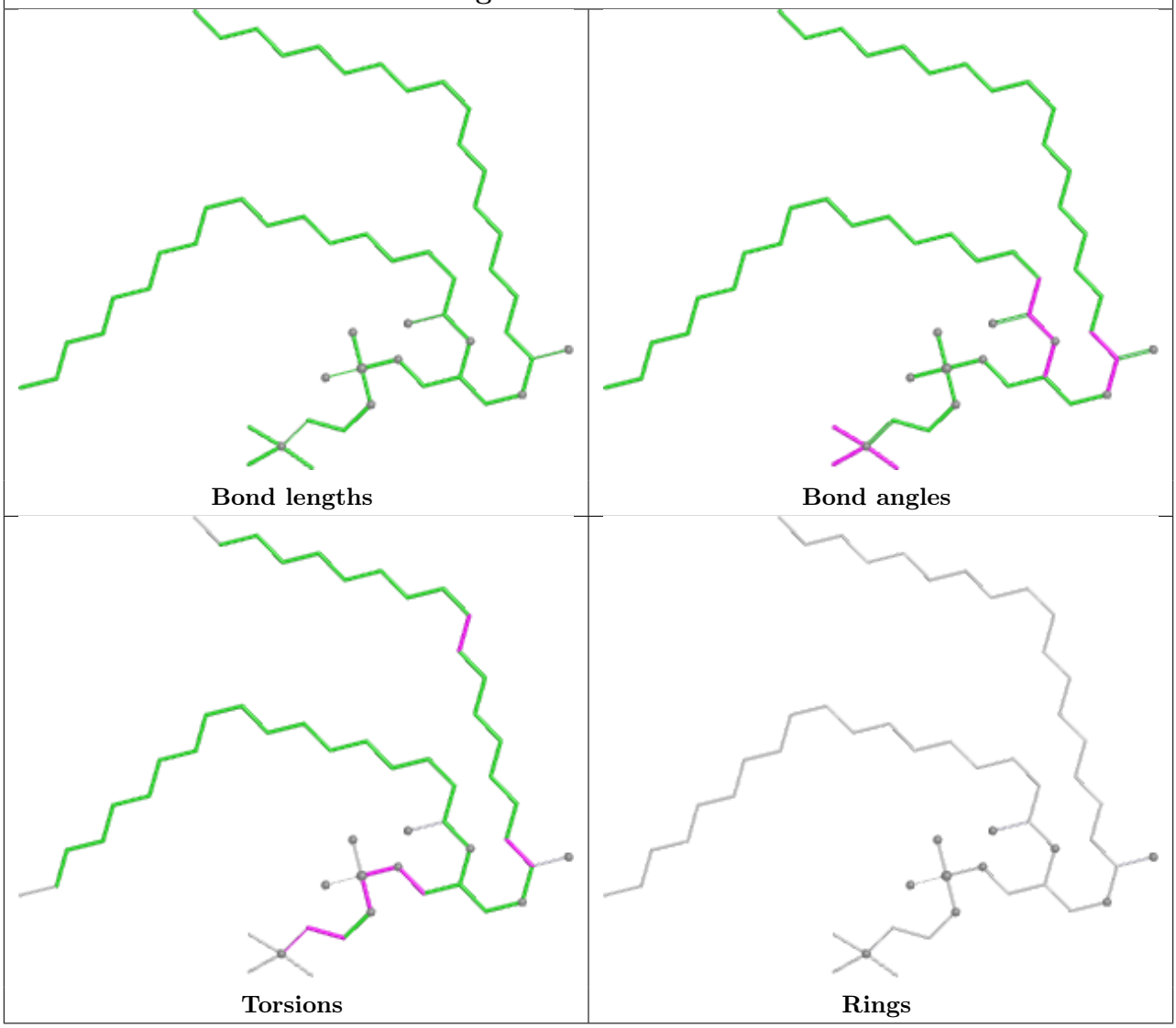


Rings

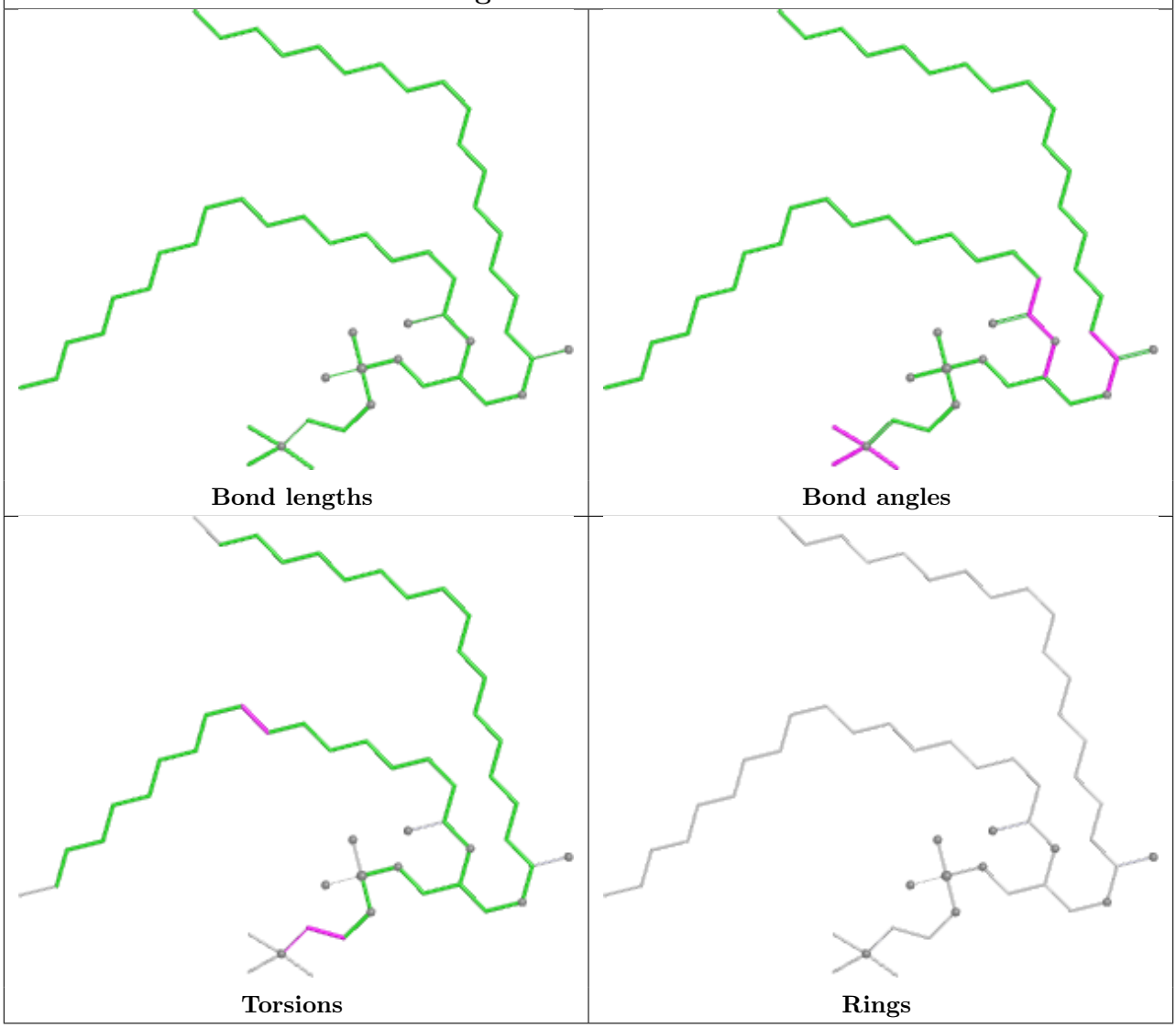
Ligand PCW D 620



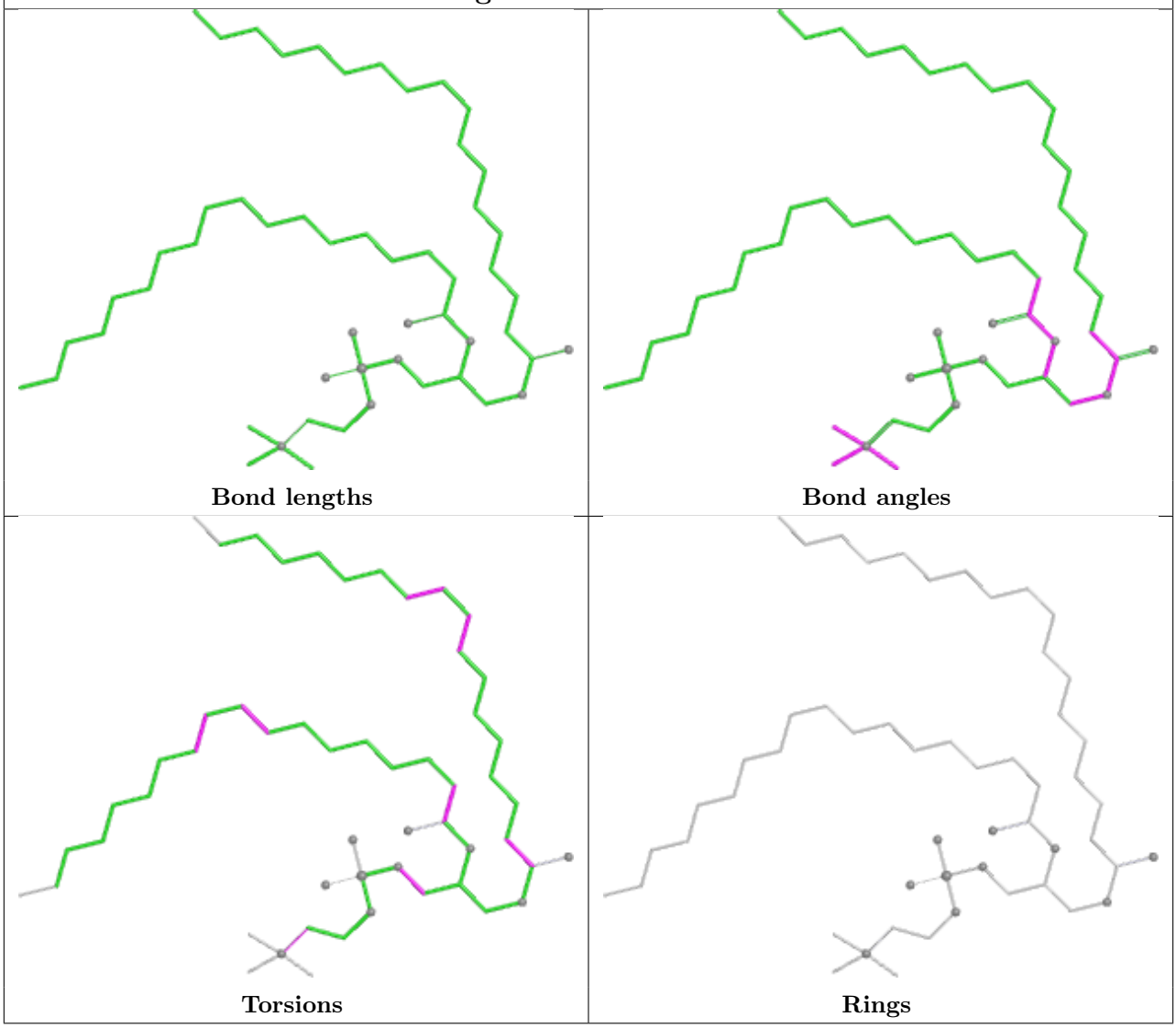
Ligand PCW B 207



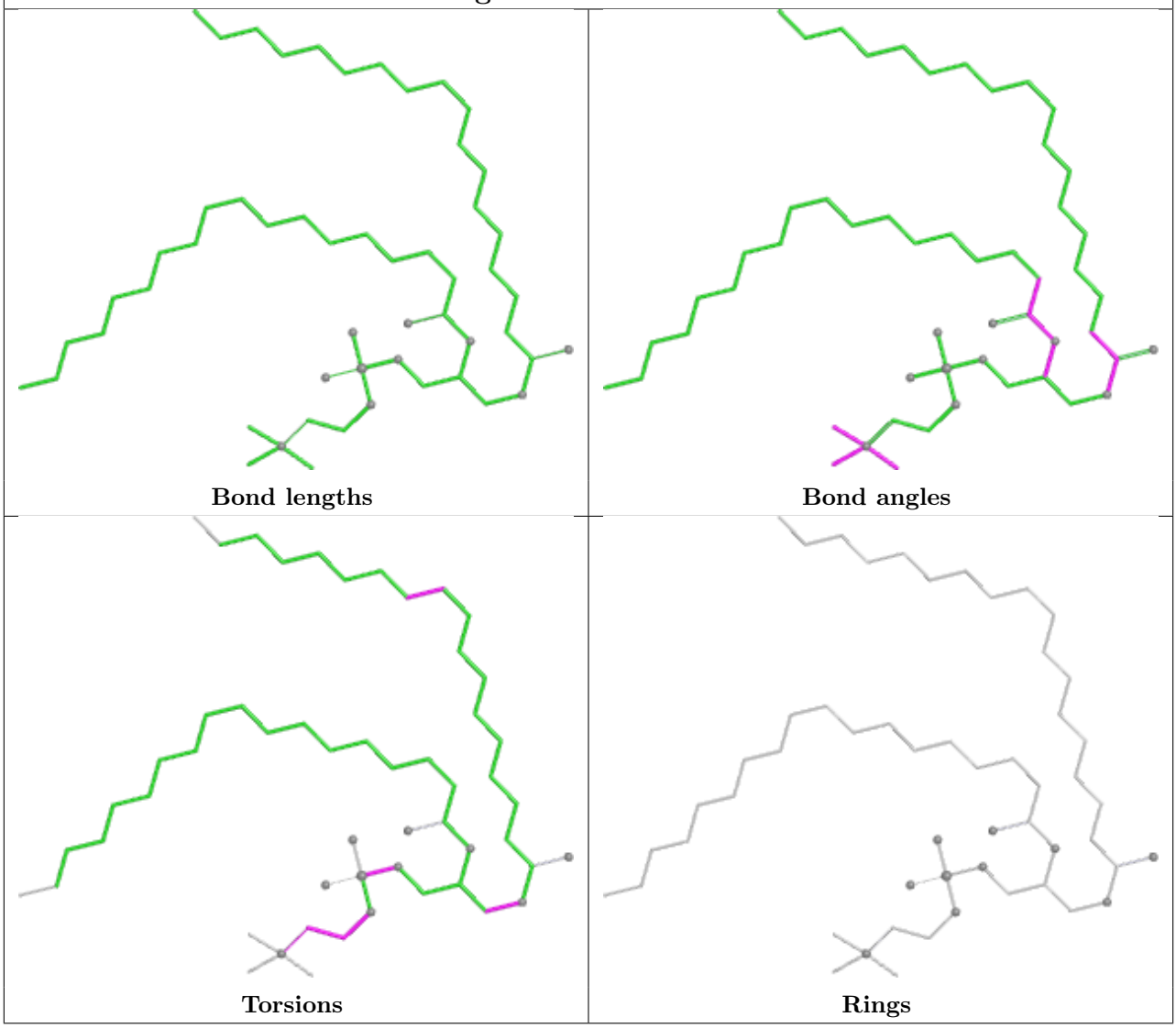
Ligand PCW A 414



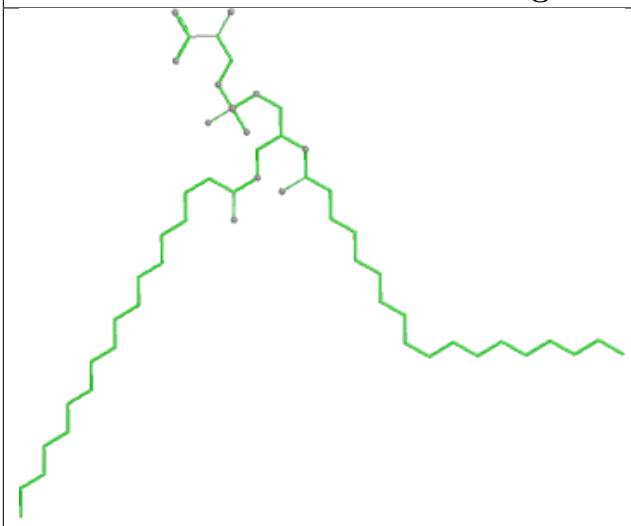
Ligand PCW C 206



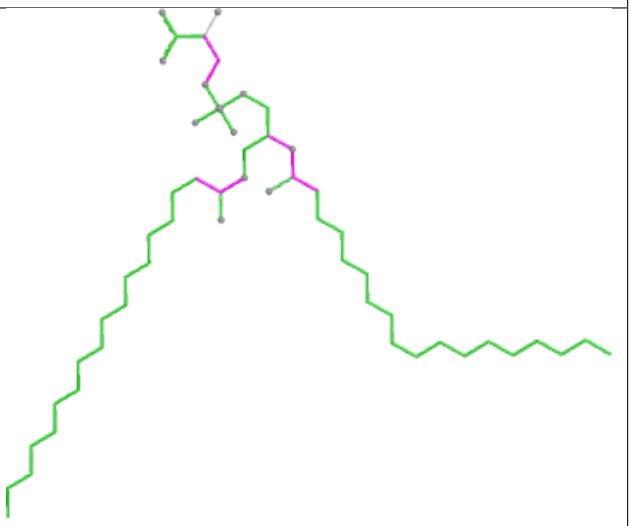
Ligand PCW A 410



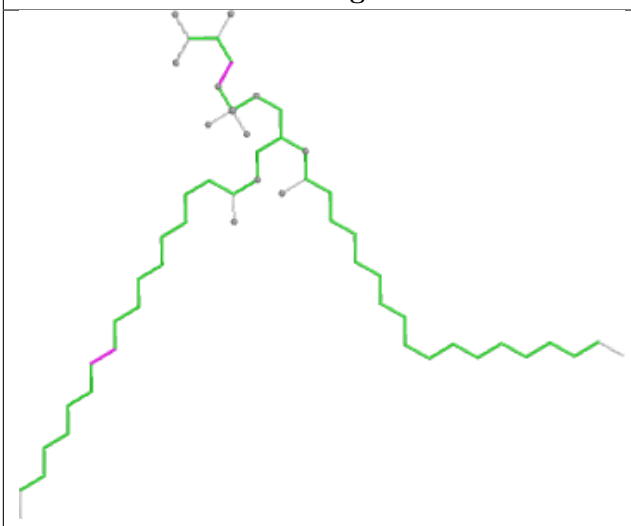
Ligand 17F A 416



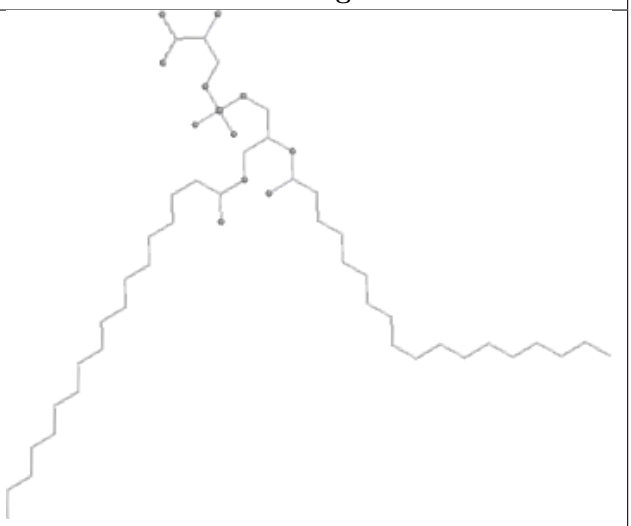
Bond lengths



Bond angles

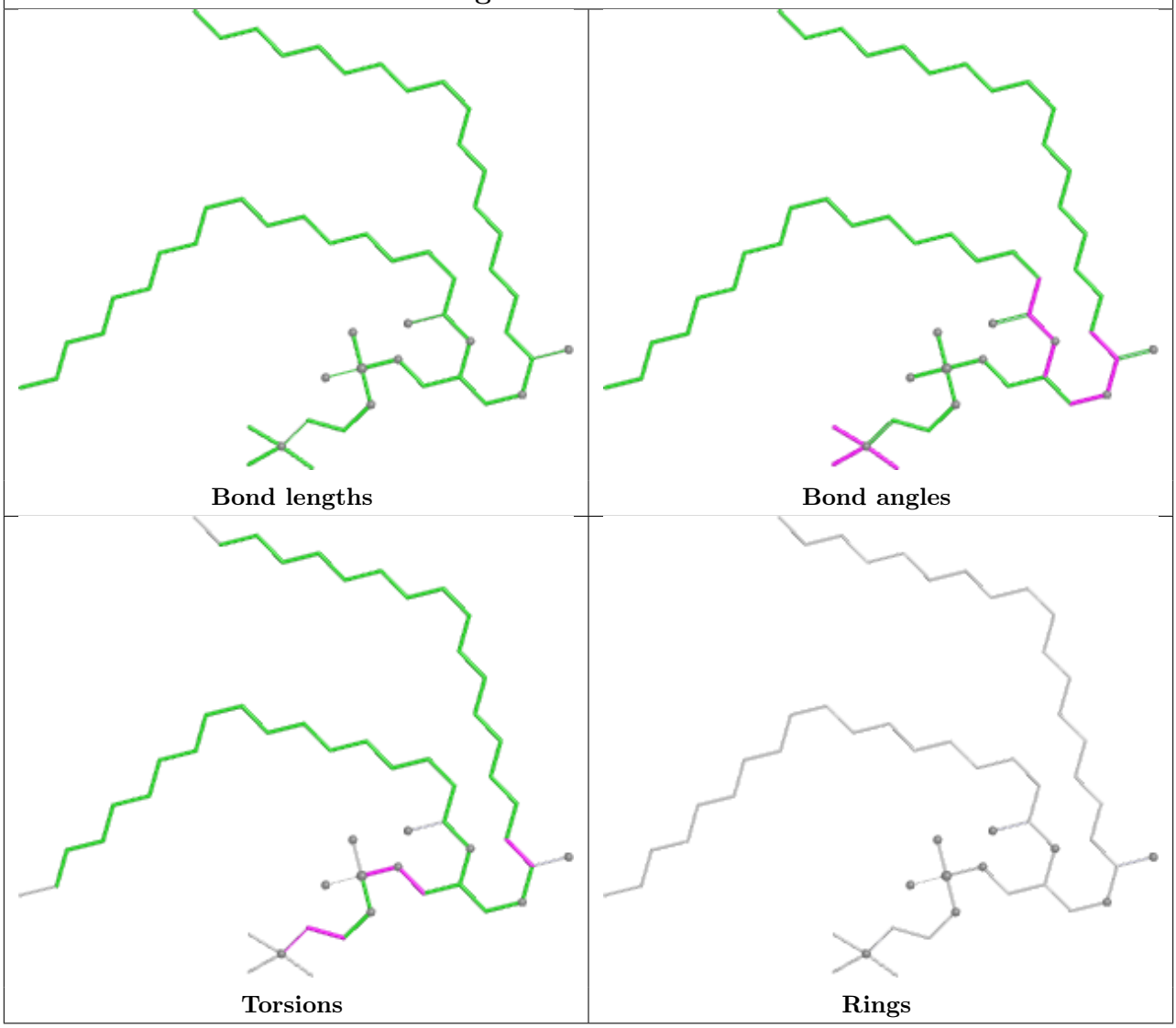


Torsions

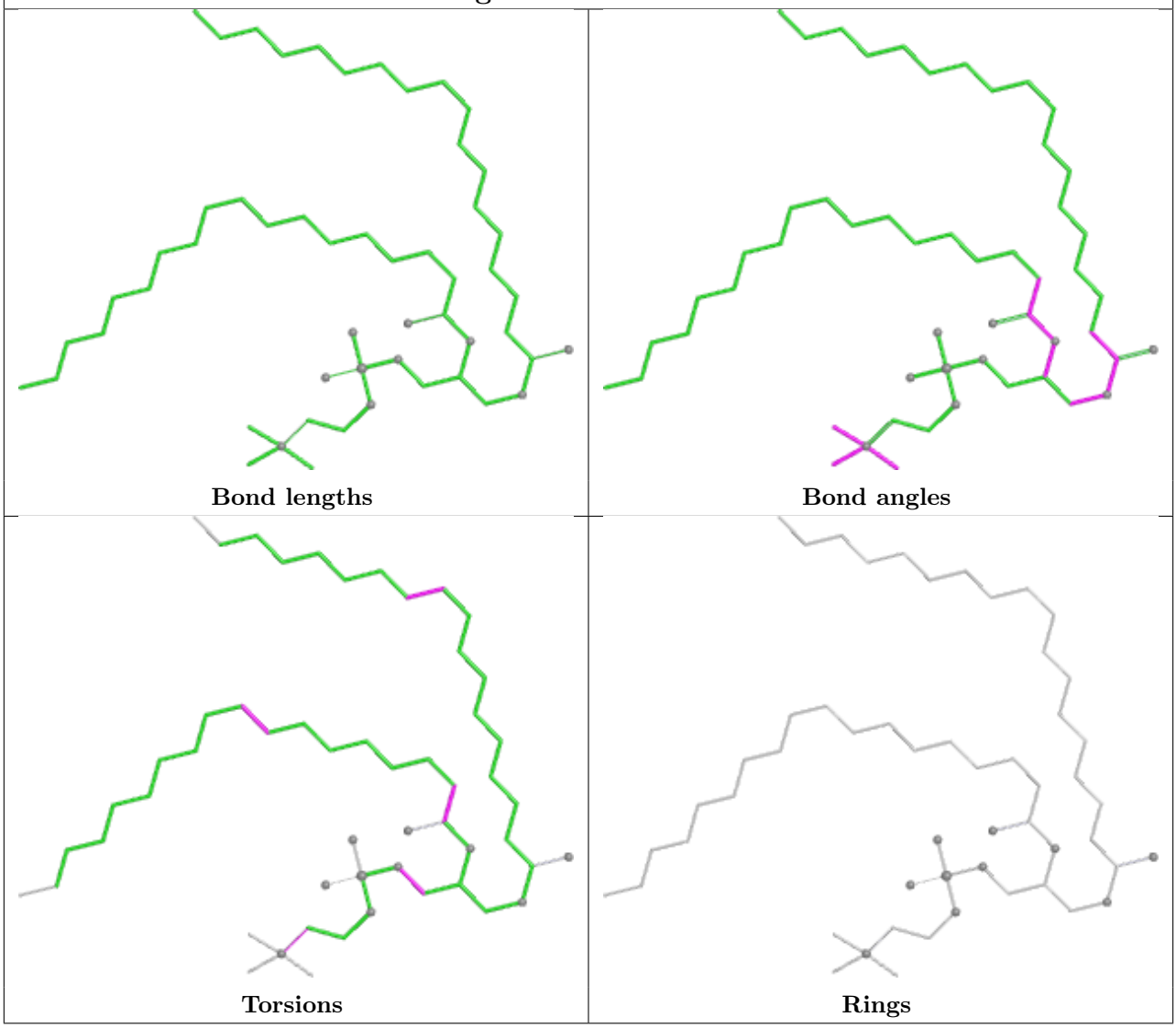


Rings

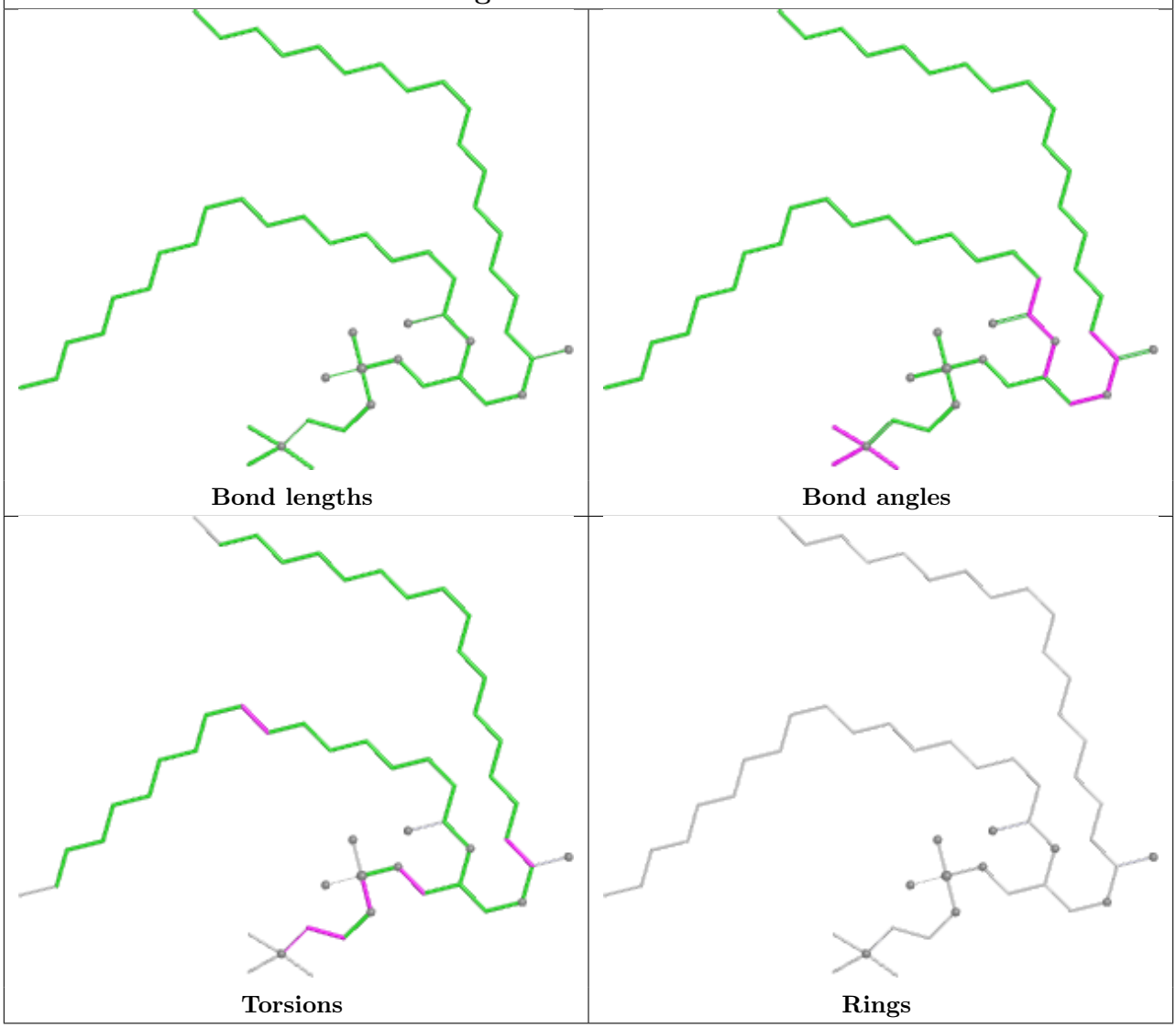
Ligand PCW A 401



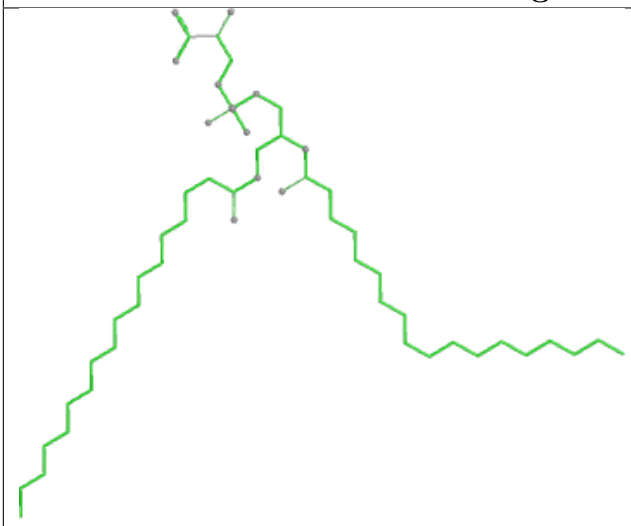
Ligand PCW C 210



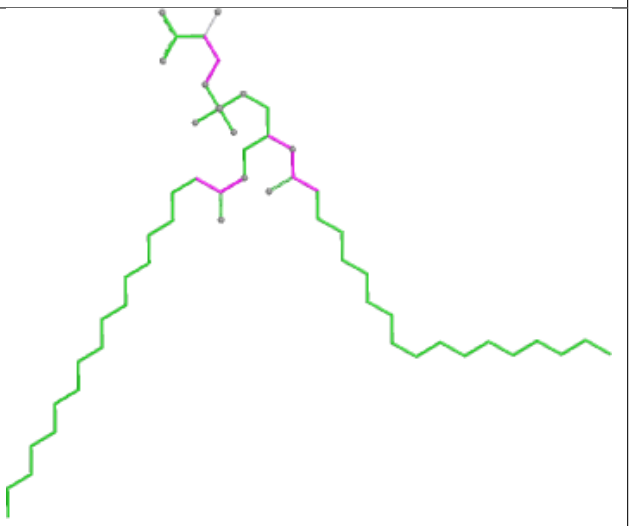
Ligand PCW D 607



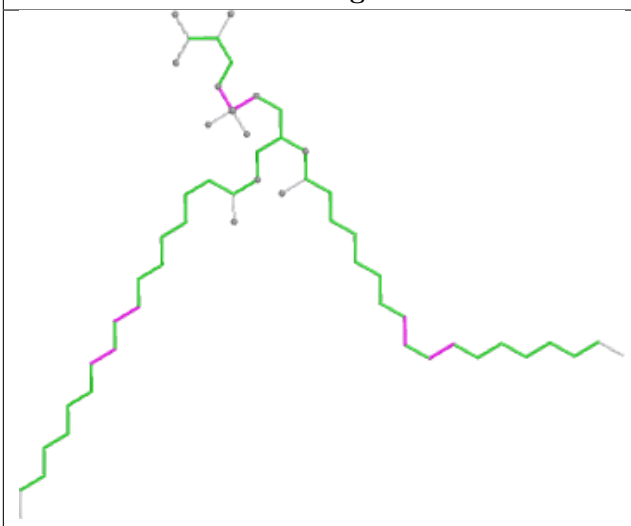
Ligand 17F D 631



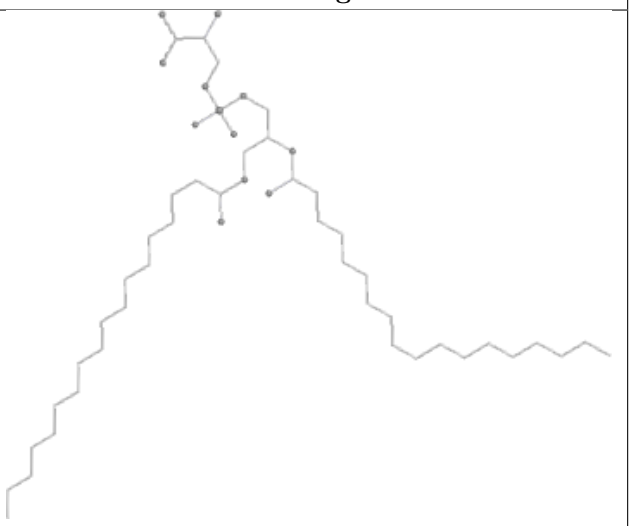
Bond lengths



Bond angles

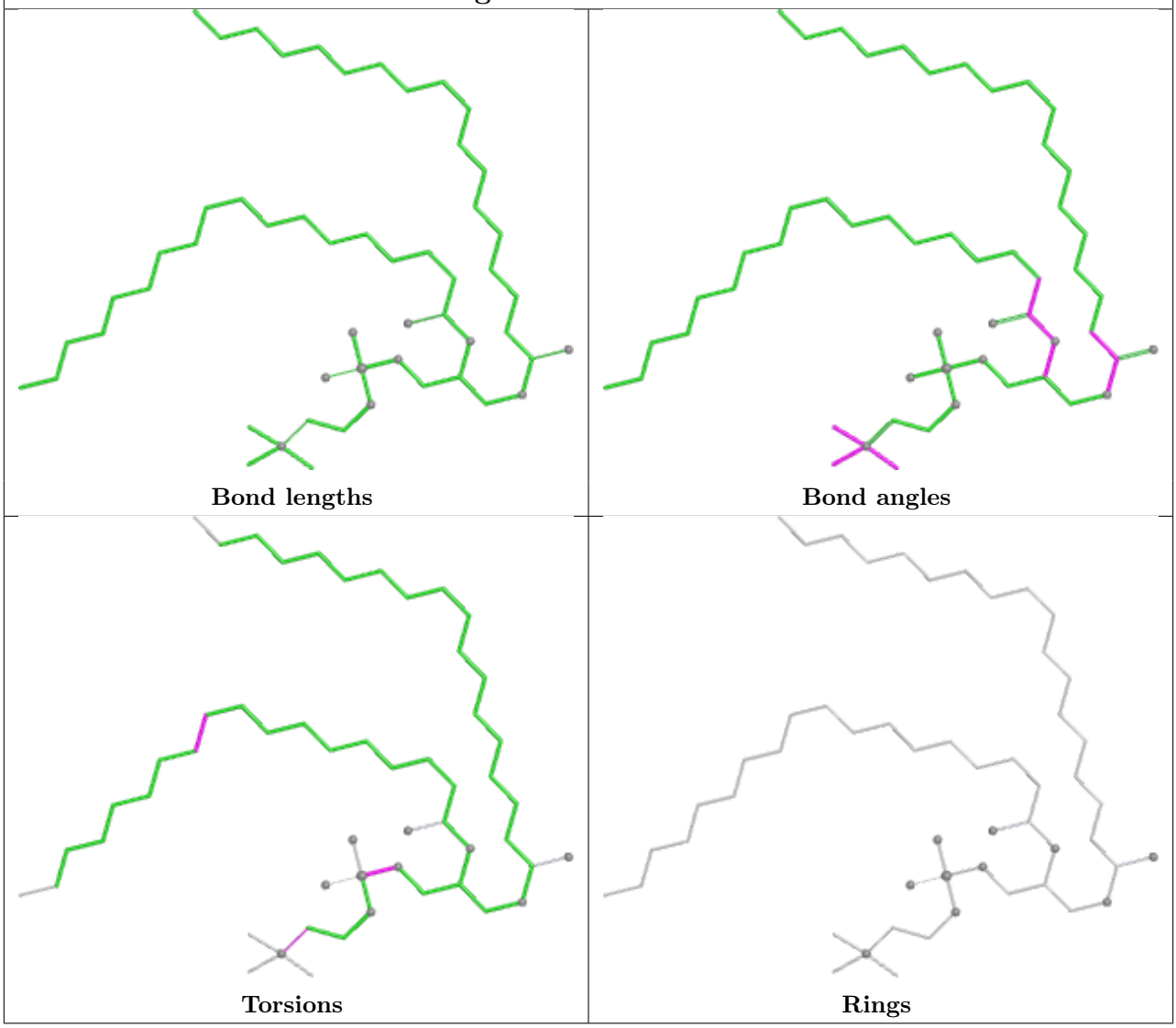


Torsions

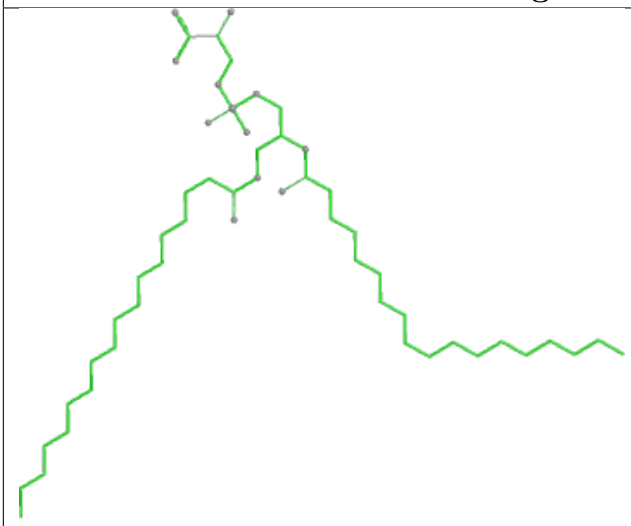


Rings

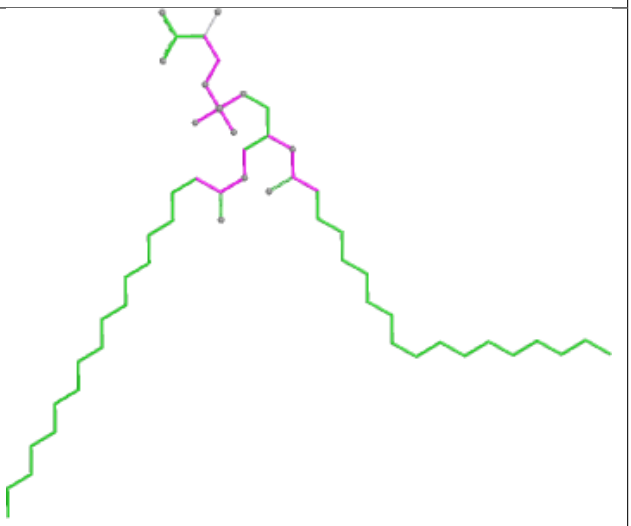
Ligand PCW D 611



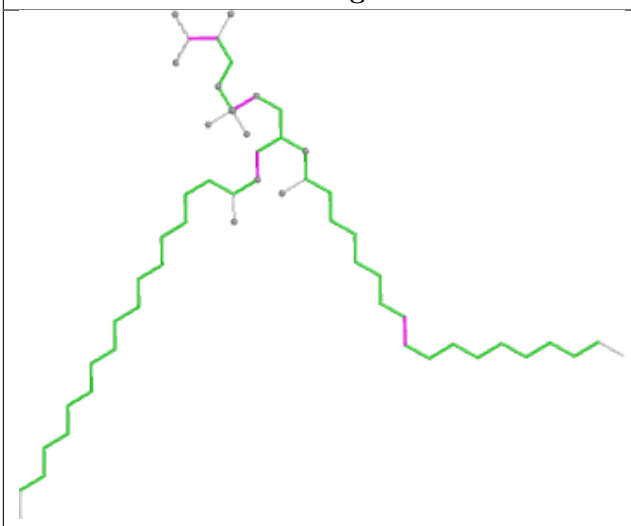
Ligand 17F D 630



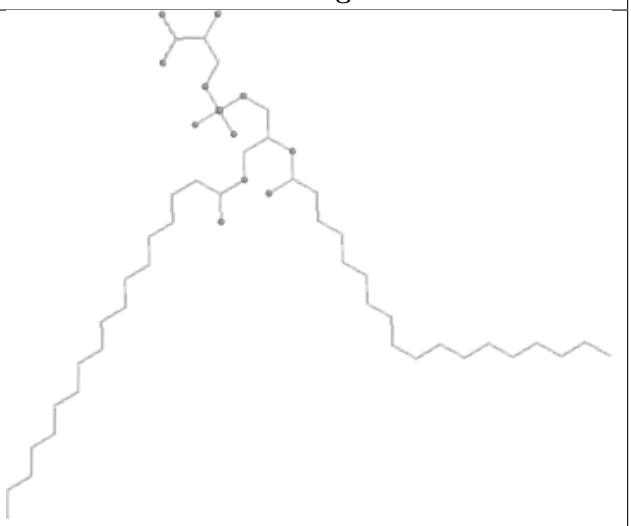
Bond lengths



Bond angles

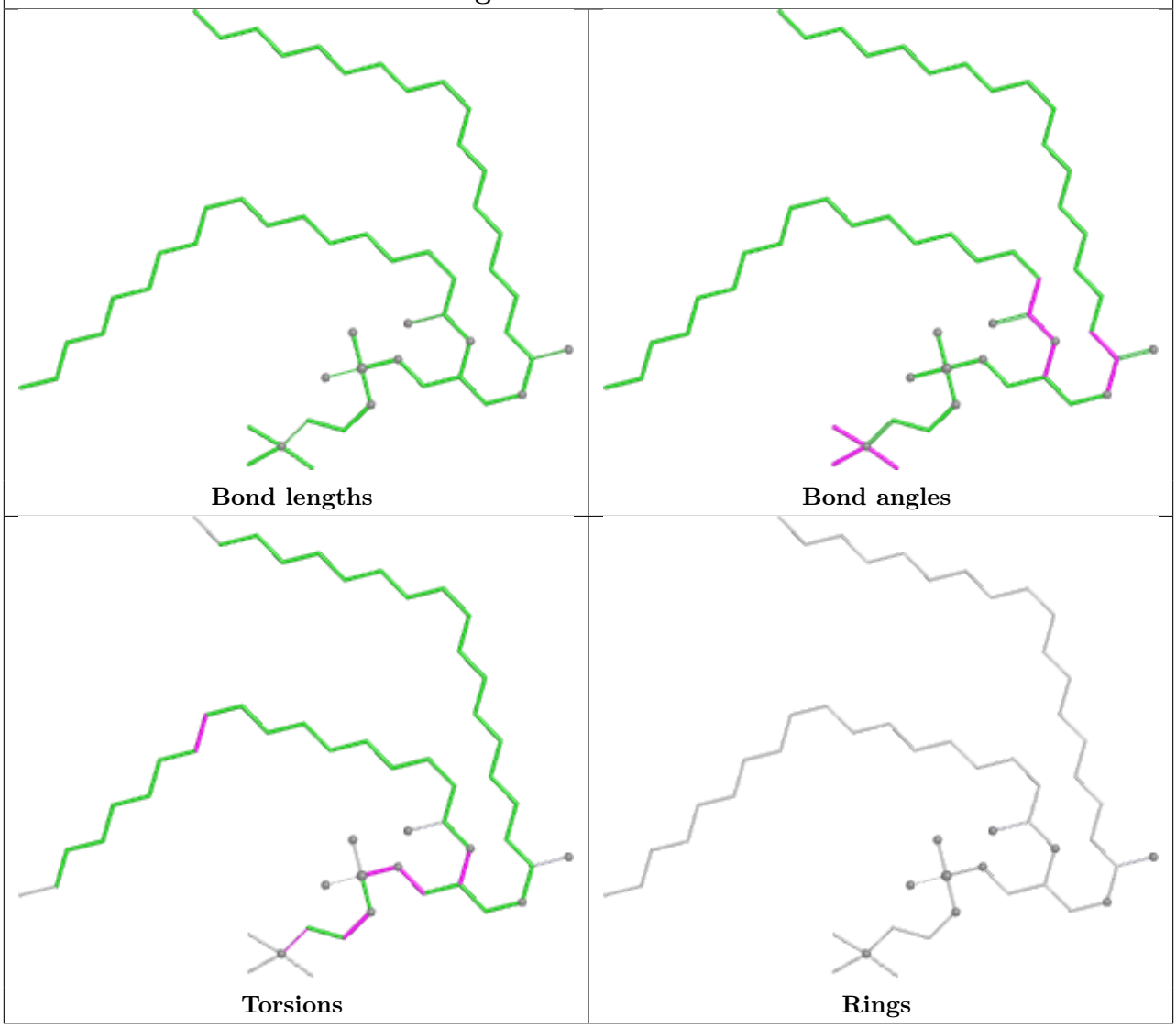


Torsions

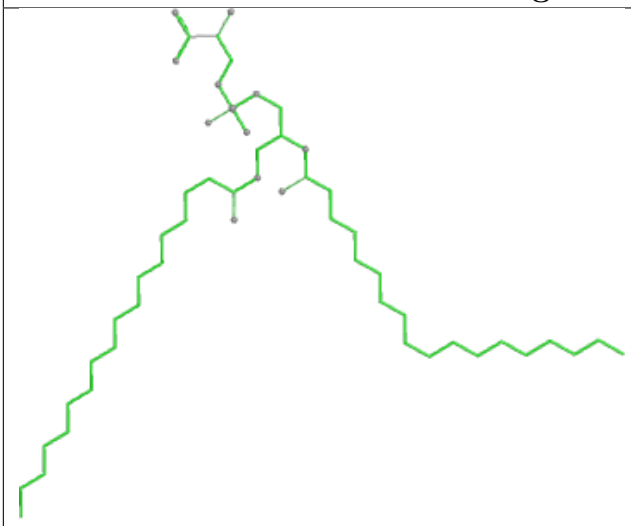


Rings

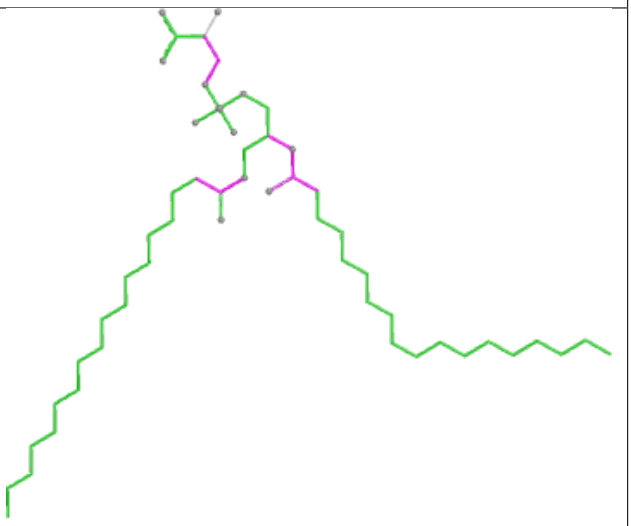
Ligand PCW A 408



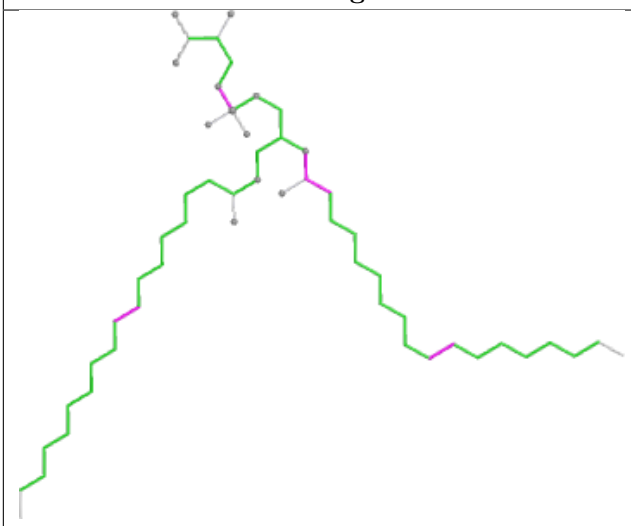
Ligand 17F C 218



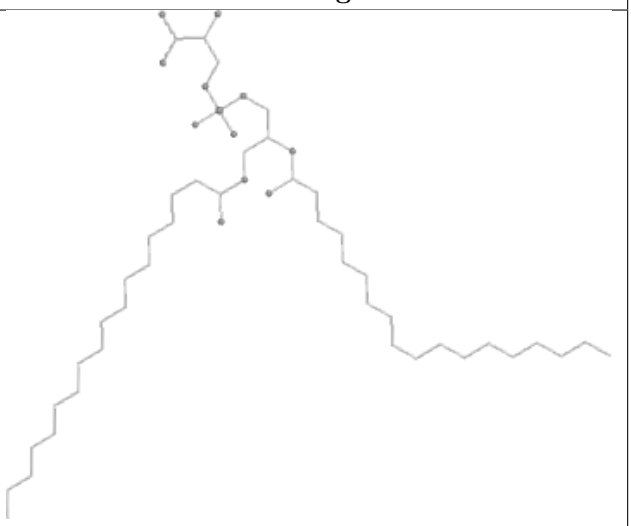
Bond lengths



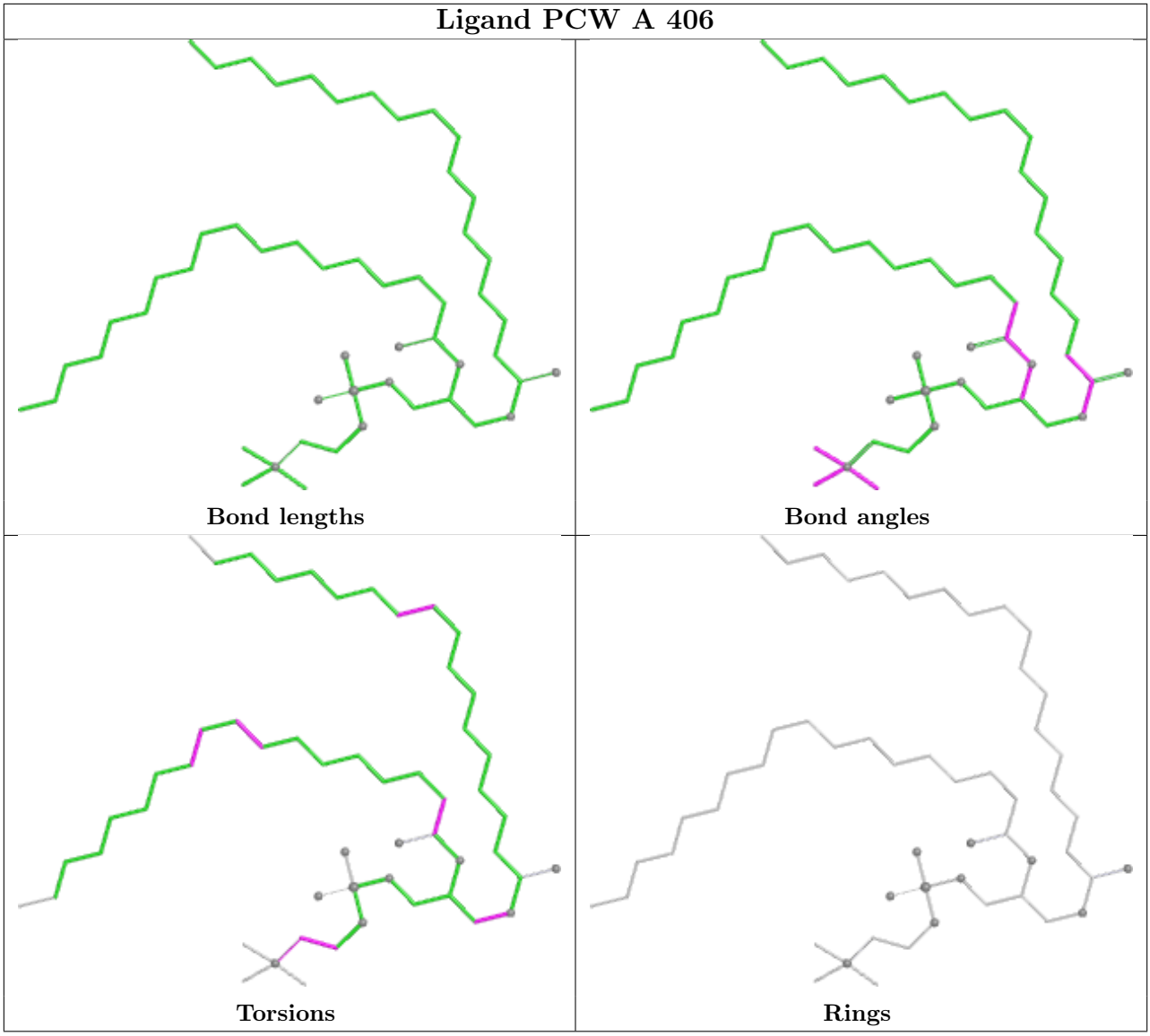
Bond angles



Torsions



Rings



6.7 Other polymers (i)

There are no such molecules in this entry.

6.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

7 Chemical shift validation (i)

The completeness of assignment taking into account all chemical shift lists is 1% for the well-defined parts and 1% for the entire structure.

7.1 Chemical shift list 1

File name: working_cs.cif

Chemical shift list name: *assigned_chem_shift_list_0*

7.1.1 Bookkeeping (i)

The following table shows the results of parsing the chemical shift list and reports the number of nuclei with statistically unusual chemical shifts.

Total number of shifts	154
Number of shifts mapped to atoms	61
Number of unparsed shifts	0
Number of shifts with mapping errors	93
Number of shifts with mapping warnings	0
Number of shift outliers (ShiftChecker)	0

The following assigned chemical shifts were not mapped to the molecules present in the coordinate file.

- No matching atom found in the structure. All 93 occurrences are reported below.

List ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
1	B	6	LEU	HD11	0.763	.	2
1	B	6	LEU	HD12	0.763	.	2
1	B	6	LEU	HD13	0.763	.	2
1	B	8	VAL	HG21	0.7528	.	2
1	B	8	VAL	HG22	0.7528	.	2
1	B	8	VAL	HG23	0.7528	.	2
1	B	14	VAL	HG21	0.9725	.	2
1	B	14	VAL	HG22	0.9725	.	2
1	B	14	VAL	HG23	0.9725	.	2
1	B	19	LEU	HD11	0.4104	.	2
1	B	19	LEU	HD12	0.4104	.	2
1	B	19	LEU	HD13	0.4104	.	2
1	B	19	LEU	HD21	0.5804	.	2
1	B	19	LEU	HD22	0.5804	.	2

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List ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
1	B	19	LEU	HD23	0.5804	.	2
1	B	21	ILE	HD11	0.4182	.	1
1	B	21	ILE	HD12	0.4182	.	1
1	B	21	ILE	HD13	0.4182	.	1
1	B	23	LEU	HD11	-0.477	.	2
1	B	23	LEU	HD12	-0.477	.	2
1	B	23	LEU	HD13	-0.477	.	2
1	B	24	ILE	HD11	0.2691	.	1
1	B	24	ILE	HD12	0.2691	.	1
1	B	24	ILE	HD13	0.2691	.	1
1	B	36	ILE	HD11	0.5397	.	1
1	B	36	ILE	HD12	0.5397	.	1
1	B	36	ILE	HD13	0.5397	.	1
1	B	44	VAL	HG11	0.5353	.	2
1	B	44	VAL	HG12	0.5353	.	2
1	B	44	VAL	HG13	0.5353	.	2
1	B	45	VAL	HG11	0.4379	.	2
1	B	45	VAL	HG12	0.4379	.	2
1	B	45	VAL	HG13	0.4379	.	2
1	B	46	ILE	HD11	0.2525	.	1
1	B	46	ILE	HD12	0.2525	.	1
1	B	46	ILE	HD13	0.2525	.	1
1	B	55	ILE	HD11	0.3369	.	1
1	B	55	ILE	HD12	0.3369	.	1
1	B	55	ILE	HD13	0.3369	.	1
1	B	56	LEU	HD11	0.5372	.	2
1	B	56	LEU	HD12	0.5372	.	2
1	B	56	LEU	HD13	0.5372	.	2
1	B	79	LEU	HD11	-0.1312	.	2
1	B	79	LEU	HD12	-0.1312	.	2
1	B	79	LEU	HD13	-0.1312	.	2
1	B	79	LEU	HD21	-0.015	.	2
1	B	79	LEU	HD22	-0.015	.	2
1	B	79	LEU	HD23	-0.015	.	2
1	B	81	VAL	HG21	0.4663	.	2
1	B	81	VAL	HG22	0.4663	.	2
1	B	81	VAL	HG23	0.4663	.	2
1	B	84	ILE	HD11	0.5865	.	1
1	B	84	ILE	HD12	0.5865	.	1
1	B	84	ILE	HD13	0.5865	.	1
1	B	93	ILE	HD11	0.6063	.	1

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List ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
1	B	93	ILE	HD12	0.6063	.	1
1	B	93	ILE	HD13	0.6063	.	1
1	B	100	ILE	HD11	0.0964	.	1
1	B	100	ILE	HD12	0.0964	.	1
1	B	100	ILE	HD13	0.0964	.	1
1	B	103	VAL	HG11	0.8243	.	2
1	B	103	VAL	HG12	0.8243	.	2
1	B	103	VAL	HG13	0.8243	.	2
1	B	112	VAL	HG11	0.5953	.	2
1	B	112	VAL	HG12	0.5953	.	2
1	B	112	VAL	HG13	0.5953	.	2
1	B	113	LEU	HD11	0.8748	.	2
1	B	113	LEU	HD12	0.8748	.	2
1	B	113	LEU	HD13	0.8748	.	2
1	B	120	LEU	HD11	0.6958	.	2
1	B	120	LEU	HD12	0.6958	.	2
1	B	120	LEU	HD13	0.6958	.	2
1	B	125	VAL	HG11	-0.3248	.	2
1	B	125	VAL	HG12	-0.3248	.	2
1	B	125	VAL	HG13	-0.3248	.	2
1	B	133	LEU	HD11	0.2014	.	2
1	B	133	LEU	HD12	0.2014	.	2
1	B	133	LEU	HD13	0.2014	.	2
1	B	139	ILE	HD11	0.7118	.	1
1	B	139	ILE	HD12	0.7118	.	1
1	B	139	ILE	HD13	0.7118	.	1
1	B	142	ILE	HD11	0.5035	.	1
1	B	142	ILE	HD12	0.5035	.	1
1	B	142	ILE	HD13	0.5035	.	1
1	B	159	LEU	HD11	0.51	.	2
1	B	159	LEU	HD12	0.51	.	2
1	B	159	LEU	HD13	0.51	.	2
1	B	160	VAL	HG11	-0.2062	.	2
1	B	160	VAL	HG12	-0.2062	.	2
1	B	160	VAL	HG13	-0.2062	.	2
1	B	163	ILE	HD11	0.5261	.	1
1	B	163	ILE	HD12	0.5261	.	1
1	B	163	ILE	HD13	0.5261	.	1

7.1.2 Chemical shift referencing (i)

No chemical shift referencing corrections were calculated (not enough data).

7.1.3 Completeness of resonance assignments (i)

The following table shows the completeness of the chemical shift assignments for the well-defined regions of the structure. The overall completeness is 1%, i.e. 138 atoms were assigned a chemical shift out of a possible 10171. 0 out of 133 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	^{1}H	^{13}C	^{15}N
Backbone	14/3625 (0%)	7/1466 (0%)	0/1454 (0%)	7/705 (1%)
Sidechain	124/5899 (2%)	93/3793 (2%)	31/1847 (2%)	0/259 (0%)
Aromatic	0/647 (0%)	0/318 (0%)	0/304 (0%)	0/25 (0%)
Overall	138/10171 (1%)	100/5577 (2%)	31/3605 (1%)	7/989 (1%)

The following table shows the completeness of the chemical shift assignments for the full structure. The overall completeness is 1%, i.e. 154 atoms were assigned a chemical shift out of a possible 10720. 0 out of 134 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	^{1}H	^{13}C	^{15}N
Backbone	30/3812 (1%)	15/1542 (1%)	0/1528 (0%)	15/742 (2%)
Sidechain	124/6254 (2%)	93/4014 (2%)	31/1960 (2%)	0/280 (0%)
Aromatic	0/654 (0%)	0/322 (0%)	0/306 (0%)	0/26 (0%)
Overall	154/10720 (1%)	108/5878 (2%)	31/3794 (1%)	15/1048 (1%)

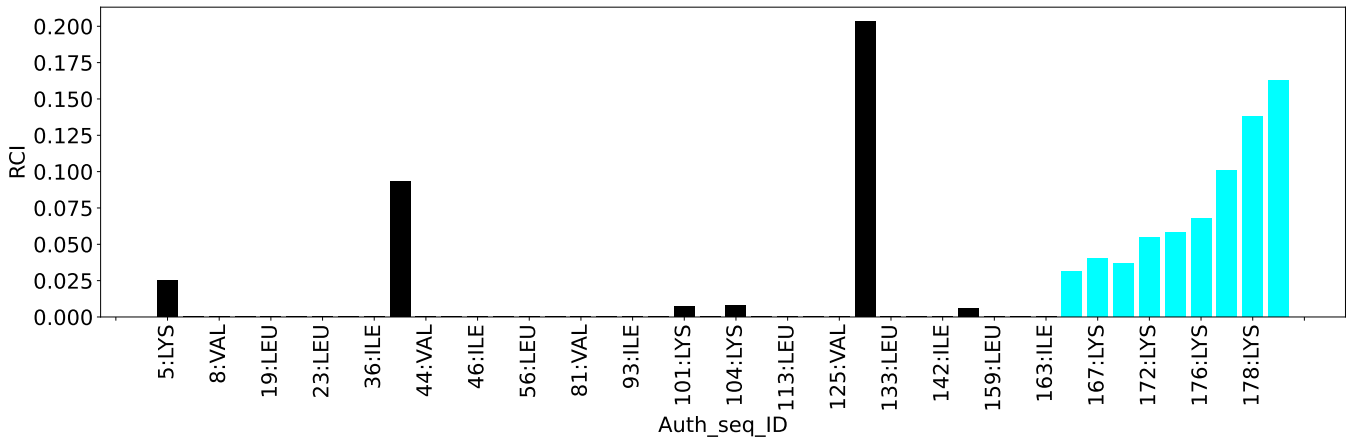
7.1.4 Statistically unusual chemical shifts (i)

There are no statistically unusual chemical shifts.

7.1.5 Random Coil Index (RCI) plots (i)

The image below reports *random coil index* values for the protein chains in the structure. The height of each bar gives a probability of a given residue to be disordered, as predicted from the available chemical shifts and the amino acid sequence. A value above 0.2 is an indication of significant predicted disorder. The colour of the bar shows whether the residue is in the well-defined core (black) or in the ill-defined residue ranges (cyan), as described in section 2 on ensemble composition.If well-defined core and ill-defined regions are not identified then it is shown as gray bars.

Random coil index (RCI) for chain B:


RCI
0.200
0.175
0.150
0.125
0.100
0.075
0.050
0.025
0.000
5:LYS
8:VAL
19:LEU
23:LEU
36:ILE
44:VAL
46:ILE
56:LEU
81:VAL
93:ILE
101:LYS
104:LYS
113:LEU
125:VAL
133:LEU
142:ILE
159:LEU
163:ILE
167:LYS
172:LYS
176:LYS
178:LYS
Auth_seq_ID