Full wwPDB X-ray Structure Validation Report (i)

Jun 25, 2024 – 04:50 PM EDT

PDB ID	:	6Q8O
Title	:	Respiratory complex I from Thermus thermophilus with bound Piericidin A
Authors	:	Gutierrez-Fernandez, J.; Minhas, G.S.; Sazanov, L.A.
Deposited on	:	2018-12-15
Resolution	:	3.60 Å(reported)

This is a Full wwPDB X-ray 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/XrayValidationReportHelp
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 (1)) were used in the production of this report:

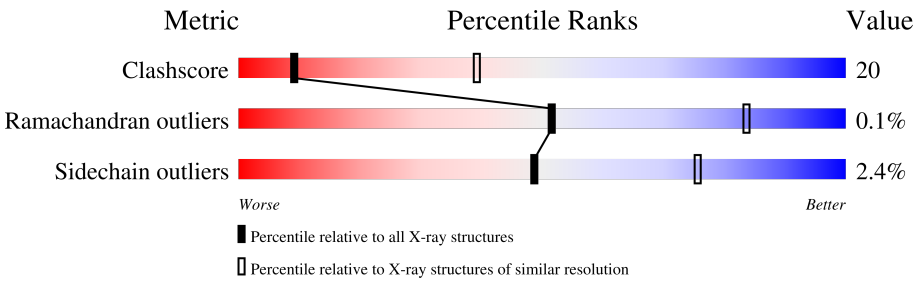
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	FAILED
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson 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:
X-RAY DIFFRACTION

The reported resolution of this entry is 3.60 Å.

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)	Similar resolution (#Entries, resolution range(Å))
Clashscore	141614	1353 (3.70-3.50)
Ramachandran outliers	138981	1307 (3.70-3.50)
Sidechain outliers	138945	1307 (3.70-3.50)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria respectively. 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%

Note EDS failed to run properly.

Mol	Chain	Length	Quality of chain
1	1	438	53% 45% •
1	B	438	51% 48% •
2	2	181	60% 38% • •
2	C	181	61% 35% • •
3	3	783	57% 39% • •
3	D	783	56% 39% • •
4	4	409	48% 45% • 6%
4	E	409	41% 52% • 6%

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Mol	Chain	Length	Quality of chain
5	5	207	61% 32% 5%
5	F	207	47% 45% 5%
6	6	181	43% 46% 8%
6	G	181	41% 48% 8%
7	9	182	65% 34%
7	O	182	53% 46%
8	7	129	59% 39%
8	I	129	63% 35%
9	W	131	71% 26%
9	X	131	66% 30%
10	A	119	55% 43%
10	P	119	52% 45%
11	J	176	51% 39% 9%
11	R	176	60% 29% 9%
12	K	95	64% 34%
12	S	95	65% 34%
13	L	606	64% 35%
13	T	606	62% 36%
14	M	469	59% 39%
14	U	469	58% 41%
15	N	427	66% 34%
15	V	427	63% 36%
16	H	365	52% 42%
16	Q	365	51% 43%

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit crite-

ria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
17	SF4	9	201	-	-	X	-
17	SF4	9	202	-	-	X	-
17	SF4	D	801	-	-	X	-
17	SF4	D	803	-	-	X	-
17	SF4	G	201	-	-	X	-
17	SF4	O	202	-	-	X	-

2 Entry composition (i)

There are 20 unique types of molecules in this entry. The entry contains 74146 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called NADH-quinone oxidoreductase subunit 1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	1	437	3417	2180	595	624	18	0	0	0
1	B	437	3417	2180	595	624	18	0	0	0

- Molecule 2 is a protein called NADH-quinone oxidoreductase subunit 2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
2	2	178	1406	895	238	265	8	0	0	0
2	C	178	1406	895	238	265	8	0	0	0

- Molecule 3 is a protein called NADH-quinone oxidoreductase subunit 3.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
3	3	756	5895	3754	1057	1053	31	0	0	0
3	D	756	5895	3754	1057	1053	31	0	0	0

- Molecule 4 is a protein called NADH-quinone oxidoreductase subunit 4.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
4	4	384	3067	1975	522	559	11	0	0	0
4	E	384	3067	1975	522	559	11	0	0	0

- Molecule 5 is a protein called NADH-quinone oxidoreductase subunit 5.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
5	5	196	1607	1043	273	288	3	0	0	0
5	F	196	1607	1043	273	288	3	0	0	0

- Molecule 6 is a protein called NADH-quinone oxidoreductase subunit 6.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
6	6	166	1289	815	235	226	13	0	0	0
6	G	166	1289	815	235	226	13	0	0	0

- Molecule 7 is a protein called NADH-quinone oxidoreductase subunit 9.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
7	9	180	1388	890	232	255	11	0	0	0
7	O	180	1388	890	232	255	11	0	0	0

- Molecule 8 is a protein called NADH-quinone oxidoreductase subunit 15.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
8	7	127	1031	664	183	181	3	0	0	0
8	I	127	1031	664	183	181	3	0	0	0

- Molecule 9 is a protein called NADH-quinone oxidoreductase subunit 16.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
9	W	127	967	623	165	175	4	0	0	0
9	X	127	967	623	165	175	4	0	0	0

- Molecule 10 is a protein called NADH-quinone oxidoreductase subunit 7.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
10	A	117	910	624	138	144	4	0	0	0

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
10	P	117	910	624	138	144	4	0	0	0

- Molecule 11 is a protein called NADH-quinone oxidoreductase subunit 10.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
11	J	160	1183	806	183	191	3	0	0	0
11	R	160	1183	806	183	191	3	0	0	0

- Molecule 12 is a protein called NADH-quinone oxidoreductase subunit 11.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
12	K	95	703	456	118	126	3	0	0	0
12	S	95	703	456	118	126	3	0	0	0

- Molecule 13 is a protein called NADH-quinone oxidoreductase subunit 12.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
13	L	605	4604	3089	740	756	19	0	0	0
13	T	605	4604	3089	740	756	19	0	0	0

- Molecule 14 is a protein called NADH-quinone oxidoreductase subunit 13.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
14	M	467	3489	2363	546	572	8	0	0	0
14	U	467	3489	2363	546	572	8	0	0	0

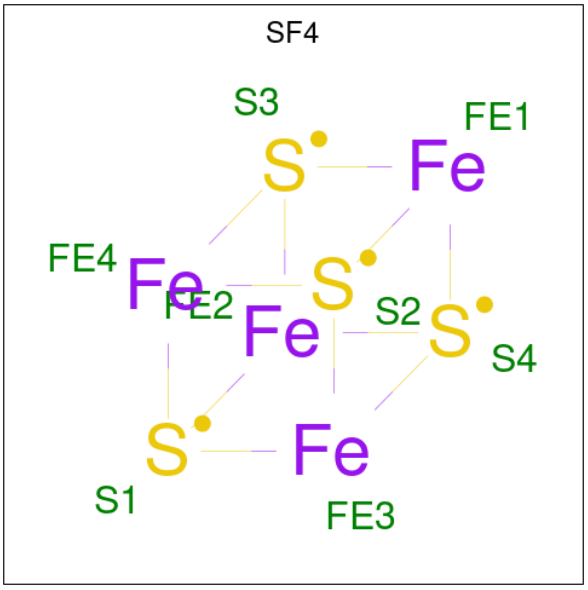
- Molecule 15 is a protein called NADH-quinone oxidoreductase subunit 14.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
15	N	427	3154	2125	505	518	6	0	0	0
15	V	427	3154	2125	505	518	6	0	0	0

- Molecule 16 is a protein called NADH-quinone oxidoreductase subunit 8.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
16	H	353	2838	1943	431	457	7	0	0	0
			Total	C	N	O	S			
16	Q	353	2838	1943	431	457	7	0	0	0

- Molecule 17 is IRON/SULFUR CLUSTER (three-letter code: SF4) (formula: Fe_4S_4).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	Fe	S		
17	1	1	8	4	4	0	0
			Total	Fe	S		
17	3	1	8	4	4	0	0
			Total	Fe	S		
17	3	1	8	4	4	0	0
			Total	Fe	S		
17	3	1	8	4	4	0	0
			Total	Fe	S		
17	6	1	8	4	4	0	0
			Total	Fe	S		
17	9	1	8	4	4	0	0
			Total	Fe	S		
17	9	1	8	4	4	0	0
			Total	Fe	S		
17	B	1	8	4	4	0	0
			Total	Fe	S		
17	D	1	8	4	4	0	0

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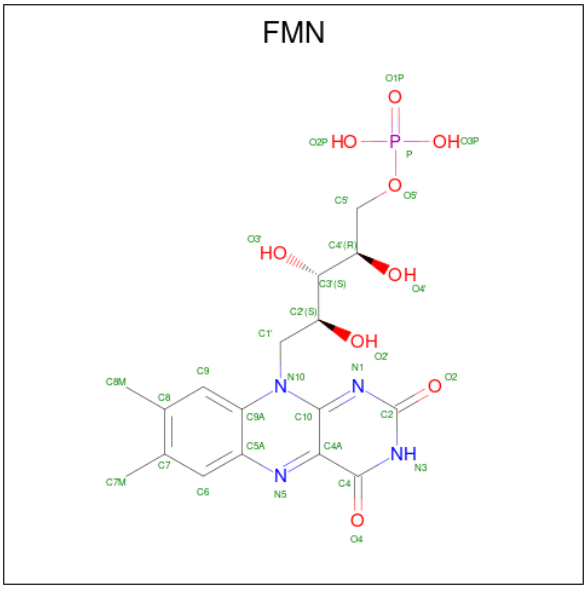
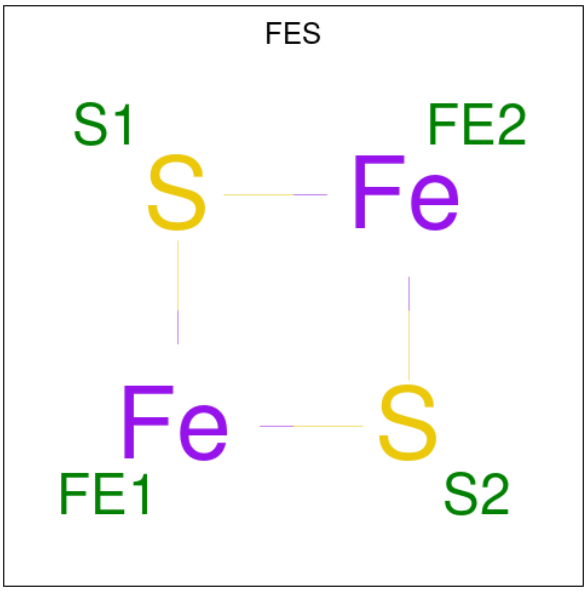
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
17	D	1	Total	Fe	S		0	0
			8	4	4			
17	D	1	Total	Fe	S		0	0
			8	4	4			
17	G	1	Total	Fe	S		0	0
			8	4	4			
17	O	1	Total	Fe	S		0	0
			8	4	4			
17	O	1	Total	Fe	S		0	0
			8	4	4			

- Molecule 18 is FLAVIN MONONUCLEOTIDE (three-letter code: FMN) (formula: $C_{17}H_{21}N_4O_9P$).



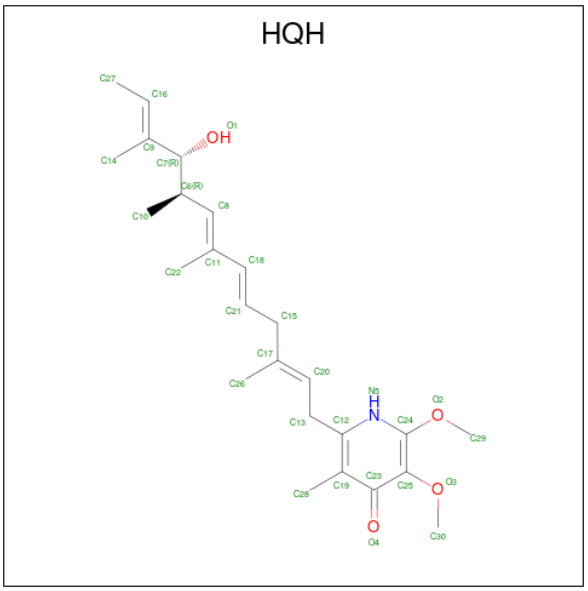
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
18	1	1	Total	C	N	O	P	0	0
			31	17	4	9	1		
18	B	1	Total	C	N	O	P	0	0
			31	17	4	9	1		

- Molecule 19 is FE2/S2 (INORGANIC) CLUSTER (three-letter code: FES) (formula: Fe_2S_2).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	Fe	S		
19	2	1	4	2	2	0	0
			Total	Fe	S		
19	3	1	4	2	2	0	0
			Total	Fe	S		
19	C	1	4	2	2	0	0
			Total	Fe	S		
19	D	1	4	2	2	0	0

- Molecule 20 is Piericidin A (three-letter code: HQH) (formula: $C_{25}H_{37}NO_4$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	C	N	O		
20	4	1	30	25	1	4	0	0
			Total	C	N	O		
20	E	1	30	25	1	4	0	0

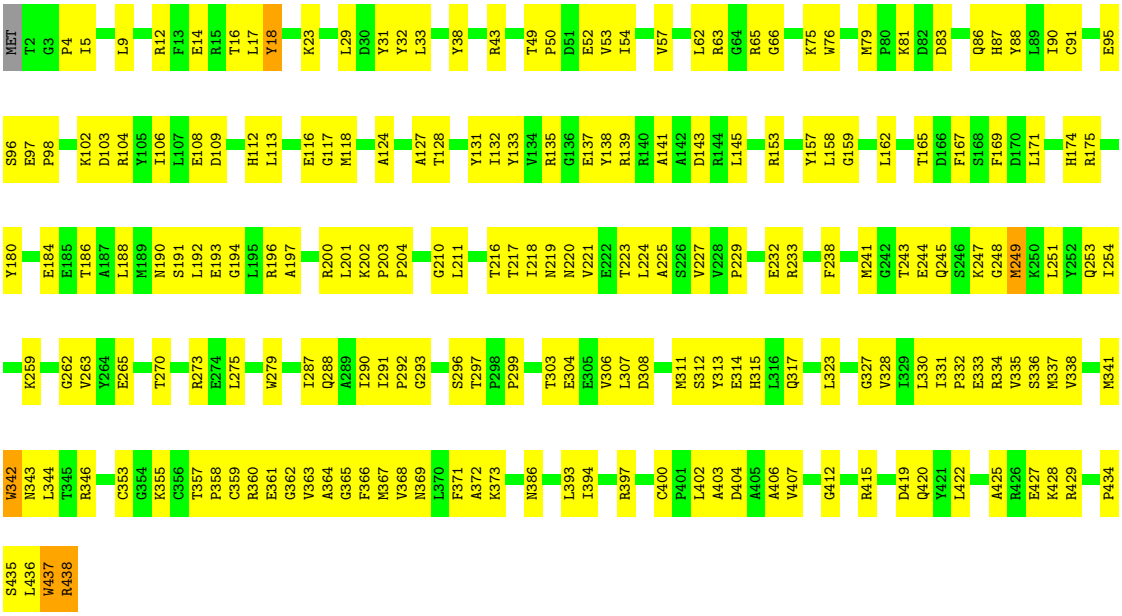
3 Residue-property plots (i)

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry. Residues are color-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 outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

Note EDS failed to run properly.

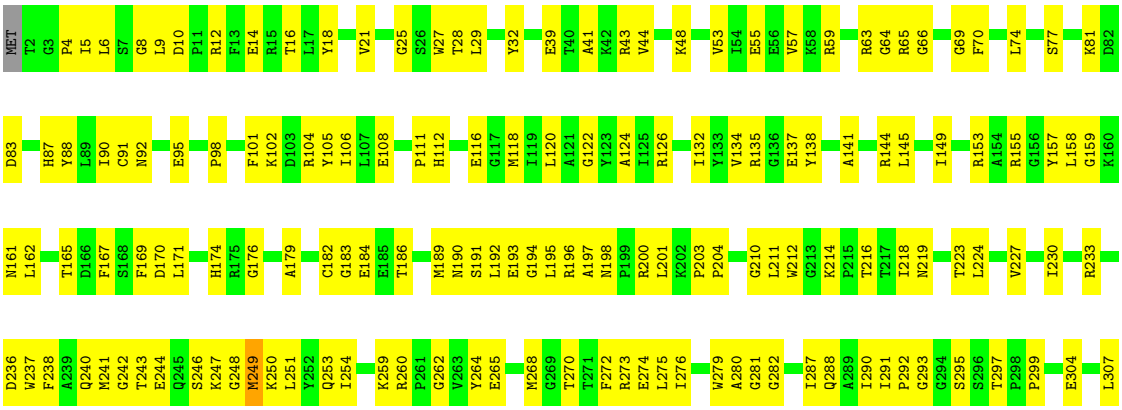
• Molecule 1: NADH-quinone oxidoreductase subunit 1

Chain 1: 53% 45%



• Molecule 1: NADH-quinone oxidoreductase subunit 1

Chain B: 51% 48%



D308 M311 S312 Y313 E314 H315 L316 Q317 M322 L323 G324 T325 G326 G327 V328 I329 L330 I331 P332 E333 M337 V338 D339 A340 M341 W342 R346 A349 S352 C353 G354 K355 C356 T357 P358 C359 R360 E361 G362 V363 A364 G365 F366 N369 L370 F371 A372 T376 E380 E381 K382

D383 V384 E385 N386 R397 C400 P401 D404 G412 R415 K418 D419 Q420 Y421 L422 A425 R426 E427 K428 R433 W437 R438

- Molecule 2: NADH-quinone oxidoreductase subunit 2

Chain 2:

MET GLY F3 K7 Q8 D9 F10 K17 Y18 R24 I27 M28 R32 R33 V34 Q35 W40 R45 I46 E47 R51 T58 E59 V60 F66 Y67 S68 Y69 Y70 Q71 P74 K77 Y78 H79 L80 Q81 T85 L86 K89 L90 A91 G92 A93 E94 T101

E102 G105 I106 G107 P108 G109 E110 V111 T112 G115 L116 F117 S118 V119 Q120 K121 V122 E123 C124 T130 A131 P132 N137 Y141 V142 E143 C144 V145 T146 R149 L153 L157 R162 L163 E164 K171 C172 G173 H174 H175 V176 H177 E178 V179 E180 VAL

- Molecule 2: NADH-quinone oxidoreductase subunit 2

Chain C:

MET GLY F3 F4 D5 D6 K7 Q8 D9 F10 L11 T14 K17 G22 R23 R24 I27 M28 P29 R32 R33 V34 Q35 W40 I41 R42 R45 E48 V53 T58 E59 V60 M61 S65 F66 Y67 Q71 H79 C83 A84 T85 L86 S87 C88 K89

E94 E95 L96 W97 D98 Y99 L100 T101 G105 I106 G109 E110 V111 T112 P113 D114 G115 L116 F117 S118 V119 Q120 K121 C124 T130 A131 P132 V133 I134 N137 Y141 V142 E143 C144 V145 T146 R147 A148 R149 L150 L154 R158 K171 E178 V179 E180 VAL

- Molecule 3: NADH-quinone oxidoreductase subunit 3

Chain 3:

M1 V2 R3 V4 K5 V6 N7 D8 R9 T17 S18 D21 A22 V23 A26 G27 Y28 D29 V30 P31 L32 F33 C34 S35 H38 L39 S40 P41 I42 C45 R46 M47 C48 L49 V50 R51 L54 P55 LYS LYS GLY PRO ASP GLY LYS PRO LEU LEU ASN GLU LYS GLY GLU PRO

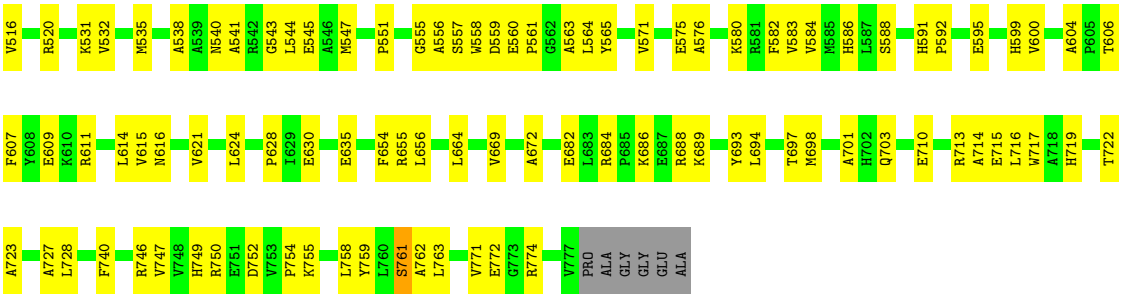
GLU I73 A81 S82 C83 V84 T85 D89 D94 S97 D98 R101 G106 M107 F110 T111 L112 L113 N114 H115 D118 C122 D123 K124 G125 G126 A127 C128 E129 L130 R133 E136 Y137 E141 K142 Y143 TYR GLN LYS GLY P148 Y154 T155 R156 F157 E158 F159

T160 R161 K166 H167 H168 P169 L170 I175 L176 E179 H183 C184 K185 R186 R189 Y190 E193 V194 P195 G196 V199 L200 D201 F202 I203 E204 R205 G206 V207 H208 T209 T213 M214 P219 F222 S223 G224 N225 I226 T227 D228 I229 G233 A234 L235 L236 D237 L238 T239

F242 R245 N246 W247 E248 M249 E250 T254 T255 C256 C259 P260 V261 I265 T269 R270 S271 G272 E273 L274 L275 R276 I277 R280 E281 V285 N286 E287 I288 W289 I290 C291 D292 A293 G294 R295 F296 G297 W300 A301 D302 R305 L306 K307 T308 P309 L310 V311 R312

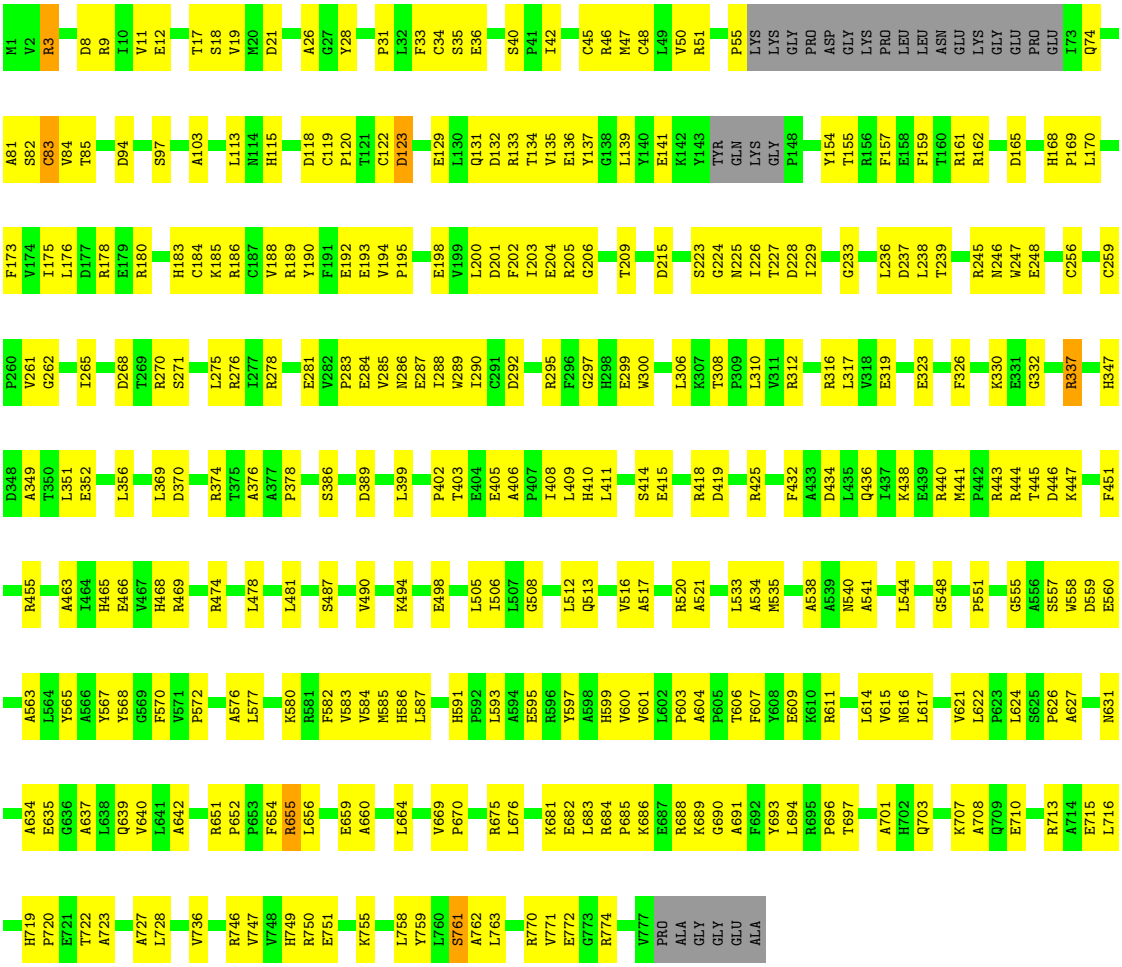
R316 L317 V318 E323 L329 R337 G338 G342 L343 Y344 L345 A349 T350 L351 L355 L356 T366 P367 H368 L369 D370 F371 Q372 G373 R374 T375 A376 S380 L381 F382 A385 S386 L387 L390 D394 F395 A396 L397 V398 L399 E404 E405 A406 L409 H410 L411

S414 E415 R418 D419 L420 H424 R425 Y426 F432 K438 E439 R440 M441 P442 R443 R444 T445 D446 K447 Y454 M459 K460 W461 A462 A463 I464 H465 E466 V467 H468 R469 E472 E473 I476 L477 L480 M489 K494 E498 N502 P503 G508 L512 Q513



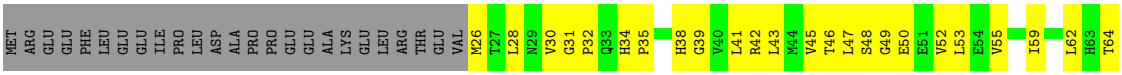
- Molecule 3: NADH-quinone oxidoreductase subunit 3

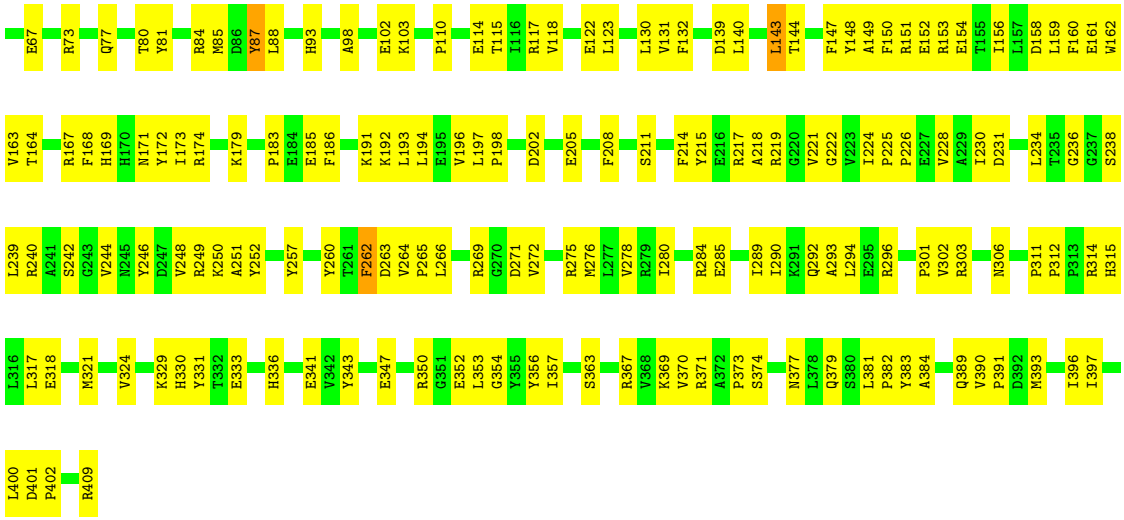
Chain D:



- Molecule 4: NADH-quinone oxidoreductase subunit 4

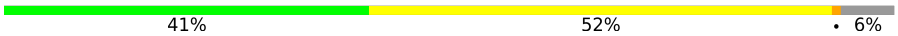
Chain 4:

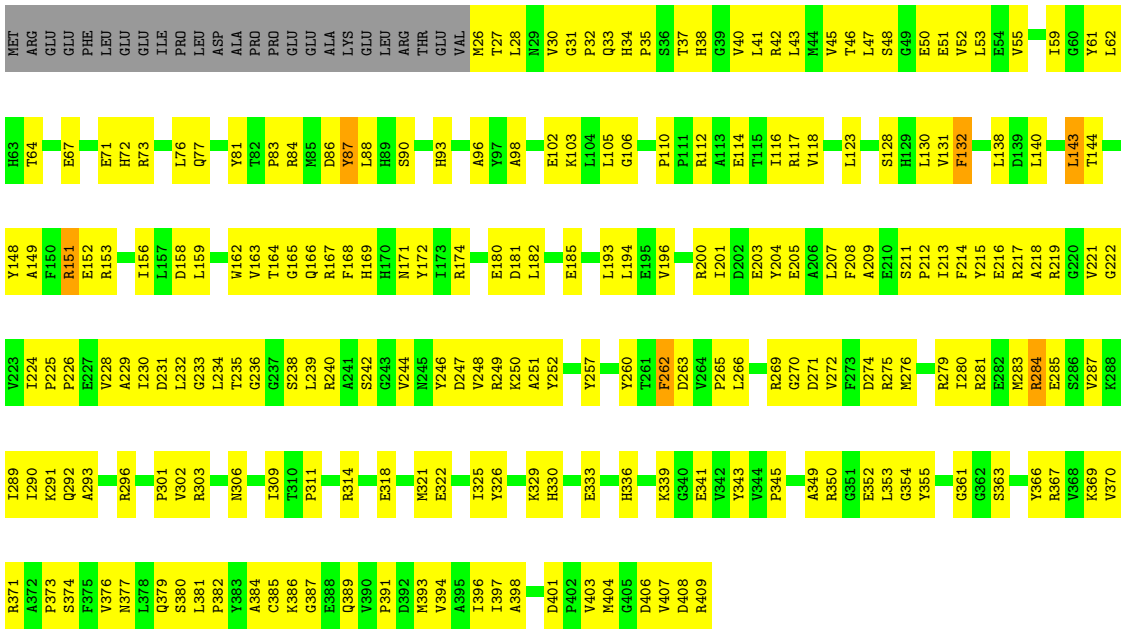




• Molecule 4: NADH-quinone oxidoreductase subunit 4

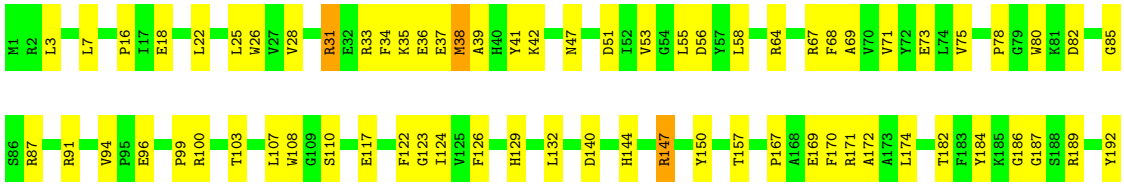
Chain E:

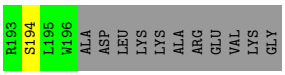




• Molecule 5: NADH-quinone oxidoreductase subunit 5

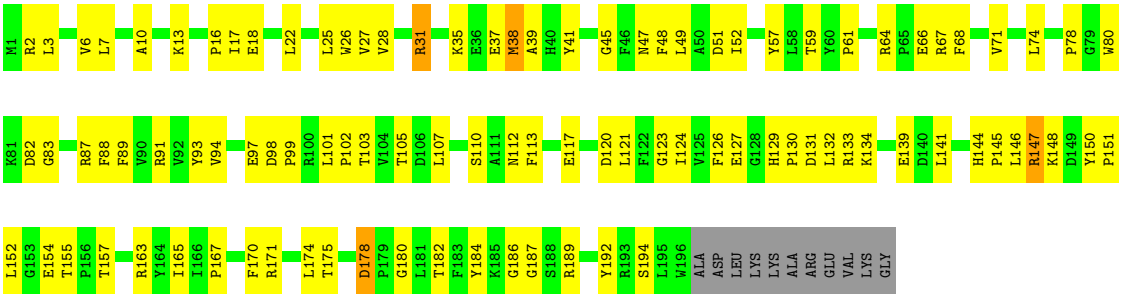
Chain 5:





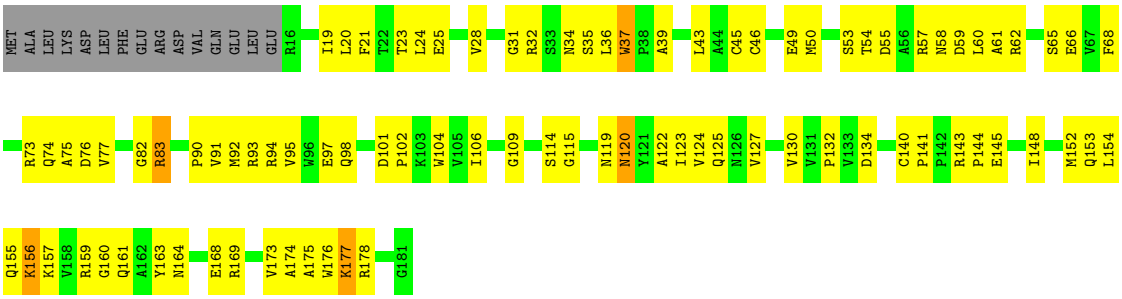
• Molecule 5: NADH-quinone oxidoreductase subunit 5

Chain F:



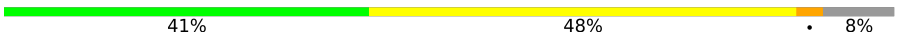
• Molecule 6: NADH-quinone oxidoreductase subunit 6

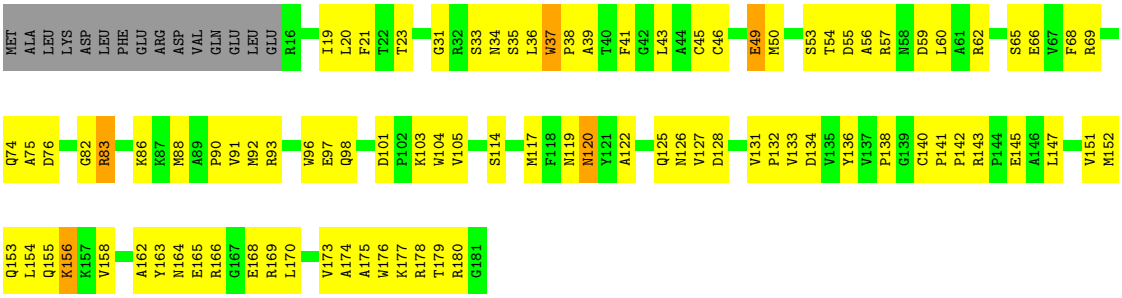
Chain 6:



• Molecule 6: NADH-quinone oxidoreductase subunit 6

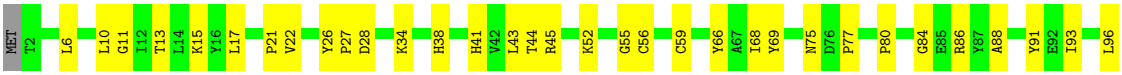
Chain G:

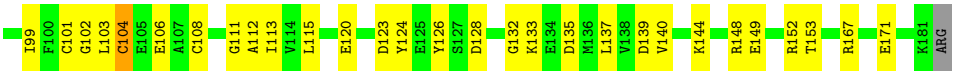




• Molecule 7: NADH-quinone oxidoreductase subunit 9

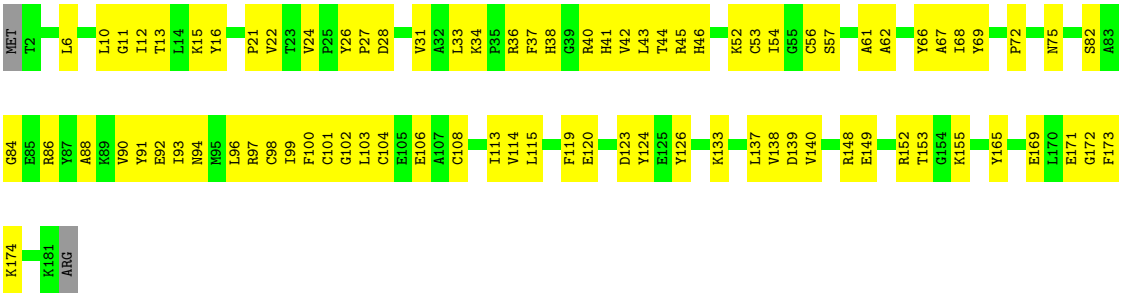
Chain 9:





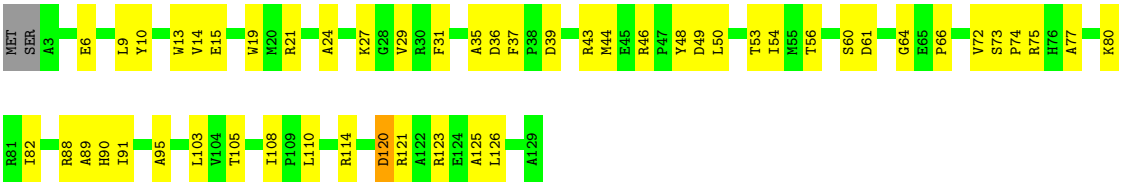
• Molecule 7: NADH-quinone oxidoreductase subunit 9

Chain O:



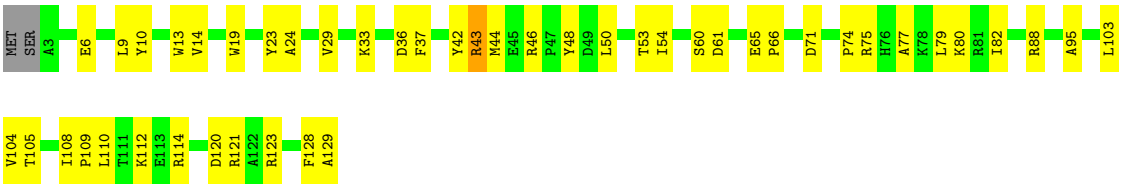
• Molecule 8: NADH-quinone oxidoreductase subunit 15

Chain 7:



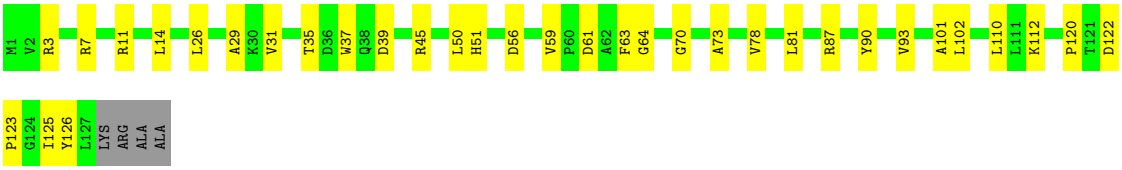
• Molecule 8: NADH-quinone oxidoreductase subunit 15

Chain I:



• Molecule 9: NADH-quinone oxidoreductase subunit 16

Chain W:

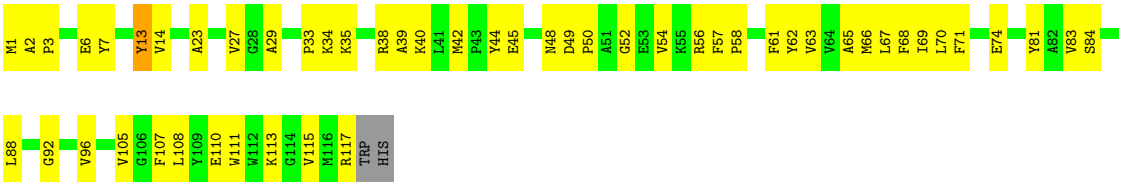


• Molecule 9: NADH-quinone oxidoreductase subunit 16

Chain X:

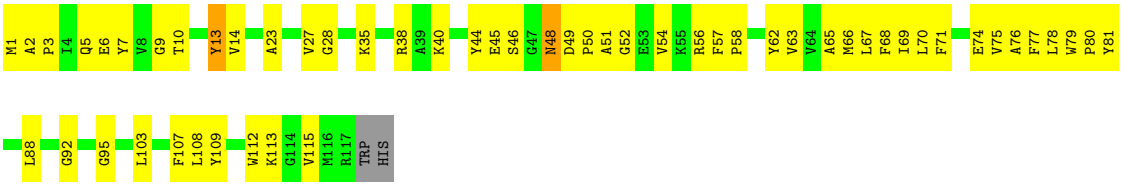
• Molecule 10: NADH-quinone oxidoreductase subunit 7

Chain A:



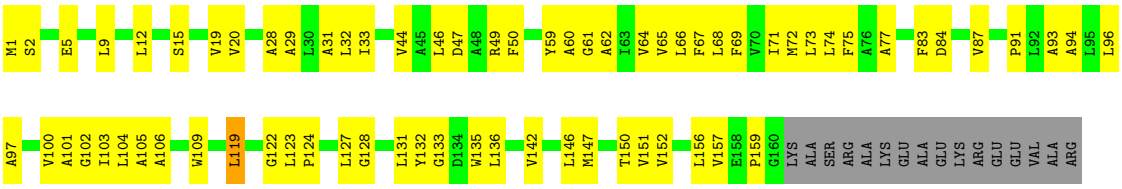
• Molecule 10: NADH-quinone oxidoreductase subunit 7

Chain P:



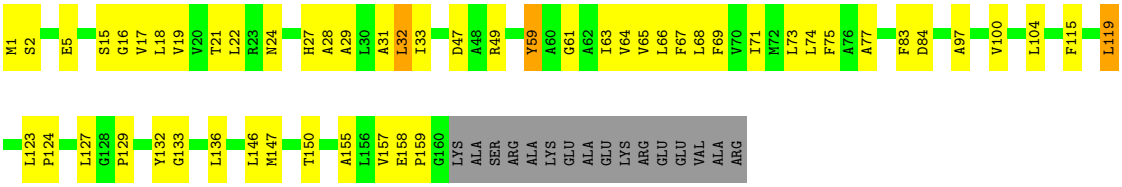
• Molecule 11: NADH-quinone oxidoreductase subunit 10

Chain J:



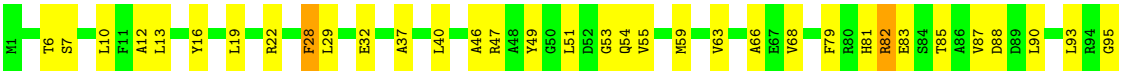
• Molecule 11: NADH-quinone oxidoreductase subunit 10

Chain R:



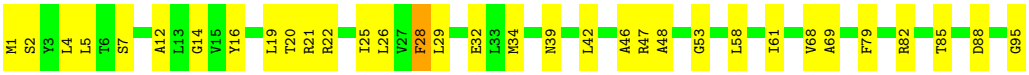
• Molecule 12: NADH-quinone oxidoreductase subunit 11

Chain K:



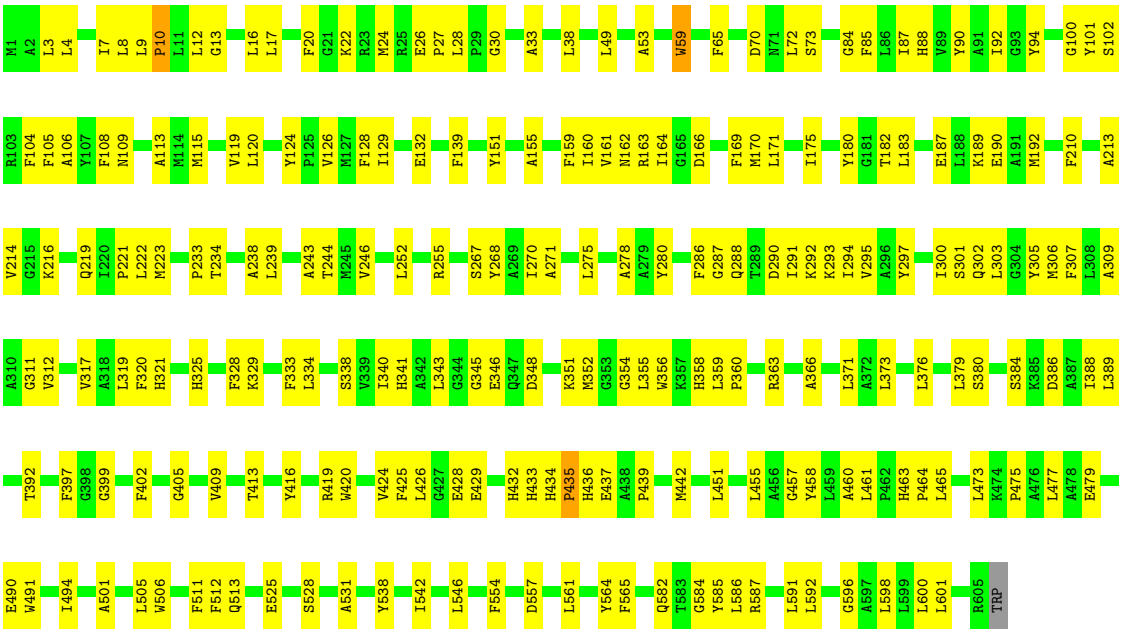
• Molecule 12: NADH-quinone oxidoreductase subunit 11

Chain S:



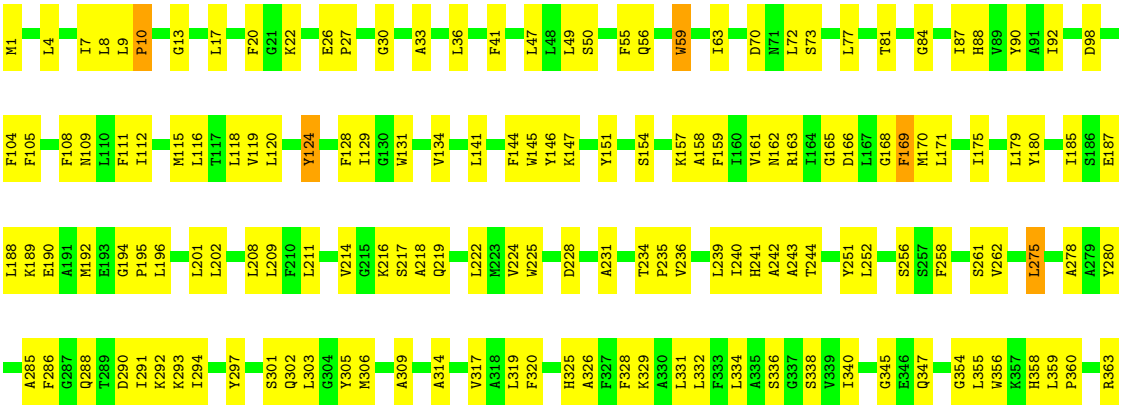
• Molecule 13: NADH-quinone oxidoreductase subunit 12

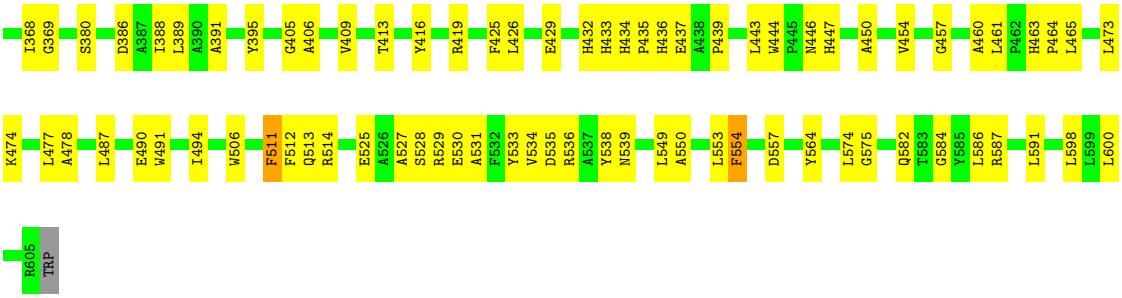
Chain L:



• Molecule 13: NADH-quinone oxidoreductase subunit 12

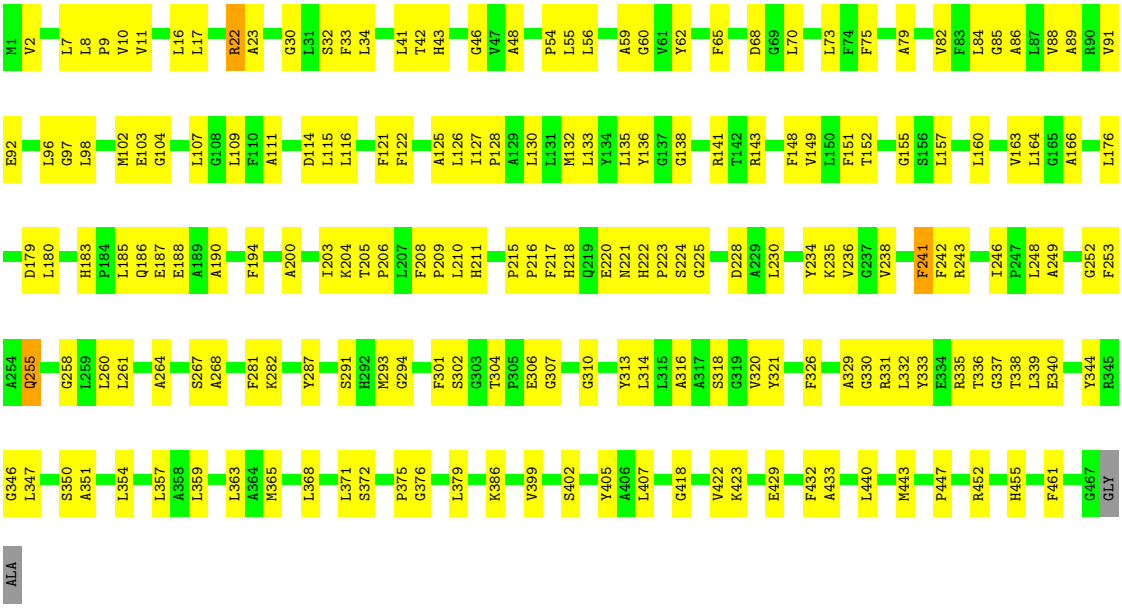
Chain T:





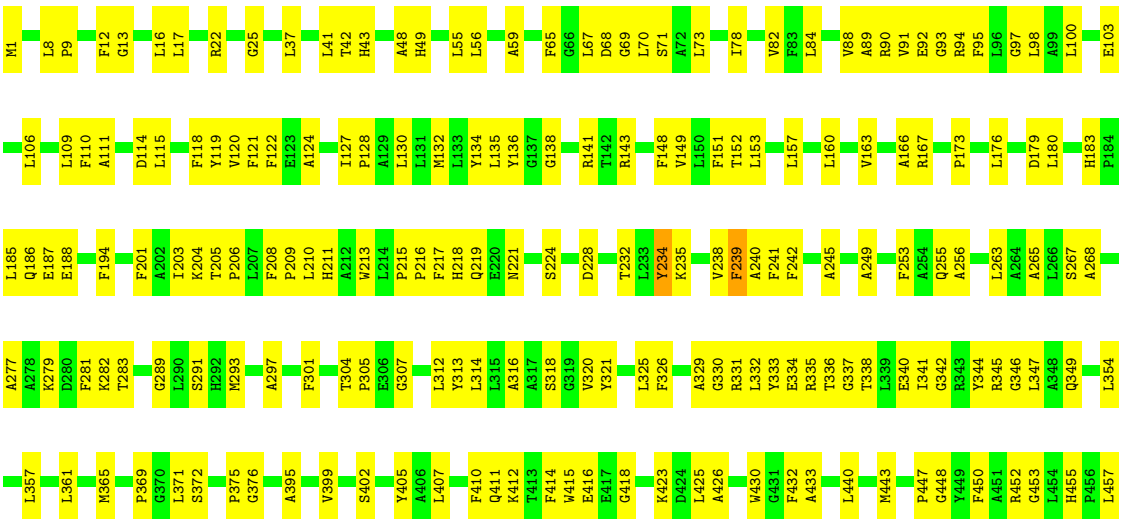
- Molecule 14: NADH-quinone oxidoreductase subunit 13

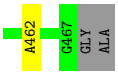
Chain M:



- Molecule 14: NADH-quinone oxidoreductase subunit 13

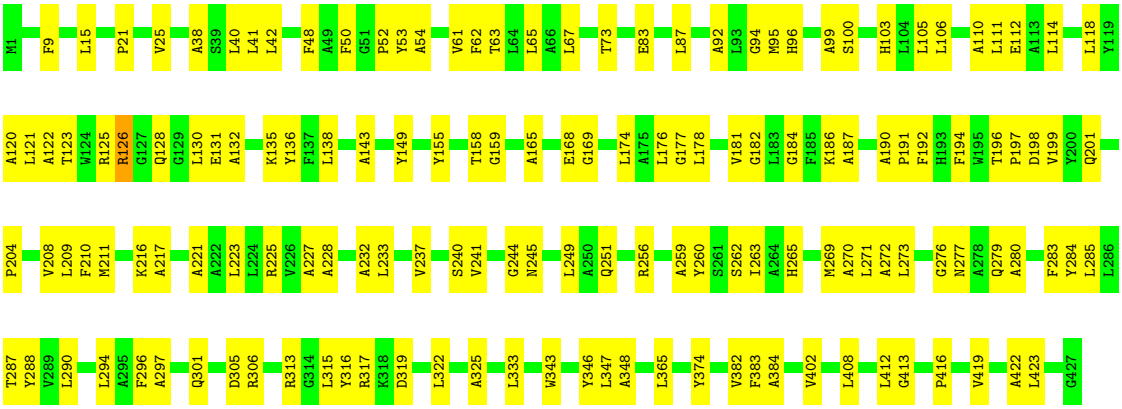
Chain U:





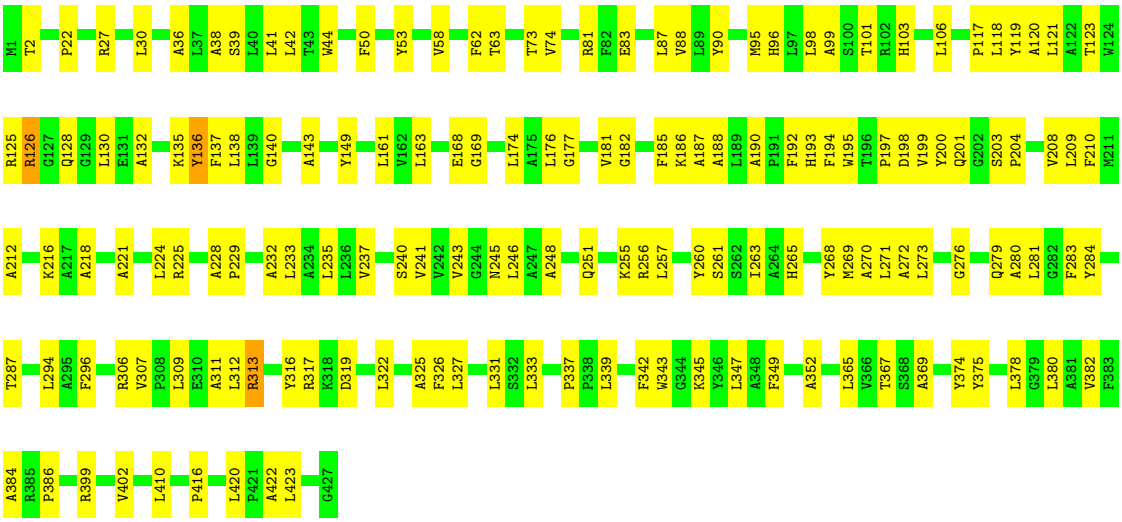
• Molecule 15: NADH-quinone oxidoreductase subunit 14

Chain N:



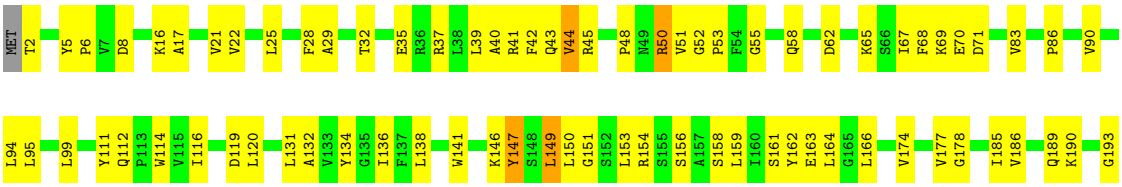
• Molecule 15: NADH-quinone oxidoreductase subunit 14

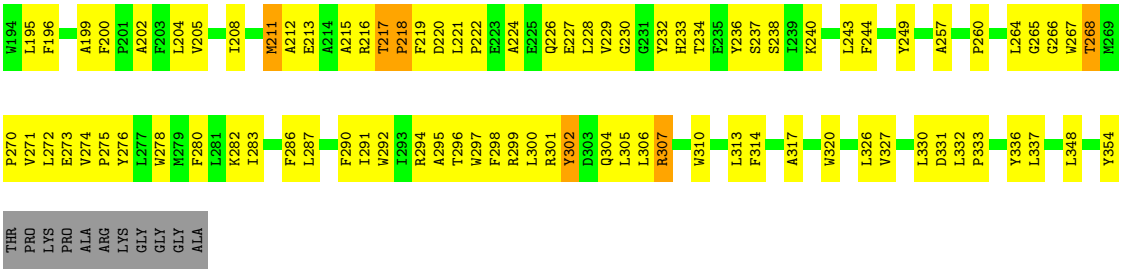
Chain V:



• Molecule 16: NADH-quinone oxidoreductase subunit 8

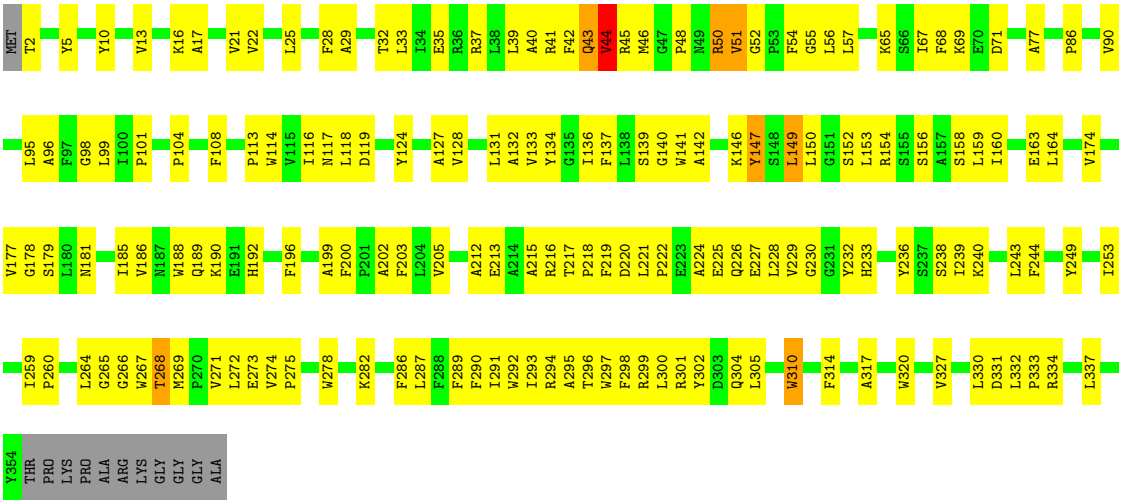
Chain H:





• Molecule 16: NADH-quinone oxidoreductase subunit 8

Chain Q:



4 Data and refinement statistics (i)

EDS failed to run properly - this section is therefore incomplete.

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	95.14Å 336.59Å 262.79Å 90.00° 100.41° 90.00°	Depositor
Resolution (Å)	49.16 – 3.60	Depositor
% Data completeness (in resolution range)	79.8 (49.16-3.60)	Depositor
R_{merge}	0.15	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.73 (at 3.57Å)	Xtriage
Refinement program	PHENIX (1.13rc1_2961: ???)	Depositor
R, R_{free}	0.218 , 0.235	Depositor
Wilson B-factor (Å^2)	107.9	Xtriage
Anisotropy	0.002	Xtriage
L-test for twinning[2]	$< \|L\| > = 0.36$, $< L^2 > = 0.18$	Xtriage
Estimated twinning fraction	0.347 for h,-k,-h-l	Xtriage
Reported twinning fraction	0.490 for -H,-K,H+L	Depositor
Outliers	0 of 148790 reflections	Xtriage
Total number of atoms	74146	wwPDB-VP
Average B, all atoms (Å^2)	111.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.58% of the height of the origin peak. No significant pseudotranslation is detected.*

[1]Intensities estimated from amplitudes.

[2]Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality (i)

5.1 Standard geometry (i)

Bond lengths and bond angles in the following residue types are not validated in this section: FMN, SF4, FES, HQH

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\#\|Z\|>5$	RMSZ	$\#\|Z\|>5$
1	1	0.27	0/3506	0.47	0/4745
1	B	0.27	0/3506	0.47	0/4745
2	2	0.27	0/1439	0.46	0/1953
2	C	0.26	0/1439	0.48	0/1953
3	3	0.28	0/6035	0.50	0/8185
3	D	0.28	0/6035	0.49	0/8185
4	4	0.28	0/3150	0.48	0/4284
4	E	0.27	0/3150	0.47	0/4284
5	5	0.27	0/1656	0.48	0/2246
5	F	0.28	0/1656	0.48	0/2246
6	6	0.30	0/1319	0.52	0/1786
6	G	0.28	0/1319	0.51	0/1786
7	9	0.32	0/1423	0.51	0/1933
7	O	0.30	0/1423	0.52	0/1933
8	7	0.27	0/1059	0.47	0/1429
8	I	0.26	0/1059	0.47	0/1429
9	W	0.26	0/985	0.47	0/1335
9	X	0.26	0/985	0.46	0/1335
10	A	0.29	0/940	0.49	0/1280
10	P	0.28	0/940	0.48	0/1280
11	J	0.26	0/1206	0.45	0/1649
11	R	0.26	0/1206	0.45	0/1649
12	K	0.28	0/710	0.44	0/962
12	S	0.25	0/710	0.44	0/962
13	L	0.26	0/4741	0.44	0/6460
13	T	0.26	0/4741	0.45	0/6460
14	M	0.27	0/3591	0.47	0/4896
14	U	0.26	0/3591	0.45	0/4896
15	N	0.27	0/3238	0.43	0/4434
15	V	0.27	0/3238	0.44	0/4434
16	H	0.30	0/2935	0.52	0/4014
16	Q	0.29	0/2935	0.51	0/4014

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#|Z| >5	RMSZ	#|Z| >5
All	All	0.28	0/75866	0.47	0/103182

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand.A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
7	9	0	1
7	O	0	1
16	H	0	2
16	Q	0	2
All	All	0	6

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (6) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
7	9	21	PRO	Peptide
16	H	217	THR	Peptide
16	H	266	GLY	Peptide
7	O	21	PRO	Peptide
16	Q	217	THR	Peptide
16	Q	266	GLY	Peptide

5.2 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 the 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 within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	1	3417	0	3388	150	0
1	B	3417	0	3388	181	0
2	2	1406	0	1373	68	0
2	C	1406	0	1373	67	0
3	3	5895	0	5930	231	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	D	5895	0	5931	253	0
4	4	3067	0	3049	164	0
4	E	3067	0	3049	217	0
5	5	1607	0	1574	65	0
5	F	1607	0	1574	93	0
6	6	1289	0	1298	80	0
6	G	1289	0	1299	106	0
7	9	1388	0	1383	61	0
7	O	1388	0	1383	82	0
8	7	1031	0	1029	57	0
8	I	1031	0	1029	40	0
9	W	967	0	1010	24	0
9	X	967	0	1010	32	0
10	A	910	0	939	59	0
10	P	910	0	939	58	0
11	J	1183	0	1286	72	0
11	R	1183	0	1286	54	0
12	K	703	0	747	36	0
12	S	703	0	747	29	0
13	L	4604	0	4734	173	0
13	T	4604	0	4734	167	0
14	M	3489	0	3606	138	0
14	U	3489	0	3606	146	0
15	N	3154	0	3343	112	0
15	V	3154	0	3343	121	0
16	H	2838	0	2903	171	0
16	Q	2838	0	2903	179	0
17	1	8	0	0	0	0
17	3	24	0	0	1	0
17	6	8	0	0	0	0
17	9	16	0	0	6	0
17	B	8	0	0	1	0
17	D	24	0	0	5	0
17	G	8	0	0	4	0
17	O	16	0	0	3	0
18	1	31	0	19	4	0
18	B	31	0	19	7	0
19	2	4	0	0	1	0
19	3	4	0	0	0	0
19	C	4	0	0	0	0
19	D	4	0	0	0	0
20	4	30	0	0	3	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
20	E	30	0	0	1	0
All	All	74146	0	75224	2994	0

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 20.

All (2994) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:L:355:LEU:HD12	13:L:359:LEU:HG	1.35	1.09
3:3:611:ARG:HA	3:3:624:LEU:O	1.62	0.98
16:Q:43:GLN:HE21	16:Q:45:ARG:NH2	1.61	0.97
16:H:146:LYS:HA	16:H:149:LEU:HB2	1.47	0.94
3:D:651:ARG:NH1	3:D:652:PRO:O	2.03	0.91
15:V:44:TRP:HE1	15:V:422:ALA:HB1	1.37	0.90
3:3:42:ILE:HD12	3:3:42:ILE:O	1.72	0.89
16:Q:39:LEU:O	16:Q:43:GLN:HG2	1.72	0.89
16:Q:146:LYS:HA	16:Q:149:LEU:HB2	1.53	0.89
4:4:263:ASP:HB2	4:4:285:GLU:HG3	1.55	0.88
1:B:437:TRP:CH2	2:C:147:ARG:HG3	2.09	0.88
2:2:132:PRO:HG2	2:2:145:VAL:HB	1.56	0.88
3:D:259:CYS:HG	17:D:803:SF4:FE4	0.91	0.87
13:T:158:ALA:HA	13:T:225:TRP:HB2	1.57	0.86
16:H:219:PHE:HB3	16:H:299:ARG:HG2	1.56	0.86
13:L:278:ALA:HA	13:L:301:SER:HA	1.57	0.85
16:H:39:LEU:O	16:H:43:GLN:HG2	1.77	0.85
16:H:216:ARG:HD2	16:H:294:ARG:HA	1.59	0.85
3:D:611:ARG:HA	3:D:624:LEU:O	1.76	0.85
13:L:59:TRP:O	14:M:452:ARG:NH2	2.10	0.84
3:3:31:PRO:HB2	3:3:47:MET:HB3	1.59	0.84
4:E:26:MET:HA	10:P:54:VAL:HG12	1.58	0.84
6:G:56:ALA:HB1	16:Q:44:VAL:CG1	2.07	0.84
16:Q:43:GLN:O	16:Q:45:ARG:N	2.10	0.84
6:G:56:ALA:CB	16:Q:44:VAL:HG12	2.08	0.84
15:V:87:LEU:HB3	15:V:117:PRO:HB2	1.59	0.83
13:T:70:ASP:H	13:T:73:SER:HB2	1.43	0.83
13:L:355:LEU:HD12	13:L:359:LEU:CG	2.08	0.83
16:H:292:TRP:O	16:H:296:THR:OG1	1.97	0.83
3:3:286:ASN:ND2	3:3:289:TRP:O	2.10	0.83
6:G:119:ASN:HA	6:G:125:GLN:HE22	1.44	0.83
4:E:151:ARG:HH22	4:E:196:VAL:HG21	1.44	0.82

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:A:35:LYS:O	10:A:40:LYS:NZ	2.12	0.82
4:4:202:ASP:HA	4:4:284:ARG:HH21	1.44	0.82
2:C:132:PRO:HG2	2:C:145:VAL:HB	1.62	0.82
5:F:66:GLU:HB2	5:F:93:TYR:HB3	1.62	0.82
7:9:41:HIS:HB3	7:9:113:ILE:HD11	1.62	0.81
16:H:189:GLN:HG2	16:H:195:LEU:H	1.46	0.81
3:3:728:LEU:HB3	3:3:747:VAL:HG11	1.59	0.81
5:F:134:LYS:NZ	5:F:141:LEU:O	2.13	0.81
10:P:35:LYS:O	10:P:40:LYS:NZ	2.14	0.81
14:U:217:PHE:O	14:U:221:ASN:ND2	2.13	0.81
3:D:188:VAL:HG11	3:D:201:ASP:HA	1.63	0.80
7:O:41:HIS:HB3	7:O:113:ILE:HD11	1.62	0.80
6:G:56:ALA:CB	16:Q:44:VAL:CG1	2.58	0.80
5:5:18:GLU:HB2	5:5:26:TRP:HB2	1.63	0.79
4:4:144:THR:HG22	4:4:148:TYR:HE1	1.46	0.79
3:3:419:ASP:OD1	3:3:447:LYS:NZ	2.13	0.79
6:6:119:ASN:HA	6:6:125:GLN:HE22	1.44	0.79
15:N:136:TYR:OH	15:N:186:LYS:NZ	2.15	0.79
3:D:31:PRO:HB2	3:D:47:MET:HB3	1.65	0.79
3:D:688:ARG:HB3	3:D:770:ARG:HB2	1.62	0.79
11:R:124:PRO:HA	11:R:127:LEU:HB2	1.66	0.78
11:J:47:ASP:O	11:J:122:GLY:N	2.16	0.78
11:J:49:ARG:NH1	16:H:119:ASP:OD2	2.17	0.78
16:Q:291:ILE:HA	16:Q:294:ARG:HG3	1.63	0.78
14:M:217:PHE:O	14:M:221:ASN:ND2	2.15	0.78
1:1:90:ILE:HB	1:1:218:ILE:HG12	1.64	0.78
5:5:167:PRO:HA	5:5:170:PHE:HB3	1.66	0.77
3:D:656:LEU:HD11	9:X:3:ARG:HD3	1.66	0.77
16:H:43:GLN:O	16:H:45:ARG:N	2.17	0.77
1:1:288:GLN:NE2	1:1:335:VAL:O	2.18	0.77
4:E:156:ILE:HA	4:E:159:LEU:HD12	1.66	0.77
1:B:88:TYR:HB2	1:B:216:THR:HG22	1.67	0.77
7:O:52:LYS:NZ	7:O:171:GLU:OE2	2.17	0.77
16:Q:50:ARG:O	16:Q:52:GLY:N	2.18	0.77
1:1:38:TYR:HH	1:1:112:HIS:HD1	1.31	0.77
3:3:614:LEU:O	3:3:621:VAL:HA	1.84	0.77
6:6:120:ASN:HD22	6:6:122:ALA:H	1.30	0.77
14:M:346:GLY:HA3	14:M:418:GLY:HA2	1.67	0.77
16:H:16:LYS:NZ	16:H:114:TRP:O	2.18	0.77
1:B:354:GLY:O	1:B:360:ARG:NH1	2.18	0.77
15:V:294:LEU:HD11	15:V:325:ALA:HB1	1.65	0.76

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:W:51:HIS:ND1	9:W:56:ASP:OD1	2.18	0.76
11:J:133:GLY:H	11:J:136:LEU:HB2	1.50	0.76
16:H:158:SER:HA	16:H:306:LEU:HD21	1.66	0.76
3:D:198:GLU:OE2	3:D:440:ARG:NH1	2.18	0.76
3:3:710:GLU:O	3:3:713:ARG:NH1	2.19	0.76
13:L:458:TYR:HB3	13:L:461:LEU:HD11	1.66	0.76
3:D:713:ARG:HH21	3:D:746:ARG:HH21	1.33	0.76
6:6:74:GLN:HE22	16:H:233:HIS:HB2	1.50	0.76
3:D:9:ARG:NH1	3:D:26:ALA:O	2.19	0.76
3:D:609:GLU:HA	3:D:627:ALA:H	1.50	0.76
4:E:26:MET:N	4:E:47:LEU:O	2.19	0.76
16:Q:224:ALA:HA	16:Q:229:VAL:HA	1.68	0.76
1:1:79:MET:SD	1:1:217:THR:OG1	2.43	0.76
7:O:68:ILE:HG12	7:O:93:ILE:HG12	1.68	0.75
1:1:437:TRP:HB3	2:2:92:GLY:HA3	1.68	0.75
16:Q:117:ASN:O	16:Q:181:ASN:ND2	2.19	0.75
2:2:105:GLY:HA2	8:7:108:ILE:HG12	1.67	0.75
16:H:332:LEU:HB2	16:H:333:PRO:HD3	1.69	0.75
13:T:278:ALA:HA	13:T:301:SER:HA	1.68	0.75
7:O:171:GLU:OE2	8:I:43:ARG:NH2	2.19	0.75
3:D:655:ARG:HH22	3:D:659:GLU:HG3	1.52	0.75
9:X:91:GLU:OE1	9:X:126:TYR:OH	2.03	0.74
16:Q:52:GLY:HA3	16:Q:55:GLY:H	1.50	0.74
13:L:288:GLN:NE2	13:L:528:SER:O	2.19	0.74
3:3:98:ASP:OD1	3:3:101:ARG:NH2	2.20	0.74
4:4:265:PRO:HB2	4:4:278:VAL:HG13	1.69	0.74
4:4:333:GLU:OE2	4:4:336:HIS:NE2	2.20	0.74
5:5:55:LEU:HB2	5:5:69:ALA:O	1.87	0.74
14:M:166:ALA:HA	14:M:185:LEU:HD21	1.70	0.74
1:B:90:ILE:HB	1:B:218:ILE:HG12	1.67	0.74
6:G:162:ALA:HB1	6:G:170:LEU:HD12	1.70	0.74
13:T:419:ARG:NH2	13:T:525:GLU:OE2	2.20	0.74
16:Q:219:PHE:HB3	16:Q:299:ARG:HG2	1.69	0.74
16:H:146:LYS:HG2	16:H:149:LEU:HD12	1.67	0.74
8:I:60:SER:HA	8:I:66:PRO:HA	1.69	0.74
3:3:694:LEU:HB3	3:3:762:ALA:HB2	1.69	0.74
10:A:3:PRO:HD2	16:H:2:THR:HB	1.68	0.74
14:M:115:LEU:HD13	14:M:163:VAL:HG23	1.70	0.74
5:5:75:VAL:HG13	5:5:87:ARG:HB2	1.70	0.74
14:M:224:SER:HA	14:M:330:GLY:HA3	1.68	0.74
3:D:119:CYS:SG	3:D:131:GLN:NE2	2.60	0.74

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:T:105:PHE:O	13:T:109:ASN:ND2	2.21	0.74
8:I:120:ASP:OD1	8:I:123:ARG:NH1	2.20	0.74
2:2:71:GLN:NE2	2:2:120:GLN:OE1	2.21	0.73
3:3:9:ARG:NH1	3:3:26:ALA:O	2.21	0.73
6:6:34:ASN:O	16:H:58:GLN:NE2	2.21	0.73
16:H:291:ILE:HA	16:H:294:ARG:HG3	1.70	0.73
16:H:177:VAL:HG11	16:H:185:ILE:HG12	1.68	0.73
4:E:200:ARG:NH2	4:E:203:GLU:OE1	2.21	0.73
7:9:75:ASN:ND2	7:9:84:GLY:O	2.22	0.73
10:P:65:ALA:HB3	11:R:66:LEU:HD13	1.70	0.73
14:U:1:MET:SD	14:U:49:HIS:ND1	2.62	0.73
7:9:22:VAL:HB	16:H:44:VAL:CG1	2.19	0.73
8:I:103:LEU:O	8:I:110:LEU:N	2.12	0.73
16:Q:43:GLN:HE21	16:Q:45:ARG:HH22	1.34	0.73
3:3:193:GLU:O	3:3:443:ARG:NH2	2.22	0.73
14:M:371:LEU:HD12	14:M:440:LEU:HB3	1.70	0.73
3:3:194:VAL:HG12	3:3:411:LEU:HD22	1.71	0.73
14:U:114:ASP:HB3	14:U:176:LEU:HD23	1.70	0.73
3:3:233:GLY:N	17:3:801:SF4:S2	2.62	0.73
14:U:166:ALA:HA	14:U:185:LEU:HD21	1.69	0.73
15:N:317:ARG:NH1	15:N:384:ALA:O	2.22	0.73
3:D:616:ASN:HD22	3:D:622:LEU:HD11	1.52	0.73
8:I:33:LYS:HG3	8:I:54:ILE:HD12	1.71	0.73
14:M:89:ALA:HB1	14:M:91:VAL:HG22	1.71	0.73
6:G:120:ASN:HD22	6:G:122:ALA:H	1.34	0.73
3:3:306:LEU:N	3:3:588:SER:O	2.21	0.72
13:L:84:GLY:O	13:L:88:HIS:ND1	2.21	0.72
15:N:128:GLN:OE1	15:N:306:ARG:NH2	2.17	0.72
5:F:182:THR:OG1	5:F:184:TYR:O	2.07	0.72
1:B:90:ILE:HD11	1:B:211:LEU:HD22	1.72	0.72
3:D:572:PRO:HD2	3:D:577:LEU:HD21	1.71	0.72
4:E:33:GLN:HB2	4:E:40:VAL:HG23	1.72	0.72
13:T:291:ILE:HD12	13:T:336:SER:HB3	1.69	0.72
16:Q:40:ALA:HB1	16:Q:45:ARG:O	1.89	0.72
1:1:118:MET:HG2	1:1:224:LEU:HD13	1.71	0.72
4:4:49:GLY:HA2	10:A:58:PRO:HD3	1.71	0.72
4:4:374:SER:HA	4:4:377:ASN:HB2	1.70	0.72
6:6:114:SER:OG	7:9:96:LEU:O	2.07	0.72
3:3:459:MET:HG2	3:3:465:HIS:HB2	1.71	0.72
7:9:28:ASP:OD2	16:H:50:ARG:NH1	2.23	0.72
3:3:414:SER:OG	3:3:443:ARG:NH2	2.23	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:6:LEU:HB2	1:B:241:MET:HA	1.71	0.72
13:T:286:PHE:O	13:T:419:ARG:NH1	2.23	0.72
7:9:128:ASP:O	7:9:144:LYS:NZ	2.22	0.72
8:I:23:TYR:OH	8:I:123:ARG:NH1	2.22	0.72
11:J:68:LEU:HD23	11:J:71:ILE:HD11	1.72	0.72
3:D:35:SER:O	3:D:186:ARG:NH2	2.22	0.72
1:1:88:TYR:HB2	1:1:216:THR:HG22	1.72	0.72
3:3:113:LEU:O	3:3:161:ARG:NH1	2.22	0.72
3:3:728:LEU:O	3:3:749:HIS:NE2	2.19	0.72
1:B:118:MET:HG2	1:B:224:LEU:HD13	1.72	0.72
3:3:8:ASP:OD2	3:3:28:TYR:OH	2.08	0.71
13:L:105:PHE:O	13:L:109:ASN:ND2	2.21	0.71
7:O:75:ASN:ND2	7:O:82:SER:OG	2.22	0.71
13:L:17:LEU:HB2	13:L:106:ALA:HB2	1.71	0.71
13:L:162:ASN:OD1	13:L:216:LYS:NZ	2.23	0.71
4:E:248:VAL:HG13	4:E:252:TYR:HD2	1.53	0.71
1:B:18:TYR:OH	1:B:102:LYS:O	2.07	0.71
4:E:262:PHE:HE1	4:E:285:GLU:HB3	1.56	0.71
5:F:94:VAL:HG11	5:F:124:ILE:HG12	1.72	0.71
7:O:75:ASN:ND2	7:O:84:GLY:O	2.24	0.71
4:E:123:LEU:HD21	4:E:159:LEU:HD13	1.73	0.71
6:G:163:TYR:O	7:O:148:ARG:NE	2.24	0.71
1:B:32:TYR:OH	1:B:116:GLU:OE1	2.05	0.71
1:B:66:GLY:HA3	18:B:502:FMN:H5'1	1.73	0.71
4:E:318:GLU:HB3	8:I:42:TYR:HB2	1.73	0.70
7:9:59:CYS:SG	7:9:91:TYR:OH	2.47	0.70
16:H:211:MET:HA	16:H:215:ALA:HB3	1.72	0.70
2:C:71:GLN:NE2	2:C:120:GLN:OE1	2.24	0.70
11:R:1:MET:O	11:R:5:GLU:N	2.22	0.70
4:4:240:ARG:HB2	4:4:266:LEU:HD23	1.72	0.70
14:M:75:PHE:HZ	14:M:111:ALA:HB2	1.57	0.70
3:D:414:SER:OG	3:D:443:ARG:NH2	2.25	0.70
5:F:6:VAL:HG13	5:F:41:TYR:HE1	1.57	0.70
10:P:95:GLY:HA3	11:R:136:LEU:HD21	1.72	0.70
13:T:217:SER:HB2	13:T:303:LEU:HD22	1.73	0.70
3:D:259:CYS:SG	17:D:803:SF4:FE4	1.82	0.70
3:D:694:LEU:HB3	3:D:762:ALA:HB2	1.73	0.70
16:H:216:ARG:NH1	16:H:294:ARG:O	2.25	0.70
1:B:92:ASN:ND2	18:B:502:FMN:O3'	2.25	0.70
4:E:83:PRO:HB2	4:E:169:HIS:HD1	1.55	0.70
6:G:56:ALA:HB1	16:Q:44:VAL:HG13	1.72	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:715:GLU:H	3:D:761:SER:HB2	1.56	0.70
3:3:576:ALA:O	3:3:580:LYS:NZ	2.22	0.70
9:W:87:ARG:HH12	10:A:38:ARG:HH12	1.39	0.70
10:P:14:VAL:HG22	16:Q:95:LEU:HD22	1.72	0.70
16:H:271:VAL:HG12	16:H:272:LEU:HG	1.74	0.69
4:E:205:GLU:OE1	4:E:284:ARG:NH2	2.25	0.69
5:F:38:MET:HA	5:F:41:TYR:HD2	1.57	0.69
6:G:153:GLN:HG3	7:O:124:TYR:CZ	2.26	0.69
6:6:102:PRO:HG2	16:H:69:LYS:HA	1.74	0.69
10:A:108:LEU:HD23	15:N:15:LEU:HD22	1.74	0.69
13:T:280:TYR:OH	13:T:531:ALA:O	2.09	0.69
14:U:345:ARG:NH1	14:U:416:GLU:OE1	2.23	0.69
15:N:343:TRP:NE1	15:N:413:GLY:O	2.24	0.69
14:U:203:ILE:HG13	14:U:210:LEU:HB3	1.73	0.69
4:4:162:TRP:CE2	7:9:34:LYS:HD2	2.28	0.69
16:H:6:PRO:HG2	16:H:112:GLN:HE22	1.57	0.69
2:2:171:LYS:NZ	2:2:178:GLU:O	2.25	0.69
8:I:23:TYR:HH	8:I:123:ARG:NH1	1.90	0.69
16:Q:71:ASP:HB2	16:Q:238:SER:HB3	1.73	0.69
6:6:102:PRO:O	16:H:69:LYS:NZ	2.25	0.69
15:N:217:ALA:HA	15:N:285:LEU:HD23	1.74	0.69
5:F:163:ARG:NE	7:O:92:GLU:OE1	2.24	0.69
6:G:143:ARG:NE	6:G:145:GLU:OE1	2.26	0.69
15:N:317:ARG:NH1	15:N:383:PHE:O	2.21	0.69
3:D:682:GLU:OE1	3:D:684:ARG:NH2	2.26	0.69
4:E:216:GLU:OE2	16:Q:304:GLN:NE2	2.26	0.69
10:P:57:PHE:HB2	11:R:73:LEU:HD22	1.74	0.69
14:U:70:LEU:O	14:U:73:LEU:HD23	1.93	0.69
15:V:58:VAL:HB	15:V:225:ARG:HH11	1.57	0.69
16:Q:140:GLY:HA3	16:Q:152:SER:HB3	1.75	0.69
16:Q:215:ALA:O	16:Q:294:ARG:NH1	2.26	0.69
4:4:50:GLU:O	4:4:389:GLN:NE2	2.25	0.69
13:L:159:PHE:HD2	14:M:407:LEU:HD11	1.55	0.69
14:U:219:GLN:NE2	14:U:283:THR:OG1	2.23	0.69
3:D:139:LEU:HD21	4:E:322:GLU:HG2	1.75	0.69
4:E:185:GLU:OE2	7:O:165:TYR:OH	2.08	0.69
13:T:305:TYR:OH	13:T:406:ALA:O	2.10	0.69
9:X:87:ARG:HH12	10:P:38:ARG:HH22	1.38	0.68
16:Q:141:TRP:HE3	16:Q:149:LEU:HD21	1.58	0.68
14:U:89:ALA:HB1	14:U:91:VAL:HG22	1.75	0.68
4:4:409:ARG:NH2	5:5:117:GLU:OE2	2.27	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:K:28:PHE:CZ	12:K:68:VAL:HA	2.29	0.68
1:B:41:ALA:HA	1:B:120:LEU:HD21	1.75	0.68
1:B:193:GLU:OE1	1:B:200:ARG:NH2	2.27	0.68
14:U:208:PHE:O	14:U:211:HIS:ND1	2.26	0.68
15:V:309:LEU:HD22	15:V:378:LEU:HD11	1.75	0.68
4:4:64:THR:OG1	6:6:83:ARG:NH1	2.25	0.68
6:6:19:ILE:HG23	6:6:20:LEU:HG	1.75	0.68
4:E:71:GLU:OE1	5:F:148:LYS:NZ	2.23	0.68
5:F:112:ASN:O	5:F:129:HIS:NE2	2.25	0.68
10:P:3:PRO:HD2	16:Q:2:THR:HB	1.75	0.68
11:R:155:ALA:O	15:V:81:ARG:NH1	2.27	0.68
13:T:529:ARG:NH2	13:T:530:GLU:OE2	2.27	0.68
3:3:40:SER:O	3:3:189:ARG:NE	2.25	0.68
4:4:333:GLU:O	4:4:363:SER:OG	2.08	0.68
14:M:194:PHE:HB2	14:M:249:ALA:HB3	1.74	0.68
16:H:205:VAL:HG21	16:H:317:ALA:HB2	1.74	0.68
4:E:33:GLN:HE22	4:E:38:HIS:HA	1.58	0.68
3:D:689:LYS:HG3	3:D:771:VAL:HA	1.75	0.68
1:1:174:HIS:ND1	2:2:18:TYR:OH	2.25	0.68
3:3:224:GLY:O	3:3:227:THR:HB	1.94	0.68
6:6:50:MET:O	6:6:53:SER:OG	2.12	0.68
8:7:120:ASP:OD1	8:7:123:ARG:NH1	2.27	0.68
13:L:419:ARG:NH2	13:L:525:GLU:OE2	2.26	0.68
14:M:268:ALA:HA	14:M:291:SER:HA	1.75	0.68
16:H:29:ALA:O	16:H:32:THR:OG1	2.10	0.68
1:B:124:ALA:O	1:B:126:ARG:NH1	2.27	0.68
6:G:90:PRO:O	6:G:93:ARG:HB3	1.93	0.68
15:V:136:TYR:OH	15:V:186:LYS:NZ	2.19	0.68
1:1:312:SER:OG	1:1:315:HIS:ND1	2.25	0.68
6:6:58:ASN:ND2	6:6:145:GLU:OE2	2.27	0.68
11:J:93:ALA:HB1	12:K:19:LEU:HB3	1.76	0.68
15:N:196:THR:HG22	15:N:259:ALA:HB1	1.75	0.68
3:D:48:CYS:SG	3:D:83:CYS:N	2.65	0.68
5:F:101:LEU:O	5:F:127:GLU:N	2.26	0.68
14:U:335:ARG:NH1	14:U:423:LYS:O	2.27	0.68
10:A:65:ALA:HB3	11:J:66:LEU:HD13	1.74	0.68
13:L:234:THR:HG23	13:L:292:LYS:HE2	1.76	0.68
14:M:203:ILE:HG13	14:M:210:LEU:HB3	1.76	0.68
5:F:78:PRO:HA	5:F:83:GLY:HA3	1.75	0.68
14:U:115:LEU:HD13	14:U:163:VAL:HG23	1.75	0.68
1:B:342:TRP:CD1	1:B:371:PHE:HB3	2.29	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:G:50:MET:O	6:G:53:SER:OG	2.10	0.67
1:1:16:THR:HG21	1:1:229:PRO:HB3	1.76	0.67
3:3:166:LYS:NZ	3:3:179:GLU:OE1	2.20	0.67
7:9:45:ARG:NH2	7:9:139:ASP:OD2	2.26	0.67
7:9:68:ILE:HG12	7:9:93:ILE:HG12	1.75	0.67
13:L:355:LEU:HD12	13:L:359:LEU:CD1	2.25	0.67
1:B:342:TRP:HZ3	1:B:346:ARG:HE	1.40	0.67
4:E:363:SER:N	5:F:174:LEU:O	2.27	0.67
16:Q:333:PRO:O	16:Q:334:ARG:NH1	2.24	0.67
14:M:208:PHE:O	14:M:211:HIS:ND1	2.27	0.67
4:E:314:ARG:NH1	7:O:106:GLU:O	2.27	0.67
15:V:188:ALA:HB3	15:V:216:LYS:HZ1	1.59	0.67
3:3:614:LEU:HD11	3:3:624:LEU:HG	1.76	0.67
6:6:43:LEU:HB2	6:6:82:GLY:HA3	1.74	0.67
4:E:341:GLU:OE2	5:F:57:TYR:OH	2.12	0.67
11:R:15:SER:OG	11:R:31:ALA:O	2.11	0.67
14:U:157:LEU:HD12	15:V:369:ALA:HB2	1.76	0.67
15:V:317:ARG:HD2	15:V:386:PRO:HG3	1.76	0.67
3:D:286:ASN:ND2	3:D:289:TRP:O	2.28	0.67
1:1:220:ASN:ND2	18:1:502:FMN:O2	2.27	0.67
7:9:26:TYR:OH	7:9:120:GLU:OE2	2.13	0.67
14:M:333:TYR:O	14:M:337:GLY:N	2.27	0.67
16:H:52:GLY:HA3	16:H:55:GLY:H	1.59	0.67
3:D:34:CYS:SG	3:D:35:SER:N	2.68	0.67
15:V:2:THR:HG23	15:V:36:ALA:HB1	1.75	0.67
3:D:403:THR:OG1	3:D:410:HIS:ND1	2.24	0.67
3:D:419:ASP:OD1	3:D:447:LYS:NZ	2.18	0.67
1:1:192:LEU:HD22	1:1:211:LEU:HD21	1.75	0.67
12:K:90:LEU:HB3	15:N:131:GLU:HG3	1.77	0.67
1:B:29:LEU:HD23	1:B:155:ARG:HD2	1.77	0.67
14:U:333:TYR:O	14:U:337:GLY:N	2.26	0.67
16:H:50:ARG:O	16:H:52:GLY:N	2.18	0.67
2:C:4:PHE:N	2:C:48:GLU:OE2	2.28	0.67
3:D:180:ARG:HH12	3:D:236:LEU:HD11	1.59	0.67
4:E:152:GLU:OE2	4:E:204:TYR:OH	2.12	0.67
11:R:19:VAL:HG21	11:R:32:LEU:HB2	1.77	0.67
16:Q:216:ARG:HB2	16:Q:294:ARG:HD2	1.77	0.67
4:4:218:ALA:HA	4:4:221:VAL:HG22	1.75	0.67
9:X:45:ARG:NH1	9:X:61:ASP:OD2	2.28	0.67
4:4:222:GLY:HA3	4:4:275:ARG:HH22	1.59	0.66
10:A:70:LEU:HD13	11:J:150:THR:HG22	1.77	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:L:358:HIS:ND1	13:L:429:GLU:OE2	2.27	0.66
15:V:143:ALA:HB1	15:V:182:GLY:HA2	1.75	0.66
3:3:682:GLU:OE1	3:3:684:ARG:NH2	2.28	0.66
4:4:218:ALA:HB1	4:4:272:VAL:HB	1.76	0.66
13:L:348:ASP:HB3	13:L:351:LYS:HB2	1.77	0.66
6:G:60:LEU:HG	6:G:65:SER:HB2	1.76	0.66
8:I:61:ASP:HB2	8:I:129:ALA:H	1.60	0.66
15:V:280:ALA:HB1	15:V:347:LEU:HB3	1.77	0.66
3:3:584:VAL:HG12	3:3:600:VAL:HB	1.76	0.66
6:6:83:ARG:HB2	6:6:123:ILE:HD12	1.77	0.66
16:Q:301:ARG:HE	16:Q:304:GLN:H	1.42	0.66
1:1:365:GLY:O	1:1:369:ASN:ND2	2.27	0.66
4:4:260:TYR:HA	4:4:292:GLN:HE22	1.58	0.66
15:N:198:ASP:OD1	15:N:256:ARG:NH2	2.29	0.66
2:2:109:GLY:O	8:7:121:ARG:NH2	2.28	0.66
11:J:103:ILE:HG12	13:L:601:LEU:HB3	1.78	0.66
3:D:139:LEU:HD11	4:E:322:GLU:HB3	1.78	0.66
6:G:45:CYS:SG	17:G:201:SF4:FE3	1.88	0.66
3:3:51:ARG:HB3	3:3:94:ASP:HB3	1.78	0.66
14:M:221:ASN:ND2	14:M:228:ASP:OD1	2.28	0.66
1:B:134:VAL:O	1:B:176:GLY:N	2.29	0.66
4:E:409:ARG:NH2	5:F:117:GLU:OE2	2.28	0.66
3:3:29:ASP:OD2	5:5:187:GLY:N	2.23	0.66
6:6:53:SER:O	6:6:60:LEU:N	2.28	0.66
10:P:63:VAL:HG11	10:P:115:VAL:HG11	1.77	0.66
2:2:102:GLU:HA	8:7:108:ILE:HD11	1.77	0.66
3:3:316:ARG:HD3	3:D:675:ARG:HD3	1.78	0.66
4:E:112:ARG:NH2	4:E:181:ASP:OD1	2.29	0.66
4:E:201:ILE:HG21	4:E:284:ARG:HG3	1.77	0.66
15:V:228:ALA:HB1	15:V:233:LEU:CD1	2.26	0.66
13:L:564:TYR:OH	14:M:209:PRO:O	2.11	0.66
1:1:165:THR:HG23	1:1:167:PHE:H	1.61	0.66
2:C:109:GLY:O	8:I:121:ARG:NH2	2.30	0.66
3:D:8:ASP:OD2	3:D:28:TYR:OH	2.14	0.66
3:D:224:GLY:N	3:D:292:ASP:OD1	2.19	0.66
4:E:336:HIS:ND1	4:E:361:GLY:O	2.28	0.66
16:H:302:TYR:HA	16:H:305:LEU:HB3	1.78	0.65
2:2:79:HIS:NE2	2:2:120:GLN:OE1	2.27	0.65
4:E:47:LEU:HA	4:E:53:LEU:HD23	1.77	0.65
4:E:333:GLU:O	4:E:363:SER:OG	2.13	0.65
2:2:7:LYS:HB2	2:2:10:PHE:HB3	1.78	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:F:35:LYS:NZ	5:F:103:THR:O	2.28	0.65
2:2:77:LYS:H	2:2:116:LEU:HA	1.61	0.65
3:3:559:ASP:OD2	3:3:686:LYS:NZ	2.29	0.65
15:N:294:LEU:HD11	15:N:325:ALA:HB1	1.79	0.65
1:B:260:ARG:O	1:B:264:TYR:OH	2.14	0.65
3:D:557:SER:H	3:D:560:GLU:HB2	1.60	0.65
13:T:151:TYR:HB3	13:T:231:ALA:HB1	1.78	0.65
13:L:246:VAL:HB	13:L:303:LEU:HD21	1.78	0.65
16:H:265:GLY:O	16:H:282:LYS:NZ	2.24	0.65
3:D:159:PHE:HE2	8:I:79:LEU:HD13	1.60	0.65
4:E:373:PRO:O	4:E:377:ASN:ND2	2.29	0.65
12:S:2:SER:HA	12:S:5:LEU:HD12	1.78	0.65
3:3:611:ARG:HH21	9:W:101:ALA:HB1	1.60	0.65
3:3:697:THR:OG1	3:3:762:ALA:O	2.11	0.65
6:6:156:LYS:NZ	6:6:161:GLN:O	2.29	0.65
4:E:374:SER:HA	4:E:377:ASN:HB2	1.79	0.65
16:Q:133:VAL:HG11	16:Q:160:ILE:HG13	1.79	0.65
1:1:139:ARG:NH1	1:1:143:ASP:OD2	2.30	0.65
4:4:41:LEU:HD13	4:4:59:ILE:HG22	1.79	0.65
7:9:52:LYS:NZ	8:7:44:MET:O	2.29	0.65
3:D:46:ARG:HH22	3:D:81:ALA:HB2	1.62	0.65
1:1:14:GLU:OE2	1:1:233:ARG:NH1	2.30	0.65
15:N:316:TYR:HB2	15:N:382:VAL:HG12	1.79	0.65
11:J:124:PRO:HA	11:J:127:LEU:HB2	1.79	0.65
1:B:219:ASN:ND2	18:B:502:FMN:O2P	2.30	0.65
3:D:55:PRO:HB3	3:D:74:GLN:HB2	1.79	0.65
3:D:297:GLY:O	3:D:300:TRP:NE1	2.30	0.65
13:T:535:ASP:HA	13:T:538:TYR:HB2	1.79	0.65
1:1:287:ILE:HA	1:1:332:PRO:HA	1.78	0.65
3:D:36:GLU:OE2	3:D:186:ARG:NH1	2.30	0.65
4:E:40:VAL:HG21	6:G:88:MET:HE1	1.79	0.65
9:X:51:HIS:ND1	9:X:56:ASP:OD1	2.29	0.65
4:4:80:THR:O	4:4:84:ARG:NH1	2.29	0.64
6:6:94:ARG:O	6:6:98:GLN:N	2.26	0.64
3:D:710:GLU:O	3:D:713:ARG:NH1	2.27	0.64
4:E:77:GLN:NE2	7:O:62:ALA:O	2.27	0.64
6:G:19:ILE:HG23	6:G:20:LEU:HG	1.79	0.64
7:O:28:ASP:OD2	16:Q:50:ARG:NH1	2.30	0.64
2:2:110:GLU:HA	8:7:121:ARG:HH22	1.62	0.64
3:3:714:ALA:HB2	3:3:763:LEU:HD11	1.79	0.64
11:J:15:SER:OG	11:J:31:ALA:O	2.13	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:E:211:SER:HB2	4:E:214:PHE:HB3	1.79	0.64
3:3:342:GLY:N	3:3:565:TYR:O	2.30	0.64
4:4:314:ARG:NH2	8:7:44:MET:SD	2.71	0.64
1:B:104:ARG:NH2	2:C:143:GLU:OE2	2.30	0.64
6:G:74:GLN:HE22	16:Q:233:HIS:HB2	1.63	0.64
11:R:83:PHE:O	12:S:22:ARG:NH1	2.30	0.64
14:M:332:LEU:O	14:M:336:THR:OG1	2.09	0.64
3:D:614:LEU:HD11	3:D:624:LEU:HG	1.79	0.64
13:T:147:LYS:NZ	14:U:349:GLN:OE1	2.29	0.64
14:U:268:ALA:HA	14:U:291:SER:HA	1.80	0.64
6:6:35:SER:O	6:6:37:TRP:HE3	1.80	0.64
6:6:66:GLU:OE1	16:H:45:ARG:NH1	2.30	0.64
3:D:351:LEU:HD11	3:D:615:VAL:HG23	1.80	0.64
16:Q:146:LYS:HG2	16:Q:149:LEU:HD12	1.79	0.64
3:3:394:ASP:OD2	3:3:502:ASN:N	2.30	0.64
16:H:267:TRP:CG	16:H:268:THR:N	2.66	0.64
1:1:186:THR:HB	1:1:200:ARG:H	1.63	0.64
11:J:1:MET:O	11:J:5:GLU:N	2.27	0.64
13:L:340:ILE:HB	13:L:345:GLY:HA2	1.77	0.64
2:C:101:THR:O	2:C:105:GLY:N	2.25	0.64
3:D:713:ARG:HE	3:D:746:ARG:HE	1.45	0.64
13:T:340:ILE:O	13:T:345:GLY:N	2.30	0.64
1:1:342:TRP:HE1	1:1:372:ALA:HA	1.61	0.64
1:B:190:ASN:ND2	1:B:198:ASN:O	2.26	0.64
11:R:69:PHE:HZ	16:Q:156:SER:HB3	1.63	0.64
14:U:224:SER:HA	14:U:330:GLY:HA3	1.79	0.64
3:3:199:VAL:HG11	3:3:219:PRO:HD2	1.80	0.64
10:A:107:PHE:HE1	16:H:310:TRP:CD1	2.16	0.64
13:L:126:VAL:HA	13:L:129:ILE:HD12	1.78	0.64
16:H:162:TYR:OH	16:H:305:LEU:O	2.10	0.64
3:3:21:ASP:OD1	3:3:432:PHE:N	2.29	0.64
14:M:335:ARG:NH2	14:M:429:GLU:OE1	2.31	0.64
3:D:559:ASP:OD2	3:D:686:LYS:NZ	2.31	0.64
3:3:285:VAL:HG13	3:3:286:ASN:H	1.63	0.63
10:A:29:ALA:O	10:A:34:LYS:NZ	2.29	0.63
3:D:228:ASP:OD1	3:D:295:ARG:NH1	2.30	0.63
14:U:55:LEU:HD11	15:V:416:PRO:HD2	1.79	0.63
14:U:402:SER:HA	14:U:405:TYR:CE2	2.33	0.63
16:Q:253:ILE:HG22	16:Q:287:LEU:HD11	1.79	0.63
6:6:39:ALA:N	6:6:77:VAL:O	2.31	0.63
8:7:88:ARG:HH21	8:7:126:LEU:HB3	1.61	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
16:Q:218:PRO:HB3	16:Q:305:LEU:HD13	1.80	0.63
3:3:715:GLU:H	3:3:761:SER:HB2	1.62	0.63
16:H:40:ALA:HB1	16:H:45:ARG:O	1.99	0.63
16:H:71:ASP:HB2	16:H:238:SER:HB3	1.80	0.63
5:F:35:LYS:HD3	5:F:102:PRO:HB2	1.80	0.63
5:F:99:PRO:HB2	5:F:124:ILE:HA	1.80	0.63
5:F:167:PRO:HA	5:F:170:PHE:HB3	1.79	0.63
1:1:438:ARG:OXT	2:2:146:THR:OG1	2.16	0.63
6:6:156:LYS:HB2	6:6:161:GLN:HB3	1.79	0.63
7:9:108:CYS:SG	7:9:112:ALA:N	2.71	0.63
9:W:35:THR:O	9:W:93:VAL:HA	1.99	0.63
16:H:189:GLN:NE2	16:H:264:LEU:O	2.30	0.63
1:1:288:GLN:HE21	1:1:331:ILE:HG22	1.63	0.63
4:E:32:PRO:O	4:E:34:HIS:ND1	2.29	0.63
2:2:110:GLU:HA	8:7:121:ARG:HH12	1.64	0.63
3:3:635:GLU:HG2	9:W:7:ARG:HD2	1.81	0.63
13:T:286:PHE:HB2	13:T:419:ARG:HD3	1.79	0.63
13:T:586:LEU:HD13	15:V:138:LEU:HD12	1.81	0.63
14:U:235:LYS:HD3	14:U:293:MET:HG3	1.81	0.63
14:M:22:ARG:HD2	14:M:23:ALA:N	2.13	0.63
1:B:4:PRO:O	1:B:5:ILE:HG13	1.99	0.63
6:G:76:ASP:HB3	16:Q:69:LYS:HZ3	1.63	0.63
7:9:88:ALA:O	7:9:133:LYS:NZ	2.29	0.63
1:B:288:GLN:NE2	1:B:332:PRO:O	2.32	0.63
6:G:169:ARG:HG3	6:G:169:ARG:HH11	1.64	0.63
15:V:63:THR:HG22	15:V:96:HIS:HA	1.81	0.63
1:1:4:PRO:HA	1:1:12:ARG:HH12	1.64	0.63
10:A:2:ALA:O	11:J:49:ARG:NH2	2.30	0.63
3:D:42:ILE:HD12	3:D:42:ILE:O	1.98	0.63
10:P:109:TYR:OH	10:P:113:LYS:NZ	2.30	0.63
16:Q:96:ALA:HB2	16:Q:128:VAL:HG21	1.81	0.63
4:4:239:LEU:HG	4:4:244:VAL:HB	1.81	0.62
1:B:253:GLN:HG2	1:B:327:GLY:HA2	1.81	0.62
1:B:293:GLY:HA3	1:B:297:THR:HG21	1.79	0.62
3:D:175:ILE:HG22	3:D:236:LEU:HB2	1.81	0.62
4:E:110:PRO:HB3	4:E:301:PRO:HG2	1.80	0.62
15:V:319:ASP:OD2	15:V:399:ARG:NH2	2.32	0.62
1:1:243:THR:HG22	1:1:244:GLU:H	1.64	0.62
13:L:340:ILE:O	13:L:345:GLY:N	2.29	0.62
14:M:313:TYR:OH	14:M:443:MET:O	2.17	0.62
1:B:18:TYR:N	1:B:265:GLU:OE1	2.31	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:419:ASP:HA	1:B:422:LEU:HD12	1.80	0.62
14:U:332:LEU:O	14:U:336:THR:OG1	2.09	0.62
3:3:34:CYS:SG	3:3:35:SER:N	2.72	0.62
3:3:168:HIS:N	3:3:176:LEU:O	2.28	0.62
3:3:195:PRO:O	3:3:410:HIS:NE2	2.29	0.62
4:E:201:ILE:HA	4:E:204:TYR:HD2	1.64	0.62
4:E:224:ILE:HD11	4:E:275:ARG:CZ	2.28	0.62
16:Q:174:VAL:O	16:Q:178:GLY:N	2.28	0.62
3:3:462:ALA:O	3:3:465:HIS:ND1	2.32	0.62
8:7:50:LEU:HD11	8:7:75:ARG:HB2	1.82	0.62
13:L:413:THR:HA	13:L:416:TYR:CE2	2.34	0.62
16:H:159:LEU:O	16:H:163:GLU:HB2	1.98	0.62
16:Q:290:PHE:O	16:Q:294:ARG:HG2	1.99	0.62
1:1:50:PRO:HB3	1:1:124:ALA:HA	1.82	0.62
1:1:95:GLU:OE1	1:1:138:TYR:OH	2.13	0.62
3:3:415:GLU:HA	3:3:420:LEU:HD12	1.82	0.62
6:6:74:GLN:NE2	16:H:233:HIS:HB2	2.13	0.62
13:L:582:GLN:HE22	15:N:197:PRO:HG2	1.63	0.62
11:R:119:LEU:HD11	12:S:47:ARG:HA	1.81	0.62
15:V:101:THR:HG21	15:V:106:LEU:HD23	1.80	0.62
1:1:275:LEU:HA	1:1:279:TRP:HD1	1.65	0.62
12:K:95:GLY:O	15:N:251:GLN:NE2	2.29	0.62
3:D:611:ARG:HB2	3:D:626:PRO:HD3	1.81	0.62
4:E:306:ASN:ND2	5:F:192:TYR:OH	2.33	0.62
16:Q:29:ALA:O	16:Q:32:THR:OG1	2.15	0.62
4:4:350:ARG:NH2	4:4:401:ASP:OD2	2.32	0.62
10:A:1:MET:HA	11:J:123:LEU:HD11	1.82	0.62
16:H:150:LEU:O	16:H:154:ARG:HG3	2.00	0.62
3:D:34:CYS:HB3	3:D:45:CYS:H	1.64	0.62
4:E:200:ARG:NH1	7:O:16:TYR:OH	2.33	0.62
13:L:439:PRO:HG2	13:L:442:MET:HE3	1.82	0.62
14:M:157:LEU:HB3	15:N:365:LEU:HB3	1.81	0.62
1:B:354:GLY:HA2	1:B:360:ARG:HB2	1.80	0.62
4:E:172:TYR:OH	4:E:180:GLU:O	2.14	0.62
14:U:221:ASN:ND2	14:U:228:ASP:OD1	2.33	0.62
7:9:56:CYS:N	17:9:202:SF4:S1	2.73	0.62
13:L:386:ASP:OD2	13:L:494:ILE:HA	2.00	0.62
7:O:13:THR:HG21	16:Q:296:THR:HG23	1.79	0.62
7:O:45:ARG:NH2	7:O:139:ASP:OD2	2.33	0.62
10:P:69:ILE:HD11	12:S:69:ALA:HB2	1.82	0.62
15:V:198:ASP:OD1	15:V:256:ARG:NH2	2.32	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:1:293:GLY:HA3	1:1:297:THR:HG21	1.81	0.61
3:3:323:GLU:OE1	9:W:11:ARG:NH1	2.33	0.61
3:3:494:LYS:O	3:3:498:GLU:HG2	2.00	0.61
13:L:312:VAL:HA	13:L:397:PHE:HD2	1.65	0.61
4:E:212:PRO:HB3	7:O:6:LEU:HG	1.81	0.61
1:1:241:MET:O	1:1:248:GLY:N	2.29	0.61
1:1:338:VAL:O	1:1:342:TRP:HB2	1.99	0.61
9:X:3:ARG:HD2	9:X:58:LEU:HD23	1.82	0.61
11:J:50:PHE:HB2	11:J:124:PRO:HD3	1.82	0.61
14:M:304:THR:O	14:M:307:GLY:N	2.33	0.61
1:B:276:ILE:O	1:B:282:GLY:N	2.27	0.61
3:D:281:GLU:HB2	3:D:288:ILE:HG22	1.82	0.61
6:G:45:CYS:HG	17:G:201:SF4:FE3	1.15	0.61
3:3:261:VAL:O	3:3:616:ASN:ND2	2.32	0.61
4:4:373:PRO:O	4:4:377:ASN:ND2	2.33	0.61
16:H:154:ARG:NH2	16:H:227:GLU:OE2	2.33	0.61
13:T:168:GLY:O	13:T:208:LEU:HB3	2.01	0.61
3:3:185:LYS:NZ	3:3:439:GLU:OE2	2.21	0.61
1:B:340:ALA:HA	2:C:86:LEU:HD13	1.81	0.61
12:S:19:LEU:HD22	13:T:591:LEU:HD12	1.82	0.61
5:5:126:PHE:HB2	5:5:132:LEU:HD11	1.83	0.61
6:6:76:ASP:OD1	16:H:65:LYS:NZ	2.32	0.61
12:K:93:LEU:HD21	15:N:128:GLN:HB2	1.82	0.61
15:N:120:ALA:O	15:N:123:THR:OG1	2.19	0.61
3:D:538:ALA:HB3	3:D:541:ALA:HB2	1.81	0.61
6:G:62:ARG:HD2	16:Q:50:ARG:HH21	1.66	0.61
14:U:187:GLU:HG2	14:U:188:GLU:HG3	1.81	0.61
16:Q:227:GLU:HG2	16:Q:228:LEU:H	1.63	0.61
11:J:93:ALA:HB2	13:L:591:LEU:HD11	1.81	0.61
8:I:23:TYR:HH	8:I:123:ARG:HH11	1.47	0.61
16:Q:267:TRP:CG	16:Q:268:THR:N	2.68	0.61
4:E:156:ILE:O	4:E:159:LEU:HB2	2.00	0.61
16:Q:332:LEU:HB2	16:Q:333:PRO:HD3	1.80	0.61
1:1:75:LYS:NZ	1:1:218:ILE:O	2.33	0.61
3:3:190:TYR:OH	3:3:222:PHE:O	2.15	0.61
3:3:397:LEU:HD21	3:3:480:LEU:HD13	1.82	0.61
3:3:538:ALA:HB3	3:3:541:ALA:HB2	1.82	0.61
10:A:105:VAL:HG13	15:N:15:LEU:HD21	1.81	0.61
16:H:43:GLN:HE21	16:H:45:ARG:NH2	1.99	0.61
12:S:95:GLY:O	15:V:251:GLN:NE2	2.19	0.61
14:U:304:THR:O	14:U:307:GLY:N	2.34	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:3:271:SER:HG	7:9:69:TYR:HH	1.45	0.61
3:3:337:ARG:HH22	3:3:564:LEU:HD22	1.65	0.61
3:3:404:GLU:OE1	3:3:698:MET:N	2.29	0.61
4:4:87:TYR:CG	6:6:45:CYS:HB3	2.36	0.61
2:C:6:ASP:HB3	2:C:7:LYS:HE3	1.82	0.60
5:F:175:THR:HG22	5:F:178:ASP:HB2	1.82	0.60
9:X:24:LEU:O	9:X:84:GLN:NE2	2.34	0.60
13:T:214:VAL:HG13	13:T:219:GLN:HB2	1.83	0.60
10:A:71:PHE:HZ	10:A:107:PHE:HB2	1.66	0.60
11:J:69:PHE:HZ	16:H:156:SER:HB3	1.66	0.60
13:L:354:GLY:HA3	13:L:428:GLU:O	2.01	0.60
1:B:27:TRP:O	1:B:112:HIS:NE2	2.33	0.60
4:E:128:SER:OG	4:E:350:ARG:NH2	2.16	0.60
7:O:44:THR:HA	7:O:138:VAL:HG13	1.83	0.60
16:Q:140:GLY:HA3	16:Q:152:SER:CB	2.31	0.60
2:2:58:THR:OG1	3:3:214:MET:N	2.35	0.60
4:4:367:ARG:NH1	4:4:369:LYS:HB2	2.17	0.60
6:6:134:ASP:OD1	6:6:157:LYS:NZ	2.35	0.60
11:J:2:SER:HA	11:J:5:GLU:HB3	1.82	0.60
16:Q:43:GLN:NE2	16:Q:45:ARG:HH22	1.99	0.60
1:1:5:ILE:H	1:1:12:ARG:HH22	1.48	0.60
1:1:104:ARG:NH2	2:2:143:GLU:OE2	2.35	0.60
3:3:229:ILE:HD11	3:3:289:TRP:HZ3	1.65	0.60
5:5:35:LYS:NZ	5:5:103:THR:O	2.30	0.60
1:B:243:THR:HG22	1:B:244:GLU:H	1.67	0.60
4:E:30:VAL:HB	4:E:43:LEU:HB2	1.84	0.60
1:1:102:LYS:NZ	1:1:103:ASP:OD1	2.32	0.60
14:M:109:LEU:HD21	14:M:236:VAL:HG21	1.82	0.60
1:B:365:GLY:O	1:B:369:ASN:ND2	2.34	0.60
3:D:237:ASP:OD1	3:D:239:THR:HG22	2.01	0.60
15:V:319:ASP:HB3	15:V:322:LEU:HB2	1.83	0.60
16:Q:137:PHE:HA	16:Q:152:SER:HB2	1.84	0.60
4:4:225:PRO:HG2	4:4:228:VAL:HB	1.82	0.60
13:L:163:ARG:HE	14:M:399:VAL:HB	1.67	0.60
4:E:103:LYS:NZ	5:F:22:LEU:O	2.29	0.60
15:V:201:GLN:OE1	15:V:256:ARG:NH1	2.35	0.60
15:V:343:TRP:CD1	15:V:416:PRO:HG3	2.36	0.60
1:1:159:GLY:H	1:1:162:LEU:HD21	1.66	0.60
2:2:106:ILE:HG22	2:2:110:GLU:HG3	1.84	0.60
4:4:87:TYR:CB	6:6:45:CYS:HB3	2.32	0.60
13:T:234:THR:HG23	13:T:292:LYS:HE2	1.83	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:L:280:TYR:OH	13:L:531:ALA:O	2.16	0.60
5:F:103:THR:N	5:F:127:GLU:O	2.32	0.60
13:T:413:THR:HA	13:T:416:TYR:CE2	2.37	0.60
1:1:54:ILE:HG12	1:1:76:TRP:HE3	1.67	0.60
2:2:110:GLU:OE2	8:7:114:ARG:NE	2.31	0.60
4:4:240:ARG:NH2	4:4:347:GLU:OE2	2.34	0.60
1:B:437:TRP:N	2:C:95:GLU:OE1	2.34	0.60
2:C:42:ARG:HB2	2:C:45:ARG:HG2	1.83	0.60
3:D:94:ASP:OD2	3:D:97:SER:OG	2.17	0.60
7:O:6:LEU:HB3	16:Q:297:TRP:CZ2	2.36	0.60
15:V:261:SER:HG	15:V:375:TYR:HH	1.39	0.60
5:5:103:THR:HG22	5:5:126:PHE:HB3	1.84	0.59
14:M:238:VAL:O	14:M:241:PHE:HB2	2.02	0.59
1:B:108:GLU:O	1:B:144:ARG:NE	2.27	0.59
1:B:372:ALA:O	1:B:376:THR:OG1	2.10	0.59
13:T:124:TYR:OH	13:T:256:SER:OG	2.16	0.59
15:V:279:GLN:NE2	15:V:420:LEU:O	2.35	0.59
1:1:4:PRO:O	1:1:5:ILE:HG13	2.02	0.59
3:3:465:HIS:N	3:3:489:MET:SD	2.72	0.59
8:7:10:TYR:O	8:7:13:TRP:HB3	2.01	0.59
3:D:180:ARG:NH1	3:D:233:GLY:O	2.31	0.59
3:D:261:VAL:O	3:D:616:ASN:ND2	2.29	0.59
4:E:341:GLU:OE1	5:F:91:ARG:NH2	2.35	0.59
12:S:39:ASN:ND2	12:S:61:ILE:HG13	2.17	0.59
13:T:157:LYS:NZ	13:T:539:ASN:OD1	2.34	0.59
13:T:474:LYS:NZ	13:T:478:ALA:O	2.27	0.59
3:3:399:LEU:O	3:3:508:GLY:N	2.35	0.59
16:H:86:PRO:HG3	16:H:244:PHE:CE2	2.37	0.59
13:T:161:VAL:HG13	13:T:222:LEU:HD22	1.85	0.59
3:D:185:LYS:HB3	3:D:189:ARG:HH11	1.68	0.59
5:F:155:THR:N	6:G:119:ASN:OD1	2.34	0.59
3:3:273:GLU:HB2	3:3:302:ASP:HB2	1.83	0.59
15:N:272:ALA:O	15:N:276:GLY:N	2.35	0.59
3:D:494:LYS:O	3:D:498:GLU:HG2	2.03	0.59
6:G:132:PRO:HG3	6:G:178:ARG:HD2	1.85	0.59
5:5:68:PHE:HB2	5:5:94:VAL:HB	1.83	0.59
11:J:100:VAL:HA	13:L:598:LEU:HD21	1.84	0.59
14:M:281:PHE:HE2	14:M:332:LEU:HD21	1.67	0.59
3:D:48:CYS:SG	3:D:82:SER:N	2.75	0.59
6:G:86:LYS:NZ	9:X:118:ALA:O	2.30	0.59
15:V:136:TYR:HB2	15:V:199:VAL:HG21	1.84	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:6:54:THR:HA	6:6:59:ASP:HA	1.84	0.59
7:9:108:CYS:HA	17:9:202:SF4:S3	2.42	0.59
11:J:104:LEU:HD23	15:N:174:LEU:HD21	1.84	0.59
14:M:102:MET:HB3	14:M:230:LEU:HD23	1.85	0.59
13:T:359:LEU:HD23	13:T:437:GLU:HB3	1.85	0.59
4:4:26:MET:N	4:4:47:LEU:O	2.36	0.59
4:4:341:GLU:OE1	5:5:91:ARG:NH2	2.36	0.59
12:K:87:VAL:HG21	13:L:586:LEU:HB2	1.84	0.59
13:L:214:VAL:HG13	13:L:219:GLN:HB2	1.85	0.59
5:F:31:ARG:NH2	5:F:98:ASP:OD2	2.29	0.59
3:3:349:ALA:HB3	3:3:544:LEU:HD21	1.85	0.59
6:6:160:GLY:O	6:6:169:ARG:NH1	2.35	0.59
10:A:39:ALA:HA	10:A:42:MET:HG3	1.84	0.59
13:L:132:GLU:OE2	13:L:163:ARG:NH1	2.36	0.59
1:1:131:TYR:OH	2:2:17:LYS:O	2.15	0.59
13:L:59:TRP:HB2	13:L:65:PHE:HB2	1.84	0.59
16:H:161:SER:HA	16:H:310:TRP:HZ3	1.67	0.59
16:H:205:VAL:HG12	16:H:313:LEU:HD22	1.85	0.59
3:D:245:ARG:NH1	7:O:56:CYS:O	2.36	0.59
14:U:218:HIS:O	14:U:282:LYS:NZ	2.32	0.59
1:B:174:HIS:HE2	2:C:28:MET:HB2	1.67	0.58
2:C:96:LEU:HD21	2:C:134:ILE:HD11	1.85	0.58
6:G:37:TRP:HB3	6:G:75:ALA:HA	1.85	0.58
10:P:62:TYR:CD2	11:R:66:LEU:HD11	2.38	0.58
15:V:120:ALA:O	15:V:123:THR:OG1	2.19	0.58
5:5:58:LEU:HB2	5:5:67:ARG:HG3	1.84	0.58
10:A:113:LYS:NZ	15:N:83:GLU:OE2	2.36	0.58
4:E:240:ARG:HB2	4:E:266:LEU:HD23	1.85	0.58
5:F:171:ARG:NE	7:O:66:TYR:OH	2.36	0.58
13:T:426:LEU:HB3	13:T:513:GLN:HE22	1.68	0.58
4:4:163:VAL:HG13	4:4:164:THR:HG23	1.84	0.58
6:6:90:PRO:O	6:6:93:ARG:HB3	2.03	0.58
6:6:169:ARG:O	6:6:169:ARG:HG2	2.02	0.58
11:J:156:LEU:HD11	15:N:123:THR:HG21	1.85	0.58
16:H:333:PRO:HG2	16:H:336:TYR:CD2	2.38	0.58
2:C:9:ASP:OD1	2:C:9:ASP:N	2.36	0.58
3:D:131:GLN:HG2	4:E:325:ILE:HG23	1.85	0.58
5:F:121:LEU:HA	5:F:145:PRO:HD2	1.85	0.58
10:P:5:GLN:OE1	16:Q:10:TYR:OH	2.14	0.58
15:V:317:ARG:NH1	15:V:384:ALA:O	2.36	0.58
16:Q:2:THR:HA	16:Q:5:TYR:HD2	1.67	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:1:303:THR:O	1:1:307:LEU:N	2.30	0.58
14:M:138:GLY:O	14:M:141:ARG:NE	2.31	0.58
6:G:76:ASP:OD1	16:Q:65:LYS:NZ	2.32	0.58
6:G:169:ARG:HG3	6:G:169:ARG:NH1	2.18	0.58
15:V:279:GLN:HG3	15:V:423:LEU:HB2	1.86	0.58
1:1:402:LEU:O	1:1:406:ALA:N	2.36	0.58
1:B:291:ILE:HG12	1:B:299:PRO:HB3	1.85	0.58
5:F:103:THR:HG22	5:F:126:PHE:HB3	1.85	0.58
5:F:134:LYS:HD2	5:F:139:GLU:HA	1.84	0.58
11:R:65:VAL:HG11	16:Q:160:ILE:HD13	1.84	0.58
15:V:38:ALA:HA	15:V:41:LEU:HD12	1.86	0.58
16:Q:48:PRO:C	16:Q:50:ARG:H	2.07	0.58
3:3:46:ARG:HH22	3:3:81:ALA:HB2	1.69	0.58
8:7:37:PHE:HE1	8:7:74:PRO:HA	1.68	0.58
3:D:719:HIS:HB3	3:D:722:THR:HG23	1.86	0.58
4:E:163:VAL:O	7:O:36:ARG:NH1	2.26	0.58
15:V:261:SER:OG	15:V:375:TYR:OH	2.15	0.58
2:2:66:PHE:O	3:3:205:ARG:NE	2.37	0.58
3:3:186:ARG:HD3	3:3:229:ILE:HG22	1.86	0.58
4:4:73:ARG:NE	4:4:81:TYR:OH	2.37	0.58
10:A:33:PRO:HD2	16:H:70:GLU:HB2	1.86	0.58
11:J:146:LEU:HD23	12:K:66:ALA:HB2	1.86	0.58
15:V:187:ALA:O	15:V:216:LYS:NZ	2.36	0.58
15:V:224:LEU:HD11	15:V:281:LEU:HD23	1.86	0.58
13:L:356:TRP:N	13:L:425:PHE:O	2.31	0.58
5:F:163:ARG:CZ	7:O:90:VAL:HG11	2.34	0.58
6:G:114:SER:OG	7:O:96:LEU:O	2.21	0.58
6:G:152:MET:SD	7:O:27:PRO:HG3	2.43	0.58
16:Q:99:LEU:HD12	16:Q:116:ILE:HG13	1.86	0.58
2:2:109:GLY:HA2	8:7:91:ILE:HD13	1.85	0.58
13:L:557:ASP:OD2	14:M:287:TYR:OH	2.22	0.58
6:G:62:ARG:HG2	16:Q:48:PRO:HA	1.86	0.58
8:I:43:ARG:NH2	8:I:44:MET:O	2.37	0.58
16:Q:221:LEU:N	16:Q:222:PRO:HA	2.18	0.58
7:9:101:CYS:N	17:9:201:SF4:S4	2.76	0.58
7:9:171:GLU:OE2	8:7:43:ARG:NH2	2.37	0.58
4:E:140:LEU:HD11	4:E:217:ARG:HH12	1.68	0.58
6:G:37:TRP:HB2	16:Q:65:LYS:HE2	1.86	0.58
12:S:95:GLY:HA2	15:V:256:ARG:HE	1.69	0.58
3:3:592:PRO:HA	3:3:595:GLU:HG2	1.84	0.57
4:4:130:LEU:HD22	4:4:149:ALA:HB1	1.83	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:586:HIS:CE1	3:D:640:VAL:HG21	2.39	0.57
16:H:274:VAL:HG12	16:H:278:TRP:CD1	2.40	0.57
7:O:108:CYS:HA	17:O:202:SF4:S3	2.44	0.57
1:1:419:ASP:HA	1:1:422:LEU:HD12	1.85	0.57
3:3:115:HIS:HB3	4:4:321:MET:HE3	1.86	0.57
3:3:227:THR:HG21	3:3:237:ASP:HB2	1.86	0.57
3:3:635:GLU:OE2	9:W:7:ARG:NH1	2.35	0.57
7:9:43:LEU:HB2	7:9:137:LEU:HD12	1.85	0.57
12:K:28:PHE:HZ	12:K:68:VAL:HA	1.69	0.57
13:L:355:LEU:HB2	13:L:425:PHE:HA	1.86	0.57
13:L:366:ALA:HB1	13:L:420:TRP:CH2	2.38	0.57
1:B:122:GLY:HA3	1:B:169:PHE:HE1	1.70	0.57
3:D:635:GLU:HB3	3:D:639:GLN:HB3	1.84	0.57
16:Q:37:ARG:O	16:Q:41:ARG:HG2	2.04	0.57
4:4:64:THR:N	4:4:409:ARG:OXT	2.36	0.57
8:7:49:ASP:OD1	8:7:75:ARG:NE	2.32	0.57
14:M:126:LEU:HD11	14:M:149:VAL:HG22	1.86	0.57
2:C:67:TYR:HA	3:D:205:ARG:HH21	1.69	0.57
9:X:3:ARG:HH21	9:X:60:PRO:HB3	1.70	0.57
13:T:290:ASP:OD1	13:T:347:GLN:HG2	2.04	0.57
13:T:358:HIS:HB3	13:T:433:HIS:CE1	2.39	0.57
14:U:70:LEU:HD13	14:U:312:LEU:HD13	1.84	0.57
15:V:99:ALA:O	15:V:225:ARG:NH1	2.38	0.57
15:V:294:LEU:HG	15:V:402:VAL:HG13	1.85	0.57
16:Q:35:GLU:OE1	16:Q:249:TYR:OH	2.20	0.57
16:Q:131:LEU:HA	16:Q:134:TYR:HB2	1.87	0.57
16:Q:291:ILE:HA	16:Q:294:ARG:CG	2.34	0.57
3:3:557:SER:OG	3:3:559:ASP:OD1	2.22	0.57
4:4:45:VAL:HG13	4:4:55:VAL:HG22	1.85	0.57
4:4:168:PHE:CE1	6:6:141:PRO:HG3	2.40	0.57
14:M:215:PRO:HG2	14:M:216:PRO:HD3	1.87	0.57
3:D:188:VAL:HG12	3:D:200:LEU:C	2.24	0.57
11:R:47:ASP:OD1	11:R:49:ARG:NH2	2.38	0.57
13:T:115:MET:HG2	13:T:244:THR:HG22	1.85	0.57
13:T:586:LEU:HD11	15:V:135:LYS:HA	1.85	0.57
1:1:128:THR:O	1:1:169:PHE:HA	2.04	0.57
14:M:56:LEU:HB3	14:M:59:ALA:HB3	1.86	0.57
15:N:249:LEU:HD23	15:N:374:TYR:HD2	1.70	0.57
3:D:188:VAL:CG1	3:D:201:ASP:HA	2.34	0.57
14:U:318:SER:HA	14:U:321:TYR:CZ	2.38	0.57
4:4:224:ILE:HD11	4:4:275:ARG:CZ	2.35	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:L:366:ALA:HB1	13:L:420:TRP:HH2	1.69	0.57
2:C:114:ASP:OD2	2:C:158:ARG:NH2	2.32	0.57
3:3:701:ALA:N	3:3:763:LEU:O	2.34	0.57
4:4:293:ALA:HA	4:4:296:ARG:HG2	1.85	0.57
4:4:367:ARG:HH12	4:4:369:LYS:HB2	1.69	0.57
10:A:2:ALA:H	11:J:49:ARG:HH12	1.50	0.57
14:M:55:LEU:HD11	15:N:416:PRO:HD2	1.87	0.57
16:Q:137:PHE:HB3	16:Q:156:SER:HB2	1.87	0.57
1:1:193:GLU:OE1	1:1:200:ARG:NH2	2.37	0.57
10:A:88:LEU:HB3	10:A:92:GLY:HA3	1.87	0.57
16:Q:274:VAL:HG12	16:Q:278:TRP:CD1	2.40	0.57
2:2:85:THR:HG22	2:2:86:LEU:H	1.69	0.57
3:3:175:ILE:HG22	3:3:236:LEU:HB2	1.85	0.57
4:4:173:ILE:O	4:4:174:ARG:NH1	2.38	0.57
4:E:148:TYR:O	4:E:151:ARG:HB3	2.04	0.57
7:O:149:GLU:O	7:O:153:THR:OG1	2.18	0.57
11:R:64:VAL:HG13	16:Q:134:TYR:OH	2.05	0.57
3:3:382:PHE:HB3	3:3:532:VAL:HB	1.86	0.56
10:A:81:TYR:CE2	10:A:96:VAL:HG11	2.40	0.56
13:L:317:VAL:HG12	13:L:388:ILE:HG12	1.87	0.56
16:H:147:TYR:CD1	16:H:229:VAL:HG22	2.40	0.56
1:B:44:VAL:HG13	1:B:48:LYS:HB2	1.87	0.56
3:D:133:ARG:NE	3:D:136:GLU:OE2	2.29	0.56
3:D:154:TYR:HB3	4:E:322:GLU:HB2	1.87	0.56
4:E:219:ARG:HD3	4:E:271:ASP:OD2	2.04	0.56
10:P:9:GLY:HA2	16:Q:13:VAL:HG11	1.87	0.56
13:T:360:PRO:HA	13:T:363:ARG:HH12	1.70	0.56
15:V:126:ARG:HH11	15:V:128:GLN:HG2	1.70	0.56
16:Q:43:GLN:NE2	16:Q:45:ARG:NH2	2.44	0.56
1:B:272:PHE:HZ	1:B:316:LEU:HD11	1.71	0.56
1:B:293:GLY:O	1:B:327:GLY:N	2.38	0.56
4:E:201:ILE:HA	4:E:204:TYR:CD2	2.39	0.56
16:Q:69:LYS:HB3	16:Q:238:SER:HA	1.86	0.56
6:6:163:TYR:OH	6:6:169:ARG:NH2	2.38	0.56
13:L:124:TYR:HB2	13:L:183:LEU:HD22	1.87	0.56
13:L:213:ALA:HB2	13:L:252:LEU:HD23	1.88	0.56
16:H:227:GLU:HB2	16:H:299:ARG:NH2	2.21	0.56
16:H:249:TYR:OH	16:H:294:ARG:NH2	2.39	0.56
1:B:287:ILE:HA	1:B:332:PRO:HA	1.86	0.56
4:E:222:GLY:HA3	4:E:275:ARG:HH22	1.70	0.56
6:G:156:LYS:NZ	7:O:152:ARG:HH21	2.04	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:G:163:TYR:CD2	6:G:169:ARG:HA	2.40	0.56
10:P:62:TYR:HD2	11:R:66:LEU:HD11	1.70	0.56
14:U:167:ARG:NH2	14:U:173:PRO:O	2.31	0.56
14:U:314:LEU:HB2	14:U:376:GLY:HA3	1.85	0.56
16:Q:71:ASP:OD1	16:Q:240:LYS:NZ	2.18	0.56
2:2:9:ASP:OD1	2:2:9:ASP:N	2.38	0.56
3:3:254:THR:O	3:3:280:ARG:NH2	2.28	0.56
13:L:325:HIS:NE2	13:L:329:LYS:HG3	2.20	0.56
14:M:205:THR:HG23	14:M:238:VAL:HG23	1.87	0.56
3:D:113:LEU:O	3:D:161:ARG:NH1	2.38	0.56
3:D:356:LEU:HD22	3:D:654:PHE:HB2	1.87	0.56
5:F:3:LEU:HD21	5:F:25:LEU:HD22	1.86	0.56
5:F:16:PRO:HD2	5:F:28:VAL:HG13	1.88	0.56
5:F:38:MET:HA	5:F:41:TYR:CD2	2.41	0.56
15:V:185:PHE:O	15:V:195:TRP:NE1	2.34	0.56
15:V:188:ALA:HB3	15:V:216:LYS:NZ	2.19	0.56
16:Q:150:LEU:O	16:Q:154:ARG:HG3	2.05	0.56
3:3:414:SER:O	3:3:418:ARG:NE	2.23	0.56
4:4:371:ARG:HG3	5:5:51:ASP:OD1	2.05	0.56
11:J:157:VAL:HG12	11:J:159:PRO:HD3	1.87	0.56
13:L:432:HIS:CE1	13:L:434:HIS:HB2	2.40	0.56
14:M:122:PHE:O	14:M:234:TYR:OH	2.14	0.56
4:E:132:PHE:CE2	4:E:279:ARG:HD2	2.40	0.56
13:T:154:SER:HB2	13:T:228:ASP:HB3	1.88	0.56
1:1:373:LYS:NZ	3:3:158:GLU:OE2	2.32	0.56
3:3:48:CYS:SG	3:3:82:SER:N	2.79	0.56
13:L:371:LEU:HB3	13:L:376:LEU:HB2	1.88	0.56
14:M:75:PHE:CZ	14:M:111:ALA:HB2	2.38	0.56
15:N:40:LEU:HD12	15:N:67:LEU:HD12	1.88	0.56
4:E:371:ARG:HG3	5:F:51:ASP:OD1	2.05	0.56
5:F:154:GLU:OE1	5:F:171:ARG:NH2	2.25	0.56
9:X:35:THR:O	9:X:93:VAL:HA	2.05	0.56
11:R:29:ALA:HA	12:S:29:LEU:HD21	1.86	0.56
16:Q:302:TYR:HA	16:Q:305:LEU:HB3	1.87	0.56
4:4:110:PRO:HB3	4:4:301:PRO:HG2	1.86	0.56
10:A:57:PHE:HB3	10:A:58:PRO:HD2	1.88	0.56
16:H:151:GLY:HA3	16:H:230:GLY:HA2	1.86	0.56
1:B:190:ASN:OD1	1:B:200:ARG:NE	2.27	0.56
4:E:167:ARG:HD3	6:G:143:ARG:NH1	2.21	0.56
6:G:127:VAL:HG12	6:G:131:VAL:HG22	1.88	0.56
6:G:138:PRO:O	6:G:142:PRO:HB3	2.05	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:G:162:ALA:CB	6:G:170:LEU:HD12	2.33	0.56
3:3:29:ASP:OD1	3:3:29:ASP:N	2.38	0.56
7:9:6:LEU:HB3	16:H:297:TRP:CZ2	2.41	0.56
7:9:13:THR:HG21	16:H:296:THR:HG23	1.88	0.56
13:L:380:SER:HB3	13:L:457:GLY:H	1.71	0.56
13:L:490:GLU:O	13:L:494:ILE:HG12	2.05	0.56
16:H:16:LYS:HZ3	16:H:112:GLN:HB2	1.71	0.56
1:B:83:ASP:CG	1:B:87:HIS:HE2	2.08	0.56
2:C:14:THR:HA	2:C:17:LYS:HE3	1.88	0.56
2:C:171:LYS:NZ	2:C:178:GLU:O	2.39	0.56
1:1:87:HIS:HB2	1:1:127:ALA:HA	1.88	0.56
2:2:130:THR:HB	2:2:143:GLU:HB3	1.87	0.56
3:3:48:CYS:SG	3:3:83:CYS:N	2.74	0.56
8:7:36:ASP:HA	8:7:54:ILE:HA	1.88	0.56
3:D:285:VAL:HG13	3:D:286:ASN:H	1.71	0.56
4:E:52:VAL:O	4:E:387:GLY:N	2.31	0.56
4:E:311:PRO:HD3	4:E:330:HIS:CE1	2.41	0.56
4:E:350:ARG:O	4:E:373:PRO:HB2	2.06	0.56
13:T:7:ILE:HD11	13:T:120:LEU:HD12	1.88	0.56
13:T:487:LEU:HA	13:T:490:GLU:HG2	1.87	0.56
6:6:73:ARG:NH2	10:A:40:LYS:O	2.35	0.56
10:A:65:ALA:O	10:A:69:ILE:HG23	2.05	0.56
11:J:105:ALA:O	11:J:109:TRP:N	2.39	0.56
11:J:119:LEU:HD23	12:K:51:LEU:HD12	1.86	0.56
13:L:267:SER:HB3	13:L:311:GLY:O	2.06	0.56
14:M:46:GLY:HA2	14:M:68:ASP:HA	1.87	0.56
4:E:163:VAL:HG13	4:E:164:THR:HG23	1.88	0.56
15:V:118:LEU:HD23	15:V:121:LEU:HD12	1.88	0.56
6:6:153:GLN:HG3	7:9:124:TYR:CZ	2.41	0.55
6:6:153:GLN:O	7:9:124:TYR:OH	2.25	0.55
10:A:67:LEU:HB3	16:H:310:TRP:HZ2	1.70	0.55
14:M:115:LEU:HD12	14:M:180:LEU:HD13	1.88	0.55
3:D:135:VAL:HA	4:E:326:TYR:CZ	2.41	0.55
8:I:109:PRO:O	8:I:114:ARG:NH1	2.38	0.55
11:R:157:VAL:HG12	11:R:159:PRO:HD3	1.88	0.55
4:4:47:LEU:HA	4:4:53:LEU:HD23	1.87	0.55
4:4:140:LEU:HD21	4:4:217:ARG:HH12	1.70	0.55
6:6:132:PRO:HG2	6:6:175:ALA:HA	1.87	0.55
15:N:63:THR:HG21	15:N:96:HIS:ND1	2.21	0.55
4:E:247:ASP:O	4:E:251:ALA:N	2.29	0.55
7:O:94:ASN:OD1	7:O:97:ARG:N	2.39	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:4:191:LYS:HE2	4:4:294:LEU:HD21	1.89	0.55
10:A:63:VAL:HG11	10:A:115:VAL:HG11	1.88	0.55
15:N:265:HIS:NE2	15:N:333:LEU:O	2.39	0.55
16:H:50:ARG:C	16:H:52:GLY:H	2.08	0.55
3:D:194:VAL:HG12	3:D:411:LEU:HD22	1.88	0.55
3:D:468:HIS:ND1	3:D:469:ARG:O	2.37	0.55
13:L:286:PHE:HD2	13:L:416:TYR:HB3	1.71	0.55
13:L:290:ASP:OD1	13:L:291:ILE:N	2.39	0.55
15:N:279:GLN:HG3	15:N:423:LEU:HB2	1.88	0.55
3:D:270:ARG:HH12	5:F:170:PHE:HE1	1.54	0.55
3:D:713:ARG:HH21	3:D:746:ARG:NH2	2.02	0.55
15:V:203:SER:O	15:V:255:LYS:NZ	2.39	0.55
1:B:161:ASN:HA	1:B:167:PHE:O	2.06	0.55
11:R:68:LEU:HD23	11:R:71:ILE:HD11	1.87	0.55
11:R:69:PHE:O	11:R:73:LEU:HG	2.07	0.55
14:U:325:LEU:HG	14:U:361:LEU:HB3	1.88	0.55
1:1:273:ARG:NH2	1:1:308:ASP:OD2	2.33	0.55
3:3:157:PHE:CZ	3:3:159:PHE:HB2	2.41	0.55
10:A:34:LYS:N	16:H:70:GLU:OE1	2.33	0.55
15:N:294:LEU:HG	15:N:402:VAL:HG13	1.87	0.55
4:E:27:THR:HA	4:E:45:VAL:O	2.05	0.55
4:E:102:GLU:OE2	4:E:117:ARG:NH2	2.40	0.55
13:T:9:LEU:HB2	13:T:10:PRO:HD3	1.88	0.55
16:H:227:GLU:HB2	16:H:299:ARG:CZ	2.37	0.55
16:H:287:LEU:O	16:H:291:ILE:HG13	2.07	0.55
1:B:165:THR:HG23	1:B:167:PHE:H	1.72	0.55
3:D:603:PRO:HG2	3:D:634:ALA:HA	1.86	0.55
3:D:697:THR:OG1	3:D:763:LEU:HA	2.06	0.55
3:D:720:PRO:HG3	3:D:749:HIS:HB3	1.88	0.55
4:E:211:SER:O	4:E:215:TYR:HB2	2.07	0.55
4:E:250:LYS:HE2	4:E:262:PHE:HB3	1.88	0.55
10:P:88:LEU:HB3	10:P:92:GLY:HA3	1.88	0.55
1:1:254:ILE:HD11	1:1:330:LEU:HD11	1.89	0.55
11:J:147:MET:O	11:J:150:THR:OG1	2.22	0.55
3:D:34:CYS:N	3:D:45:CYS:SG	2.75	0.55
3:D:557:SER:OG	3:D:559:ASP:OD1	2.21	0.55
4:4:62:LEU:HD11	6:6:43:LEU:O	2.06	0.55
14:M:91:VAL:HG23	14:M:92:GLU:H	1.71	0.55
15:N:118:LEU:HD13	15:N:211:MET:HG2	1.89	0.55
3:D:256:CYS:HB2	3:D:265:ILE:HD13	1.89	0.55
4:E:73:ARG:NH1	5:F:171:ARG:HH21	2.05	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:F:123:GLY:HA2	5:F:144:HIS:CE1	2.41	0.55
16:Q:301:ARG:HE	16:Q:304:GLN:N	2.04	0.55
7:9:102:GLY:HA2	7:9:115:LEU:HD11	1.90	0.55
4:E:248:VAL:HA	4:E:251:ALA:HB3	1.89	0.55
14:U:91:VAL:HB	14:U:95:PHE:HE1	1.72	0.55
14:U:95:PHE:HB2	14:U:98:LEU:HD12	1.88	0.55
1:1:275:LEU:HA	1:1:279:TRP:CD1	2.41	0.54
4:4:336:HIS:ND1	5:5:189:ARG:O	2.40	0.54
5:5:144:HIS:HB2	5:5:147:ARG:HD3	1.89	0.54
14:M:318:SER:HA	14:M:321:TYR:CZ	2.42	0.54
16:H:226:GLN:HB2	16:H:299:ARG:NH2	2.22	0.54
3:D:157:PHE:CE1	3:D:159:PHE:HB2	2.42	0.54
10:P:66:MET:HG3	12:S:69:ALA:HB1	1.89	0.54
13:T:163:ARG:HH21	14:U:399:VAL:HB	1.72	0.54
14:U:321:TYR:CE1	14:U:365:MET:HA	2.42	0.54
2:2:112:THR:HB	2:2:117:PHE:HB2	1.90	0.54
3:3:48:CYS:O	3:3:82:SER:OG	2.15	0.54
4:4:194:LEU:HD21	4:4:290:ILE:HG22	1.87	0.54
4:4:285:GLU:O	4:4:289:ILE:HG12	2.06	0.54
4:4:384:ALA:HB1	4:4:396:ILE:HD11	1.90	0.54
8:7:88:ARG:NH2	8:7:126:LEU:HB3	2.23	0.54
11:J:122:GLY:HA3	12:K:54:GLN:HE22	1.72	0.54
13:L:187:GLU:HA	13:L:190:GLU:HG2	1.90	0.54
3:D:129:GLU:O	3:D:133:ARG:HG2	2.07	0.54
13:T:490:GLU:O	13:T:494:ILE:HG12	2.07	0.54
14:U:13:GLY:HA2	14:U:97:GLY:HA2	1.87	0.54
3:3:349:ALA:O	3:3:540:ASN:ND2	2.34	0.54
5:5:39:ALA:HA	5:5:107:LEU:HD21	1.88	0.54
11:J:94:ALA:O	11:J:97:ALA:HB3	2.08	0.54
14:M:314:LEU:HB2	14:M:376:GLY:HA3	1.87	0.54
3:D:11:VAL:HG21	3:D:26:ALA:HB2	1.89	0.54
3:D:310:LEU:N	3:D:601:VAL:O	2.35	0.54
16:Q:90:VAL:HG21	16:Q:243:LEU:HB3	1.89	0.54
1:1:362:GLY:O	1:1:367:MET:N	2.29	0.54
7:9:133:LYS:O	7:9:137:LEU:HD13	2.08	0.54
13:L:287:GLY:HA3	13:L:528:SER:HB2	1.90	0.54
15:N:53:TYR:HE1	15:N:96:HIS:HE2	1.54	0.54
1:B:342:TRP:HE1	1:B:372:ALA:HA	1.72	0.54
8:I:6:GLU:O	8:I:9:LEU:HB3	2.07	0.54
14:U:281:PHE:CD1	14:U:341:ILE:HG22	2.43	0.54
3:3:656:LEU:HD11	9:W:3:ARG:HD3	1.89	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:4:314:ARG:HB3	8:7:44:MET:HE3	1.89	0.54
10:A:81:TYR:HB2	11:J:132:TYR:CZ	2.42	0.54
11:J:128:GLY:O	11:J:132:TYR:N	2.36	0.54
13:L:352:MET:HB3	13:L:424:VAL:HA	1.90	0.54
14:M:338:THR:HG22	14:M:340:GLU:H	1.71	0.54
15:N:122:ALA:HA	15:N:204:PRO:HD2	1.89	0.54
1:B:437:TRP:CZ3	2:C:147:ARG:HA	2.41	0.54
3:D:123:ASP:HB3	3:D:236:LEU:HD22	1.90	0.54
3:D:576:ALA:O	3:D:580:LYS:NZ	2.28	0.54
3:D:603:PRO:HB2	3:D:634:ALA:HB2	1.90	0.54
4:E:379:GLN:HG2	5:F:113:PHE:CD2	2.42	0.54
7:O:43:LEU:HB2	7:O:137:LEU:HD12	1.89	0.54
14:U:41:LEU:O	14:U:42:THR:HG22	2.06	0.54
14:U:138:GLY:O	14:U:141:ARG:NE	2.35	0.54
1:1:65:ARG:NH1	1:1:249:MET:O	2.41	0.54
1:1:313:TYR:HD1	1:1:323:LEU:HB3	1.73	0.54
13:L:433:HIS:ND1	13:L:433:HIS:O	2.41	0.54
4:E:260:TYR:HA	4:E:292:GLN:HE22	1.72	0.54
6:G:101:ASP:OD1	6:G:180:ARG:NH2	2.40	0.54
13:T:564:TYR:OH	14:U:209:PRO:O	2.18	0.54
14:U:346:GLY:HA3	14:U:418:GLY:HA2	1.89	0.54
2:2:58:THR:HG23	3:3:213:THR:HA	1.89	0.54
14:M:16:LEU:HD22	14:M:97:GLY:H	1.73	0.54
14:M:82:VAL:HG21	14:M:103:GLU:HB2	1.89	0.54
1:B:195:LEU:HD23	2:C:24:ARG:NH1	2.22	0.54
1:B:425:ALA:O	1:B:428:LYS:NZ	2.28	0.54
1:B:437:TRP:HH2	2:C:147:ARG:HG3	1.64	0.54
10:P:57:PHE:HB3	10:P:58:PRO:HD2	1.88	0.54
12:S:7:SER:OG	15:V:149:TYR:OH	2.24	0.54
15:V:168:GLU:HG2	15:V:169:GLY:H	1.73	0.54
16:Q:99:LEU:HA	16:Q:116:ILE:O	2.08	0.54
16:Q:218:PRO:HA	16:Q:300:LEU:HD22	1.90	0.54
1:1:18:TYR:N	1:1:265:GLU:OE1	2.37	0.54
1:1:153:ARG:NH2	1:1:171:LEU:O	2.41	0.54
4:4:263:ASP:HB2	4:4:285:GLU:CG	2.32	0.54
3:D:728:LEU:HB3	3:D:747:VAL:HG11	1.89	0.54
4:E:196:VAL:O	4:E:200:ARG:HG2	2.08	0.54
12:S:88:ASP:OD2	13:T:587:ARG:NH1	2.41	0.54
14:U:357:LEU:HD22	14:U:433:ALA:HB2	1.90	0.54
10:A:69:ILE:HG22	11:J:62:ALA:HB1	1.89	0.54
11:J:12:LEU:HD22	12:K:10:LEU:HD11	1.89	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:J:152:VAL:HG22	15:N:87:LEU:HD13	1.90	0.54
14:M:114:ASP:HB3	14:M:176:LEU:HD23	1.90	0.54
16:H:326:LEU:HD12	16:H:330:LEU:HD23	1.88	0.54
4:E:64:THR:OG1	6:G:83:ARG:HD2	2.07	0.54
13:T:175:ILE:HG23	13:T:201:LEU:HG	1.90	0.54
14:U:338:THR:HG22	14:U:340:GLU:H	1.72	0.54
16:Q:218:PRO:C	16:Q:220:ASP:H	2.11	0.54
3:3:414:SER:HG	3:3:443:ARG:NH2	2.06	0.54
4:4:211:SER:HB2	4:4:214:PHE:HB3	1.89	0.54
11:J:146:LEU:O	11:J:150:THR:HG23	2.07	0.54
16:H:276:TYR:HD2	16:H:280:PHE:HE2	1.54	0.54
1:B:18:TYR:HB2	1:B:265:GLU:HB2	1.88	0.54
1:B:241:MET:O	1:B:248:GLY:N	2.40	0.54
4:E:64:THR:N	4:E:409:ARG:OXT	2.38	0.54
11:R:64:VAL:HA	11:R:67:PHE:HB2	1.89	0.54
13:T:358:HIS:HB3	13:T:433:HIS:NE2	2.22	0.54
14:U:228:ASP:OD2	14:U:282:LYS:NZ	2.34	0.54
15:V:422:ALA:O	15:V:423:LEU:HD23	2.08	0.54
3:3:469:ARG:HB3	3:3:754:PRO:HG3	1.90	0.53
10:A:56:ARG:HD3	11:J:73:LEU:O	2.07	0.53
1:B:25:GLY:O	1:B:28:THR:OG1	2.16	0.53
3:D:583:VAL:HG21	3:D:597:TYR:O	2.08	0.53
6:G:93:ARG:NH1	9:X:122:ASP:OD2	2.41	0.53
6:G:179:THR:HB	9:X:127:LEU:HB2	1.91	0.53
7:O:46:HIS:CD2	7:O:52:LYS:HG2	2.43	0.53
3:3:583:VAL:HG23	3:3:599:HIS:H	1.74	0.53
3:3:713:ARG:HH21	3:3:746:ARG:HH21	1.57	0.53
6:6:106:ILE:HD11	6:6:154:LEU:HD22	1.91	0.53
14:M:41:LEU:O	14:M:42:THR:HG22	2.06	0.53
3:D:17:THR:HG22	3:D:18:SER:O	2.08	0.53
4:E:73:ARG:NH2	6:G:117:MET:O	2.41	0.53
4:E:86:ASP:HA	4:E:403:VAL:HG11	1.89	0.53
6:G:39:ALA:HB2	6:G:75:ALA:HB3	1.90	0.53
9:X:7:ARG:NE	9:X:61:ASP:OD2	2.41	0.53
13:T:285:ALA:O	13:T:294:ILE:HG13	2.08	0.53
16:Q:39:LEU:O	16:Q:43:GLN:CG	2.53	0.53
15:N:54:ALA:N	15:N:100:SER:O	2.28	0.53
3:D:190:TYR:O	3:D:195:PRO:HD2	2.08	0.53
3:D:300:TRP:HE1	3:D:703:GLN:HE21	1.55	0.53
14:U:93:GLY:HA3	14:U:136:TYR:HE1	1.74	0.53
1:1:393:LEU:HD22	3:3:106:GLY:HA3	1.91	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:5:3:LEU:HD21	5:5:25:LEU:HD22	1.90	0.53
10:A:68:PHE:CD2	16:H:164:LEU:HB2	2.43	0.53
1:B:287:ILE:HG12	1:B:330:LEU:HB3	1.91	0.53
2:C:61:MET:O	2:C:65:SER:OG	2.23	0.53
2:C:79:HIS:H	2:C:137:ASN:HD21	1.56	0.53
20:E:501:HQH:O1	16:Q:226:GLN:NE2	2.41	0.53
6:G:163:TYR:HD1	7:O:152:ARG:HH11	1.55	0.53
12:S:28:PHE:CZ	12:S:68:VAL:HA	2.43	0.53
13:T:88:HIS:O	13:T:92:ILE:HG13	2.08	0.53
14:U:289:GLY:O	14:U:293:MET:HG2	2.08	0.53
1:1:259:LYS:NZ	2:2:178:GLU:OE2	2.42	0.53
2:2:173:GLY:HA3	2:2:176:VAL:O	2.08	0.53
3:3:225:ASN:O	3:3:229:ILE:HG13	2.08	0.53
3:3:439:GLU:HG2	3:3:440:ARG:HG2	1.91	0.53
12:K:79:PHE:CD2	12:K:85:THR:HA	2.44	0.53
13:L:87:ILE:HD12	13:L:239:LEU:HD13	1.90	0.53
14:M:281:PHE:CE2	14:M:332:LEU:HD21	2.44	0.53
14:M:335:ARG:NH1	14:M:423:LYS:O	2.41	0.53
15:N:262:SER:HG	15:N:288:TYR:HH	1.56	0.53
16:H:177:VAL:HG21	16:H:185:ILE:HG23	1.91	0.53
1:B:437:TRP:O	2:C:147:ARG:NH2	2.40	0.53
3:D:224:GLY:O	3:D:227:THR:HB	2.09	0.53
4:E:225:PRO:HG2	4:E:228:VAL:HB	1.90	0.53
7:O:101:CYS:N	17:O:201:SF4:S4	2.81	0.53
13:T:108:PHE:HE1	13:T:236:VAL:HG22	1.74	0.53
2:2:101:THR:O	2:2:105:GLY:N	2.29	0.53
4:4:52:VAL:HG21	4:4:393:MET:HB2	1.91	0.53
8:7:35:ALA:HB3	8:7:56:THR:HB	1.91	0.53
14:M:128:PRO:O	14:M:132:MET:HG2	2.09	0.53
14:M:235:LYS:HD3	14:M:293:MET:HG3	1.90	0.53
15:N:245:ASN:OD1	15:N:374:TYR:OH	2.26	0.53
1:B:8:GLY:HA2	1:B:270:THR:HG22	1.89	0.53
3:D:686:LYS:HD3	3:D:688:ARG:NH2	2.22	0.53
4:E:168:PHE:CE1	6:G:141:PRO:HG3	2.42	0.53
4:E:171:ASN:OD1	4:E:174:ARG:NH1	2.32	0.53
14:U:128:PRO:O	14:U:132:MET:HG2	2.09	0.53
1:1:303:THR:HB	1:1:306:VAL:HB	1.90	0.53
3:3:129:GLU:O	3:3:133:ARG:HG2	2.09	0.53
3:3:183:HIS:NE2	3:3:209:THR:O	2.38	0.53
4:4:306:ASN:ND2	5:5:192:TYR:OH	2.26	0.53
15:N:187:ALA:O	15:N:216:LYS:NZ	2.40	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
16:H:190:LYS:NZ	16:H:270:PRO:HA	2.23	0.53
3:D:690:GLY:HA2	3:D:770:ARG:HB3	1.91	0.53
5:F:131:ASP:OD2	5:F:133:ARG:NH2	2.37	0.53
3:3:141:GLU:OE2	3:3:143:TYR:OH	2.26	0.53
4:4:352:GLU:OE2	5:5:87:ARG:NH1	2.35	0.53
12:K:93:LEU:HD22	15:N:201:GLN:HB3	1.91	0.53
13:L:70:ASP:OD2	13:L:255:ARG:NH2	2.40	0.53
2:C:89:LYS:HG3	2:C:94:GLU:HG2	1.91	0.53
6:G:56:ALA:HB2	16:Q:44:VAL:HG12	1.87	0.53
13:T:77:LEU:HD12	13:T:116:LEU:HD22	1.91	0.53
15:V:272:ALA:O	15:V:276:GLY:N	2.42	0.53
16:Q:265:GLY:O	16:Q:282:LYS:NZ	2.29	0.53
16:Q:271:VAL:HG12	16:Q:272:LEU:HG	1.91	0.53
3:3:196:GLY:HA3	3:3:461:TRP:HZ2	1.73	0.53
10:A:66:MET:O	10:A:69:ILE:HG12	2.08	0.53
11:J:64:VAL:HG13	16:H:134:TYR:OH	2.09	0.53
13:L:9:LEU:HB2	13:L:10:PRO:HD3	1.91	0.53
15:N:283:PHE:O	15:N:287:THR:HG23	2.09	0.53
4:E:47:LEU:HD12	4:E:48:SER:N	2.24	0.53
4:E:73:ARG:NE	4:E:81:TYR:OH	2.42	0.53
6:G:97:GLU:O	10:P:40:LYS:HG3	2.09	0.53
13:T:187:GLU:HA	13:T:190:GLU:HG2	1.90	0.53
13:L:356:TRP:CE3	13:L:363:ARG:HD2	2.43	0.53
3:D:175:ILE:HB	3:D:238:LEU:HD13	1.91	0.53
4:E:130:LEU:HD22	4:E:149:ALA:HB1	1.90	0.53
11:R:19:VAL:O	12:S:21:ARG:NH2	2.29	0.53
14:U:426:ALA:O	14:U:430:TRP:N	2.41	0.53
1:1:291:ILE:O	1:1:328:VAL:HA	2.08	0.52
3:3:444:ARG:NH2	3:3:446:ASP:OD2	2.35	0.52
5:5:182:THR:OG1	5:5:184:TYR:O	2.27	0.52
7:9:55:GLY:O	7:9:86:ARG:NE	2.37	0.52
10:A:13:TYR:CZ	16:H:95:LEU:HA	2.44	0.52
10:A:71:PHE:CZ	10:A:107:PHE:HB2	2.45	0.52
13:L:388:ILE:O	13:L:392:THR:OG1	2.27	0.52
1:B:304:GLU:O	1:B:308:ASP:N	2.35	0.52
4:E:235:THR:HG21	4:E:352:GLU:HB2	1.91	0.52
6:G:62:ARG:HB3	16:Q:50:ARG:HB2	1.90	0.52
8:I:50:LEU:HD11	8:I:75:ARG:HB2	1.91	0.52
13:T:288:GLN:NE2	13:T:528:SER:O	2.42	0.52
15:V:128:GLN:OE1	15:V:306:ARG:NH2	2.42	0.52
15:V:265:HIS:NE2	15:V:333:LEU:O	2.36	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:2:74:PRO:HD3	8:7:125:ALA:HB2	1.90	0.52
2:2:146:THR:HG23	2:2:149:ARG:H	1.74	0.52
3:3:190:TYR:O	3:3:195:PRO:HD2	2.10	0.52
11:J:93:ALA:HA	11:J:96:LEU:HD12	1.91	0.52
4:E:185:GLU:OE1	4:E:185:GLU:N	2.41	0.52
5:F:145:PRO:HA	5:F:150:TYR:CG	2.44	0.52
6:G:53:SER:O	6:G:60:LEU:N	2.42	0.52
8:I:104:VAL:HA	8:I:109:PRO:HA	1.90	0.52
14:U:16:LEU:HD22	14:U:97:GLY:H	1.73	0.52
16:Q:37:ARG:HH11	16:Q:41:ARG:HH22	1.56	0.52
13:L:20:PHE:O	13:L:22:LYS:N	2.43	0.52
1:B:250:LYS:NZ	1:B:325:THR:O	2.40	0.52
1:B:437:TRP:CH2	2:C:147:ARG:CG	2.90	0.52
3:D:558:TRP:HB2	3:D:570:PHE:HZ	1.74	0.52
4:E:214:PHE:HA	4:E:217:ARG:HB2	1.92	0.52
4:E:222:GLY:HA3	4:E:275:ARG:NH2	2.25	0.52
4:E:367:ARG:NH1	4:E:369:LYS:HB2	2.24	0.52
8:I:77:ALA:O	8:I:80:LYS:NZ	2.40	0.52
10:P:6:GLU:OE1	16:Q:117:ASN:N	2.37	0.52
14:U:17:LEU:HD21	14:U:98:LEU:HG	1.91	0.52
14:U:90:ARG:HG2	14:U:334:GLU:HG3	1.90	0.52
15:V:270:ALA:O	15:V:273:LEU:HB2	2.09	0.52
2:2:101:THR:HG22	8:7:108:ILE:HD13	1.92	0.52
4:4:341:GLU:OE1	4:4:356:TYR:OH	2.21	0.52
11:J:60:ALA:O	16:H:134:TYR:OH	2.10	0.52
3:D:284:GLU:OE2	3:D:425:ARG:NH2	2.43	0.52
4:E:72:HIS:ND1	5:F:152:LEU:HD22	2.25	0.52
4:E:231:ASP:O	5:F:110:SER:OG	2.24	0.52
7:O:11:GLY:O	7:O:15:LYS:HG3	2.10	0.52
13:T:275:LEU:HD11	13:T:405:GLY:HA3	1.91	0.52
1:1:97:GLU:OE2	1:1:296:SER:N	2.40	0.52
4:4:280:ILE:HG22	4:4:284:ARG:HH12	1.74	0.52
3:D:609:GLU:HA	3:D:627:ALA:N	2.24	0.52
4:E:276:MET:O	4:E:280:ILE:HG13	2.09	0.52
13:T:286:PHE:HB3	13:T:416:TYR:HB2	1.90	0.52
13:T:380:SER:HB3	13:T:457:GLY:H	1.73	0.52
14:U:119:TYR:CZ	14:U:160:LEU:HB2	2.45	0.52
14:U:179:ASP:O	14:U:183:HIS:ND1	2.39	0.52
1:1:9:LEU:HD13	1:1:279:TRP:CH2	2.45	0.52
1:1:32:TYR:OH	1:1:116:GLU:OE1	2.18	0.52
3:3:185:LYS:HB3	3:3:189:ARG:HH11	1.74	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:3:356:LEU:HD13	3:3:654:PHE:HB2	1.91	0.52
10:A:62:TYR:CD2	11:J:66:LEU:HD11	2.44	0.52
13:L:343:LEU:HB3	13:L:346:GLU:HB2	1.92	0.52
14:M:331:ARG:O	14:M:335:ARG:HG2	2.08	0.52
1:B:63:ARG:NE	1:B:69:GLY:O	2.31	0.52
1:B:196:ARG:NH2	3:D:204:GLU:O	2.40	0.52
1:B:270:THR:O	1:B:311:MET:HG3	2.09	0.52
3:D:516:VAL:O	3:D:520:ARG:HG3	2.09	0.52
6:G:57:ARG:O	7:O:24:VAL:HG22	2.09	0.52
8:I:36:ASP:HA	8:I:54:ILE:HA	1.92	0.52
13:T:189:LYS:HD2	13:T:477:LEU:HD11	1.92	0.52
3:3:175:ILE:O	3:3:235:LEU:HA	2.08	0.52
4:4:84:ARG:NE	4:4:169:HIS:HB3	2.25	0.52
6:6:19:ILE:HG12	6:6:20:LEU:H	1.75	0.52
6:6:62:ARG:HG2	16:H:48:PRO:HA	1.92	0.52
8:7:82:ILE:HG23	8:7:95:ALA:HB3	1.92	0.52
13:L:433:HIS:ND1	13:L:437:GLU:OE2	2.32	0.52
16:H:227:GLU:HB2	16:H:299:ARG:NH1	2.24	0.52
1:B:18:TYR:OH	1:B:105:TYR:HB2	2.09	0.52
14:U:124:ALA:HB2	15:V:337:PRO:HB2	1.90	0.52
16:Q:227:GLU:HG2	16:Q:228:LEU:N	2.24	0.52
3:3:46:ARG:NH2	3:3:81:ALA:HB2	2.25	0.52
16:H:333:PRO:HG2	16:H:336:TYR:CG	2.45	0.52
1:B:401:PRO:O	1:B:404:ASP:HB2	2.09	0.52
5:F:157:THR:OG1	5:F:165:ILE:HB	2.10	0.52
6:G:169:ARG:HG2	6:G:169:ARG:O	2.10	0.52
10:P:49:ASP:CG	10:P:52:GLY:HA3	2.30	0.52
13:T:325:HIS:NE2	13:T:329:LYS:HG3	2.24	0.52
13:T:331:LEU:HD22	13:T:450:ALA:HA	1.92	0.52
14:U:130:LEU:HD13	15:V:380:LEU:HD11	1.89	0.52
15:V:63:THR:HG21	15:V:96:HIS:ND1	2.25	0.52
1:1:394:ILE:HG22	1:1:403:ALA:HB1	1.92	0.52
4:4:183:PRO:HG2	4:4:186:PHE:HB2	1.92	0.52
4:4:205:GLU:HB2	4:4:284:ARG:HH22	1.75	0.52
8:7:74:PRO:HG2	8:7:77:ALA:HB2	1.90	0.52
13:L:3:LEU:HD22	13:L:53:ALA:HB3	1.92	0.52
1:B:149:ILE:HG22	1:B:153:ARG:HE	1.75	0.52
3:D:567:TYR:HA	3:D:584:VAL:HG23	1.92	0.52
14:U:69:GLY:HA3	14:U:453:GLY:HA3	1.91	0.52
14:U:134:TYR:O	14:U:141:ARG:NH1	2.42	0.52
3:3:723:ALA:O	3:3:727:ALA:N	2.43	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:J:32:LEU:HD13	12:K:29:LEU:HG	1.92	0.52
13:L:24:MET:HB3	13:L:28:LEU:HB3	1.91	0.52
13:L:275:LEU:HD23	13:L:275:LEU:C	2.31	0.52
14:M:85:GLY:O	14:M:89:ALA:HB2	2.10	0.52
14:M:321:TYR:CE1	14:M:365:MET:HA	2.44	0.52
1:B:203:PRO:HB2	1:B:204:PRO:HD3	1.92	0.52
10:P:65:ALA:HB1	11:R:66:LEU:HB2	1.92	0.52
13:T:258:PHE:O	13:T:261:SER:OG	2.27	0.52
13:T:439:PRO:HD2	13:T:443:LEU:HD13	1.91	0.52
3:3:716:LEU:HD21	3:3:758:LEU:HD23	1.92	0.51
4:4:84:ARG:CZ	4:4:169:HIS:HB3	2.41	0.51
4:4:148:TYR:OH	16:H:42:PHE:O	2.18	0.51
6:6:163:TYR:O	7:9:148:ARG:NE	2.43	0.51
13:L:355:LEU:HB3	13:L:359:LEU:HD12	1.93	0.51
3:D:131:GLN:NE2	17:D:801:SF4:S3	2.82	0.51
5:F:71:VAL:HG11	5:F:89:PHE:HD2	1.75	0.51
13:T:162:ASN:OD1	13:T:216:LYS:NZ	2.42	0.51
13:T:356:TRP:CZ3	13:T:363:ARG:HD2	2.45	0.51
11:J:75:PHE:O	11:J:77:ALA:N	2.43	0.51
1:B:98:PRO:HA	2:C:124:CYS:SG	2.50	0.51
1:B:381:GLU:OE1	1:B:426:ARG:NE	2.35	0.51
1:B:438:ARG:HA	2:C:147:ARG:HH21	1.75	0.51
3:D:203:ILE:HG22	3:D:204:GLU:HG3	1.92	0.51
6:G:21:PHE:HD1	6:G:23:THR:H	1.59	0.51
6:G:31:GLY:O	6:G:35:SER:HB3	2.10	0.51
6:G:145:GLU:HB3	7:O:26:TYR:CZ	2.45	0.51
7:O:172:GLY:O	7:O:174:LYS:NZ	2.34	0.51
13:T:41:PHE:HB2	13:T:81:THR:HB	1.92	0.51
14:U:115:LEU:HD12	14:U:180:LEU:HD13	1.93	0.51
16:H:208:ILE:O	16:H:212:ALA:N	2.35	0.51
1:B:380:GLU:N	1:B:383:ASP:OD2	2.35	0.51
1:B:382:LYS:O	1:B:386:ASN:ND2	2.43	0.51
2:C:88:CYS:SG	2:C:133:VAL:HG23	2.50	0.51
3:D:585:MET:HB3	3:D:587:LEU:HD13	1.92	0.51
4:E:366:TYR:CZ	5:F:148:LYS:HE3	2.46	0.51
13:T:119:VAL:O	13:T:251:TYR:OH	2.21	0.51
1:1:133:TYR:HB3	1:1:188:LEU:HD11	1.93	0.51
4:4:302:VAL:HG23	4:4:303:ARG:HG2	1.93	0.51
6:6:97:GLU:O	10:A:40:LYS:HG3	2.10	0.51
13:L:70:ASP:H	13:L:73:SER:HB2	1.75	0.51
14:M:179:ASP:O	14:M:183:HIS:ND1	2.38	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
14:M:350:SER:HB3	14:M:422:VAL:H	1.75	0.51
15:N:62:PHE:HE2	15:N:285:LEU:HD22	1.74	0.51
15:N:262:SER:OG	15:N:288:TYR:OH	2.26	0.51
16:H:212:ALA:HA	16:H:218:PRO:HD3	1.92	0.51
16:H:306:LEU:O	16:H:310:TRP:HB2	2.11	0.51
2:C:106:ILE:HG22	2:C:110:GLU:HG3	1.91	0.51
3:D:349:ALA:O	3:D:540:ASN:ND2	2.32	0.51
14:U:194:PHE:HB2	14:U:249:ALA:HB3	1.90	0.51
14:U:215:PRO:HG2	14:U:216:PRO:HD3	1.93	0.51
16:Q:232:TYR:HB2	16:Q:244:PHE:CD1	2.46	0.51
16:Q:330:LEU:HB3	16:Q:332:LEU:HD12	1.92	0.51
1:1:412:GLY:HA2	1:1:415:ARG:HB3	1.91	0.51
4:4:230:ILE:HG21	5:5:47:ASN:HB3	1.91	0.51
15:N:52:PRO:HB2	15:N:106:LEU:HD23	1.92	0.51
2:C:4:PHE:HB3	2:C:11:LEU:HD11	1.91	0.51
2:C:85:THR:HG22	2:C:86:LEU:H	1.75	0.51
3:D:716:LEU:HD21	3:D:758:LEU:HD23	1.92	0.51
8:I:43:ARG:HA	8:I:46:ARG:HH21	1.74	0.51
8:I:44:MET:HE3	8:I:46:ARG:HH12	1.74	0.51
14:U:331:ARG:O	14:U:335:ARG:HG2	2.11	0.51
3:3:200:LEU:HD12	3:3:213:THR:HB	1.93	0.51
3:3:250:GLU:HG3	5:5:169:GLU:HG3	1.91	0.51
4:4:114:GLU:O	4:4:118:VAL:HG13	2.10	0.51
14:M:22:ARG:HD2	14:M:22:ARG:C	2.30	0.51
2:C:99:TYR:HE2	2:C:150:LEU:HD11	1.75	0.51
13:T:490:GLU:HG3	13:T:491:TRP:N	2.25	0.51
16:Q:212:ALA:HA	16:Q:218:PRO:HG3	1.92	0.51
1:1:273:ARG:NH1	1:1:304:GLU:OE1	2.41	0.51
4:4:276:MET:O	4:4:280:ILE:HG13	2.10	0.51
7:9:108:CYS:HB2	7:9:113:ILE:HG22	1.93	0.51
9:W:45:ARG:NH1	9:W:61:ASP:OD2	2.43	0.51
16:H:150:LEU:HD21	16:H:154:ARG:HH11	1.74	0.51
3:D:223:SER:O	3:D:226:ILE:HG12	2.11	0.51
5:F:144:HIS:HB2	5:F:147:ARG:HD3	1.93	0.51
10:P:70:LEU:HD13	11:R:150:THR:HG22	1.91	0.51
1:1:427:GLU:OE1	1:1:429:ARG:NH1	2.44	0.51
8:7:48:TYR:CZ	8:7:50:LEU:HB2	2.46	0.51
14:M:56:LEU:HD11	15:N:416:PRO:HG2	1.93	0.51
15:N:209:LEU:HB2	15:N:296:PHE:HB3	1.93	0.51
3:D:225:ASN:HD21	3:D:290:ILE:H	1.57	0.51
3:D:248:GLU:CD	7:O:57:SER:HG	2.14	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:434:ASP:OD2	3:D:436:GLN:NE2	2.44	0.51
4:E:143:LEU:HD23	4:E:143:LEU:H	1.76	0.51
6:6:21:PHE:HB3	6:6:24:LEU:HB2	1.93	0.51
13:L:160:ILE:O	13:L:164:ILE:HG13	2.11	0.51
13:L:490:GLU:HG3	13:L:491:TRP:N	2.25	0.51
15:N:313:ARG:HB2	15:N:384:ALA:HB3	1.93	0.51
15:N:422:ALA:O	15:N:423:LEU:HD23	2.10	0.51
2:C:66:PHE:O	3:D:205:ARG:NE	2.44	0.51
3:D:51:ARG:HB3	3:D:94:ASP:HB3	1.93	0.51
4:E:114:GLU:O	4:E:118:VAL:HG13	2.11	0.51
4:E:403:VAL:HG12	4:E:406:ASP:H	1.76	0.51
7:O:53:CYS:SG	7:O:88:ALA:HB2	2.50	0.51
10:P:13:TYR:CZ	16:Q:95:LEU:HA	2.46	0.51
14:U:411:GLN:NE2	14:U:416:GLU:OE2	2.41	0.51
3:3:606:THR:OG1	3:3:609:GLU:OE1	2.27	0.51
15:N:316:TYR:HB2	15:N:382:VAL:CG1	2.41	0.51
1:B:223:THR:O	1:B:227:VAL:HG23	2.11	0.51
3:D:40:SER:O	3:D:189:ARG:NE	2.40	0.51
4:E:363:SER:HB3	5:F:174:LEU:H	1.75	0.51
1:1:91:CYS:SG	1:1:221:VAL:HG22	2.51	0.50
2:2:40:TRP:CD1	2:2:74:PRO:HA	2.45	0.50
5:5:38:MET:HA	5:5:41:TYR:HD2	1.75	0.50
7:9:149:GLU:O	7:9:153:THR:OG1	2.17	0.50
13:L:17:LEU:O	13:L:102:SER:HB2	2.10	0.50
13:L:189:LYS:HD2	13:L:477:LEU:HD11	1.92	0.50
14:M:264:ALA:HB1	14:M:294:GLY:O	2.11	0.50
16:H:260:PRO:HG3	16:H:286:PHE:CD2	2.46	0.50
1:B:418:LYS:O	1:B:421:TYR:HB2	2.11	0.50
2:C:40:TRP:CH2	2:C:42:ARG:HG2	2.46	0.50
3:D:283:PRO:HA	3:D:287:GLU:HA	1.93	0.50
4:E:47:LEU:HD13	4:E:51:GLU:O	2.11	0.50
6:G:69:ARG:NH2	16:Q:225:GLU:OE2	2.43	0.50
13:T:59:TRP:HB3	13:T:63:ILE:O	2.11	0.50
13:T:87:ILE:HD12	13:T:239:LEU:HD13	1.92	0.50
16:Q:222:PRO:HG2	16:Q:230:GLY:HA2	1.94	0.50
3:3:185:LYS:O	3:3:189:ARG:HB2	2.11	0.50
3:3:740:PHE:HE2	3:3:771:VAL:HG11	1.77	0.50
4:4:139:ASP:O	16:H:226:GLN:HB3	2.12	0.50
7:9:126:TYR:HB3	9:W:39:ASP:CG	2.32	0.50
11:J:9:LEU:HD22	12:K:6:THR:HG21	1.93	0.50
13:L:371:LEU:HD22	13:L:376:LEU:HD13	1.93	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:G:19:ILE:HG12	6:G:20:LEU:H	1.75	0.50
13:T:104:PHE:HZ	13:T:235:PRO:HG2	1.76	0.50
1:1:106:ILE:HD11	1:1:251:LEU:HD21	1.94	0.50
2:2:28:MET:O	2:2:70:TYR:OH	2.29	0.50
4:4:226:PRO:HG3	4:4:242:SER:HB2	1.92	0.50
16:H:22:VAL:HA	16:H:25:LEU:HD12	1.92	0.50
1:B:197:ALA:HB3	2:C:66:PHE:CE2	2.46	0.50
2:C:24:ARG:HH21	2:C:59:GLU:HB3	1.76	0.50
3:D:376:ALA:N	3:D:513:GLN:OE1	2.38	0.50
10:P:10:THR:OG1	16:Q:118:LEU:HD21	2.12	0.50
10:P:65:ALA:O	10:P:69:ILE:HG23	2.11	0.50
13:T:433:HIS:ND1	13:T:433:HIS:O	2.45	0.50
13:T:463:HIS:CG	13:T:464:PRO:HD3	2.46	0.50
16:Q:159:LEU:O	16:Q:163:GLU:HB2	2.10	0.50
16:Q:216:ARG:NH1	16:Q:294:ARG:HB3	2.27	0.50
1:1:386:ASN:OD1	3:3:156:ARG:NE	2.37	0.50
16:H:300:LEU:HB3	16:H:305:LEU:HB2	1.92	0.50
16:H:302:TYR:O	16:H:306:LEU:HG	2.12	0.50
1:B:433:ARG:HH12	2:C:89:LYS:HE2	1.76	0.50
3:D:270:ARG:HB3	3:D:275:LEU:HD11	1.94	0.50
3:D:399:LEU:O	3:D:508:GLY:N	2.44	0.50
3:D:512:LEU:HD21	3:D:534:ALA:HB1	1.94	0.50
6:G:156:LYS:HZ2	7:O:152:ARG:HH21	1.59	0.50
11:R:158:GLU:OE1	15:V:81:ARG:NH1	2.44	0.50
12:S:16:TYR:O	12:S:20:THR:OG1	2.25	0.50
14:U:68:ASP:HB3	14:U:457:LEU:HD21	1.93	0.50
15:V:132:ALA:HB1	15:V:199:VAL:HA	1.93	0.50
16:Q:50:ARG:C	16:Q:52:GLY:H	2.12	0.50
16:Q:108:PHE:HB2	16:Q:113:PRO:HA	1.93	0.50
3:3:305:ARG:HH22	3:3:606:THR:H	1.58	0.50
4:4:26:MET:HA	10:A:54:VAL:HB	1.93	0.50
4:4:154:GLU:OE2	4:4:167:ARG:NH2	2.44	0.50
7:9:137:LEU:O	7:9:140:VAL:HG12	2.12	0.50
15:N:280:ALA:HA	15:N:347:LEU:HD13	1.93	0.50
16:H:8:ASP:OD2	16:H:111:TYR:HB3	2.12	0.50
6:G:54:THR:HA	6:G:59:ASP:HA	1.94	0.50
6:G:104:TRP:HE1	6:G:173:VAL:HA	1.76	0.50
4:4:32:PRO:O	4:4:34:HIS:ND1	2.43	0.50
4:4:123:LEU:HD23	4:4:160:PHE:CE1	2.47	0.50
6:6:148:ILE:O	6:6:152:MET:HG3	2.11	0.50
8:7:37:PHE:N	8:7:53:THR:O	2.41	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
14:M:186:GLN:HG2	14:M:187:GLU:H	1.77	0.50
16:H:16:LYS:HZ3	16:H:112:GLN:CB	2.25	0.50
16:H:190:LYS:HD3	16:H:268:THR:HG22	1.93	0.50
1:B:190:ASN:HD21	1:B:200:ARG:HG2	1.77	0.50
3:D:81:ALA:O	3:D:85:THR:OG1	2.22	0.50
6:6:21:PHE:HD1	6:6:23:THR:H	1.59	0.50
7:9:22:VAL:HB	16:H:44:VAL:HG11	1.90	0.50
13:L:584:GLY:O	15:N:135:LYS:NZ	2.24	0.50
14:M:402:SER:HA	14:M:405:TYR:CE2	2.47	0.50
3:D:50:VAL:HG22	3:D:82:SER:HB3	1.94	0.50
6:G:96:TRP:CZ2	6:G:103:LYS:HE3	2.47	0.50
9:X:3:ARG:NH2	9:X:60:PRO:HB3	2.27	0.50
10:P:80:PRO:HA	11:R:124:PRO:HB2	1.93	0.50
15:V:193:HIS:CD2	15:V:263:ILE:HD13	2.46	0.50
16:Q:199:ALA:HA	16:Q:320:TRP:CZ2	2.46	0.50
16:Q:292:TRP:HD1	16:Q:296:THR:OG1	1.95	0.50
3:3:351:LEU:HD11	3:3:543:GLY:HA3	1.94	0.50
6:6:153:GLN:HG3	7:9:124:TYR:OH	2.11	0.50
13:L:88:HIS:O	13:L:92:ILE:HG13	2.12	0.50
14:M:218:HIS:HA	14:M:228:ASP:OD1	2.12	0.50
16:H:186:VAL:HG11	16:H:267:TRP:CZ3	2.46	0.50
3:D:378:PRO:HD2	3:D:683:LEU:HD23	1.92	0.50
13:T:185:ILE:HA	13:T:188:LEU:HB3	1.93	0.50
3:3:563:ALA:O	3:3:580:LYS:HG2	2.11	0.50
11:J:64:VAL:HA	11:J:67:PHE:HB2	1.93	0.50
2:C:112:THR:HB	2:C:117:PHE:HB2	1.92	0.50
3:D:136:GLU:HB3	5:F:187:GLY:HA3	1.94	0.50
13:T:165:GLY:HA2	13:T:211:LEU:HD23	1.93	0.50
15:V:245:ASN:ND2	15:V:367:THR:HB	2.27	0.50
2:2:46:ILE:HG23	2:2:60:VAL:HG12	1.94	0.49
3:3:34:CYS:N	3:3:45:CYS:SG	2.83	0.49
3:3:228:ASP:OD1	3:3:295:ARG:NH1	2.45	0.49
4:4:73:ARG:NH1	5:5:171:ARG:HH21	2.10	0.49
4:4:315:HIS:HA	8:7:46:ARG:CZ	2.42	0.49
13:L:30:GLY:HA2	13:L:105:PHE:CD1	2.47	0.49
2:C:27:ILE:HG13	2:C:53:VAL:HG21	1.93	0.49
14:U:78:ILE:HG22	14:U:103:GLU:HG3	1.92	0.49
1:1:63:ARG:HD3	1:1:313:TYR:HD2	1.76	0.49
3:3:237:ASP:OD1	3:3:239:THR:HG22	2.12	0.49
10:A:7:TYR:HD2	11:J:44:VAL:HG11	1.77	0.49
10:A:110:GLU:HG3	10:A:111:TRP:N	2.26	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:L:426:LEU:HB3	13:L:513:GLN:NE2	2.27	0.49
1:B:14:GLU:OE1	1:B:237:TRP:NE1	2.45	0.49
1:B:437:TRP:CE3	1:B:438:ARG:O	2.65	0.49
3:D:505:LEU:HD21	3:D:521:ALA:HB1	1.94	0.49
4:E:343:TYR:CZ	4:E:354:GLY:HA3	2.47	0.49
6:G:66:GLU:OE1	16:Q:45:ARG:NH1	2.46	0.49
13:T:290:ASP:OD1	13:T:291:ILE:N	2.44	0.49
15:V:98:LEU:HD23	15:V:218:ALA:HB1	1.93	0.49
15:V:265:HIS:HA	15:V:268:TYR:CD2	2.47	0.49
1:1:53:VAL:O	1:1:57:VAL:HG23	2.11	0.49
3:3:136:GLU:HG2	5:5:186:GLY:O	2.12	0.49
2:C:146:THR:HG23	2:C:149:ARG:H	1.77	0.49
4:E:285:GLU:O	4:E:289:ILE:HG12	2.12	0.49
13:T:582:GLN:HE22	15:V:197:PRO:HB2	1.77	0.49
14:U:56:LEU:HB3	14:U:59:ALA:HB3	1.94	0.49
14:U:91:VAL:HG23	14:U:92:GLU:H	1.77	0.49
1:1:238:PHE:CZ	1:1:248:GLY:HA3	2.47	0.49
3:3:345:LEU:O	3:3:372:GLN:N	2.45	0.49
4:4:215:TYR:OH	4:4:219:ARG:NH2	2.43	0.49
4:4:249:ARG:HD2	4:4:262:PHE:HE2	1.77	0.49
11:J:97:ALA:HB1	12:K:16:TYR:HB2	1.94	0.49
13:L:13:GLY:O	13:L:17:LEU:HG	2.12	0.49
13:L:163:ARG:NE	14:M:399:VAL:HB	2.26	0.49
16:H:43:GLN:HE21	16:H:45:ARG:CZ	2.25	0.49
1:B:186:THR:HB	1:B:200:ARG:H	1.77	0.49
3:D:540:ASN:HB2	3:D:614:LEU:HD23	1.94	0.49
6:G:154:LEU:O	6:G:158:VAL:HG13	2.11	0.49
13:T:340:ILE:HB	13:T:345:GLY:HA2	1.94	0.49
14:U:218:HIS:HA	14:U:228:ASP:OD1	2.12	0.49
14:U:232:THR:HA	14:U:235:LYS:NZ	2.27	0.49
15:V:53:TYR:HA	15:V:101:THR:HG22	1.95	0.49
16:Q:289:PHE:O	16:Q:293:ILE:HG12	2.13	0.49
3:3:312:ARG:HA	3:3:316:ARG:O	2.12	0.49
4:4:39:GLY:H	20:4:501:HQH:C19	2.25	0.49
4:4:47:LEU:HD12	4:4:48:SER:N	2.27	0.49
5:5:75:VAL:HG11	5:5:87:ARG:HH21	1.77	0.49
1:B:4:PRO:HA	1:B:12:ARG:HH12	1.76	0.49
3:D:656:LEU:HD21	9:X:3:ARG:HH11	1.77	0.49
3:D:686:LYS:HD3	3:D:688:ARG:HH22	1.78	0.49
4:E:33:GLN:HB2	4:E:40:VAL:CG2	2.41	0.49
4:E:246:TYR:CD1	5:F:78:PRO:HD2	2.47	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:E:353:LEU:HD12	4:E:354:GLY:H	1.77	0.49
15:V:181:VAL:HA	15:V:192:PHE:CE2	2.47	0.49
16:Q:101:PRO:HA	16:Q:114:TRP:HB3	1.95	0.49
3:3:247:TRP:CD1	5:5:172:ALA:HB2	2.47	0.49
4:4:43:LEU:HD13	4:4:55:VAL:HG11	1.95	0.49
13:L:542:ILE:O	13:L:546:LEU:HG	2.12	0.49
2:C:130:THR:HB	2:C:143:GLU:HB3	1.94	0.49
3:D:185:LYS:O	3:D:189:ARG:HB2	2.12	0.49
13:T:180:TYR:CZ	13:T:192:MET:HG2	2.47	0.49
14:U:263:LEU:O	14:U:267:SER:OG	2.22	0.49
16:Q:158:SER:HB2	16:Q:305:LEU:HD21	1.94	0.49
16:Q:189:GLN:NE2	16:Q:264:LEU:O	2.45	0.49
1:1:191:SER:HB2	1:1:197:ALA:HB2	1.95	0.49
1:1:203:PRO:HB2	1:1:204:PRO:HD3	1.93	0.49
1:1:223:THR:O	1:1:227:VAL:HG23	2.13	0.49
1:1:343:ASN:HA	1:1:346:ARG:HG2	1.95	0.49
1:1:343:ASN:HB2	2:2:89:LYS:NZ	2.27	0.49
5:5:16:PRO:HD2	5:5:28:VAL:HG13	1.94	0.49
7:9:43:LEU:HD12	7:9:133:LYS:HG3	1.95	0.49
10:A:67:LEU:HD21	10:A:110:GLU:OE2	2.11	0.49
11:J:151:VAL:HG12	15:N:87:LEU:HD21	1.95	0.49
13:L:356:TRP:O	13:L:363:ARG:HD3	2.13	0.49
16:H:131:LEU:HA	16:H:134:TYR:HB2	1.94	0.49
1:B:276:ILE:HA	1:B:280:ALA:HB3	1.93	0.49
1:B:352:SER:OG	1:B:359:CYS:SG	2.61	0.49
3:D:135:VAL:HG11	4:E:329:LYS:HG2	1.93	0.49
13:T:239:LEU:HD12	13:T:243:ALA:HB3	1.93	0.49
3:3:338:GLY:O	3:3:366:THR:HB	2.12	0.49
3:3:571:VAL:HG21	3:3:591:HIS:CD2	2.48	0.49
7:9:10:LEU:HA	16:H:296:THR:HG21	1.93	0.49
16:H:6:PRO:HG2	16:H:112:GLN:NE2	2.26	0.49
1:B:95:GLU:O	1:B:135:ARG:NH1	2.33	0.49
3:D:268:ASP:OD2	3:D:278:ARG:NH1	2.40	0.49
3:D:506:ILE:HG12	3:D:533:LEU:HB2	1.95	0.49
3:D:637:ALA:HA	3:D:640:VAL:HB	1.95	0.49
4:E:45:VAL:HG13	4:E:55:VAL:HG22	1.93	0.49
4:E:218:ALA:HA	4:E:221:VAL:HG22	1.95	0.49
7:O:56:CYS:N	17:O:202:SF4:S1	2.85	0.49
13:T:129:ILE:HG12	14:U:369:PRO:HB2	1.95	0.49
1:1:363:VAL:O	1:1:368:VAL:HG12	2.13	0.49
3:3:50:VAL:HG22	3:3:82:SER:HB3	1.94	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:3:94:ASP:OD2	3:3:97:SER:OG	2.20	0.49
6:6:155:GLN:O	6:6:159:ARG:HG3	2.13	0.49
6:6:163:TYR:HD1	7:9:152:ARG:HH11	1.61	0.49
6:6:169:ARG:HH11	6:6:169:ARG:HG3	1.78	0.49
7:9:41:HIS:NE2	17:9:201:SF4:S1	2.86	0.49
13:L:463:HIS:CG	13:L:464:PRO:HD3	2.48	0.49
15:N:99:ALA:O	15:N:225:ARG:NH1	2.45	0.49
4:E:144:THR:HG22	4:E:148:TYR:HE1	1.78	0.49
5:F:17:ILE:HD12	5:F:27:VAL:HG22	1.95	0.49
8:I:71:ASP:O	8:I:82:ILE:HG13	2.13	0.49
9:X:98:GLU:O	9:X:101:ALA:N	2.46	0.49
15:V:2:THR:OG1	15:V:39:SER:OG	2.24	0.49
15:V:200:TYR:CE2	15:V:212:ALA:HB2	2.48	0.49
3:3:33:PHE:HB2	3:3:45:CYS:SG	2.52	0.49
4:4:31:GLY:HA3	10:A:45:GLU:OE2	2.13	0.49
4:4:122:GLU:OE1	4:4:257:TYR:OH	2.30	0.49
4:4:150:PHE:O	4:4:153:ARG:HB3	2.13	0.49
4:4:167:ARG:HD3	6:6:143:ARG:NH1	2.28	0.49
7:9:111:GLY:N	8:7:44:MET:HG2	2.27	0.49
10:A:1:MET:HG2	11:J:49:ARG:NH1	2.27	0.49
3:D:168:HIS:NE2	8:I:65:GLU:HG2	2.28	0.49
3:D:347:HIS:HB2	3:D:538:ALA:HB1	1.95	0.49
4:E:302:VAL:HG23	4:E:303:ARG:HG2	1.95	0.49
6:G:175:ALA:O	6:G:180:ARG:NH2	2.37	0.49
13:T:214:VAL:O	13:T:218:ALA:N	2.46	0.49
16:Q:259:ILE:HB	16:Q:260:PRO:HD3	1.95	0.49
3:3:6:VAL:HG21	3:3:23:VAL:HA	1.95	0.48
3:3:154:TYR:CZ	4:4:312:PRO:HB3	2.48	0.48
6:6:91:VAL:O	6:6:95:VAL:HG23	2.13	0.48
13:L:26:GLU:HB3	13:L:27:PRO:HD3	1.94	0.48
13:L:461:LEU:HD13	13:L:465:LEU:HD13	1.95	0.48
15:N:280:ALA:CB	15:N:347:LEU:HB3	2.42	0.48
16:H:232:TYR:HB2	16:H:244:PHE:CD1	2.48	0.48
1:B:179:ALA:HB3	1:B:182:CYS:SG	2.53	0.48
13:T:90:TYR:OH	13:T:338:SER:N	2.46	0.48
16:Q:17:ALA:O	16:Q:21:VAL:HG23	2.12	0.48
1:1:18:TYR:OH	1:1:102:LYS:O	2.22	0.48
1:1:91:CYS:HB3	1:1:132:ILE:HG12	1.95	0.48
3:3:271:SER:OG	7:9:69:TYR:OH	2.17	0.48
3:3:329:LEU:HD11	3:3:584:VAL:HG11	1.95	0.48
4:4:38:HIS:HB2	20:4:501:HQH:C24	2.42	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:L:182:THR:HB	13:L:187:GLU:HG3	1.96	0.48
14:M:215:PRO:HG3	14:M:287:TYR:OH	2.13	0.48
15:N:38:ALA:HA	15:N:41:LEU:HD12	1.95	0.48
1:B:223:THR:OG1	18:B:502:FMN:O3P	2.24	0.48
3:D:247:TRP:HE1	7:O:61:ALA:HB2	1.78	0.48
4:E:272:VAL:N	4:E:275:ARG:HH21	2.12	0.48
4:4:260:TYR:HA	4:4:292:GLN:NE2	2.28	0.48
6:6:124:VAL:HG22	9:W:120:PRO:HD2	1.95	0.48
8:7:6:GLU:O	8:7:9:LEU:HB3	2.14	0.48
10:A:23:ALA:O	10:A:27:VAL:HG23	2.12	0.48
13:L:166:ASP:O	13:L:170:MET:HG3	2.13	0.48
13:L:291:ILE:O	13:L:294:ILE:HG22	2.14	0.48
14:M:208:PHE:N	14:M:267:SER:OG	2.46	0.48
1:B:98:PRO:HB2	1:B:295:SER:HB2	1.95	0.48
1:B:174:HIS:CE1	2:C:29:PRO:HD3	2.49	0.48
1:B:312:SER:OG	1:B:315:HIS:ND1	2.22	0.48
3:D:326:PHE:CZ	3:D:330:LYS:HE3	2.48	0.48
13:T:354:GLY:HA3	13:T:429:GLU:HG2	1.96	0.48
14:U:219:GLN:HA	14:U:282:LYS:HG3	1.95	0.48
15:V:119:TYR:CZ	15:V:137:PHE:HA	2.48	0.48
1:1:291:ILE:HG12	1:1:299:PRO:HB3	1.95	0.48
3:3:406:ALA:HB2	3:3:535:MET:HG2	1.95	0.48
4:4:171:ASN:CG	4:4:174:ARG:HH22	2.17	0.48
13:L:128:PHE:CE1	13:L:166:ASP:HB3	2.48	0.48
14:M:17:LEU:HD21	14:M:98:LEU:HG	1.95	0.48
14:M:260:LEU:HB3	14:M:301:PHE:CE2	2.48	0.48
16:H:274:VAL:HG12	16:H:278:TRP:HD1	1.77	0.48
3:D:693:TYR:HB3	3:D:759:TYR:CD1	2.48	0.48
4:E:87:TYR:HA	4:E:169:HIS:HE1	1.78	0.48
4:E:88:LEU:C	4:E:128:SER:HB2	2.34	0.48
10:P:66:MET:O	10:P:69:ILE:HG12	2.13	0.48
1:B:106:ILE:HD11	1:B:251:LEU:HD21	1.95	0.48
3:D:159:PHE:CE2	8:I:79:LEU:HD13	2.45	0.48
3:D:664:LEU:HD22	3:D:669:VAL:HG11	1.94	0.48
5:F:174:LEU:HB3	5:F:178:ASP:HB3	1.95	0.48
6:G:101:ASP:O	6:G:103:LYS:N	2.46	0.48
10:P:2:ALA:HB2	16:Q:119:ASP:HB3	1.96	0.48
11:R:17:VAL:O	11:R:21:THR:OG1	2.18	0.48
14:U:372:SER:O	14:U:375:PRO:HD2	2.14	0.48
15:V:176:LEU:HD13	15:V:229:PRO:HD3	1.93	0.48
16:Q:177:VAL:HG11	16:Q:185:ILE:HG12	1.95	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:3:8:ASP:OD1	3:3:9:ARG:HG3	2.14	0.48
3:3:376:ALA:N	3:3:513:GLN:OE1	2.42	0.48
6:6:90:PRO:HA	6:6:93:ARG:HB3	1.96	0.48
7:9:11:GLY:O	7:9:15:LYS:HG3	2.13	0.48
8:7:44:MET:HE2	8:7:46:ARG:HH22	1.78	0.48
14:M:70:LEU:O	14:M:73:LEU:HD23	2.14	0.48
15:N:168:GLU:HG2	15:N:169:GLY:H	1.78	0.48
15:N:280:ALA:HB1	15:N:347:LEU:HB3	1.94	0.48
1:B:65:ARG:NH2	1:B:247:LYS:O	2.34	0.48
2:C:79:HIS:H	2:C:137:ASN:ND2	2.11	0.48
9:X:102:LEU:HD12	9:X:105:LEU:HD12	1.96	0.48
11:R:29:ALA:O	11:R:33:ILE:HG13	2.13	0.48
11:R:63:ILE:HG23	12:S:68:VAL:HG11	1.95	0.48
13:T:158:ALA:HA	13:T:225:TRP:CB	2.38	0.48
13:T:386:ASP:HA	13:T:389:LEU:HB2	1.96	0.48
15:V:87:LEU:HA	15:V:90:TYR:CD2	2.48	0.48
16:Q:216:ARG:CB	16:Q:294:ARG:HD2	2.42	0.48
3:3:287:GLU:OE1	3:3:289:TRP:NE1	2.39	0.48
3:3:565:TYR:HD1	3:3:582:PHE:HB3	1.79	0.48
6:6:93:ARG:NH1	6:6:130:VAL:O	2.47	0.48
13:L:115:MET:HG2	13:L:244:THR:HG22	1.96	0.48
1:B:433:ARG:NH1	2:C:89:LYS:HE2	2.29	0.48
4:E:239:LEU:HG	4:E:244:VAL:HB	1.95	0.48
11:R:22:LEU:HB2	11:R:28:ALA:HB2	1.95	0.48
14:U:151:PHE:HD2	14:U:213:TRP:CD1	2.31	0.48
1:1:29:LEU:O	1:1:33:LEU:HG	2.14	0.48
3:3:750:ARG:HB3	3:3:752:ASP:OD1	2.14	0.48
6:6:92:MET:HE1	6:6:127:VAL:HG13	1.95	0.48
13:L:105:PHE:HA	13:L:108:PHE:HB2	1.95	0.48
14:M:10:VAL:HG23	14:M:104:GLY:HA3	1.95	0.48
14:M:306:GLU:OE2	14:M:386:LYS:NZ	2.42	0.48
16:H:147:TYR:HD1	16:H:229:VAL:HG22	1.79	0.48
3:D:300:TRP:NE1	3:D:703:GLN:HG2	2.28	0.48
3:D:352:GLU:HG2	3:D:660:ALA:HB1	1.96	0.48
4:E:64:THR:OG1	6:G:83:ARG:NH1	2.42	0.48
4:E:229:ALA:HB1	4:E:234:LEU:HB3	1.96	0.48
10:P:76:ALA:HA	10:P:79:TRP:HE3	1.78	0.48
13:T:168:GLY:HA3	13:T:211:LEU:HD22	1.96	0.48
13:T:527:ALA:HA	13:T:533:TYR:CZ	2.49	0.48
1:1:18:TYR:CZ	1:1:263:VAL:HG11	2.49	0.48
2:2:112:THR:HG22	2:2:117:PHE:H	1.78	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:3:31:PRO:HG3	3:3:137:TYR:CD2	2.48	0.48
7:9:132:GLY:H	7:9:135:ASP:HB2	1.79	0.48
10:A:61:PHE:HE1	16:H:302:TYR:HE2	1.62	0.48
13:L:475:PRO:HA	13:L:479:GLU:OE2	2.14	0.48
15:N:94:GLY:O	15:N:110:ALA:HB1	2.14	0.48
16:H:218:PRO:C	16:H:220:ASP:H	2.16	0.48
3:D:310:LEU:HB2	3:D:601:VAL:HB	1.94	0.48
3:D:481:LEU:HD11	3:D:520:ARG:HB3	1.96	0.48
3:D:642:ALA:HA	3:D:652:PRO:HB3	1.96	0.48
11:R:18:LEU:HG	11:R:22:LEU:HD21	1.95	0.48
13:T:214:VAL:HG12	13:T:222:LEU:HB2	1.95	0.48
14:U:149:VAL:HG12	14:U:153:LEU:HD22	1.96	0.48
14:U:201:PHE:CE2	14:U:245:ALA:HB2	2.48	0.48
15:V:190:ALA:N	15:V:240:SER:OG	2.47	0.48
2:2:7:LYS:HB2	2:2:10:PHE:CB	2.44	0.48
3:3:123:ASP:OD2	3:3:242:PHE:N	2.26	0.48
4:4:98:ALA:O	4:4:102:GLU:HG3	2.14	0.48
4:4:225:PRO:HA	4:4:269:ARG:HH12	1.79	0.48
13:L:239:LEU:HD12	13:L:243:ALA:HB3	1.96	0.48
14:M:363:LEU:HD22	14:M:368:LEU:HD13	1.96	0.48
1:B:274:GLU:HG2	1:B:279:TRP:CD1	2.49	0.48
4:E:47:LEU:HD13	4:E:51:GLU:C	2.34	0.48
10:P:48:ASN:OD1	10:P:49:ASP:HB2	2.13	0.48
11:R:16:GLY:HA2	11:R:19:VAL:HG12	1.96	0.48
11:R:146:LEU:O	11:R:150:THR:HG23	2.14	0.48
13:T:26:GLU:HB3	13:T:27:PRO:HD3	1.95	0.48
13:T:314:ALA:HB1	13:T:317:VAL:HB	1.96	0.48
16:Q:43:GLN:C	16:Q:45:ARG:H	2.12	0.48
3:3:693:TYR:HB3	3:3:759:TYR:CD1	2.49	0.47
5:5:3:LEU:O	5:5:7:LEU:HG	2.14	0.47
5:5:82:ASP:OD1	5:5:82:ASP:N	2.45	0.47
11:J:46:LEU:HD22	12:K:47:ARG:HD3	1.96	0.47
11:J:102:GLY:O	11:J:106:ALA:N	2.37	0.47
14:M:331:ARG:HA	14:M:331:ARG:HH11	1.79	0.47
15:N:270:ALA:O	15:N:273:LEU:HB2	2.14	0.47
1:B:55:GLU:OE2	1:B:59:ARG:NH2	2.47	0.47
1:B:184:GLU:OE1	1:B:186:THR:OG1	2.20	0.47
3:D:337:ARG:NH1	3:D:565:TYR:OH	2.47	0.47
9:X:21:LEU:HD11	9:X:26:LEU:HD11	1.95	0.47
13:T:242:ALA:HB1	13:T:326:ALA:HA	1.96	0.47
3:3:374:ARG:HB3	3:3:558:TRP:CD1	2.49	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:3:395:PHE:HB3	3:3:503:PRO:HB3	1.97	0.47
4:4:103:LYS:HB3	5:5:22:LEU:HD13	1.96	0.47
6:6:31:GLY:O	6:6:35:SER:HB3	2.14	0.47
9:W:122:ASP:O	9:W:125:ILE:HG12	2.14	0.47
3:D:83:CYS:SG	3:D:84:VAL:HG13	2.54	0.47
5:F:49:LEU:HD21	5:F:52:ILE:HD11	1.96	0.47
10:P:56:ARG:HD3	11:R:73:LEU:O	2.12	0.47
13:T:90:TYR:CD1	13:T:334:LEU:HD22	2.49	0.47
13:T:291:ILE:HG13	13:T:292:LYS:N	2.28	0.47
13:T:302:GLN:O	13:T:306:MET:HG3	2.14	0.47
13:T:444:TRP:O	13:T:447:HIS:HB2	2.14	0.47
16:Q:300:LEU:O	16:Q:301:ARG:HG2	2.14	0.47
3:3:118:ASP:O	3:3:122:CYS:N	2.47	0.47
4:4:117:ARG:CZ	4:4:173:ILE:HD11	2.44	0.47
4:4:156:ILE:O	4:4:159:LEU:HB2	2.14	0.47
4:4:343:TYR:CZ	4:4:354:GLY:HA3	2.49	0.47
10:A:44:TYR:O	10:A:50:PRO:HG3	2.15	0.47
13:L:305:TYR:HB3	13:L:321:HIS:CD2	2.49	0.47
3:D:609:GLU:OE2	3:D:631:ASN:HB3	2.14	0.47
5:F:120:ASP:OD2	5:F:134:LYS:HG3	2.14	0.47
6:G:104:TRP:NE1	6:G:173:VAL:HA	2.30	0.47
10:P:68:PHE:CE2	16:Q:164:LEU:HB2	2.49	0.47
13:T:88:HIS:NE2	13:T:108:PHE:HB3	2.28	0.47
13:T:436:HIS:ND1	13:T:436:HIS:O	2.47	0.47
2:2:77:LYS:HB3	2:2:116:LEU:HB2	1.96	0.47
3:3:445:THR:HB	3:3:463:ALA:HB2	1.97	0.47
4:4:30:VAL:HG13	4:4:35:PRO:HD3	1.95	0.47
4:4:202:ASP:OD1	4:4:284:ARG:NE	2.27	0.47
4:4:222:GLY:HA3	4:4:275:ARG:NH2	2.28	0.47
5:5:157:THR:HG21	7:9:66:TYR:O	2.14	0.47
10:A:2:ALA:N	11:J:49:ARG:HH12	2.12	0.47
13:L:221:PRO:O	13:L:538:TYR:OH	2.30	0.47
13:L:586:LEU:HD13	15:N:138:LEU:HD12	1.95	0.47
16:H:70:GLU:O	16:H:237:SER:OG	2.27	0.47
8:I:10:TYR:O	8:I:13:TRP:HB3	2.14	0.47
13:T:391:ALA:O	13:T:395:TYR:HB2	2.14	0.47
14:U:56:LEU:HD11	15:V:416:PRO:HG2	1.96	0.47
1:1:361:GLU:HB3	3:3:113:LEU:HD22	1.96	0.47
3:3:248:GLU:HB3	3:3:270:ARG:NH1	2.30	0.47
3:3:713:ARG:HE	3:3:746:ARG:HH21	1.62	0.47
5:5:150:TYR:HA	9:W:112:LYS:HE2	1.96	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:L:90:TYR:CD1	13:L:334:LEU:HD22	2.49	0.47
16:H:48:PRO:C	16:H:50:ARG:H	2.16	0.47
16:H:332:LEU:HB2	16:H:333:PRO:CD	2.43	0.47
1:B:194:GLY:O	2:C:24:ARG:NH1	2.48	0.47
1:B:210:GLY:HA3	1:B:216:THR:OG1	2.15	0.47
1:B:422:LEU:O	1:B:426:ARG:N	2.27	0.47
3:D:225:ASN:ND2	3:D:290:ILE:H	2.12	0.47
3:D:474:ARG:HB3	3:D:517:ALA:HB2	1.96	0.47
13:T:4:LEU:HG	13:T:8:LEU:HG	1.97	0.47
13:T:331:LEU:HD12	13:T:446:ASN:OD1	2.13	0.47
14:U:281:PHE:CE2	14:U:332:LEU:HD21	2.50	0.47
15:V:233:LEU:HD21	15:V:273:LEU:HB3	1.97	0.47
15:V:260:TYR:HA	15:V:263:ILE:HD12	1.97	0.47
1:1:9:LEU:HD13	1:1:279:TRP:HH2	1.79	0.47
3:3:136:GLU:HB3	5:5:187:GLY:HA3	1.95	0.47
3:3:607:PHE:O	3:3:624:LEU:HD22	2.15	0.47
6:6:25:GLU:HA	6:6:28:VAL:HG12	1.95	0.47
12:K:46:ALA:HA	15:N:155:TYR:HE2	1.79	0.47
13:L:373:LEU:HD21	13:L:416:TYR:HE1	1.80	0.47
15:N:343:TRP:CE2	15:N:416:PRO:HG3	2.49	0.47
1:B:179:ALA:HB2	2:C:67:TYR:HD1	1.79	0.47
8:I:37:PHE:N	8:I:53:THR:O	2.36	0.47
14:U:106:LEU:O	14:U:110:PHE:HD1	1.97	0.47
14:U:149:VAL:CG1	14:U:153:LEU:HD22	2.44	0.47
16:Q:141:TRP:CE3	16:Q:149:LEU:HD21	2.45	0.47
1:1:43:ARG:NH1	1:1:232:GLU:O	2.48	0.47
3:3:2:VAL:HG13	3:3:89:ASP:HA	1.95	0.47
3:3:717:TRP:HB2	3:3:759:TYR:HB2	1.97	0.47
4:4:144:THR:OG1	16:H:295:ALA:O	2.24	0.47
4:4:353:LEU:HD12	4:4:354:GLY:H	1.79	0.47
5:5:99:PRO:HB2	5:5:124:ILE:HA	1.96	0.47
7:9:17:LEU:HD12	16:H:42:PHE:CZ	2.50	0.47
10:A:40:LYS:HB2	10:A:40:LYS:HE3	1.79	0.47
14:M:33:PHE:HA	14:M:79:ALA:HB1	1.97	0.47
14:M:242:PHE:CZ	14:M:461:PHE:HB2	2.50	0.47
14:M:246:ILE:HG23	14:M:253:PHE:CG	2.49	0.47
1:B:212:TRP:CZ2	2:C:22:GLY:HA3	2.50	0.47
1:B:214:LYS:O	1:B:216:THR:HG23	2.14	0.47
1:B:230:ILE:HG12	1:B:238:PHE:CG	2.50	0.47
1:B:236:ASP:O	1:B:240:GLN:N	2.47	0.47
3:D:134:THR:HG22	4:E:326:TYR:HE1	1.80	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:451:PHE:CE1	3:D:466:GLU:HB3	2.49	0.47
4:E:233:GLY:HA2	5:F:48:PHE:HE1	1.79	0.47
4:E:263:ASP:O	4:E:285:GLU:HG3	2.15	0.47
4:E:339:LYS:HD3	5:F:61:PRO:HG2	1.96	0.47
4:E:382:PRO:O	4:E:386:LYS:HB2	2.15	0.47
6:G:163:TYR:H	7:O:152:ARG:HH12	1.63	0.47
13:T:166:ASP:O	13:T:170:MET:HG3	2.14	0.47
13:T:179:LEU:HD13	13:T:202:LEU:HD13	1.97	0.47
14:U:88:VAL:HG22	14:U:331:ARG:HE	1.80	0.47
16:Q:16:LYS:NZ	16:Q:114:TRP:O	2.27	0.47
1:1:201:LEU:O	1:1:204:PRO:HD2	2.15	0.47
3:3:81:ALA:O	3:3:85:THR:OG1	2.25	0.47
3:3:285:VAL:HA	3:3:387:LEU:HD12	1.96	0.47
3:3:297:GLY:HA3	3:3:703:GLN:NE2	2.29	0.47
4:4:252:TYR:OH	5:5:85:GLY:O	2.31	0.47
13:L:319:LEU:HD12	13:L:473:LEU:HD13	1.97	0.47
16:H:327:VAL:HG21	16:H:337:LEU:HD21	1.96	0.47
4:E:76:LEU:HD22	4:E:330:HIS:CE1	2.49	0.47
7:O:6:LEU:HD23	16:Q:297:TRP:CE2	2.49	0.47
14:U:204:LYS:HE3	14:U:234:TYR:O	2.15	0.47
14:U:232:THR:HA	14:U:235:LYS:HZ2	1.78	0.47
16:Q:150:LEU:HD23	16:Q:154:ARG:HD2	1.96	0.47
3:3:375:THR:HB	3:3:512:LEU:O	2.15	0.47
5:5:33:ARG:NH1	5:5:36:GLU:OE2	2.48	0.47
6:6:62:ARG:HB3	16:H:50:ARG:HB2	1.97	0.47
15:N:52:PRO:HB3	15:N:103:HIS:HB2	1.97	0.47
1:B:53:VAL:O	1:B:57:VAL:HG23	2.14	0.47
1:B:111:PRO:HB3	1:B:145:LEU:HD23	1.95	0.47
1:B:197:ALA:HB3	2:C:66:PHE:CZ	2.50	0.47
14:U:316:ALA:O	14:U:320:VAL:HG23	2.15	0.47
3:3:141:GLU:OE1	5:5:194:SER:HA	2.15	0.47
6:6:35:SER:OG	16:H:62:ASP:HA	2.15	0.47
14:M:7:LEU:O	14:M:11:VAL:HG12	2.15	0.47
14:M:187:GLU:HG2	14:M:188:GLU:HG3	1.96	0.47
15:N:260:TYR:HA	15:N:263:ILE:HD12	1.96	0.47
1:B:101:PHE:CZ	1:B:253:GLN:HB2	2.50	0.47
4:E:67:GLU:OE2	4:E:409:ARG:NE	2.42	0.47
7:O:42:VAL:HG11	7:O:173:PHE:CD1	2.50	0.47
10:P:81:TYR:HB2	11:R:132:TYR:CE1	2.50	0.47
10:P:107:PHE:HE1	16:Q:310:TRP:CD1	2.33	0.47
15:V:38:ALA:O	15:V:42:LEU:HG	2.15	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
15:V:73:THR:HG21	15:V:210:PHE:CG	2.49	0.47
15:V:209:LEU:HD12	15:V:296:PHE:HB2	1.95	0.47
16:Q:40:ALA:HA	16:Q:43:GLN:HG3	1.97	0.47
16:Q:186:VAL:HG11	16:Q:267:TRP:CZ3	2.50	0.47
1:1:336:SER:OG	1:1:420:GLN:NE2	2.49	0.46
3:3:33:PHE:HZ	3:3:130:LEU:HA	1.80	0.46
4:4:143:LEU:H	4:4:143:LEU:HD23	1.79	0.46
4:4:228:VAL:HG21	4:4:383:TYR:CZ	2.50	0.46
9:W:14:LEU:HD22	9:W:73:ALA:HA	1.97	0.46
13:L:59:TRP:NE1	14:M:447:PRO:HD2	2.31	0.46
13:L:291:ILE:HG13	13:L:292:LYS:N	2.30	0.46
13:L:312:VAL:HA	13:L:397:PHE:CD2	2.48	0.46
16:H:90:VAL:HG21	16:H:243:LEU:HD22	1.97	0.46
1:B:159:GLY:H	1:B:162:LEU:HD21	1.80	0.46
3:D:225:ASN:O	3:D:229:ILE:HG13	2.15	0.46
3:D:455:ARG:CZ	3:D:750:ARG:HH22	2.28	0.46
3:D:635:GLU:HG2	9:X:7:ARG:HD2	1.97	0.46
4:E:352:GLU:HB3	4:E:371:ARG:CZ	2.45	0.46
13:T:533:TYR:HB3	13:T:536:ARG:HE	1.80	0.46
2:2:153:LEU:HD21	2:2:163:LEU:HD12	1.96	0.46
11:J:131:LEU:HA	11:J:135:TRP:HB2	1.97	0.46
3:D:463:ALA:O	3:D:465:HIS:ND1	2.47	0.46
3:D:568:TYR:CD1	3:D:572:PRO:HG3	2.50	0.46
4:E:87:TYR:CZ	4:E:403:VAL:HG13	2.51	0.46
4:E:404:MET:HA	4:E:407:VAL:HB	1.97	0.46
5:F:74:LEU:HD12	5:F:88:PHE:CE1	2.50	0.46
6:G:164:ASN:HD21	6:G:168:GLU:CD	2.17	0.46
7:O:102:GLY:HA2	7:O:115:LEU:HD11	1.97	0.46
9:X:37:TRP:HD1	9:X:40:LYS:HB2	1.80	0.46
10:P:77:PHE:O	10:P:80:PRO:HD2	2.15	0.46
10:P:81:TYR:HB2	11:R:132:TYR:CZ	2.51	0.46
11:R:2:SER:HA	11:R:5:GLU:HB3	1.97	0.46
13:T:59:TRP:NE1	14:U:447:PRO:HD2	2.31	0.46
13:T:98:ASP:HB3	13:T:145:TRP:HE1	1.79	0.46
14:U:127:ILE:O	14:U:130:LEU:HG	2.15	0.46
14:U:241:PHE:HA	14:U:245:ALA:HB3	1.97	0.46
14:U:354:LEU:HD13	14:U:425:LEU:HG	1.97	0.46
1:1:275:LEU:O	1:1:279:TRP:HB2	2.16	0.46
4:4:185:GLU:OE1	4:4:185:GLU:N	2.48	0.46
4:4:317:LEU:HD11	4:4:324:VAL:HA	1.98	0.46
9:W:64:GLY:O	9:W:70:GLY:HA3	2.16	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:A:117:ARG:HD2	11:J:159:PRO:HG2	1.98	0.46
15:N:176:LEU:HD11	15:N:227:ALA:HB3	1.96	0.46
16:H:190:LYS:HZ3	16:H:270:PRO:HA	1.81	0.46
1:B:95:GLU:OE1	1:B:138:TYR:OH	2.18	0.46
1:B:219:ASN:HD22	18:B:502:FMN:P	2.37	0.46
1:B:342:TRP:HZ3	1:B:346:ARG:NE	2.12	0.46
1:B:437:TRP:HZ3	2:C:147:ARG:HA	1.80	0.46
5:F:132:LEU:HD23	5:F:132:LEU:HA	1.81	0.46
10:P:76:ALA:HA	10:P:79:TRP:CE3	2.50	0.46
13:T:433:HIS:O	13:T:433:HIS:CG	2.68	0.46
14:U:37:LEU:O	14:U:41:LEU:HG	2.16	0.46
1:1:138:TYR:HB3	1:1:141:ALA:HB3	1.97	0.46
1:1:253:GLN:HA	1:1:262:GLY:O	2.14	0.46
1:1:357:THR:HG23	1:1:360:ARG:NH2	2.30	0.46
3:3:387:LEU:O	3:3:390:LEU:HB3	2.15	0.46
6:6:53:SER:HA	6:6:144:PRO:HB3	1.97	0.46
8:7:10:TYR:HA	8:7:13:TRP:HB3	1.96	0.46
13:L:598:LEU:HA	13:L:598:LEU:HD23	1.74	0.46
15:N:204:PRO:O	15:N:208:VAL:HG23	2.15	0.46
16:H:200:PHE:HE2	16:H:348:LEU:HD12	1.79	0.46
1:B:338:VAL:HG22	1:B:421:TYR:CE2	2.50	0.46
6:G:126:ASN:HB2	9:X:38:GLN:HE21	1.80	0.46
7:O:101:CYS:HB2	7:O:103:LEU:H	1.81	0.46
15:V:237:VAL:O	15:V:241:VAL:HG23	2.16	0.46
3:3:371:PHE:CZ	3:3:374:ARG:HA	2.50	0.46
3:3:382:PHE:CD2	3:3:532:VAL:HG11	2.50	0.46
3:3:722:THR:HG21	3:3:755:LYS:HA	1.98	0.46
4:4:140:LEU:HD21	4:4:217:ARG:NH1	2.29	0.46
5:5:80:TRP:HA	5:5:80:TRP:CE3	2.51	0.46
15:N:61:VAL:O	15:N:65:LEU:HG	2.16	0.46
15:N:184:GLY:HA2	15:N:187:ALA:HB3	1.97	0.46
1:B:201:LEU:HG	1:B:203:PRO:HD2	1.98	0.46
1:B:246:SER:HB3	1:B:268:MET:HG2	1.96	0.46
1:B:352:SER:O	3:D:206:GLY:N	2.46	0.46
3:D:115:HIS:HB3	4:E:321:MET:CE	2.46	0.46
3:D:587:LEU:O	3:D:604:ALA:N	2.48	0.46
4:E:87:TYR:HB3	6:G:45:CYS:HB3	1.96	0.46
6:G:128:ASP:O	6:G:178:ARG:NH2	2.48	0.46
12:S:21:ARG:CZ	12:S:26:LEU:HD23	2.45	0.46
13:T:104:PHE:HB2	13:T:144:PHE:CE1	2.51	0.46
13:T:240:ILE:HG22	13:T:241:HIS:HD2	1.79	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
16:Q:22:VAL:HA	16:Q:25:LEU:HD12	1.98	0.46
16:Q:293:ILE:HD12	16:Q:297:TRP:CZ3	2.51	0.46
3:3:385:ALA:HB2	3:3:531:LYS:HB3	1.98	0.46
4:4:352:GLU:O	4:4:373:PRO:HB3	2.15	0.46
5:5:31:ARG:HH21	5:5:100:ARG:HB2	1.81	0.46
6:6:36:LEU:HB3	6:6:77:VAL:HG21	1.96	0.46
12:K:7:SER:HB2	12:K:37:ALA:O	2.16	0.46
13:L:94:TYR:HE1	13:L:341:HIS:HB2	1.81	0.46
14:M:316:ALA:O	14:M:320:VAL:HG23	2.15	0.46
15:N:143:ALA:HB1	15:N:182:GLY:HA2	1.97	0.46
16:H:327:VAL:O	16:H:331:ASP:N	2.48	0.46
3:D:136:GLU:HG2	5:F:186:GLY:O	2.15	0.46
3:D:414:SER:O	3:D:418:ARG:NE	2.31	0.46
4:E:165:GLY:HA3	7:O:36:ARG:O	2.15	0.46
13:T:84:GLY:O	13:T:88:HIS:ND1	2.40	0.46
13:T:111:PHE:CE1	13:T:134:VAL:HG13	2.51	0.46
15:V:87:LEU:HB2	15:V:121:LEU:HD11	1.97	0.46
2:2:40:TRP:CZ2	2:2:74:PRO:HG3	2.51	0.46
13:L:210:PHE:CD1	13:L:270:ILE:HG12	2.50	0.46
14:M:115:LEU:HD11	14:M:248:LEU:HD21	1.96	0.46
14:M:127:ILE:O	14:M:130:LEU:HG	2.16	0.46
16:H:290:PHE:O	16:H:294:ARG:HG2	2.16	0.46
1:B:437:TRP:HD1	2:C:95:GLU:OE1	1.98	0.46
4:E:384:ALA:HB1	4:E:396:ILE:HD11	1.97	0.46
5:F:174:LEU:HD22	5:F:180:GLY:HA2	1.98	0.46
6:G:125:GLN:OE1	7:O:97:ARG:NH2	2.40	0.46
7:O:114:VAL:HG21	7:O:169:GLU:O	2.15	0.46
11:R:24:ASN:HB3	11:R:27:HIS:HB2	1.98	0.46
1:1:63:ARG:HD3	1:1:313:TYR:CD2	2.51	0.46
1:1:249:MET:SD	1:1:249:MET:N	2.79	0.46
3:3:713:ARG:NE	3:3:746:ARG:HE	2.13	0.46
4:4:88:LEU:HD21	4:4:131:VAL:HG11	1.98	0.46
6:6:130:VAL:HA	9:W:122:ASP:HB2	1.97	0.46
13:L:437:GLU:O	13:L:439:PRO:HD3	2.16	0.46
1:B:242:GLY:HA3	1:B:246:SER:O	2.15	0.46
3:D:223:SER:N	3:D:292:ASP:OD2	2.44	0.46
3:D:616:ASN:ND2	3:D:622:LEU:HD11	2.27	0.46
4:E:50:GLU:CD	16:Q:154:ARG:HH12	2.19	0.46
4:E:131:VAL:HG23	4:E:153:ARG:HD2	1.98	0.46
8:I:82:ILE:HG23	8:I:95:ALA:HB3	1.98	0.46
13:T:1:MET:HA	13:T:55:PHE:HE2	1.80	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
14:U:127:ILE:HB	14:U:128:PRO:HD3	1.97	0.46
3:3:297:GLY:O	3:3:300:TRP:NE1	2.49	0.46
4:4:314:ARG:HB3	8:7:44:MET:CE	2.46	0.46
5:5:140:ASP:OD2	9:W:90:TYR:OH	2.32	0.46
6:6:59:ASP:HB3	16:H:45:ARG:HG3	1.96	0.46
6:6:74:GLN:NE2	16:H:234:THR:H	2.14	0.46
12:K:87:VAL:HA	12:K:90:LEU:HD13	1.97	0.46
15:N:177:GLY:O	15:N:181:VAL:HG23	2.15	0.46
16:H:17:ALA:O	16:H:21:VAL:HG23	2.16	0.46
16:H:132:ALA:O	16:H:136:ILE:HG13	2.16	0.46
1:B:4:PRO:HA	1:B:12:ARG:NH1	2.31	0.46
1:B:137:GLU:HB3	2:C:141:TYR:OH	2.16	0.46
5:F:10:ALA:HB3	5:F:17:ILE:HD11	1.98	0.46
6:G:145:GLU:HG2	7:O:31:VAL:HG21	1.97	0.46
15:V:123:THR:HG22	15:V:130:LEU:HD21	1.98	0.46
15:V:257:LEU:HD11	15:V:374:TYR:HB2	1.97	0.46
1:1:337:MET:O	1:1:341:MET:HG2	2.15	0.46
6:6:140:CYS:SG	7:9:99:ILE:HG13	2.56	0.46
11:J:29:ALA:O	11:J:33:ILE:HG13	2.16	0.46
13:L:72:LEU:HB3	13:L:255:ARG:NH1	2.31	0.46
15:N:123:THR:HG22	15:N:130:LEU:HD23	1.98	0.46
16:H:268:THR:HA	16:H:273:GLU:OE1	2.16	0.46
1:B:14:GLU:OE2	1:B:233:ARG:NH1	2.49	0.46
4:E:38:HIS:CE1	4:E:398:ALA:HA	2.51	0.46
4:E:166:GLN:NE2	7:O:100:PHE:O	2.49	0.46
4:E:231:ASP:O	5:F:110:SER:N	2.49	0.46
5:F:103:THR:HG23	5:F:127:GLU:O	2.15	0.46
8:I:61:ASP:OD2	8:I:128:PHE:HD1	1.99	0.46
13:T:72:LEU:HD13	13:T:473:LEU:HD22	1.98	0.46
13:T:360:PRO:HA	13:T:363:ARG:NH1	2.31	0.46
14:U:281:PHE:CE1	14:U:341:ILE:HG22	2.50	0.46
15:V:27:ARG:HA	15:V:30:LEU:HD12	1.96	0.46
1:1:253:GLN:HG2	1:1:327:GLY:HA2	1.97	0.45
5:5:42:LYS:HB2	5:5:108:TRP:CZ2	2.51	0.45
7:9:41:HIS:NE2	7:9:104:CYS:SG	2.89	0.45
14:M:133:LEU:HD11	14:M:220:GLU:HB2	1.97	0.45
15:N:92:ALA:HA	15:N:95:MET:HE2	1.98	0.45
15:N:190:ALA:N	15:N:240:SER:OG	2.47	0.45
16:H:217:THR:HG23	16:H:298:PHE:O	2.17	0.45
3:D:563:ALA:HB3	3:D:580:LYS:HE3	1.99	0.45
4:E:93:HIS:HA	4:E:353:LEU:HD21	1.97	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:F:151:PRO:HD3	9:X:112:LYS:HE2	1.98	0.45
10:P:68:PHE:CD2	16:Q:164:LEU:HB2	2.51	0.45
13:T:432:HIS:CE1	13:T:434:HIS:HB2	2.51	0.45
1:1:23:LYS:HG3	1:1:31:TYR:OH	2.16	0.45
1:1:137:GLU:HB3	2:2:141:TYR:OH	2.16	0.45
1:1:157:TYR:O	1:1:158:LEU:HD23	2.16	0.45
3:3:713:ARG:NH2	3:3:746:ARG:HH21	2.13	0.45
4:4:161:GLU:HG2	7:9:34:LYS:HG2	1.96	0.45
4:4:246:TYR:CD1	5:5:78:PRO:HD2	2.51	0.45
14:M:30:GLY:O	14:M:34:LEU:HG	2.16	0.45
14:M:318:SER:HA	14:M:321:TYR:CE1	2.50	0.45
1:B:192:LEU:HD22	1:B:211:LEU:HD21	1.98	0.45
4:E:350:ARG:NH2	4:E:401:ASP:OD2	2.49	0.45
5:F:163:ARG:NH2	7:O:92:GLU:OE2	2.49	0.45
14:U:143:ARG:HD3	14:U:143:ARG:HA	1.71	0.45
14:U:218:HIS:HA	14:U:221:ASN:HD22	1.81	0.45
15:V:339:LEU:HD23	15:V:410:LEU:HA	1.97	0.45
1:1:66:GLY:HA3	18:1:502:FMN:H3'	1.98	0.45
2:2:142:VAL:HG21	2:2:163:LEU:HD11	1.98	0.45
3:3:269:THR:HG21	3:3:628:PRO:HD2	1.98	0.45
9:W:31:VAL:HG22	9:W:50:LEU:HD13	1.97	0.45
12:K:88:ASP:HA	13:L:585:TYR:HD1	1.81	0.45
13:L:90:TYR:CG	13:L:334:LEU:HD13	2.52	0.45
15:N:412:LEU:HD13	15:N:419:VAL:HG21	1.98	0.45
16:H:267:TRP:CD1	16:H:275:PRO:HA	2.51	0.45
1:B:138:TYR:HB3	1:B:141:ALA:HB3	1.97	0.45
1:B:275:LEU:HA	1:B:279:TRP:CD1	2.52	0.45
1:B:297:THR:HG22	1:B:322:MET:HG3	1.98	0.45
3:D:256:CYS:O	3:D:262:GLY:HA2	2.16	0.45
3:D:308:THR:OG1	3:D:319:GLU:HG2	2.17	0.45
3:D:688:ARG:HD3	3:D:688:ARG:HA	1.48	0.45
3:D:689:LYS:H	3:D:689:LYS:HG2	1.55	0.45
5:F:64:ARG:HD3	5:F:64:ARG:HA	1.69	0.45
13:T:128:PHE:HD1	13:T:169:PHE:CD2	2.34	0.45
13:T:554:PHE:CZ	14:U:283:THR:HG21	2.51	0.45
14:U:329:ALA:O	14:U:332:LEU:HG	2.17	0.45
14:U:347:LEU:HB2	14:U:414:PHE:HA	1.98	0.45
3:3:561:PRO:HG3	3:3:575:GLU:HG3	1.98	0.45
6:6:39:ALA:HB2	6:6:75:ALA:HB3	1.98	0.45
6:6:46:CYS:SG	6:6:109:GLY:HA3	2.56	0.45
6:6:93:ARG:NH2	9:W:122:ASP:OD1	2.50	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
14:M:306:GLU:O	14:M:379:LEU:HB3	2.17	0.45
4:E:30:VAL:HG21	4:E:393:MET:HE1	1.98	0.45
4:E:76:LEU:HD22	4:E:330:HIS:HE1	1.80	0.45
7:O:72:PRO:HG3	7:O:86:ARG:HH21	1.81	0.45
7:O:94:ASN:O	7:O:98:CYS:N	2.40	0.45
14:U:16:LEU:HD22	14:U:97:GLY:N	2.32	0.45
16:Q:274:VAL:HG22	16:Q:275:PRO:HD2	1.98	0.45
3:3:183:HIS:HE2	3:3:209:THR:C	2.19	0.45
4:4:28:LEU:HD21	16:H:228:LEU:HD11	1.98	0.45
4:4:271:ASP:C	4:4:275:ARG:HE	2.20	0.45
5:5:33:ARG:O	5:5:37:GLU:HB2	2.17	0.45
7:9:17:LEU:HA	16:H:41:ARG:O	2.16	0.45
15:N:126:ARG:HG3	15:N:305:ASP:OD1	2.16	0.45
3:D:31:PRO:HG3	3:D:137:TYR:CD2	2.52	0.45
3:D:188:VAL:HG11	3:D:201:ASP:CA	2.40	0.45
3:D:444:ARG:HH21	3:D:446:ASP:CG	2.20	0.45
4:E:33:GLN:H	4:E:41:LEU:H	1.63	0.45
4:E:366:TYR:HE1	5:F:59:THR:HB	1.82	0.45
11:R:133:GLY:H	11:R:136:LEU:HB2	1.82	0.45
13:T:159:PHE:HD2	14:U:407:LEU:HD11	1.80	0.45
13:T:293:LYS:O	13:T:297:TYR:HD1	1.98	0.45
13:T:325:HIS:CD2	13:T:329:LYS:HG3	2.51	0.45
13:T:557:ASP:OD1	14:U:211:HIS:NE2	2.26	0.45
13:T:574:LEU:HD22	15:V:246:LEU:HD13	1.98	0.45
15:V:193:HIS:CE1	15:V:243:VAL:HG11	2.51	0.45
3:3:468:HIS:CE1	3:3:473:GLU:HG3	2.51	0.45
7:9:44:THR:OG1	7:9:52:LYS:HD2	2.17	0.45
7:9:113:ILE:HB	17:9:202:SF4:S4	2.57	0.45
14:M:204:LYS:HE3	14:M:234:TYR:O	2.16	0.45
15:N:126:ARG:HE	15:N:305:ASP:CG	2.19	0.45
1:B:276:ILE:HG22	1:B:282:GLY:HA2	1.99	0.45
1:B:357:THR:N	1:B:358:PRO:HD2	2.32	0.45
3:D:376:ALA:HB1	3:D:685:PRO:HA	1.98	0.45
4:E:240:ARG:HA	4:E:244:VAL:H	1.81	0.45
6:G:92:MET:O	6:G:96:TRP:N	2.38	0.45
10:P:113:LYS:NZ	15:V:83:GLU:OE2	2.47	0.45
12:S:39:ASN:HD22	12:S:61:ILE:HG13	1.79	0.45
13:T:171:LEU:HB3	13:T:208:LEU:HD13	1.98	0.45
16:Q:260:PRO:HG3	16:Q:286:PHE:CD2	2.51	0.45
1:1:167:PHE:CE2	1:1:169:PHE:HB2	2.52	0.45
13:L:355:LEU:N	13:L:425:PHE:O	2.49	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:L:557:ASP:OD1	14:M:211:HIS:NE2	2.36	0.45
3:D:297:GLY:HA3	3:D:703:GLN:NE2	2.32	0.45
3:D:444:ARG:NH2	3:D:446:ASP:OD2	2.47	0.45
4:E:376:VAL:HG12	4:E:379:GLN:HE21	1.80	0.45
5:F:13:LYS:NZ	5:F:37:GLU:OE2	2.28	0.45
6:G:91:VAL:HG22	10:P:46:SER:HB3	1.98	0.45
9:X:3:ARG:NH1	9:X:103:LEU:HB3	2.31	0.45
10:P:28:GLY:HA2	16:Q:67:ILE:HG22	1.99	0.45
13:T:320:PHE:CE2	13:T:460:ALA:HB3	2.52	0.45
15:V:119:TYR:HE1	15:V:136:TYR:CD2	2.35	0.45
16:Q:65:LYS:O	16:Q:69:LYS:HB2	2.16	0.45
16:Q:77:ALA:HB1	16:Q:142:ALA:O	2.16	0.45
10:A:57:PHE:HB2	11:J:73:LEU:HD23	1.99	0.45
10:A:61:PHE:HE1	16:H:302:TYR:CE2	2.35	0.45
13:L:12:LEU:O	13:L:16:LEU:HG	2.16	0.45
13:L:119:VAL:HG23	13:L:120:LEU:HG	1.99	0.45
13:L:320:PHE:CZ	13:L:460:ALA:HB3	2.52	0.45
14:M:157:LEU:O	15:N:365:LEU:HD13	2.16	0.45
15:N:315:LEU:O	15:N:319:ASP:N	2.40	0.45
16:H:199:ALA:HA	16:H:320:TRP:CZ2	2.52	0.45
16:H:300:LEU:O	16:H:301:ARG:HG2	2.17	0.45
16:H:310:TRP:CE3	16:H:314:PHE:HE2	2.35	0.45
4:E:46:THR:O	4:E:53:LEU:HB2	2.17	0.45
5:F:101:LEU:HD23	5:F:126:PHE:CE2	2.51	0.45
6:G:177:LYS:HB2	6:G:177:LYS:HE3	1.51	0.45
13:T:600:LEU:HD11	15:V:232:ALA:HB1	1.98	0.45
14:U:235:LYS:HD3	14:U:293:MET:CG	2.46	0.45
4:4:193:LEU:HA	4:4:196:VAL:HG12	1.98	0.45
4:4:231:ASP:O	5:5:110:SER:OG	2.31	0.45
4:4:381:LEU:HB3	4:4:382:PRO:HD3	1.98	0.45
16:H:212:ALA:HA	16:H:218:PRO:HG3	1.99	0.45
1:B:91:CYS:HB3	1:B:132:ILE:HG23	1.99	0.45
1:B:167:PHE:CE2	1:B:169:PHE:HB2	2.52	0.45
1:B:349:ALA:HB2	1:B:363:VAL:HG12	1.99	0.45
1:B:412:GLY:HA2	1:B:415:ARG:HB3	1.99	0.45
1:B:438:ARG:HA	2:C:147:ARG:NH2	2.32	0.45
3:D:299:GLU:OE2	3:D:707:LYS:HG3	2.17	0.45
3:D:332:GLY:HA3	3:D:582:PHE:CE1	2.52	0.45
3:D:438:LYS:O	3:D:441:MET:HG3	2.17	0.45
4:E:86:ASP:HB3	4:E:93:HIS:CD2	2.51	0.45
4:E:132:PHE:CD1	4:E:401:ASP:HB2	2.52	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:E:167:ARG:NE	6:G:49:GLU:OE2	2.36	0.45
4:E:287:VAL:O	4:E:291:LYS:HG3	2.16	0.45
6:G:34:ASN:HA	6:G:155:GLN:HE21	1.81	0.45
10:P:23:ALA:O	10:P:27:VAL:HG23	2.17	0.45
13:T:461:LEU:HB3	13:T:465:LEU:HB2	1.98	0.45
1:1:342:TRP:CD1	1:1:371:PHE:HB3	2.51	0.45
3:3:201:ASP:OD1	3:3:202:PHE:N	2.45	0.45
6:6:153:GLN:O	6:6:156:LYS:HG2	2.16	0.45
7:9:101:CYS:HB2	7:9:103:LEU:H	1.81	0.45
8:7:103:LEU:O	8:7:110:LEU:N	2.30	0.45
14:M:351:ALA:HB1	14:M:354:LEU:HB2	1.99	0.45
16:H:67:ILE:HG13	16:H:68:PHE:CD1	2.52	0.45
16:H:221:LEU:N	16:H:222:PRO:HA	2.31	0.45
4:E:105:LEU:HD13	4:E:309:ILE:HD13	1.98	0.45
4:E:193:LEU:HA	4:E:196:VAL:HG12	1.98	0.45
6:G:82:GLY:HA2	17:G:201:SF4:S4	2.57	0.45
6:G:104:TRP:HD1	6:G:134:ASP:OD1	2.00	0.45
10:P:1:MET:HG2	10:P:2:ALA:H	1.81	0.45
11:R:97:ALA:O	12:S:12:ALA:HB1	2.17	0.45
14:U:93:GLY:HA3	14:U:136:TYR:CE1	2.52	0.45
14:U:122:PHE:O	14:U:234:TYR:OH	2.33	0.45
16:Q:150:LEU:HD21	16:Q:154:ARG:HH11	1.81	0.45
3:3:399:LEU:HD22	3:3:477:LEU:HD11	1.98	0.44
3:3:557:SER:H	3:3:560:GLU:HB2	1.82	0.44
3:3:664:LEU:HD22	3:3:669:VAL:HG11	1.99	0.44
4:4:85:MET:CE	4:4:370:VAL:HG21	2.47	0.44
6:6:120:ASN:HD22	6:6:122:ALA:N	2.05	0.44
13:L:30:GLY:HA3	13:L:92:ILE:HG12	1.99	0.44
3:D:606:THR:OG1	3:D:609:GLU:OE1	2.35	0.44
3:D:713:ARG:NE	3:D:746:ARG:HE	2.14	0.44
4:E:50:GLU:OE1	16:Q:154:ARG:NH1	2.44	0.44
4:E:367:ARG:HH22	4:E:369:LYS:HG3	1.82	0.44
5:F:2:ARG:NH1	5:F:45:GLY:O	2.50	0.44
6:G:166:ARG:HD3	6:G:168:GLU:OE2	2.17	0.44
8:I:24:ALA:HA	8:I:29:VAL:HG12	1.98	0.44
14:U:448:GLY:O	14:U:452:ARG:HG2	2.17	0.44
16:Q:177:VAL:HG12	16:Q:179:SER:H	1.82	0.44
1:1:109:ASP:OD2	2:2:174:HIS:NE2	2.38	0.44
3:3:409:LEU:HD23	3:3:409:LEU:HA	1.79	0.44
15:N:297:ALA:O	15:N:301:GLN:HG3	2.17	0.44
1:B:9:LEU:HD13	1:B:279:TRP:CZ2	2.52	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:242:GLY:HA2	1:B:268:MET:O	2.17	0.44
2:C:154:LEU:HD23	2:C:154:LEU:HA	1.84	0.44
7:O:94:ASN:HB3	7:O:97:ARG:HB2	1.99	0.44
8:I:43:ARG:NH1	8:I:46:ARG:O	2.50	0.44
12:S:46:ALA:HB2	12:S:53:GLY:HA3	1.99	0.44
14:U:16:LEU:HD12	14:U:25:GLY:HA3	1.99	0.44
14:U:242:PHE:CE2	14:U:312:LEU:HD11	2.53	0.44
16:Q:267:TRP:CD1	16:Q:275:PRO:HA	2.52	0.44
1:1:117:GLY:HA3	1:1:224:LEU:O	2.16	0.44
3:3:444:ARG:HH21	3:3:446:ASP:CG	2.17	0.44
4:4:46:THR:O	4:4:53:LEU:HB2	2.18	0.44
4:4:131:VAL:HG23	4:4:153:ARG:HD2	1.99	0.44
4:4:379:GLN:NE2	5:5:110:SER:O	2.49	0.44
12:K:28:PHE:O	12:K:32:GLU:HG2	2.17	0.44
13:L:600:LEU:HD11	15:N:232:ALA:HB1	1.99	0.44
14:M:452:ARG:HD3	14:M:452:ARG:HA	1.71	0.44
15:N:21:PRO:O	15:N:25:VAL:HG23	2.16	0.44
1:B:259:LYS:HB3	1:B:281:GLY:HA3	1.98	0.44
3:D:33:PHE:HB2	3:D:45:CYS:SG	2.58	0.44
3:D:120:PRO:HB2	7:O:54:ILE:HD11	1.99	0.44
4:E:343:TYR:HA	4:E:355:TYR:O	2.17	0.44
5:F:3:LEU:O	5:F:7:LEU:HG	2.17	0.44
6:G:104:TRP:CD1	6:G:154:LEU:HD11	2.52	0.44
13:T:179:LEU:HD11	13:T:201:LEU:HB3	1.98	0.44
15:V:126:ARG:HD3	15:V:126:ARG:HA	1.60	0.44
1:1:190:ASN:HD21	1:1:200:ARG:HG2	1.82	0.44
3:3:472:GLU:O	3:3:476:ILE:HD12	2.16	0.44
5:5:132:LEU:HD23	5:5:132:LEU:HA	1.82	0.44
7:9:34:LYS:HA	7:9:34:LYS:HD3	1.85	0.44
7:9:123:ASP:CG	7:9:148:ARG:HH22	2.20	0.44
8:7:24:ALA:HA	8:7:29:VAL:HG12	1.99	0.44
8:7:77:ALA:O	8:7:80:LYS:NZ	2.41	0.44
11:J:83:PHE:O	12:K:22:ARG:NH1	2.50	0.44
13:L:33:ALA:HB2	13:L:109:ASN:HD21	1.83	0.44
13:L:270:ILE:HG23	13:L:307:PHE:HD2	1.83	0.44
13:L:286:PHE:HB2	13:L:419:ARG:HD3	2.00	0.44
13:L:433:HIS:O	13:L:433:HIS:CG	2.71	0.44
13:L:435:PRO:HG2	13:L:436:HIS:CD2	2.53	0.44
15:N:62:PHE:CG	15:N:221:ALA:HB2	2.52	0.44
1:B:253:GLN:HA	1:B:262:GLY:O	2.17	0.44
4:E:62:LEU:HD11	6:G:43:LEU:O	2.18	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:F:18:GLU:HB2	5:F:26:TRP:HB2	1.99	0.44
13:T:30:GLY:HA3	13:T:92:ILE:HG12	1.99	0.44
14:U:70:LEU:HD21	14:U:239:PHE:HD1	1.83	0.44
15:V:327:LEU:O	15:V:331:LEU:HG	2.17	0.44
1:1:167:PHE:HE2	1:1:169:PHE:HB2	1.82	0.44
3:3:373:GLY:HA3	3:3:538:ALA:HB2	2.00	0.44
8:7:10:TYR:OH	8:7:73:SER:O	2.21	0.44
10:A:68:PHE:HD2	16:H:164:LEU:HB2	1.83	0.44
12:K:82:ARG:HG2	12:K:83:GLU:N	2.33	0.44
13:L:94:TYR:HA	13:L:442:MET:HE1	1.99	0.44
15:N:73:THR:HG21	15:N:210:PHE:HB2	1.99	0.44
15:N:319:ASP:HB3	15:N:322:LEU:HB2	2.00	0.44
16:H:174:VAL:O	16:H:178:GLY:N	2.38	0.44
3:D:34:CYS:O	3:D:189:ARG:NH2	2.45	0.44
4:E:98:ALA:O	4:E:102:GLU:HG3	2.17	0.44
4:E:265:PRO:HB3	4:E:281:ARG:HB2	2.00	0.44
13:T:47:LEU:O	13:T:50:SER:OG	2.29	0.44
13:T:112:ILE:O	13:T:116:LEU:HG	2.17	0.44
16:Q:139:SER:HG	16:Q:236:TYR:HH	1.46	0.44
1:1:194:GLY:O	2:2:24:ARG:NH1	2.51	0.44
3:3:565:TYR:HA	3:3:582:PHE:O	2.17	0.44
3:3:688:ARG:HD3	3:3:688:ARG:HA	1.58	0.44
3:3:750:ARG:NE	3:3:752:ASP:OD1	2.50	0.44
4:4:77:GLN:O	4:4:80:THR:OG1	2.18	0.44
4:4:159:LEU:O	4:4:163:VAL:HG12	2.18	0.44
13:L:223:MET:HB2	13:L:300:ILE:HD13	1.98	0.44
13:L:358:HIS:O	13:L:360:PRO:HD3	2.18	0.44
14:M:218:HIS:O	14:M:282:LYS:NZ	2.41	0.44
15:N:38:ALA:O	15:N:42:LEU:HG	2.17	0.44
16:H:99:LEU:HD12	16:H:116:ILE:HG13	1.99	0.44
8:I:23:TYR:OH	8:I:120:ASP:HA	2.17	0.44
8:I:105:THR:OG1	8:I:114:ARG:NH2	2.44	0.44
10:P:67:LEU:HD23	16:Q:310:TRP:CZ2	2.53	0.44
13:T:534:VAL:O	13:T:538:TYR:N	2.36	0.44
14:U:84:LEU:HB3	14:U:432:PHE:CE1	2.52	0.44
15:V:177:GLY:O	15:V:181:VAL:HG23	2.18	0.44
16:Q:287:LEU:O	16:Q:291:ILE:HG13	2.17	0.44
3:3:689:LYS:HG3	3:3:772:GLU:HG2	2.00	0.44
12:K:59:MET:HB2	15:N:105:LEU:HD21	1.99	0.44
13:L:139:PHE:CD2	13:L:155:ALA:HB1	2.52	0.44
13:L:491:TRP:HA	13:L:494:ILE:HG12	1.99	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
14:M:160:LEU:O	14:M:163:VAL:HG12	2.18	0.44
2:C:97:TRP:CH2	2:C:119:VAL:HB	2.52	0.44
4:E:116:ILE:HG12	4:E:182:LEU:HD11	1.99	0.44
5:F:145:PRO:O	5:F:150:TYR:HB3	2.18	0.44
11:R:100:VAL:HA	13:T:598:LEU:HD21	2.00	0.44
13:T:359:LEU:HD12	13:T:425:PHE:HE2	1.83	0.44
1:1:364:ALA:HB3	3:3:207:VAL:HG13	1.99	0.44
4:4:147:PHE:HE2	16:H:45:ARG:HD3	1.83	0.44
11:J:61:GLY:O	11:J:65:VAL:HG21	2.17	0.44
11:J:71:ILE:HA	11:J:74:LEU:O	2.18	0.44
13:L:356:TRP:O	13:L:363:ARG:NH1	2.50	0.44
13:L:386:ASP:HA	13:L:389:LEU:HB2	1.99	0.44
15:N:223:LEU:HB3	15:N:273:LEU:HD11	1.99	0.44
15:N:271:LEU:HB2	15:N:348:ALA:HB1	1.99	0.44
1:B:293:GLY:HA2	1:B:323:LEU:HD12	2.00	0.44
3:D:134:THR:HG22	4:E:326:TYR:CE1	2.53	0.44
3:D:723:ALA:O	3:D:727:ALA:N	2.51	0.44
4:E:42:ARG:HD2	4:E:61:TYR:OH	2.17	0.44
4:E:229:ALA:O	4:E:234:LEU:N	2.41	0.44
7:O:149:GLU:O	7:O:153:THR:CB	2.66	0.44
11:R:115:PHE:CD1	12:S:48:ALA:HB2	2.52	0.44
13:T:224:VAL:HG11	13:T:538:TYR:HD2	1.82	0.44
13:T:444:TRP:HE3	13:T:447:HIS:HD2	1.66	0.44
14:U:224:SER:HA	14:U:330:GLY:CA	2.48	0.44
15:V:269:MET:HB3	15:V:281:LEU:HD11	1.99	0.44
1:1:17:LEU:H	1:1:265:GLU:CD	2.20	0.44
3:3:343:LEU:HB2	3:3:369:LEU:HB3	2.00	0.44
4:4:272:VAL:N	4:4:275:ARG:HH21	2.16	0.44
4:4:331:TYR:OH	7:9:106:GLU:HG2	2.18	0.44
5:5:71:VAL:HG22	5:5:91:ARG:HA	1.99	0.44
5:5:103:THR:CG2	5:5:126:PHE:HB3	2.45	0.44
6:6:169:ARG:NH1	6:6:169:ARG:HG3	2.33	0.44
11:J:142:VAL:O	11:J:146:LEU:HG	2.18	0.44
13:L:293:LYS:O	13:L:297:TYR:HD1	2.01	0.44
13:L:405:GLY:O	13:L:409:VAL:HG23	2.17	0.44
16:H:35:GLU:HG3	16:H:291:ILE:HD13	2.00	0.44
16:H:224:ALA:HB2	16:H:233:HIS:CE1	2.53	0.44
1:B:16:THR:OG1	1:B:233:ARG:NH2	2.50	0.44
1:B:212:TRP:CE2	2:C:22:GLY:HA3	2.53	0.44
1:B:275:LEU:HA	1:B:279:TRP:HD1	1.83	0.44
4:E:162:TRP:NE1	7:O:34:LYS:HD2	2.33	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:E:194:LEU:HD21	4:E:290:ILE:HG22	2.00	0.44
7:O:33:LEU:HD11	7:O:119:PHE:CE2	2.53	0.44
15:V:312:LEU:HD13	15:V:326:PHE:CZ	2.53	0.44
16:Q:188:TRP:CZ3	16:Q:192:HIS:HB2	2.52	0.44
16:Q:239:ILE:O	16:Q:243:LEU:N	2.43	0.44
3:3:621:VAL:HG23	3:3:672:ALA:HA	2.00	0.43
13:L:22:LYS:NZ	13:L:100:GLY:HA2	2.33	0.43
14:M:2:VAL:HG21	14:M:65:PHE:HB3	2.00	0.43
14:M:357:LEU:HD22	14:M:433:ALA:HB2	1.99	0.43
1:B:191:SER:OG	2:C:28:MET:SD	2.72	0.43
4:E:329:LYS:HD2	4:E:329:LYS:HA	1.73	0.43
8:I:48:TYR:CZ	8:I:50:LEU:HB2	2.53	0.43
11:R:75:PHE:O	11:R:77:ALA:N	2.51	0.43
14:U:135:LEU:H	14:U:135:LEU:HD23	1.81	0.43
15:V:204:PRO:O	15:V:208:VAL:HG23	2.18	0.43
16:Q:86:PRO:HG3	16:Q:244:PHE:CE2	2.53	0.43
1:1:90:ILE:HD11	1:1:211:LEU:HD22	2.00	0.43
1:1:184:GLU:OE1	1:1:186:THR:OG1	2.26	0.43
1:1:314:GLU:HA	1:1:317:GLN:HB3	2.00	0.43
2:2:74:PRO:HD3	8:7:125:ALA:CB	2.48	0.43
3:3:33:PHE:CZ	3:3:130:LEU:HA	2.53	0.43
3:3:368:HIS:CB	3:3:556:ALA:HB3	2.48	0.43
4:4:73:ARG:HH11	5:5:171:ARG:HH21	1.66	0.43
11:J:5:GLU:O	11:J:9:LEU:HG	2.17	0.43
13:L:271:ALA:HB2	13:L:311:GLY:HA3	2.00	0.43
13:L:419:ARG:HB2	13:L:512:PHE:CD2	2.54	0.43
14:M:223:PRO:HB3	14:M:339:LEU:HD11	2.00	0.43
15:N:131:GLU:HG2	15:N:135:LYS:HE2	1.99	0.43
1:B:397:ARG:HH21	3:D:103:ALA:HB2	1.82	0.43
3:D:317:LEU:HD21	3:D:595:GLU:HA	2.00	0.43
4:E:53:LEU:O	4:E:386:LYS:HG3	2.18	0.43
11:R:104:LEU:HD23	15:V:174:LEU:HD21	2.00	0.43
14:U:152:THR:OG1	14:U:153:LEU:HD13	2.17	0.43
15:V:63:THR:HG21	15:V:96:HIS:HD1	1.83	0.43
15:V:313:ARG:HB2	15:V:384:ALA:HB3	2.00	0.43
1:1:83:ASP:OD1	1:1:87:HIS:NE2	2.51	0.43
1:1:98:PRO:HG3	2:2:124:CYS:HB2	1.99	0.43
3:3:586:HIS:NE2	3:3:604:ALA:HA	2.34	0.43
6:6:61:ALA:O	16:H:48:PRO:HG3	2.18	0.43
10:A:44:TYR:CD2	10:A:45:GLU:HB2	2.53	0.43
14:M:54:PRO:HA	14:M:62:TYR:HD1	1.82	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
15:N:265:HIS:O	15:N:269:MET:HG3	2.17	0.43
16:H:224:ALA:HA	16:H:229:VAL:HA	2.00	0.43
3:D:115:HIS:CE1	17:D:801:SF4:S2	2.84	0.43
3:D:192:GLU:CD	3:D:440:ARG:HD2	2.39	0.43
4:E:207:LEU:HD21	7:O:12:ILE:HD11	2.01	0.43
6:G:41:PHE:CE2	6:G:43:LEU:HD21	2.53	0.43
6:G:46:CYS:HB2	6:G:82:GLY:HA2	2.00	0.43
7:O:26:TYR:OH	7:O:120:GLU:HG2	2.18	0.43
12:S:14:GLY:HA3	12:S:34:MET:HG3	2.00	0.43
13:T:209:LEU:HD22	13:T:252:LEU:HD11	2.00	0.43
13:T:368:ILE:HG21	13:T:450:ALA:HB1	2.00	0.43
14:U:8:LEU:HB3	14:U:9:PRO:HD3	1.99	0.43
15:V:307:VAL:HG13	15:V:311:ALA:HB3	2.01	0.43
15:V:316:TYR:HB2	15:V:382:VAL:CG1	2.48	0.43
16:Q:185:ILE:HG22	16:Q:189:GLN:OE1	2.19	0.43
3:3:228:ASP:OD2	3:3:295:ARG:NH2	2.33	0.43
4:4:48:SER:H	4:4:53:LEU:HD23	1.83	0.43
5:5:38:MET:HA	5:5:41:TYR:HB2	2.00	0.43
11:J:103:ILE:HG21	13:L:601:LEU:HD23	2.01	0.43
13:L:38:LEU:HB2	13:L:85:PHE:CD1	2.53	0.43
14:M:86:ALA:HA	14:M:96:LEU:HD11	2.00	0.43
14:M:91:VAL:HG12	14:M:222:HIS:CE1	2.53	0.43
14:M:151:PHE:O	14:M:203:ILE:HD13	2.18	0.43
15:N:237:VAL:O	15:N:241:VAL:HG23	2.18	0.43
1:B:249:MET:SD	1:B:249:MET:N	2.87	0.43
3:D:141:GLU:OE1	4:E:306:ASN:ND2	2.51	0.43
3:D:352:GLU:CG	3:D:660:ALA:HB1	2.48	0.43
3:D:478:LEU:HD12	3:D:520:ARG:NH2	2.33	0.43
4:E:140:LEU:HD21	4:E:217:ARG:NH1	2.34	0.43
4:E:394:VAL:HG11	16:Q:226:GLN:O	2.19	0.43
6:G:147:LEU:O	6:G:151:VAL:HG13	2.17	0.43
9:X:102:LEU:HG	9:X:110:LEU:HD13	1.99	0.43
10:P:7:TYR:CD1	16:Q:118:LEU:HD22	2.53	0.43
15:V:140:GLY:HA2	15:V:185:PHE:CE2	2.53	0.43
2:2:162:ARG:HE	2:2:164:GLU:CD	2.22	0.43
3:3:370:ASP:OD2	3:3:558:TRP:HD1	2.02	0.43
6:6:115:GLY:HA3	6:6:125:GLN:OE1	2.19	0.43
13:L:161:VAL:HG13	13:L:222:LEU:HD13	2.01	0.43
14:M:155:GLY:O	14:M:200:ALA:HB2	2.18	0.43
14:M:344:TYR:O	14:M:347:LEU:HD23	2.19	0.43
15:N:48:PHE:CD1	15:N:53:TYR:HE2	2.36	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:10:ASP:OD2	1:B:12:ARG:NE	2.52	0.43
18:B:502:FMN:H9	18:B:502:FMN:H1'1	1.69	0.43
3:D:204:GLU:O	3:D:209:THR:HG23	2.18	0.43
3:D:445:THR:HB	3:D:463:ALA:HB2	2.01	0.43
3:D:583:VAL:HG22	3:D:599:HIS:CE1	2.53	0.43
14:U:203:ILE:HB	14:U:210:LEU:HD13	1.99	0.43
14:U:206:PRO:HD2	14:U:293:MET:HG3	2.00	0.43
15:V:74:VAL:HG23	15:V:88:VAL:HG11	2.00	0.43
16:Q:127:ALA:O	16:Q:131:LEU:HG	2.18	0.43
16:Q:220:ASP:CG	16:Q:301:ARG:H	2.21	0.43
16:Q:224:ALA:HB2	16:Q:233:HIS:CE1	2.53	0.43
3:3:285:VAL:HG13	3:3:286:ASN:N	2.29	0.43
10:A:49:ASP:CG	10:A:52:GLY:HA3	2.39	0.43
13:L:592:LEU:HB3	15:N:194:PHE:CZ	2.54	0.43
15:N:111:LEU:O	15:N:114:LEU:HG	2.19	0.43
16:H:189:GLN:O	16:H:193:GLY:HA2	2.17	0.43
2:C:10:PHE:CZ	2:C:33:ARG:HG3	2.53	0.43
3:D:402:PRO:HA	3:D:535:MET:HE2	2.00	0.43
4:E:232:LEU:HD13	4:E:380:SER:HA	1.99	0.43
4:E:281:ARG:HD3	4:E:284:ARG:NH1	2.34	0.43
5:F:82:ASP:OD1	5:F:82:ASP:N	2.46	0.43
5:F:101:LEU:HD12	5:F:101:LEU:HA	1.88	0.43
6:G:92:MET:HE1	6:G:127:VAL:HG13	1.99	0.43
11:R:61:GLY:O	11:R:65:VAL:HG21	2.18	0.43
14:U:109:LEU:HD11	14:U:118:PHE:CD1	2.54	0.43
14:U:281:PHE:HE2	14:U:332:LEU:HD21	1.83	0.43
15:V:103:HIS:HE1	15:V:161:LEU:HD13	1.83	0.43
16:Q:104:PRO:HD3	16:Q:267:TRP:NE1	2.34	0.43
16:Q:222:PRO:O	16:Q:230:GLY:HA3	2.18	0.43
1:1:358:PRO:HB3	3:3:107:MET:SD	2.59	0.43
2:2:81:GLN:HB3	2:2:122:VAL:HG21	2.00	0.43
3:3:125:GLY:HA2	3:3:245:ARG:HH21	1.81	0.43
7:9:68:ILE:HD11	17:9:201:SF4:S1	2.58	0.43
13:L:451:LEU:HG	13:L:455:LEU:HD23	2.00	0.43
14:M:109:LEU:HB2	14:M:121:PHE:HB3	2.01	0.43
14:M:190:ALA:HB1	14:M:249:ALA:HB1	2.01	0.43
3:D:584:VAL:HG12	3:D:600:VAL:HB	2.01	0.43
3:D:606:THR:O	3:D:609:GLU:HG2	2.19	0.43
3:D:722:THR:HG21	3:D:755:LYS:HA	2.01	0.43
4:E:30:VAL:HG13	4:E:35:PRO:HD2	1.99	0.43
5:F:80:TRP:CE3	5:F:80:TRP:HA	2.52	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:S:79:PHE:CD2	12:S:85:THR:HA	2.53	0.43
14:U:12:PHE:HB3	14:U:100:LEU:HD13	2.01	0.43
2:2:112:THR:HG23	2:2:115:GLY:H	1.83	0.43
3:3:281:GLU:HB2	3:3:288:ILE:HG22	1.99	0.43
3:3:615:VAL:HG22	3:3:621:VAL:HG12	2.01	0.43
3:3:719:HIS:HB3	3:3:722:THR:HG23	2.01	0.43
5:5:51:ASP:H	5:5:73:GLU:HB3	1.84	0.43
5:5:64:ARG:HA	5:5:64:ARG:HD3	1.72	0.43
9:W:102:LEU:HG	9:W:110:LEU:HD13	1.99	0.43
11:J:19:VAL:HA	11:J:28:ALA:HB1	2.01	0.43
14:M:329:ALA:O	14:M:332:LEU:HG	2.18	0.43
16:H:141:TRP:HA	16:H:149:LEU:HD21	2.01	0.43
2:C:83:CYS:SG	2:C:124:CYS:HA	2.58	0.43
3:D:192:GLU:OE1	3:D:193:GLU:HG3	2.18	0.43
3:D:478:LEU:HB2	3:D:520:ARG:NH1	2.34	0.43
3:D:691:ALA:HB3	3:D:772:GLU:HA	2.00	0.43
4:E:37:THR:OG1	4:E:397:ILE:HG21	2.18	0.43
6:G:173:VAL:HG12	6:G:174:ALA:O	2.19	0.43
15:V:176:LEU:HD23	15:V:176:LEU:HA	1.87	0.43
1:1:314:GLU:O	1:1:317:GLN:HB3	2.19	0.43
1:1:394:ILE:CG2	1:1:403:ALA:HB1	2.48	0.43
2:2:85:THR:HG21	2:2:124:CYS:HB2	2.01	0.43
3:3:571:VAL:HG11	3:3:591:HIS:CD2	2.54	0.43
6:6:32:ARG:HD2	6:6:104:TRP:HH2	1.83	0.43
8:7:27:LYS:HD3	8:7:27:LYS:HA	1.84	0.43
12:K:55:VAL:O	12:K:59:MET:HG2	2.19	0.43
14:M:84:LEU:HB3	14:M:432:PHE:CE1	2.54	0.43
16:H:299:ARG:O	16:H:300:LEU:HD12	2.18	0.43
16:H:304:GLN:HE22	16:H:307:ARG:HD2	1.83	0.43
1:B:183:GLY:HA3	18:B:502:FMN:N5	2.34	0.43
3:D:246:ASN:ND2	3:D:276:ARG:HH12	2.17	0.43
3:D:261:VAL:HG21	3:D:408:ILE:HG12	1.99	0.43
3:D:408:ILE:HG23	17:D:803:SF4:S1	2.59	0.43
3:D:591:HIS:CE1	3:D:593:LEU:HD23	2.54	0.43
4:E:213:ILE:O	4:E:217:ARG:HG2	2.19	0.43
13:T:600:LEU:HA	15:V:235:LEU:HD23	2.01	0.43
14:U:69:GLY:O	14:U:73:LEU:HD22	2.19	0.43
3:3:225:ASN:ND2	3:3:290:ILE:H	2.17	0.43
3:3:256:CYS:HB2	3:3:265:ILE:HD13	2.00	0.43
3:3:272:GLY:O	3:3:630:GLU:N	2.49	0.43
5:5:123:GLY:H	5:5:147:ARG:HH11	1.66	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:5:174:LEU:HD11	5:5:189:ARG:HH21	1.83	0.43
8:7:13:TRP:HE3	8:7:82:ILE:HD12	1.84	0.43
9:W:78:VAL:HA	9:W:81:LEU:HD12	2.01	0.43
11:J:87:VAL:O	11:J:91:PRO:HD3	2.19	0.43
13:L:59:TRP:HE1	14:M:447:PRO:HD2	1.84	0.43
13:L:286:PHE:HA	13:L:294:ILE:HD11	2.01	0.43
16:H:218:PRO:HA	16:H:300:LEU:HB2	2.00	0.43
1:B:145:LEU:HD23	1:B:145:LEU:HA	1.77	0.43
3:D:190:TYR:CE1	3:D:195:PRO:HD3	2.54	0.43
3:D:248:GLU:HG2	5:F:170:PHE:CE1	2.54	0.43
4:E:62:LEU:N	4:E:408:ASP:OD2	2.51	0.43
5:F:39:ALA:HA	5:F:107:LEU:HD21	2.00	0.43
10:P:71:PHE:O	10:P:75:VAL:HG23	2.19	0.43
13:T:1:MET:HA	13:T:55:PHE:CE2	2.54	0.43
13:T:194:GLY:HA3	13:T:195:PRO:HD3	1.82	0.43
13:T:461:LEU:HD13	13:T:465:LEU:HB3	2.00	0.43
14:U:17:LEU:HD23	14:U:17:LEU:HA	1.77	0.43
14:U:67:LEU:HA	14:U:71:SER:HB2	2.01	0.43
14:U:186:GLN:HG2	14:U:187:GLU:H	1.82	0.43
14:U:205:THR:HG23	14:U:238:VAL:HG23	2.01	0.43
14:U:410:PHE:HE2	14:U:415:TRP:CE2	2.37	0.43
15:V:118:LEU:HD21	15:V:210:PHE:CE2	2.54	0.43
15:V:283:PHE:O	15:V:287:THR:HG23	2.18	0.43
16:Q:51:VAL:O	16:Q:57:LEU:HB2	2.18	0.43
16:Q:298:PHE:N	16:Q:298:PHE:CD1	2.86	0.43
1:1:262:GLY:HA3	2:2:175:HIS:O	2.19	0.42
1:1:436:LEU:HD23	2:2:90:LEU:HA	2.01	0.42
10:A:67:LEU:HD23	16:H:310:TRP:CZ2	2.54	0.42
13:L:171:LEU:O	13:L:175:ILE:HG13	2.19	0.42
15:N:158:THR:HG21	15:N:165:ALA:HB2	2.00	0.42
15:N:290:LEU:HD11	15:N:408:LEU:HD23	2.01	0.42
16:H:304:GLN:NE2	16:H:307:ARG:HD2	2.33	0.42
1:B:211:LEU:HD12	1:B:211:LEU:HA	1.84	0.42
1:B:384:VAL:HG12	1:B:418:LYS:HE3	2.01	0.42
4:E:158:ASP:CG	6:G:57:ARG:HH12	2.23	0.42
4:E:249:ARG:HB3	4:E:257:TYR:CD2	2.54	0.42
5:F:120:ASP:O	5:F:145:PRO:HD2	2.19	0.42
7:O:33:LEU:HD13	7:O:37:PHE:CD2	2.54	0.42
14:U:65:PHE:HA	14:U:111:ALA:O	2.18	0.42
14:U:443:MET:HA	14:U:450:PHE:CE2	2.54	0.42
1:1:16:THR:HG23	1:1:233:ARG:HH21	1.83	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:1:219:ASN:HD22	18:1:502:FMN:P	2.41	0.42
1:1:288:GLN:HB3	1:1:333:GLU:HA	2.01	0.42
3:3:110:PHE:O	3:3:113:LEU:HB2	2.18	0.42
3:3:310:LEU:HA	3:3:318:VAL:O	2.19	0.42
3:3:438:LYS:O	3:3:441:MET:HG3	2.20	0.42
4:4:191:LYS:HG2	4:4:294:LEU:HD11	2.01	0.42
8:7:15:GLU:HG3	8:7:19:TRP:NE1	2.33	0.42
10:A:57:PHE:HB2	11:J:73:LEU:CD2	2.48	0.42
12:K:19:LEU:HD22	13:L:591:LEU:HD12	2.00	0.42
14:M:43:HIS:CD2	14:M:48:ALA:HB2	2.54	0.42
14:M:54:PRO:HA	14:M:62:TYR:CD1	2.54	0.42
14:M:135:LEU:HG	14:M:136:TYR:CD2	2.54	0.42
14:M:203:ILE:HB	14:M:210:LEU:HD13	2.00	0.42
14:M:252:GLY:HA2	14:M:255:GLN:NE2	2.34	0.42
16:H:8:ASP:CG	16:H:112:GLN:HG2	2.39	0.42
1:B:64:GLY:N	1:B:70:PHE:O	2.47	0.42
1:B:273:ARG:HH22	1:B:304:GLU:CD	2.22	0.42
1:B:290:ILE:HD12	1:B:292:PRO:HD3	2.00	0.42
3:D:21:ASP:OD1	3:D:432:PHE:N	2.43	0.42
3:D:544:LEU:O	3:D:548:GLY:N	2.53	0.42
4:E:211:SER:CB	4:E:214:PHE:HB3	2.46	0.42
4:E:271:ASP:OD1	4:E:274:ASP:HB2	2.18	0.42
5:F:105:THR:HG21	5:F:130:PRO:HD3	2.00	0.42
6:G:60:LEU:O	6:G:65:SER:HB2	2.20	0.42
6:G:140:CYS:SG	7:O:99:ILE:HG13	2.59	0.42
8:I:19:TRP:CD1	8:I:112:LYS:HE3	2.54	0.42
11:R:147:MET:O	11:R:150:THR:OG1	2.29	0.42
13:T:291:ILE:HA	13:T:294:ILE:HG22	2.00	0.42
14:U:345:ARG:HG2	14:U:412:LYS:O	2.19	0.42
16:Q:132:ALA:O	16:Q:136:ILE:HG13	2.19	0.42
16:Q:216:ARG:HD2	16:Q:294:ARG:HD2	2.01	0.42
1:1:65:ARG:NH2	1:1:247:LYS:O	2.52	0.42
1:1:334:ARG:O	1:1:434:PRO:HG3	2.18	0.42
2:2:27:ILE:HD13	2:2:60:VAL:HG22	2.01	0.42
3:3:223:SER:N	3:3:292:ASP:OD2	2.46	0.42
3:3:274:LEU:HD21	3:3:277:ILE:HD11	2.01	0.42
4:4:115:THR:O	4:4:118:VAL:HG22	2.19	0.42
5:5:129:HIS:HB3	5:5:132:LEU:HG	2.00	0.42
8:7:13:TRP:CE3	8:7:72:VAL:HB	2.54	0.42
14:M:215:PRO:CG	14:M:216:PRO:HD3	2.48	0.42
16:H:204:LEU:HD12	16:H:348:LEU:HD13	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
16:H:226:GLN:C	16:H:299:ARG:HH22	2.22	0.42
3:D:614:LEU:O	3:D:621:VAL:HA	2.19	0.42
4:E:52:VAL:HB	4:E:385:CYS:O	2.19	0.42
4:E:84:ARG:O	6:G:83:ARG:NH2	2.52	0.42
4:E:352:GLU:HB3	4:E:371:ARG:NE	2.34	0.42
7:O:44:THR:OG1	7:O:52:LYS:HD2	2.18	0.42
7:O:126:TYR:HB3	9:X:39:ASP:CG	2.39	0.42
9:X:52:THR:HG1	9:X:55:LYS:H	1.67	0.42
10:P:56:ARG:HD3	11:R:74:LEU:HA	2.00	0.42
10:P:74:GLU:HB2	10:P:103:LEU:HD23	2.01	0.42
10:P:77:PHE:CE1	12:S:58:LEU:HD22	2.54	0.42
13:T:13:GLY:O	13:T:17:LEU:HG	2.19	0.42
13:T:355:LEU:HB3	13:T:359:LEU:HD12	2.02	0.42
13:T:550:ALA:HB1	14:U:277:ALA:HB2	2.00	0.42
15:V:130:LEU:HD23	15:V:130:LEU:HA	1.81	0.42
15:V:163:LEU:HD23	15:V:163:LEU:HA	1.89	0.42
3:3:17:THR:HG22	3:3:18:SER:O	2.20	0.42
3:3:203:ILE:HG22	3:3:204:GLU:HG3	2.00	0.42
4:4:234:LEU:O	4:4:239:LEU:HB2	2.20	0.42
7:9:115:LEU:O	7:9:167:ARG:NH2	2.52	0.42
14:M:56:LEU:O	14:M:60:GLY:N	2.47	0.42
15:N:40:LEU:HD23	15:N:40:LEU:HA	1.93	0.42
16:H:301:ARG:O	16:H:302:TYR:CD1	2.72	0.42
16:H:314:PHE:N	16:H:314:PHE:CD1	2.85	0.42
1:B:189:MET:HB3	1:B:211:LEU:HD13	2.01	0.42
1:B:437:TRP:CZ3	2:C:147:ARG:CA	3.03	0.42
3:D:716:LEU:HD12	3:D:736:VAL:HG21	2.01	0.42
4:E:236:GLY:O	4:E:238:SER:N	2.52	0.42
6:G:38:PRO:HG2	6:G:65:SER:HB3	2.02	0.42
8:I:10:TYR:O	8:I:14:VAL:HG23	2.19	0.42
13:T:13:GLY:HA3	13:T:36:LEU:HD13	2.01	0.42
13:T:20:PHE:O	13:T:22:LYS:N	2.53	0.42
13:T:286:PHE:HD2	13:T:416:TYR:HB3	1.83	0.42
13:T:584:GLY:O	15:V:135:LYS:NZ	2.41	0.42
16:Q:267:TRP:O	16:Q:269:MET:N	2.52	0.42
1:1:334:ARG:NH1	1:1:435:SER:O	2.39	0.42
3:3:290:ILE:HG21	3:3:295:ARG:HB2	2.02	0.42
3:3:305:ARG:NH1	3:3:609:GLU:OE1	2.31	0.42
4:4:329:LYS:HD2	4:4:329:LYS:HA	1.82	0.42
6:6:173:VAL:HG12	6:6:174:ALA:O	2.19	0.42
7:9:149:GLU:HA	7:9:152:ARG:NE	2.34	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:L:376:LEU:HD23	13:L:379:LEU:HG	2.02	0.42
13:L:392:THR:O	13:L:399:GLY:HA3	2.20	0.42
13:L:596:GLY:HA3	15:N:191:PRO:CG	2.49	0.42
14:M:8:LEU:HD23	14:M:32:SER:HA	2.01	0.42
14:M:8:LEU:HB3	14:M:9:PRO:HD3	2.02	0.42
15:N:277:ASN:C	15:N:279:GLN:H	2.22	0.42
3:D:201:ASP:OD1	3:D:202:PHE:N	2.51	0.42
3:D:406:ALA:O	3:D:409:LEU:HB2	2.19	0.42
3:D:593:LEU:O	3:D:597:TYR:HB2	2.19	0.42
4:E:86:ASP:HB2	4:E:406:ASP:OD2	2.20	0.42
4:E:106:GLY:O	5:F:194:SER:HB3	2.19	0.42
6:G:60:LEU:HD21	6:G:151:VAL:HG11	2.00	0.42
7:O:34:LYS:HA	7:O:34:LYS:HD3	1.96	0.42
7:O:43:LEU:HD23	7:O:43:LEU:HA	1.86	0.42
10:P:9:GLY:CA	16:Q:13:VAL:HG11	2.48	0.42
13:T:419:ARG:HD2	13:T:512:PHE:CZ	2.54	0.42
14:U:157:LEU:HB3	15:V:365:LEU:HB3	2.02	0.42
16:Q:67:ILE:HG13	16:Q:68:PHE:CD1	2.55	0.42
16:Q:205:VAL:HG21	16:Q:317:ALA:HB2	2.01	0.42
3:3:247:TRP:CG	5:5:172:ALA:HB2	2.54	0.42
4:4:390:VAL:HB	4:4:391:PRO:HD3	2.01	0.42
5:5:56:ASP:HB2	5:5:122:PHE:HE2	1.84	0.42
11:J:68:LEU:HA	11:J:71:ILE:HG12	2.02	0.42
13:L:384:SER:O	13:L:388:ILE:HG13	2.20	0.42
14:M:157:LEU:HA	14:M:157:LEU:HD23	1.82	0.42
15:N:118:LEU:HA	15:N:121:LEU:HB2	2.01	0.42
15:N:233:LEU:HD12	15:N:233:LEU:HA	1.91	0.42
1:B:170:ASP:OD1	1:B:171:LEU:N	2.52	0.42
2:C:97:TRP:CE2	2:C:121:LYS:HE2	2.55	0.42
3:D:228:ASP:OD2	3:D:295:ARG:NH2	2.39	0.42
3:D:681:LYS:HE3	3:D:681:LYS:HB3	1.79	0.42
4:E:381:LEU:HB3	4:E:382:PRO:HD3	2.01	0.42
5:F:145:PRO:HA	5:F:150:TYR:CD1	2.53	0.42
14:U:157:LEU:HD23	14:U:157:LEU:HA	1.74	0.42
14:U:297:ALA:HB1	14:U:301:PHE:CE2	2.55	0.42
1:1:49:THR:OG1	1:1:52:GLU:HG3	2.19	0.42
1:1:245:GLN:HB2	1:1:314:GLU:OE2	2.20	0.42
3:3:124:LYS:HD2	3:3:127:ALA:O	2.20	0.42
4:4:311:PRO:HD3	4:4:330:HIS:CE1	2.54	0.42
13:L:104:PHE:HE1	13:L:233:PRO:HG3	1.85	0.42
13:L:180:TYR:CZ	13:L:192:MET:HG2	2.54	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
15:N:132:ALA:HB1	15:N:199:VAL:HA	2.02	0.42
16:H:202:ALA:O	16:H:205:VAL:HG22	2.19	0.42
1:B:361:GLU:OE2	3:D:162:ARG:NH2	2.53	0.42
3:D:719:HIS:HA	3:D:750:ARG:O	2.18	0.42
4:E:263:ASP:HB2	4:E:285:GLU:CD	2.40	0.42
5:F:184:TYR:HE2	5:F:186:GLY:HA3	1.85	0.42
6:G:133:VAL:HG11	6:G:136:TYR:CE1	2.54	0.42
8:I:66:PRO:O	8:I:88:ARG:NH2	2.51	0.42
9:X:1:MET:HG3	9:X:56:ASP:HB2	2.00	0.42
11:R:65:VAL:HG11	16:Q:160:ILE:CD1	2.48	0.42
13:T:141:LEU:HB3	13:T:236:VAL:CG2	2.50	0.42
14:U:92:GLU:C	14:U:94:ARG:H	2.23	0.42
14:U:305:PRO:HD3	14:U:462:ALA:CB	2.50	0.42
16:Q:150:LEU:HD21	16:Q:154:ARG:NH1	2.35	0.42
16:Q:200:PHE:O	16:Q:203:PHE:HB3	2.19	0.42
1:1:104:ARG:O	1:1:108:GLU:HG3	2.20	0.42
18:1:502:FMN:H9	18:1:502:FMN:H1'1	1.67	0.42
5:5:31:ARG:O	5:5:34:PHE:HB3	2.20	0.42
13:L:268:TYR:CZ	13:L:402:PHE:HZ	2.37	0.42
13:L:286:PHE:O	13:L:419:ARG:NH1	2.53	0.42
13:L:291:ILE:O	13:L:295:VAL:HG23	2.19	0.42
13:L:309:ALA:HB2	13:L:388:ILE:HD13	2.02	0.42
13:L:561:LEU:HG	13:L:565:PHE:CE2	2.54	0.42
14:M:84:LEU:O	14:M:88:VAL:HG12	2.19	0.42
14:M:88:VAL:HG23	14:M:429:GLU:HG2	2.02	0.42
14:M:125:ALA:HB3	14:M:234:TYR:CE1	2.54	0.42
14:M:222:HIS:O	14:M:225:GLY:N	2.48	0.42
14:M:258:GLY:HA2	14:M:261:LEU:HD12	2.02	0.42
14:M:302:SER:O	14:M:304:THR:HG23	2.20	0.42
16:H:163:GLU:O	16:H:166:LEU:HB2	2.19	0.42
3:D:370:ASP:OD2	3:D:374:ARG:HD3	2.19	0.42
4:E:33:GLN:HE22	4:E:38:HIS:CA	2.30	0.42
7:O:123:ASP:CG	7:O:148:ARG:HH22	2.22	0.42
7:O:137:LEU:O	7:O:140:VAL:HG12	2.19	0.42
10:P:74:GLU:O	10:P:78:LEU:HG	2.20	0.42
13:T:224:VAL:HG11	13:T:538:TYR:CD2	2.55	0.42
14:U:43:HIS:CD2	14:U:48:ALA:HB2	2.55	0.42
14:U:120:VAL:HG22	15:V:342:PHE:CE2	2.55	0.42
14:U:341:ILE:HG13	14:U:342:GLY:N	2.34	0.42
14:U:371:LEU:HD12	14:U:440:LEU:HB3	2.02	0.42
16:Q:35:GLU:CD	16:Q:294:ARG:HH21	2.22	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:4:87:TYR:HB3	6:6:45:CYS:HB3	2.01	0.42
4:4:341:GLU:HA	4:4:357:ILE:O	2.20	0.42
8:7:15:GLU:HG3	8:7:19:TRP:CE2	2.55	0.42
13:L:399:GLY:HA2	13:L:402:PHE:CD2	2.54	0.42
14:M:148:PHE:O	14:M:152:THR:HG23	2.20	0.42
16:H:163:GLU:HG2	16:H:166:LEU:HD12	2.02	0.42
16:H:236:TYR:HB3	16:H:240:LYS:HB2	2.01	0.42
1:B:18:TYR:CD2	1:B:21:VAL:HG21	2.55	0.42
3:D:170:LEU:HD11	3:D:176:LEU:HD22	2.01	0.42
4:E:30:VAL:HG13	4:E:35:PRO:CD	2.50	0.42
4:E:33:GLN:CB	4:E:40:VAL:HG23	2.45	0.42
4:E:84:ARG:HG2	17:G:201:SF4:S2	2.59	0.42
4:E:90:SER:O	4:E:93:HIS:HB2	2.20	0.42
5:F:64:ARG:HH12	5:F:91:ARG:HH12	1.67	0.42
7:O:153:THR:HG22	7:O:155:LYS:HB2	2.00	0.42
9:X:95:SER:OG	9:X:98:GLU:HB2	2.20	0.42
10:P:51:ALA:HB3	16:Q:146:LYS:HB2	2.02	0.42
13:T:319:LEU:HD12	13:T:473:LEU:HD13	2.01	0.42
16:Q:327:VAL:HG21	16:Q:337:LEU:HD21	2.01	0.42
2:2:110:GLU:HA	8:7:121:ARG:NH1	2.32	0.42
4:4:144:THR:HG22	4:4:148:TYR:CE1	2.37	0.42
4:4:248:VAL:HA	4:4:251:ALA:HB3	2.01	0.42
4:4:249:ARG:NH1	4:4:262:PHE:HZ	2.17	0.42
9:W:26:LEU:HB3	9:W:29:ALA:HB3	2.00	0.42
10:A:71:PHE:O	10:A:74:GLU:HB3	2.19	0.42
12:K:93:LEU:HB3	15:N:198:ASP:HA	2.02	0.42
14:M:206:PRO:HD2	14:M:293:MET:HG3	2.02	0.42
14:M:260:LEU:HD13	14:M:301:PHE:CE1	2.55	0.42
14:M:359:LEU:O	14:M:363:LEU:HG	2.20	0.42
15:N:244:GLY:O	15:N:260:TYR:HB3	2.19	0.42
16:H:222:PRO:HG2	16:H:230:GLY:HA2	2.01	0.42
3:D:312:ARG:HA	3:D:316:ARG:O	2.19	0.42
4:E:102:GLU:O	4:E:106:GLY:N	2.50	0.42
5:F:38:MET:HA	5:F:41:TYR:HB2	2.01	0.42
5:F:68:PHE:HB3	5:F:124:ILE:HD11	2.01	0.42
6:G:104:TRP:CZ2	6:G:173:VAL:HG22	2.54	0.42
6:G:162:ALA:HA	7:O:152:ARG:NH1	2.35	0.42
13:T:163:ARG:HE	14:U:399:VAL:C	2.24	0.42
14:U:265:ALA:HA	14:U:395:ALA:HB2	2.01	0.42
15:V:62:PHE:CD2	15:V:221:ALA:HB2	2.55	0.42
15:V:138:LEU:HD23	15:V:138:LEU:HA	1.84	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
16:Q:273:GLU:OE1	16:Q:273:GLU:HA	2.20	0.42
2:2:68:SER:HA	8:7:90:HIS:NE2	2.35	0.41
3:3:226:ILE:HD12	3:3:235:LEU:HD13	2.01	0.41
3:3:270:ARG:HB3	3:3:275:LEU:HD11	2.02	0.41
4:4:39:GLY:H	20:4:501:HQH:C12	2.33	0.41
4:4:244:VAL:HG22	5:5:80:TRP:CE3	2.55	0.41
6:6:164:ASN:HD21	6:6:168:GLU:CD	2.23	0.41
11:J:135:TRP:CG	12:K:55:VAL:HG11	2.55	0.41
12:K:49:TYR:HB3	15:N:159:GLY:HA2	2.01	0.41
2:C:42:ARG:HD2	2:C:45:ARG:NE	2.35	0.41
3:D:261:VAL:HG21	3:D:408:ILE:CG1	2.50	0.41
3:D:568:TYR:O	3:D:585:MET:HA	2.20	0.41
3:D:716:LEU:HA	3:D:759:TYR:O	2.19	0.41
10:P:108:LEU:HD21	10:P:112:TRP:CH2	2.55	0.41
12:S:42:LEU:HD23	12:S:42:LEU:HA	1.93	0.41
14:U:91:VAL:HB	14:U:95:PHE:CE1	2.51	0.41
14:U:201:PHE:CZ	14:U:240:ALA:HB1	2.55	0.41
15:V:345:LYS:HB3	15:V:349:PHE:CE2	2.55	0.41
16:Q:331:ASP:CG	16:Q:334:ARG:HH22	2.23	0.41
1:1:259:LYS:NZ	2:2:179:VAL:O	2.53	0.41
1:1:290:ILE:HG22	1:1:330:LEU:HD22	2.02	0.41
3:3:415:GLU:O	3:3:420:LEU:HB2	2.21	0.41
3:3:516:VAL:O	3:3:520:ARG:HG3	2.19	0.41
4:4:318:GLU:HB2	8:7:39:ASP:CB	2.50	0.41
13:L:234:THR:OG1	13:L:340:ILE:HD11	2.20	0.41
14:M:310:GLY:HA2	14:M:376:GLY:HA2	2.00	0.41
16:H:83:VAL:O	16:H:86:PRO:HD2	2.20	0.41
2:C:146:THR:HG22	2:C:149:ARG:HB2	2.02	0.41
4:E:226:PRO:HG3	4:E:242:SER:OG	2.20	0.41
4:E:293:ALA:HA	4:E:296:ARG:HG2	2.02	0.41
10:P:88:LEU:HD11	11:R:129:PRO:N	2.35	0.41
13:T:196:LEU:HD21	13:T:262:VAL:HG21	2.02	0.41
14:U:279:LYS:HD3	14:U:279:LYS:HA	1.79	0.41
15:V:271:LEU:HD23	15:V:352:ALA:HB2	2.02	0.41
16:Q:190:LYS:HB2	16:Q:268:THR:HG21	2.01	0.41
1:1:133:TYR:HB2	1:1:188:LEU:HD21	2.02	0.41
1:1:404:ASP:HA	1:1:407:VAL:HG22	2.01	0.41
2:2:108:PRO:HA	2:2:119:VAL:HG23	2.03	0.41
2:2:110:GLU:HA	8:7:121:ARG:NH2	2.31	0.41
3:3:551:PRO:HB2	3:3:555:GLY:HA2	2.02	0.41
4:4:85:MET:HE1	4:4:370:VAL:HG21	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:4:202:ASP:CA	4:4:284:ARG:HH21	2.25	0.41
12:K:7:SER:HB3	12:K:40:LEU:HD23	2.03	0.41
12:K:81:HIS:CD2	12:K:81:HIS:H	2.37	0.41
13:L:4:LEU:HG	13:L:8:LEU:HG	2.03	0.41
13:L:477:LEU:HD12	13:L:477:LEU:HA	1.72	0.41
13:L:587:ARG:O	13:L:591:LEU:HD13	2.19	0.41
14:M:143:ARG:HA	14:M:143:ARG:HD3	1.69	0.41
14:M:372:SER:O	14:M:375:PRO:HD2	2.20	0.41
15:N:181:VAL:HA	15:N:192:PHE:CE2	2.55	0.41
3:D:19:VAL:HG23	3:D:85:THR:O	2.20	0.41
4:E:31:GLY:HA3	10:P:45:GLU:OE2	2.21	0.41
4:E:138:LEU:HD13	4:E:143:LEU:HA	2.03	0.41
4:E:205:GLU:HG3	4:E:209:ALA:HB2	2.02	0.41
4:E:345:PRO:HB3	5:F:87:ARG:NH1	2.35	0.41
11:R:59:TYR:CD1	11:R:63:ILE:HD12	2.56	0.41
13:T:328:PHE:O	13:T:331:LEU:HB3	2.20	0.41
13:T:409:VAL:O	13:T:413:THR:HG23	2.20	0.41
15:V:126:ARG:NH1	15:V:128:GLN:HG2	2.34	0.41
16:Q:216:ARG:HD2	16:Q:294:ARG:HB3	2.02	0.41
16:Q:310:TRP:CE3	16:Q:314:PHE:HE2	2.37	0.41
1:1:98:PRO:HA	2:2:124:CYS:SG	2.61	0.41
1:1:357:THR:N	1:1:358:PRO:HD2	2.35	0.41
3:3:466:GLU:HB2	3:3:489:MET:HB2	2.02	0.41
4:4:158:ASP:OD1	6:6:57:ARG:NH1	2.38	0.41
4:4:197:LEU:N	4:4:198:PRO:HD2	2.35	0.41
4:4:352:GLU:CD	5:5:87:ARG:HH22	2.24	0.41
10:A:14:VAL:HG22	16:H:95:LEU:HD22	2.01	0.41
13:L:355:LEU:CD1	13:L:359:LEU:HG	2.27	0.41
16:H:190:LYS:HB2	16:H:268:THR:HG21	2.01	0.41
1:B:250:LYS:NZ	1:B:251:LEU:O	2.52	0.41
3:D:405:GLU:HG2	3:D:696:PRO:HB2	2.02	0.41
3:D:411:LEU:O	3:D:415:GLU:HG3	2.20	0.41
8:I:105:THR:N	8:I:108:ILE:O	2.38	0.41
3:3:380:SER:OG	3:3:545:GLU:OE1	2.27	0.41
3:3:454:TYR:HB2	3:3:752:ASP:OD2	2.21	0.41
4:4:236:GLY:C	4:4:238:SER:H	2.24	0.41
4:4:400:LEU:HD23	4:4:400:LEU:HA	1.91	0.41
7:9:6:LEU:HD23	16:H:297:TRP:CE2	2.56	0.41
10:A:6:GLU:OE2	16:H:2:THR:OG1	2.36	0.41
10:A:83:VAL:HG23	10:A:84:SER:H	1.86	0.41
1:B:162:LEU:O	1:B:165:THR:HG22	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:118:ASP:O	3:D:122:CYS:N	2.54	0.41
3:D:169:PRO:HA	3:D:175:ILE:HA	2.02	0.41
3:D:607:PHE:O	3:D:624:LEU:HD22	2.20	0.41
4:E:143:LEU:HD21	16:Q:216:ARG:NH1	2.35	0.41
4:E:389:GLN:HG3	4:E:391:PRO:HD2	2.02	0.41
6:G:128:ASP:HA	6:G:131:VAL:O	2.19	0.41
14:U:151:PHE:HD2	14:U:213:TRP:HD1	1.69	0.41
14:U:253:PHE:HA	14:U:256:ALA:HB3	2.03	0.41
16:Q:310:TRP:HA	16:Q:314:PHE:CD2	2.55	0.41
1:1:287:ILE:HG12	1:1:330:LEU:HB3	2.02	0.41
2:2:89:LYS:HE3	2:2:94:GLU:HG3	2.02	0.41
3:3:476:ILE:O	3:3:480:LEU:HG	2.21	0.41
3:3:689:LYS:H	3:3:689:LYS:HG2	1.60	0.41
9:W:123:PRO:HA	9:W:126:TYR:HD2	1.86	0.41
11:J:49:ARG:HD2	11:J:123:LEU:HD21	2.02	0.41
11:J:72:MET:HE2	16:H:153:LEU:HD21	2.03	0.41
13:L:94:TYR:HA	13:L:442:MET:CE	2.50	0.41
13:L:501:ALA:O	13:L:505:LEU:HG	2.21	0.41
15:N:228:ALA:HB1	15:N:233:LEU:HD13	2.02	0.41
16:H:138:LEU:HD23	16:H:138:LEU:HA	1.89	0.41
1:B:356:CYS:N	17:B:501:SF4:S3	2.85	0.41
1:B:421:TYR:O	1:B:425:ALA:N	2.40	0.41
4:E:165:GLY:O	7:O:37:PHE:HA	2.21	0.41
6:G:33:SER:O	6:G:36:LEU:HG	2.20	0.41
6:G:98:GLN:OE1	10:P:44:TYR:HA	2.20	0.41
11:R:123:LEU:O	11:R:127:LEU:HD13	2.20	0.41
13:T:118:LEU:HD11	13:T:131:TRP:CD1	2.55	0.41
14:U:78:ILE:O	14:U:82:VAL:HG23	2.20	0.41
14:U:313:TYR:OH	14:U:443:MET:O	2.37	0.41
1:1:425:ALA:O	1:1:428:LYS:NZ	2.29	0.41
3:3:5:LYS:HA	3:3:9:ARG:O	2.20	0.41
4:4:87:TYR:HB3	4:4:169:HIS:HE1	1.85	0.41
4:4:224:ILE:HD11	4:4:275:ARG:NH1	2.36	0.41
6:6:94:ARG:HB3	6:6:98:GLN:NE2	2.36	0.41
8:7:21:ARG:HG2	8:7:31:PHE:CE2	2.55	0.41
8:7:48:TYR:CE2	8:7:50:LEU:HB2	2.55	0.41
11:J:64:VAL:HA	11:J:67:PHE:HD2	1.86	0.41
13:L:49:LEU:HD23	13:L:49:LEU:HA	1.86	0.41
13:L:419:ARG:HB2	13:L:512:PHE:CE2	2.55	0.41
16:H:2:THR:HA	16:H:5:TYR:HD2	1.86	0.41
16:H:213:GLU:OE1	16:H:213:GLU:N	2.53	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:167:PHE:HE2	1:B:169:PHE:HB2	1.86	0.41
1:B:292:PRO:HA	1:B:328:VAL:HG13	2.01	0.41
1:B:360:ARG:CZ	3:D:183:HIS:HB2	2.50	0.41
3:D:173:PHE:HZ	3:D:708:ALA:HA	1.85	0.41
3:D:720:PRO:HG2	3:D:751:GLU:HG3	2.01	0.41
4:E:41:LEU:HD13	4:E:59:ILE:HG22	2.03	0.41
4:E:283:MET:O	4:E:287:VAL:HG23	2.21	0.41
4:E:349:ALA:HB3	4:E:350:ARG:HH12	1.86	0.41
6:G:153:GLN:HG3	7:O:124:TYR:CE1	2.56	0.41
13:T:33:ALA:HB2	13:T:109:ASN:HD21	1.85	0.41
13:T:511:PHE:CD1	13:T:514:ARG:HD2	2.55	0.41
13:T:533:TYR:HD1	13:T:536:ARG:HD3	1.85	0.41
13:T:549:LEU:O	13:T:553:LEU:HG	2.21	0.41
13:T:575:GLY:HA2	15:V:246:LEU:HB3	2.01	0.41
15:V:95:MET:HB3	15:V:218:ALA:HB2	2.01	0.41
15:V:194:PHE:O	15:V:197:PRO:HD2	2.20	0.41
1:1:404:ASP:N	1:1:404:ASP:OD1	2.54	0.41
2:2:85:THR:HB	19:2:201:FES:S2	2.61	0.41
3:3:715:GLU:HA	3:3:746:ARG:O	2.21	0.41
4:4:318:GLU:OE1	8:7:46:ARG:NE	2.53	0.41
5:5:35:LYS:HA	5:5:35:LYS:HD2	1.90	0.41
7:9:102:GLY:CA	7:9:115:LEU:HD11	2.51	0.41
8:7:49:ASP:CG	8:7:75:ARG:HE	2.21	0.41
13:L:88:HIS:NE2	13:L:108:PHE:HB3	2.36	0.41
14:M:68:ASP:OD2	14:M:243:ARG:NH2	2.54	0.41
14:M:116:LEU:HD12	14:M:116:LEU:HA	1.96	0.41
15:N:118:LEU:HD23	15:N:121:LEU:HD12	2.02	0.41
1:B:157:TYR:O	1:B:158:LEU:HD23	2.21	0.41
13:T:309:ALA:HB2	13:T:388:ILE:HG12	2.03	0.41
16:Q:98:GLY:O	16:Q:114:TRP:HB2	2.20	0.41
1:1:96:SER:HB2	1:1:180:TYR:HD1	1.86	0.41
1:1:96:SER:HA	1:1:135:ARG:NH1	2.36	0.41
1:1:113:LEU:HD21	1:1:225:ALA:HB1	2.02	0.41
1:1:175:ARG:NH1	2:2:32:ARG:HD3	2.36	0.41
1:1:196:ARG:NH2	3:3:204:GLU:O	2.54	0.41
1:1:202:LYS:N	1:1:203:PRO:HD2	2.36	0.41
2:2:47:GLU:O	2:2:51:ARG:HG3	2.20	0.41
3:3:582:PHE:HA	3:3:599:HIS:ND1	2.36	0.41
5:5:123:GLY:HA2	5:5:144:HIS:CE1	2.56	0.41
6:6:60:LEU:HG	6:6:65:SER:HB2	2.03	0.41
6:6:177:LYS:O	6:6:178:ARG:HG3	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:7:105:THR:OG1	8:7:114:ARG:NH1	2.50	0.41
12:K:46:ALA:HB2	12:K:53:GLY:HA3	2.02	0.41
13:L:7:ILE:HG23	13:L:113:ALA:HB1	2.02	0.41
13:L:139:PHE:CZ	14:M:407:LEU:HD22	2.56	0.41
13:L:356:TRP:HB2	13:L:426:LEU:HD12	2.02	0.41
14:M:89:ALA:HB3	14:M:92:GLU:OE2	2.21	0.41
16:H:149:LEU:O	16:H:153:LEU:HG	2.20	0.41
16:H:215:ALA:O	16:H:294:ARG:HD3	2.21	0.41
1:B:74:LEU:HD12	1:B:77:SER:OG	2.20	0.41
1:B:273:ARG:NH1	1:B:307:LEU:HD13	2.36	0.41
3:D:337:ARG:CD	3:D:337:ARG:H	2.34	0.41
3:D:670:PRO:HD3	3:D:676:LEU:HD23	2.02	0.41
4:E:62:LEU:HD23	4:E:62:LEU:HA	1.94	0.41
4:E:148:TYR:OH	16:Q:42:PHE:O	2.19	0.41
4:E:168:PHE:CZ	6:G:141:PRO:HG3	2.56	0.41
6:G:165:GLU:HG2	7:O:148:ARG:NH1	2.35	0.41
9:X:61:ASP:OD1	9:X:61:ASP:N	2.50	0.41
13:T:598:LEU:HD23	13:T:598:LEU:HA	1.79	0.41
15:V:248:ALA:HB2	15:V:260:TYR:CB	2.51	0.41
16:Q:216:ARG:CG	16:Q:294:ARG:HD2	2.51	0.41
1:1:313:TYR:CD1	1:1:323:LEU:HB3	2.55	0.41
2:2:78:TYR:CE2	2:2:157:LEU:HB3	2.56	0.41
3:3:355:LEU:HB2	3:3:547:MET:SD	2.61	0.41
4:4:93:HIS:CE1	4:4:353:LEU:HD11	2.56	0.41
4:4:240:ARG:HD3	4:4:265:PRO:O	2.21	0.41
4:4:315:HIS:HA	8:7:46:ARG:NH1	2.35	0.41
9:W:59:VAL:HG11	9:W:63:PHE:CE2	2.56	0.41
10:A:7:TYR:N	10:A:7:TYR:CD1	2.89	0.41
11:J:20:VAL:HG11	12:K:13:LEU:O	2.20	0.41
12:K:63:VAL:CG1	15:N:112:GLU:HG3	2.51	0.41
13:L:302:GLN:O	13:L:306:MET:HG3	2.21	0.41
14:M:331:ARG:HA	14:M:331:ARG:HD2	1.66	0.41
15:N:138:LEU:HD23	15:N:138:LEU:HA	1.87	0.41
16:H:257:ALA:HA	16:H:283:ILE:HG12	2.03	0.41
1:B:201:LEU:O	1:B:204:PRO:HD2	2.21	0.41
1:B:273:ARG:NH2	1:B:304:GLU:OE1	2.53	0.41
1:B:288:GLN:HB3	1:B:333:GLU:CG	2.51	0.41
3:D:165:ASP:HB2	8:I:66:PRO:HG2	2.03	0.41
3:D:271:SER:OG	7:O:69:TYR:OH	2.29	0.41
3:D:323:GLU:OE1	9:X:11:ARG:HB2	2.20	0.41
3:D:551:PRO:HB2	3:D:555:GLY:HA2	2.03	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:E:224:ILE:HB	4:E:270:GLY:HA3	2.03	0.41
5:F:165:ILE:HG23	5:F:170:PHE:CG	2.55	0.41
5:F:192:TYR:OH	5:F:194:SER:HB2	2.21	0.41
6:G:153:GLN:O	7:O:124:TYR:OH	2.29	0.41
8:I:74:PRO:HG2	8:I:77:ALA:HB2	2.02	0.41
12:S:1:MET:HA	12:S:4:LEU:HD23	2.03	0.41
13:T:49:LEU:HD23	13:T:49:LEU:HA	1.90	0.41
14:U:452:ARG:HA	14:U:452:ARG:HD3	1.83	0.41
15:V:119:TYR:HE1	15:V:136:TYR:CG	2.39	0.41
15:V:190:ALA:HB3	15:V:240:SER:HA	2.02	0.41
1:1:62:LEU:HD21	1:1:223:THR:HG23	2.02	0.40
1:1:210:GLY:HA3	1:1:216:THR:OG1	2.21	0.40
1:1:344:LEU:HD21	2:2:86:LEU:HD22	2.01	0.40
3:3:424:HIS:HB2	3:3:426:TYR:CE1	2.56	0.40
4:4:367:ARG:HH12	5:5:53:VAL:HG23	1.85	0.40
5:5:67:ARG:HD3	5:5:96:GLU:HG3	2.03	0.40
7:9:26:TYR:CD1	7:9:27:PRO:HA	2.56	0.40
8:7:89:ALA:O	8:7:90:HIS:ND1	2.54	0.40
14:M:115:LEU:HD11	14:M:248:LEU:CD2	2.51	0.40
16:H:149:LEU:HD23	16:H:149:LEU:HA	1.78	0.40
1:B:6:LEU:HD12	1:B:241:MET:HG3	2.03	0.40
1:B:39:GLU:O	1:B:43:ARG:HG2	2.20	0.40
1:B:63:ARG:HD3	1:B:313:TYR:CD2	2.56	0.40
1:B:314:GLU:HA	1:B:317:GLN:HB3	2.03	0.40
3:D:306:LEU:HD11	3:D:308:THR:O	2.21	0.40
3:D:487:SER:OG	3:D:490:VAL:HG23	2.21	0.40
4:E:50:GLU:HB3	4:E:389:GLN:NE2	2.36	0.40
5:F:146:LEU:HD23	5:F:146:LEU:HA	1.85	0.40
13:T:450:ALA:O	13:T:454:VAL:HG23	2.22	0.40
13:T:477:LEU:HD12	13:T:477:LEU:HA	1.74	0.40
14:U:242:PHE:CD2	14:U:312:LEU:HD11	2.57	0.40
16:Q:147:TYR:HD1	16:Q:229:VAL:HG22	1.85	0.40
3:3:291:CYS:SG	3:3:294:GLY:N	2.88	0.40
4:4:236:GLY:O	4:4:238:SER:N	2.53	0.40
4:4:317:LEU:HD12	4:4:317:LEU:HA	1.87	0.40
8:7:61:ASP:OD1	8:7:64:GLY:N	2.53	0.40
10:A:68:PHE:CE2	16:H:164:LEU:HB2	2.57	0.40
13:L:104:PHE:HE1	13:L:233:PRO:CG	2.34	0.40
13:L:238:ALA:HB2	13:L:333:PHE:HB3	2.03	0.40
14:M:215:PRO:HG3	14:M:287:TYR:CZ	2.57	0.40
15:N:176:LEU:HD23	15:N:176:LEU:HA	1.90	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
16:H:119:ASP:OD1	16:H:120:LEU:HG	2.20	0.40
1:B:437:TRP:CD1	2:C:95:GLU:CB	3.04	0.40
1:B:437:TRP:CD1	2:C:95:GLU:HB3	2.57	0.40
2:C:58:THR:OG1	3:D:215:ASP:OD2	2.31	0.40
3:D:178:ARG:HH22	8:I:65:GLU:CD	2.24	0.40
4:E:96:ALA:HB3	4:E:355:TYR:HE1	1.85	0.40
4:E:214:PHE:HB2	16:Q:298:PHE:CD2	2.57	0.40
7:O:40:ARG:NH1	7:O:42:VAL:HG12	2.36	0.40
12:S:25:ILE:H	12:S:25:ILE:HG13	1.68	0.40
14:U:109:LEU:HB2	14:U:121:PHE:HB3	2.04	0.40
15:V:256:ARG:HG2	15:V:260:TYR:CE2	2.57	0.40
15:V:270:ALA:HA	15:V:273:LEU:HD23	2.04	0.40
16:Q:159:LEU:HD11	16:Q:221:LEU:HD21	2.03	0.40
16:Q:213:GLU:N	16:Q:213:GLU:OE1	2.55	0.40
16:Q:216:ARG:CD	16:Q:294:ARG:HD2	2.51	0.40
1:1:357:THR:HG21	3:3:111:THR:OG1	2.22	0.40
3:3:463:ALA:C	3:3:465:HIS:HD1	2.25	0.40
4:4:197:LEU:HA	4:4:197:LEU:HD23	1.85	0.40
4:4:318:GLU:HB2	8:7:39:ASP:HB2	2.03	0.40
11:J:69:PHE:O	11:J:73:LEU:HG	2.20	0.40
14:M:9:PRO:HG2	14:M:107:LEU:HD12	2.03	0.40
15:N:63:THR:HG22	15:N:96:HIS:HA	2.02	0.40
3:D:3:ARG:HD2	3:D:12:GLU:OE2	2.22	0.40
3:D:386:SER:HB3	3:D:389:ASP:OD2	2.20	0.40
4:E:112:ARG:O	4:E:116:ILE:HG13	2.21	0.40
4:E:230:ILE:HG21	5:F:47:ASN:HB3	2.03	0.40
4:E:269:ARG:HA	4:E:269:ARG:HD3	1.98	0.40
4:E:336:HIS:ND1	5:F:189:ARG:O	2.54	0.40
4:E:369:LYS:HD3	4:E:370:VAL:N	2.35	0.40
6:G:56:ALA:O	7:O:22:VAL:HG12	2.20	0.40
11:R:59:TYR:O	11:R:64:VAL:HG12	2.22	0.40
12:S:28:PHE:O	12:S:32:GLU:HG2	2.21	0.40
13:T:305:TYR:HE1	13:T:406:ALA:HB1	1.86	0.40
13:T:332:LEU:HD12	13:T:369:GLY:HA3	2.03	0.40
16:Q:45:ARG:HG2	16:Q:46:MET:N	2.34	0.40
1:1:86:GLN:NE2	1:1:128:THR:OG1	2.48	0.40
1:1:145:LEU:HD23	1:1:145:LEU:HA	1.85	0.40
1:1:270:THR:O	1:1:311:MET:HG3	2.22	0.40
2:2:77:LYS:HE3	2:2:78:TYR:OH	2.21	0.40
3:3:306:LEU:HD11	3:3:308:THR:O	2.21	0.40
3:3:713:ARG:NE	3:3:746:ARG:HH21	2.19	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:4:67:GLU:OE2	4:4:369:LYS:HG2	2.20	0.40
4:4:250:LYS:HG3	4:4:264:VAL:HG21	2.02	0.40
7:9:77:PRO:O	7:9:80:PRO:HD3	2.22	0.40
8:7:60:SER:HA	8:7:66:PRO:HA	2.03	0.40
11:J:101:ALA:HB2	12:K:12:ALA:HB2	2.03	0.40
13:L:90:TYR:OH	13:L:334:LEU:O	2.29	0.40
13:L:325:HIS:HA	13:L:328:PHE:CE2	2.56	0.40
14:M:164:LEU:HD21	15:N:346:TYR:CE1	2.57	0.40
16:H:21:VAL:HG13	16:H:94:LEU:HD13	2.03	0.40
16:H:35:GLU:CD	16:H:294:ARG:HH21	2.23	0.40
3:D:34:CYS:HB3	3:D:45:CYS:SG	2.61	0.40
3:D:155:THR:HB	4:E:322:GLU:OE1	2.20	0.40
3:D:701:ALA:HB2	3:D:763:LEU:HB2	2.03	0.40
4:E:28:LEU:HD12	10:P:50:PRO:O	2.22	0.40
4:E:144:THR:OG1	16:Q:295:ALA:HB1	2.22	0.40
7:O:67:ALA:O	7:O:93:ILE:HA	2.21	0.40
11:R:19:VAL:CG2	11:R:32:LEU:HB2	2.50	0.40
13:T:90:TYR:CE2	13:T:334:LEU:HB3	2.57	0.40
16:Q:96:ALA:HA	16:Q:124:TYR:HE2	1.86	0.40
16:Q:202:ALA:O	16:Q:205:VAL:HG22	2.21	0.40
1:1:290:ILE:HD12	1:1:292:PRO:HD3	2.03	0.40
2:2:137:ASN:OD1	2:2:137:ASN:N	2.55	0.40
3:3:38:HIS:ND1	3:3:287:GLU:OE2	2.55	0.40
3:3:54:LEU:HD12	3:3:54:LEU:HA	1.91	0.40
3:3:170:LEU:HD23	3:3:170:LEU:HA	1.80	0.40
4:4:42:ARG:O	4:4:43:LEU:HD23	2.22	0.40
4:4:172:TYR:CD1	4:4:179:LYS:HB3	2.56	0.40
4:4:397:ILE:O	4:4:402:PRO:HD3	2.21	0.40
8:7:10:TYR:O	8:7:14:VAL:HG23	2.22	0.40
11:J:105:ALA:O	11:J:109:TRP:HB2	2.21	0.40
13:L:90:TYR:OH	13:L:338:SER:N	2.55	0.40
15:N:149:TYR:HB3	15:N:178:LEU:HD13	2.03	0.40
16:H:274:VAL:HG22	16:H:275:PRO:HD2	2.03	0.40
1:B:6:LEU:HD23	1:B:6:LEU:HA	1.84	0.40
1:B:101:PHE:CE1	1:B:253:GLN:HB2	2.57	0.40
1:B:176:GLY:O	2:C:32:ARG:NH2	2.51	0.40
1:B:254:ILE:HG22	1:B:264:TYR:HE2	1.86	0.40
3:D:170:LEU:HD23	3:D:170:LEU:HA	1.89	0.40
3:D:577:LEU:HB3	3:D:597:TYR:HB3	2.04	0.40
3:D:642:ALA:HB2	3:D:654:PHE:O	2.22	0.40
5:F:67:ARG:NH2	5:F:147:ARG:HB2	2.37	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:G:105:VAL:HB	6:G:132:PRO:O	2.21	0.40
7:O:10:LEU:HD12	16:Q:296:THR:HG21	2.03	0.40
7:O:91:TYR:O	7:O:133:LYS:N	2.54	0.40
9:X:41:ARG:HA	9:X:44:ALA:HB2	2.03	0.40
9:X:41:ARG:HD3	9:X:46:TYR:OH	2.21	0.40
11:R:97:ALA:CB	12:S:16:TYR:HB2	2.52	0.40
13:T:59:TRP:CD1	14:U:447:PRO:HD2	2.57	0.40
13:T:444:TRP:CE3	13:T:447:HIS:HD2	2.40	0.40
16:Q:33:LEU:HD11	16:Q:56:LEU:HA	2.04	0.40
16:Q:149:LEU:O	16:Q:153:LEU:HG	2.22	0.40

There are no symmetry-related clashes.

5.3 Torsion angles (i)

5.3.1 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 X-ray entries followed by that with respect to entries of similar resolution.

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	1	435/438 (99%)	410 (94%)	25 (6%)	0	100	100
1	B	435/438 (99%)	405 (93%)	30 (7%)	0	100	100
2	2	176/181 (97%)	167 (95%)	9 (5%)	0	100	100
2	C	176/181 (97%)	169 (96%)	7 (4%)	0	100	100
3	3	750/783 (96%)	702 (94%)	48 (6%)	0	100	100
3	D	750/783 (96%)	699 (93%)	51 (7%)	0	100	100
4	4	382/409 (93%)	358 (94%)	24 (6%)	0	100	100
4	E	382/409 (93%)	357 (94%)	25 (6%)	0	100	100
5	5	194/207 (94%)	187 (96%)	7 (4%)	0	100	100
5	F	194/207 (94%)	186 (96%)	8 (4%)	0	100	100
6	6	164/181 (91%)	153 (93%)	11 (7%)	0	100	100
6	G	164/181 (91%)	149 (91%)	15 (9%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
7	9	178/182 (98%)	167 (94%)	11 (6%)	0	100	100
7	O	178/182 (98%)	168 (94%)	10 (6%)	0	100	100
8	7	125/129 (97%)	117 (94%)	8 (6%)	0	100	100
8	I	125/129 (97%)	114 (91%)	11 (9%)	0	100	100
9	W	125/131 (95%)	121 (97%)	4 (3%)	0	100	100
9	X	125/131 (95%)	120 (96%)	5 (4%)	0	100	100
10	A	115/119 (97%)	103 (90%)	12 (10%)	0	100	100
10	P	115/119 (97%)	103 (90%)	12 (10%)	0	100	100
11	J	158/176 (90%)	143 (90%)	15 (10%)	0	100	100
11	R	158/176 (90%)	144 (91%)	14 (9%)	0	100	100
12	K	93/95 (98%)	88 (95%)	5 (5%)	0	100	100
12	S	93/95 (98%)	90 (97%)	3 (3%)	0	100	100
13	L	603/606 (100%)	568 (94%)	34 (6%)	1 (0%)	47	79
13	T	603/606 (100%)	572 (95%)	30 (5%)	1 (0%)	47	79
14	M	465/469 (99%)	435 (94%)	30 (6%)	0	100	100
14	U	465/469 (99%)	434 (93%)	31 (7%)	0	100	100
15	N	425/427 (100%)	400 (94%)	25 (6%)	0	100	100
15	V	425/427 (100%)	403 (95%)	22 (5%)	0	100	100
16	H	351/365 (96%)	297 (85%)	48 (14%)	6 (2%)	9	45
16	Q	351/365 (96%)	298 (85%)	49 (14%)	4 (1%)	14	53
All	All	9478/9796 (97%)	8827 (93%)	639 (7%)	12 (0%)	51	83

All (12) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
16	H	51	VAL
16	Q	44	VAL
16	Q	51	VAL
16	H	44	VAL
16	H	50	ARG
16	Q	50	ARG
16	H	268	THR
13	L	435	PRO
16	Q	268	THR
13	T	435	PRO

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Mol	Chain	Res	Type
16	H	218	PRO
16	H	53	PRO

5.3.2 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 X-ray entries followed by that with respect to entries of similar resolution.

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	1	355/356 (100%)	343 (97%)	12 (3%)	37	69
1	B	355/356 (100%)	344 (97%)	11 (3%)	40	71
2	2	150/152 (99%)	146 (97%)	4 (3%)	44	73
2	C	150/152 (99%)	144 (96%)	6 (4%)	31	65
3	3	609/628 (97%)	599 (98%)	10 (2%)	62	83
3	D	609/628 (97%)	598 (98%)	11 (2%)	59	81
4	4	332/355 (94%)	324 (98%)	8 (2%)	49	75
4	E	332/355 (94%)	325 (98%)	7 (2%)	53	78
5	5	167/175 (95%)	164 (98%)	3 (2%)	59	81
5	F	167/175 (95%)	162 (97%)	5 (3%)	41	71
6	6	135/149 (91%)	125 (93%)	10 (7%)	13	46
6	G	135/149 (91%)	127 (94%)	8 (6%)	19	55
7	9	148/150 (99%)	146 (99%)	2 (1%)	67	85
7	O	148/150 (99%)	146 (99%)	2 (1%)	67	85
8	7	104/106 (98%)	103 (99%)	1 (1%)	76	88
8	I	104/106 (98%)	103 (99%)	1 (1%)	76	88
9	W	99/101 (98%)	98 (99%)	1 (1%)	76	88
9	X	99/101 (98%)	97 (98%)	2 (2%)	55	79
10	A	90/92 (98%)	88 (98%)	2 (2%)	52	77
10	P	90/92 (98%)	88 (98%)	2 (2%)	52	77
11	J	118/130 (91%)	115 (98%)	3 (2%)	47	75
11	R	118/130 (91%)	114 (97%)	4 (3%)	37	69

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
12	K	71/71 (100%)	69 (97%)	2 (3%)	43	72
12	S	71/71 (100%)	69 (97%)	2 (3%)	43	72
13	L	453/454 (100%)	445 (98%)	8 (2%)	59	81
13	T	453/454 (100%)	443 (98%)	10 (2%)	52	77
14	M	332/332 (100%)	327 (98%)	5 (2%)	65	84
14	U	332/332 (100%)	324 (98%)	8 (2%)	49	75
15	N	302/302 (100%)	297 (98%)	5 (2%)	60	82
15	V	302/302 (100%)	295 (98%)	7 (2%)	50	76
16	H	293/300 (98%)	284 (97%)	9 (3%)	40	71
16	Q	293/300 (98%)	285 (97%)	8 (3%)	44	73
All	All	7516/7706 (98%)	7337 (98%)	179 (2%)	49	75

All (179) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	1	18	TYR
1	1	81	LYS
1	1	249	MET
1	1	342	TRP
1	1	353	CYS
1	1	355	LYS
1	1	359	CYS
1	1	366	PHE
1	1	397	ARG
1	1	400	CYS
1	1	437	TRP
1	1	438	ARG
2	2	33	ARG
2	2	35	GLN
2	2	45	ARG
2	2	116	LEU
3	3	3	ARG
3	3	34	CYS
3	3	123	ASP
3	3	184	CYS
3	3	259	CYS
3	3	337	ARG
3	3	425	ARG

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Mol	Chain	Res	Type
3	3	655	ARG
3	3	761	SER
3	3	774	ARG
4	4	87	TYR
4	4	132	PHE
4	4	143	LEU
4	4	151	ARG
4	4	152	GLU
4	4	192	LYS
4	4	208	PHE
4	4	262	PHE
5	5	31	ARG
5	5	38	MET
5	5	147	ARG
6	6	37	TRP
6	6	49	GLU
6	6	55	ASP
6	6	68	PHE
6	6	83	ARG
6	6	101	ASP
6	6	120	ASN
6	6	156	LYS
6	6	176	TRP
6	6	177	LYS
7	9	38	HIS
7	9	104	CYS
8	7	120	ASP
9	W	37	TRP
10	A	13	TYR
10	A	48	ASN
11	J	59	TYR
11	J	84	ASP
11	J	119	LEU
12	K	28	PHE
12	K	82	ARG
13	L	10	PRO
13	L	59	TRP
13	L	101	TYR
13	L	151	TYR
13	L	169	PHE
13	L	506	TRP
13	L	511	PHE

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Mol	Chain	Res	Type
13	L	554	PHE
14	M	22	ARG
14	M	241	PHE
14	M	255	GLN
14	M	326	PHE
14	M	455	HIS
15	N	9	PHE
15	N	50	PHE
15	N	125	ARG
15	N	126	ARG
15	N	284	TYR
16	H	28	PHE
16	H	37	ARG
16	H	147	TYR
16	H	149	LEU
16	H	196	PHE
16	H	211	MET
16	H	302	TYR
16	H	307	ARG
16	H	354	TYR
1	B	81	LYS
1	B	249	MET
1	B	337	MET
1	B	342	TRP
1	B	346	ARG
1	B	353	CYS
1	B	355	LYS
1	B	359	CYS
1	B	366	PHE
1	B	397	ARG
1	B	400	CYS
2	C	7	LYS
2	C	33	ARG
2	C	35	GLN
2	C	45	ARG
2	C	116	LEU
2	C	147	ARG
3	D	3	ARG
3	D	83	CYS
3	D	123	ASP
3	D	132	ASP
3	D	184	CYS

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Mol	Chain	Res	Type
3	D	337	ARG
3	D	369	LEU
3	D	617	LEU
3	D	655	ARG
3	D	761	SER
3	D	774	ARG
4	E	87	TYR
4	E	132	PHE
4	E	143	LEU
4	E	151	ARG
4	E	208	PHE
4	E	262	PHE
4	E	284	ARG
5	F	31	ARG
5	F	38	MET
5	F	97	GLU
5	F	147	ARG
5	F	178	ASP
6	G	37	TRP
6	G	49	GLU
6	G	55	ASP
6	G	68	PHE
6	G	83	ARG
6	G	120	ASN
6	G	156	LYS
6	G	176	TRP
7	O	38	HIS
7	O	104	CYS
8	I	43	ARG
9	X	37	TRP
9	X	43	GLN
10	P	13	TYR
10	P	48	ASN
11	R	32	LEU
11	R	59	TYR
11	R	84	ASP
11	R	119	LEU
12	S	28	PHE
12	S	82	ARG
13	T	10	PRO
13	T	56	GLN
13	T	59	TRP

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Mol	Chain	Res	Type
13	T	124	TYR
13	T	146	TYR
13	T	169	PHE
13	T	275	LEU
13	T	506	TRP
13	T	511	PHE
13	T	554	PHE
14	U	22	ARG
14	U	148	PHE
14	U	234	TYR
14	U	239	PHE
14	U	255	GLN
14	U	326	PHE
14	U	344	TYR
14	U	455	HIS
15	V	22	PRO
15	V	50	PHE
15	V	125	ARG
15	V	126	ARG
15	V	136	TYR
15	V	284	TYR
15	V	313	ARG
16	Q	28	PHE
16	Q	43	GLN
16	Q	44	VAL
16	Q	54	PHE
16	Q	147	TYR
16	Q	149	LEU
16	Q	196	PHE
16	Q	310	TRP

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (57) such sidechains are listed below:

Mol	Chain	Res	Type
1	1	219	ASN
1	1	288	GLN
1	1	420	GLN
2	2	71	GLN
3	3	104	GLN
3	3	208	HIS
3	3	613	HIS
3	3	661	GLN

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Mol	Chain	Res	Type
4	4	38	HIS
4	4	292	GLN
4	4	330	HIS
5	5	144	HIS
6	6	74	GLN
6	6	98	GLN
6	6	120	ASN
6	6	153	GLN
9	W	43	GLN
9	W	84	GLN
12	K	54	GLN
12	K	81	HIS
13	L	341	HIS
13	L	513	GLN
13	L	544	ASN
13	L	582	GLN
14	M	221	ASN
14	M	255	GLN
15	N	245	ASN
16	H	43	GLN
16	H	112	GLN
1	B	219	ASN
1	B	220	ASN
2	C	71	GLN
2	C	81	GLN
2	C	120	GLN
3	D	246	ASN
3	D	703	GLN
4	E	33	GLN
4	E	292	GLN
4	E	330	HIS
6	G	74	GLN
6	G	120	ASN
6	G	153	GLN
6	G	155	GLN
9	X	38	GLN
9	X	43	GLN
10	P	60	HIS
12	S	81	HIS
13	T	288	GLN
13	T	341	HIS
13	T	358	HIS

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Mol	Chain	Res	Type
13	T	513	GLN
13	T	544	ASN
14	U	221	ASN
15	V	245	ASN
16	Q	43	GLN
16	Q	117	ASN
16	Q	304	GLN

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

22 ligands are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or 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 length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
17	SF4	D	803	3	0,12,12	-	-	-		
19	FES	2	201	2	0,4,4	-	-	-		
20	HQH	4	501	-	29,30,30	0.39	0	28,40,40	0.65	2 (7%)
17	SF4	O	202	7	0,12,12	-	-	-		
17	SF4	3	803	3	0,12,12	-	-	-		
17	SF4	6	201	6	0,12,12	-	-	-		
17	SF4	9	201	7	0,12,12	-	-	-		

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
17	SF4	3	801	3	0,12,12	-	-	-		
19	FES	C	201	2	0,4,4	-	-	-		
17	SF4	B	501	1	0,12,12	-	-	-		
19	FES	D	804	3	0,4,4	-	-	-		
17	SF4	O	201	7	0,12,12	-	-	-		
17	SF4	G	201	6	0,12,12	-	-	-		
17	SF4	D	802	3	0,12,12	-	-	-		
17	SF4	1	501	1	0,12,12	-	-	-		
18	FMN	B	502	-	33,33,33	1.09	2 (6%)	48,50,50	1.32	10 (20%)
19	FES	3	804	3	0,4,4	-	-	-		
18	FMN	1	502	-	33,33,33	1.12	2 (6%)	48,50,50	1.33	10 (20%)
17	SF4	9	202	7	0,12,12	-	-	-		
20	HQH	E	501	-	29,30,30	0.37	0	28,40,40	0.45	0
17	SF4	3	802	3	0,12,12	-	-	-		
17	SF4	D	801	3	0,12,12	-	-	-		

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
17	SF4	D	803	3	-	-	0/6/5/5
19	FES	2	201	2	-	-	0/1/1/1
20	HQH	4	501	-	-	10/27/29/29	0/1/1/1
17	SF4	O	202	7	-	-	0/6/5/5
17	SF4	3	803	3	-	-	0/6/5/5
17	SF4	6	201	6	-	-	0/6/5/5
17	SF4	9	201	7	-	-	0/6/5/5
17	SF4	3	801	3	-	-	0/6/5/5
19	FES	C	201	2	-	-	0/1/1/1
17	SF4	B	501	1	-	-	0/6/5/5
19	FES	D	804	3	-	-	0/1/1/1
17	SF4	G	201	6	-	-	0/6/5/5
17	SF4	O	201	7	-	-	0/6/5/5
17	SF4	D	802	3	-	-	0/6/5/5
17	SF4	1	501	1	-	-	0/6/5/5
18	FMN	B	502	-	-	8/18/18/18	0/3/3/3
19	FES	3	804	3	-	-	0/1/1/1
18	FMN	1	502	-	-	8/18/18/18	0/3/3/3
17	SF4	9	202	7	-	-	0/6/5/5

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
20	HQH	E	501	-	-	12/27/29/29	0/1/1/1
17	SF4	3	802	3	-	-	0/6/5/5
17	SF4	D	801	3	-	-	0/6/5/5

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
18	1	502	FMN	C4A-N5	3.89	1.38	1.30
18	B	502	FMN	C4A-N5	3.79	1.38	1.30
18	1	502	FMN	C10-N1	2.66	1.38	1.33
18	B	502	FMN	C10-N1	2.57	1.38	1.33

All (22) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
18	B	502	FMN	C4-N3-C2	-3.22	119.69	125.64
18	1	502	FMN	C4-N3-C2	-3.16	119.79	125.64
18	1	502	FMN	O4-C4-C4A	-2.86	119.02	126.60
18	1	502	FMN	C4A-C4-N3	2.74	120.14	113.19
18	B	502	FMN	C4A-C4-N3	2.65	119.92	113.19
18	B	502	FMN	O4-C4-C4A	-2.63	119.62	126.60
18	B	502	FMN	C4A-C10-N1	-2.60	118.70	124.73
18	1	502	FMN	C9A-C5A-N5	-2.54	119.67	122.43
18	B	502	FMN	C5A-C9A-N10	2.47	120.50	117.95
18	1	502	FMN	C4A-C10-N1	-2.46	119.01	124.73
18	1	502	FMN	C5A-C9A-N10	2.46	120.49	117.95
18	B	502	FMN	C9A-C5A-N5	-2.30	119.94	122.43
18	B	502	FMN	C4-C4A-C10	2.23	120.54	116.79
18	B	502	FMN	C5'-C4'-C3'	-2.23	107.90	112.20
18	B	502	FMN	C4A-C10-N10	2.19	119.68	116.48
18	B	502	FMN	C10-C4A-N5	-2.17	120.25	124.86
20	4	501	HQH	C15-C21-C18	-2.14	120.85	124.18
20	4	501	HQH	C7-C6-C8	-2.10	106.65	110.80
18	1	502	FMN	C10-C4A-N5	-2.08	120.45	124.86
18	1	502	FMN	C4-C4A-C10	2.06	120.25	116.79
18	1	502	FMN	C4A-C10-N10	2.02	119.44	116.48
18	1	502	FMN	C10-N1-C2	2.00	120.90	116.90

There are no chirality outliers.

All (38) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
18	1	502	FMN	N10-C1'-C2'-O2'
18	1	502	FMN	N10-C1'-C2'-C3'
18	1	502	FMN	C1'-C2'-C3'-O3'
18	1	502	FMN	C1'-C2'-C3'-C4'
18	1	502	FMN	O4'-C4'-C5'-O5'
18	B	502	FMN	N10-C1'-C2'-O2'
18	B	502	FMN	N10-C1'-C2'-C3'
18	B	502	FMN	C1'-C2'-C3'-O3'
18	B	502	FMN	C1'-C2'-C3'-C4'
18	B	502	FMN	O4'-C4'-C5'-O5'
20	4	501	HQH	C17-C15-C21-C18
20	4	501	HQH	C19-C12-C13-C20
20	4	501	HQH	C21-C15-C17-C26
20	4	501	HQH	C21-C15-C17-C20
20	4	501	HQH	C6-C7-C9-C14
20	4	501	HQH	C6-C7-C9-C16
20	E	501	HQH	C17-C15-C21-C18
20	E	501	HQH	C19-C12-C13-C20
20	E	501	HQH	N5-C12-C13-C20
20	E	501	HQH	C21-C15-C17-C26
20	E	501	HQH	C21-C15-C17-C20
20	E	501	HQH	C6-C7-C9-C14
20	E	501	HQH	C6-C7-C9-C16
18	1	502	FMN	O2'-C2'-C3'-O3'
18	1	502	FMN	O2'-C2'-C3'-C4'
20	4	501	HQH	C22-C11-C18-C21
20	E	501	HQH	C22-C11-C18-C21
20	4	501	HQH	C8-C11-C18-C21
20	E	501	HQH	C8-C11-C18-C21
18	B	502	FMN	O2'-C2'-C3'-C4'
18	B	502	FMN	O2'-C2'-C3'-O3'
18	1	502	FMN	C3'-C4'-C5'-O5'
20	4	501	HQH	O1-C7-C9-C14
20	E	501	HQH	O1-C7-C9-C14
20	4	501	HQH	O1-C7-C9-C16
20	E	501	HQH	O1-C7-C9-C16
20	E	501	HQH	C12-C13-C20-C17
18	B	502	FMN	C3'-C4'-C5'-O5'

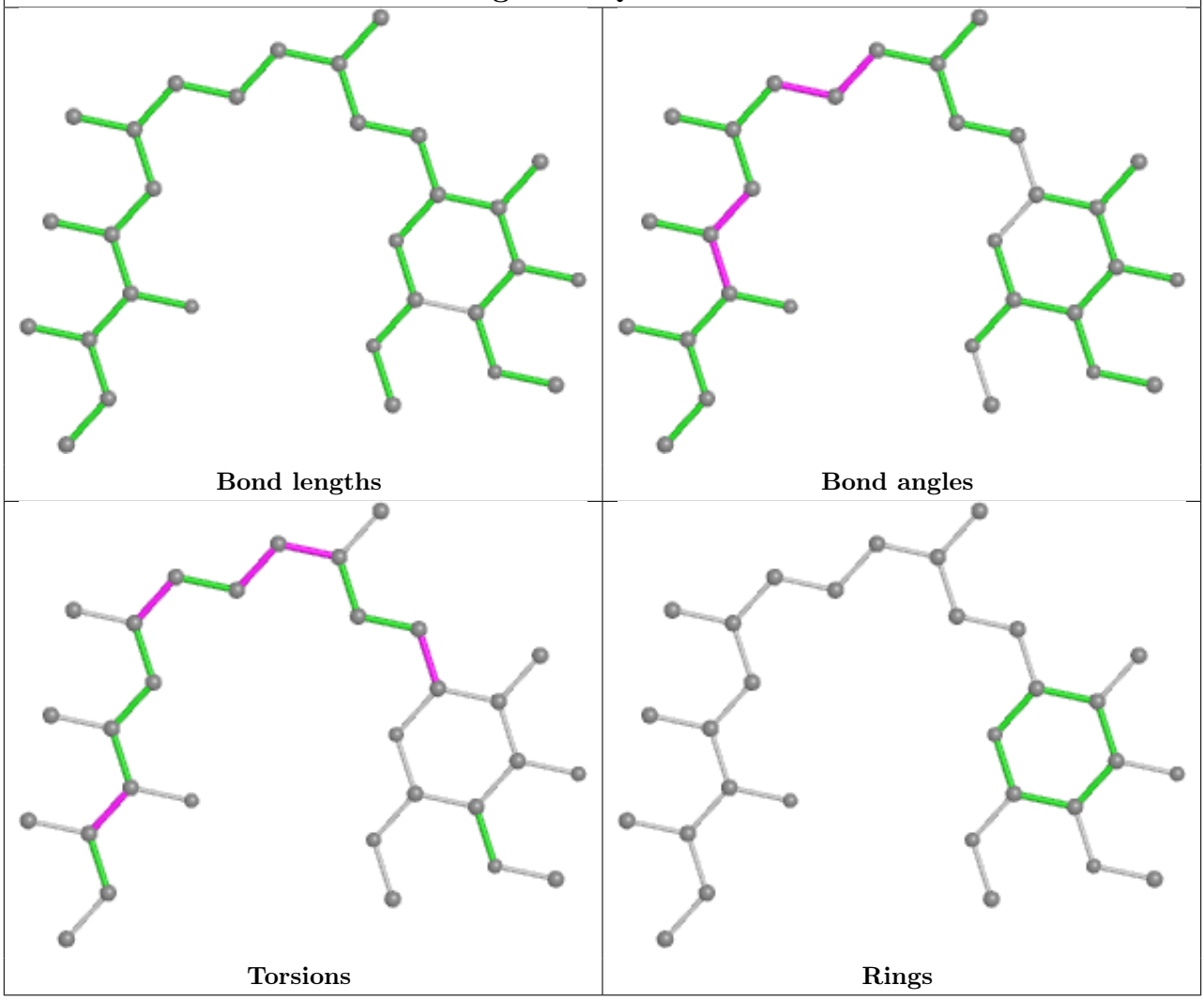
There are no ring outliers.

14 monomers are involved in 36 short contacts:

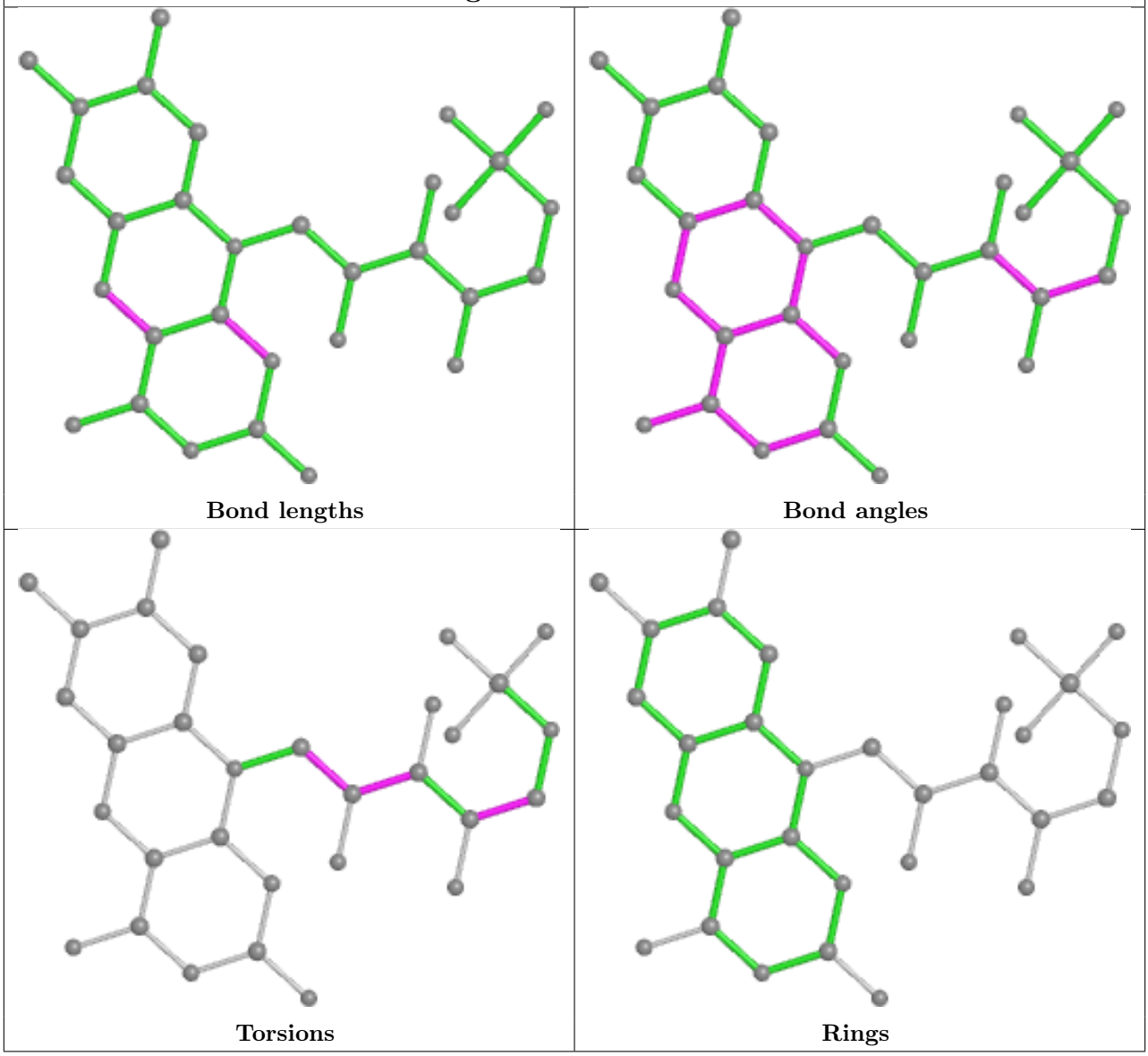
Mol	Chain	Res	Type	Clashes	Symm-Clashes
17	D	803	SF4	3	0
19	2	201	FES	1	0
20	4	501	HQH	3	0
17	O	202	SF4	2	0
17	9	201	SF4	3	0
17	3	801	SF4	1	0
17	B	501	SF4	1	0
17	O	201	SF4	1	0
17	G	201	SF4	4	0
18	B	502	FMN	7	0
18	1	502	FMN	4	0
17	9	202	SF4	3	0
20	E	501	HQH	1	0
17	D	801	SF4	2	0

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.

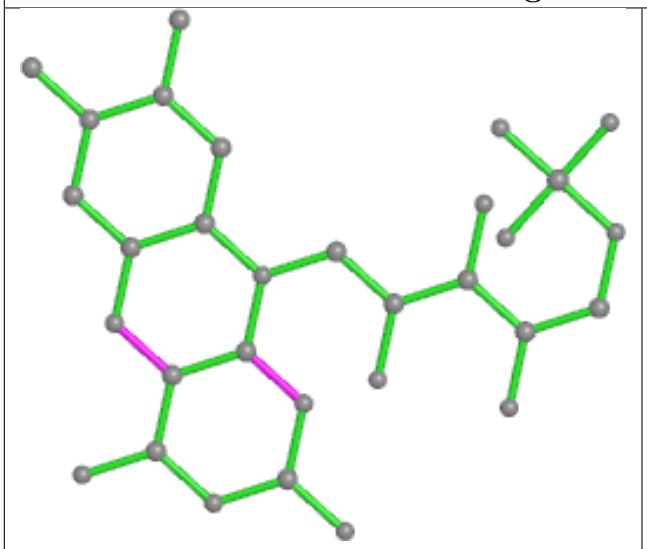
Ligand HQH 4 501



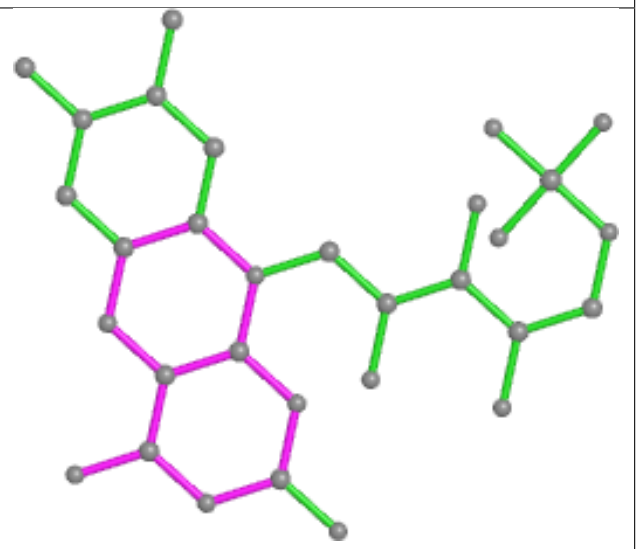
Ligand FMN B 502



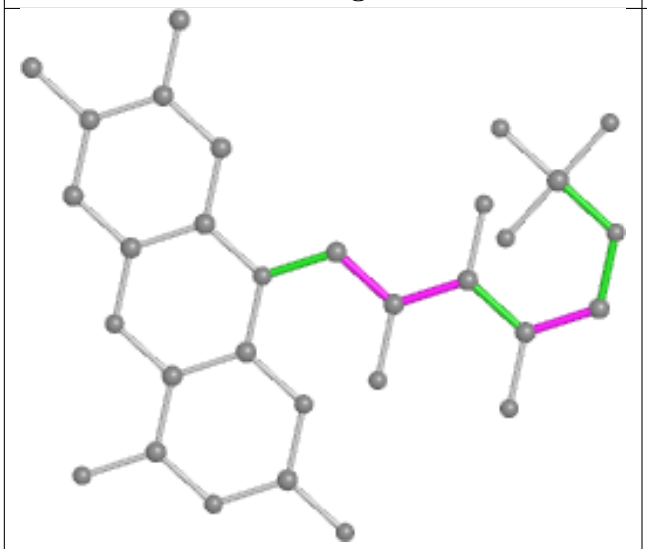
Ligand FMN 1 502



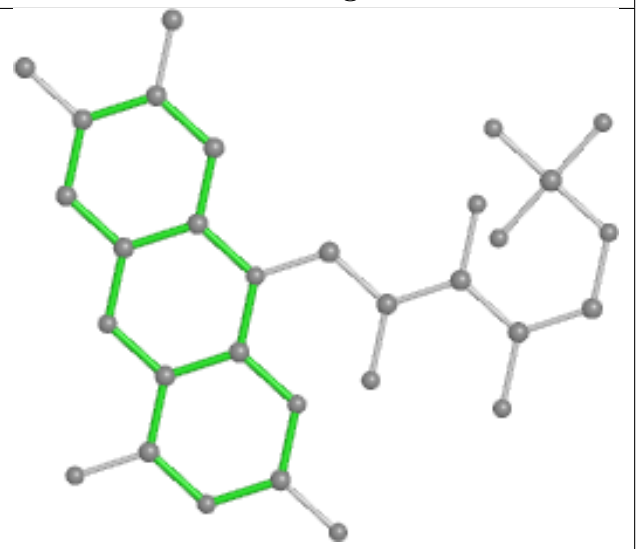
Bond lengths



Bond angles

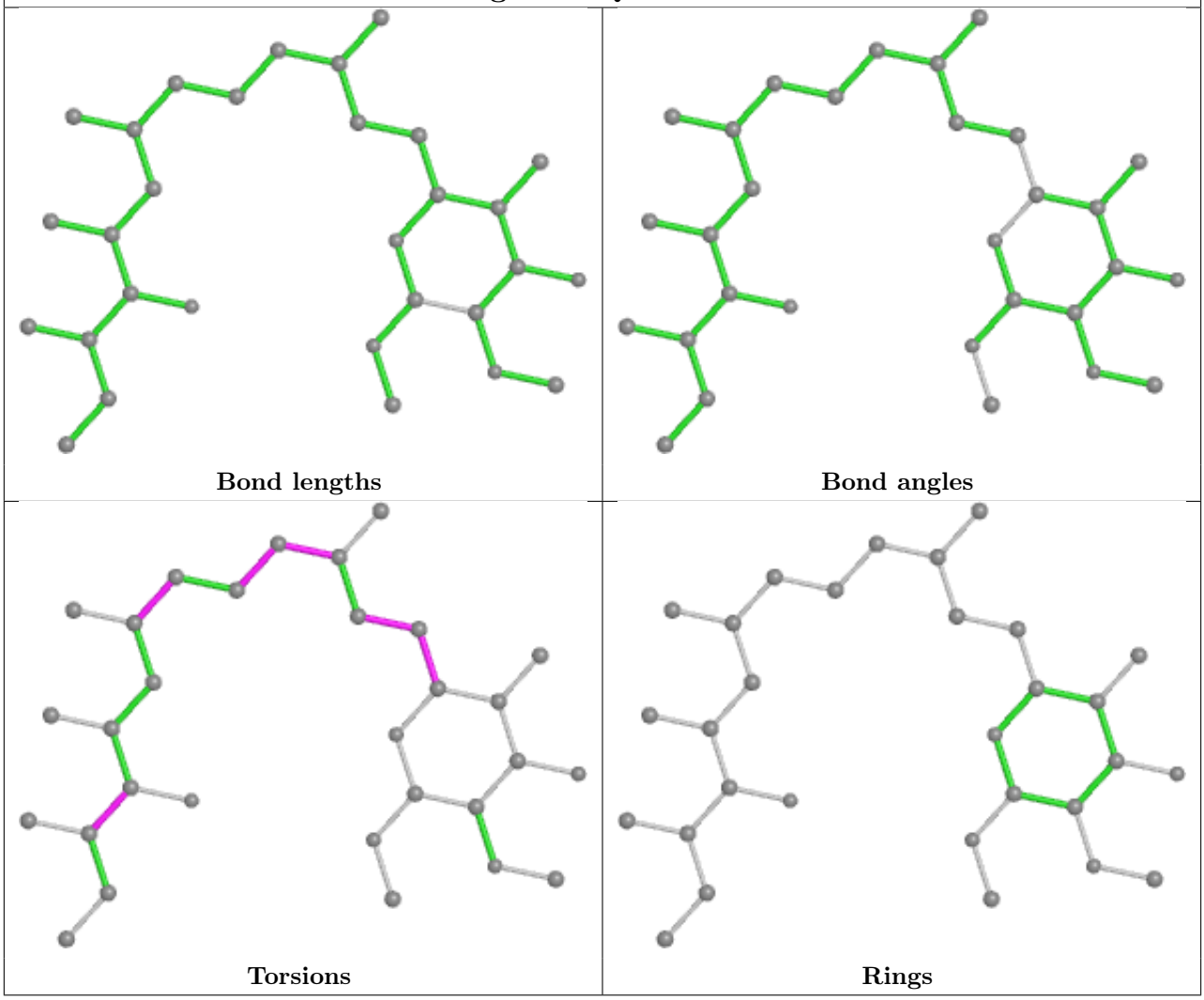


Torsions



Rings

Ligand HQH E 501



5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

6 Fit of model and data (i)

6.1 Protein, DNA and RNA chains (i)

EDS failed to run properly - this section is therefore empty.

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

EDS failed to run properly - this section is therefore empty.

6.3 Carbohydrates (i)

EDS failed to run properly - this section is therefore empty.

6.4 Ligands (i)

EDS failed to run properly - this section is therefore empty.

6.5 Other polymers (i)

EDS failed to run properly - this section is therefore empty.