Full wwPDB X-ray Structure Validation Report (i)

Jun 25, 2024 – 05:15 PM EDT

PDB ID	:	6Q8W
Title	:	Respiratory complex I from Thermus thermophilus with bound Aureothin.
Authors	:	Gutierrez-Fernandez, J.; Minhas, G.S.; Sazanov, L.A.
Deposited on	:	2018-12-16
Resolution	:	3.40 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:

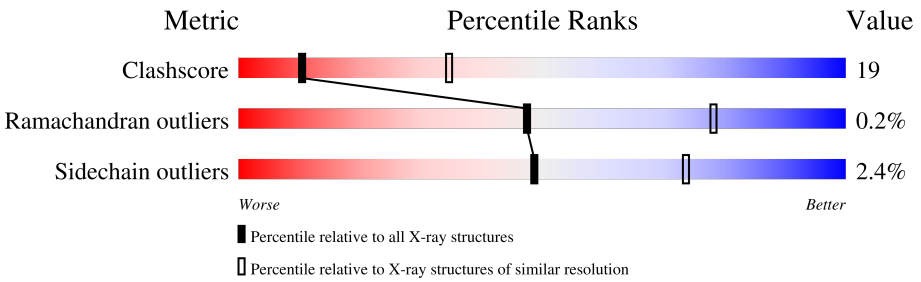
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	FAILED
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson 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 3.40 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	1055 (3.48-3.32)
Ramachandran outliers	138981	1038 (3.48-3.32)
Sidechain outliers	138945	1038 (3.48-3.32)

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	64% 34% •
1	B	438	57% 41% •
2	2	181	66% 30% • •
2	C	181	62% 34% • •
3	3	783	59% 37% • •
3	D	783	62% 34% • •
4	4	409	51% 43% 6%
4	E	409	50% 42% • 6%

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Mol	Chain	Length	Quality of chain
5	5	207	57% 36% 5%
5	F	207	60% 33% 5%
6	6	181	35% 54% 8%
6	G	181	44% 45% 8%
7	9	182	61% 37%
7	O	182	60% 38%
8	7	129	71% 27%
8	I	129	70% 28%
9	W	131	68% 28%
9	X	131	76% 20%
10	A	119	51% 45%
10	P	119	55% 40%
11	J	176	53% 37% 9%
11	R	176	55% 35% 9%
12	K	95	64% 34%
12	S	95	69% 29%
13	L	606	66% 33%
13	T	606	66% 33%
14	M	469	65% 34%
14	U	469	64% 35%
15	N	427	67% 32%
15	V	427	69% 30%
16	H	365	50% 43%
16	Q	365	50% 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	1	501	-	-	X	-
17	SF4	B	501	-	-	X	-
19	FES	3	804	-	-	X	-
19	FES	C	201	-	-	X	-
19	FES	D	804	-	-	X	-

2 Entry composition (i)

There are 20 unique types of molecules in this entry. The entry contains 74144 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 Uncharacterized protein.

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

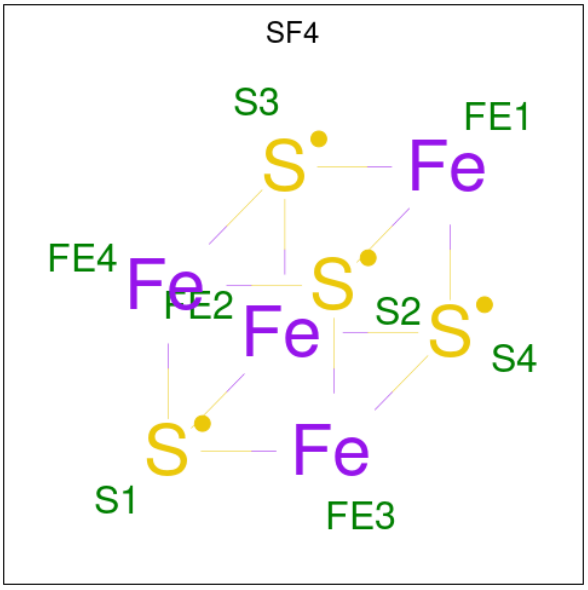
- Molecule 15 is a protein called NADH-quinone oxidoreductase subunit 14.

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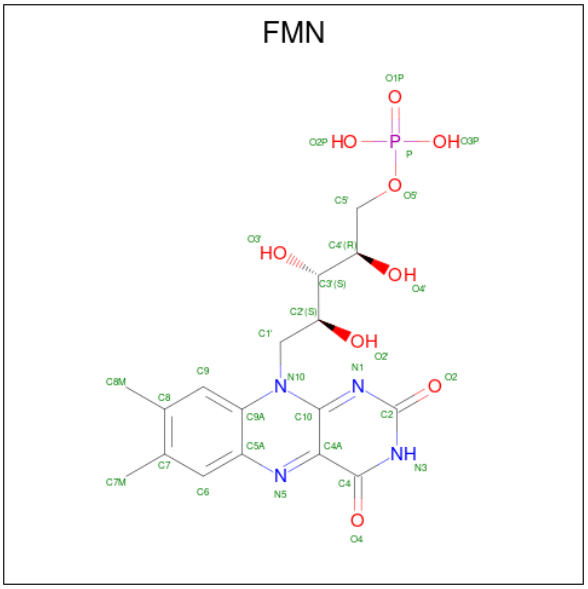
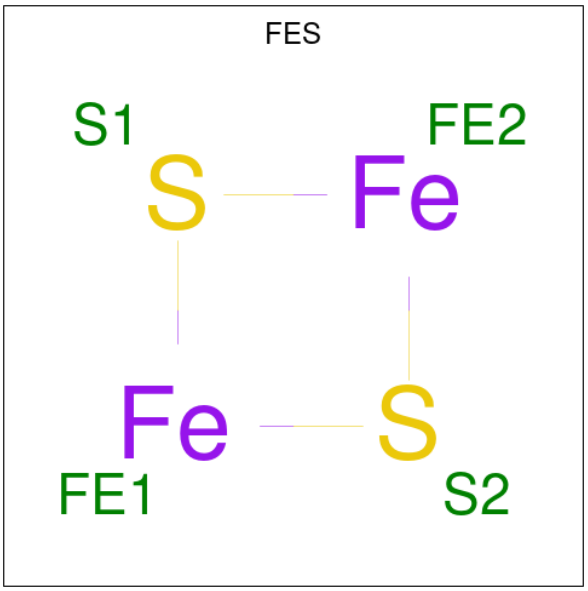
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
17	D	1	Total	Fe	S		0	0
			8	4	4			
17	D	1	Total	Fe	S		0	0
			8	4	4			
17	G	1	Total	Fe	S		0	0
			8	4	4			
17	O	1	Total	Fe	S		0	0
			8	4	4			
17	O	1	Total	Fe	S		0	0
			8	4	4			

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



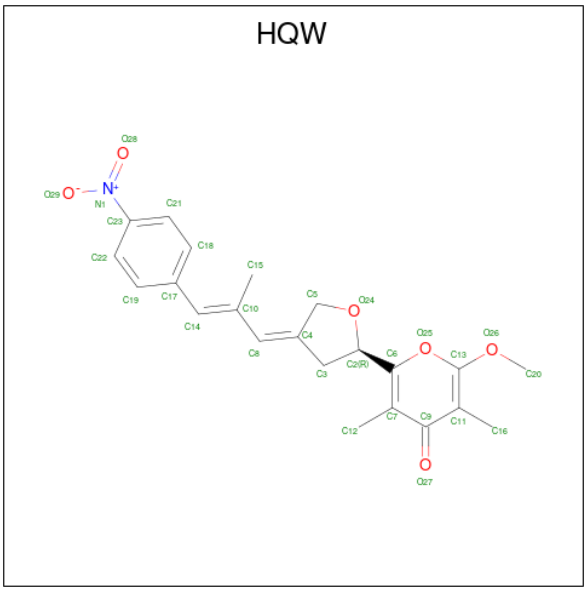
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
18	1	1	Total	C	N	O	P	0	0
			31	17	4	9	1		
18	B	1	Total	C	N	O	P	0	0
			31	17	4	9	1		

- 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 Aureothin (three-letter code: HQW) (formula: $C_{22}H_{23}NO_6$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	C	N	O		
20	4	1	29	22	1	6	0	0
			Total	C	N	O		
20	E	1	29	22	1	6	0	0

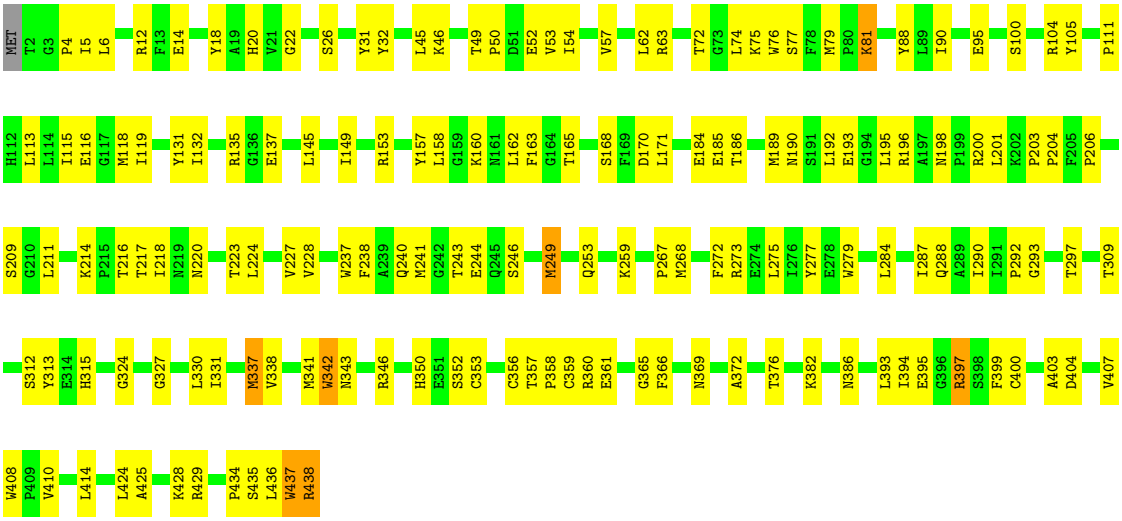
3 Residue-property plots (i)

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.

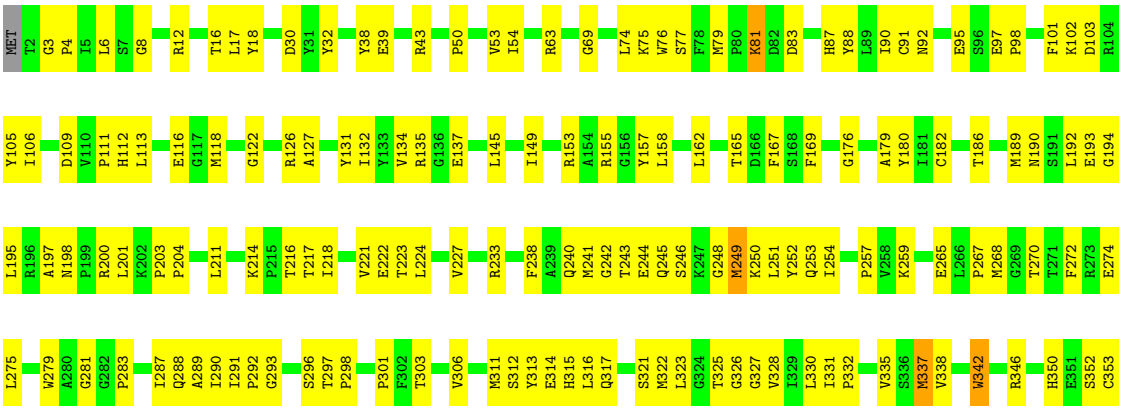
• Molecule 1: NADH-quinone oxidoreductase subunit 1

Chain 1:



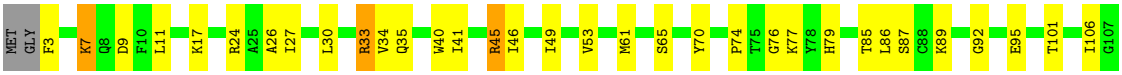
• Molecule 1: NADH-quinone oxidoreductase subunit 1

Chain B:



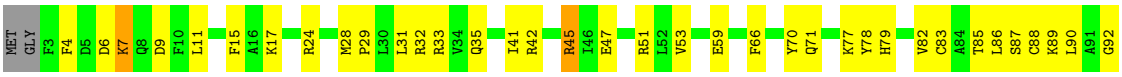
- Molecule 2: NADH-quinone oxidoreductase subunit 2

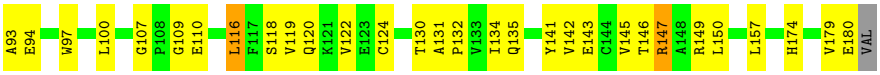
Chain 2:



- Molecule 2: NADH-quinone oxidoreductase subunit 2

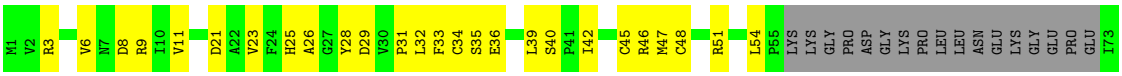
Chain C:

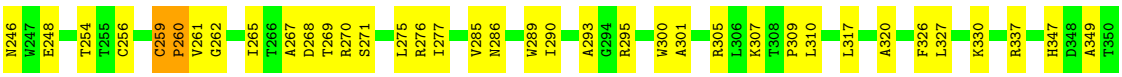


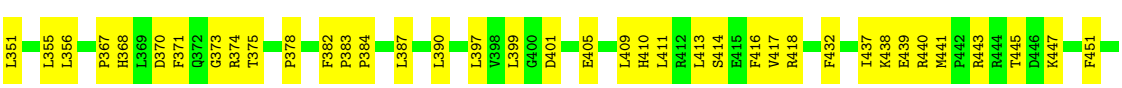


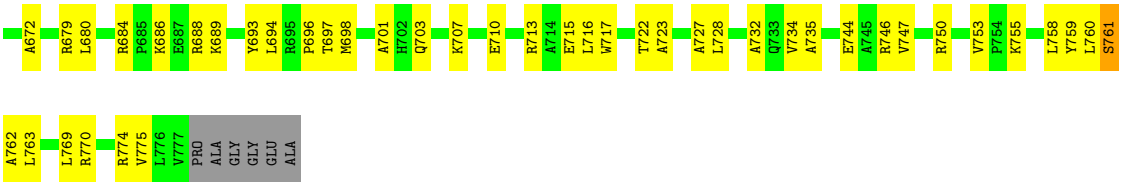
- Molecule 3: NADH-quinone oxidoreductase subunit 3

Chain 3:



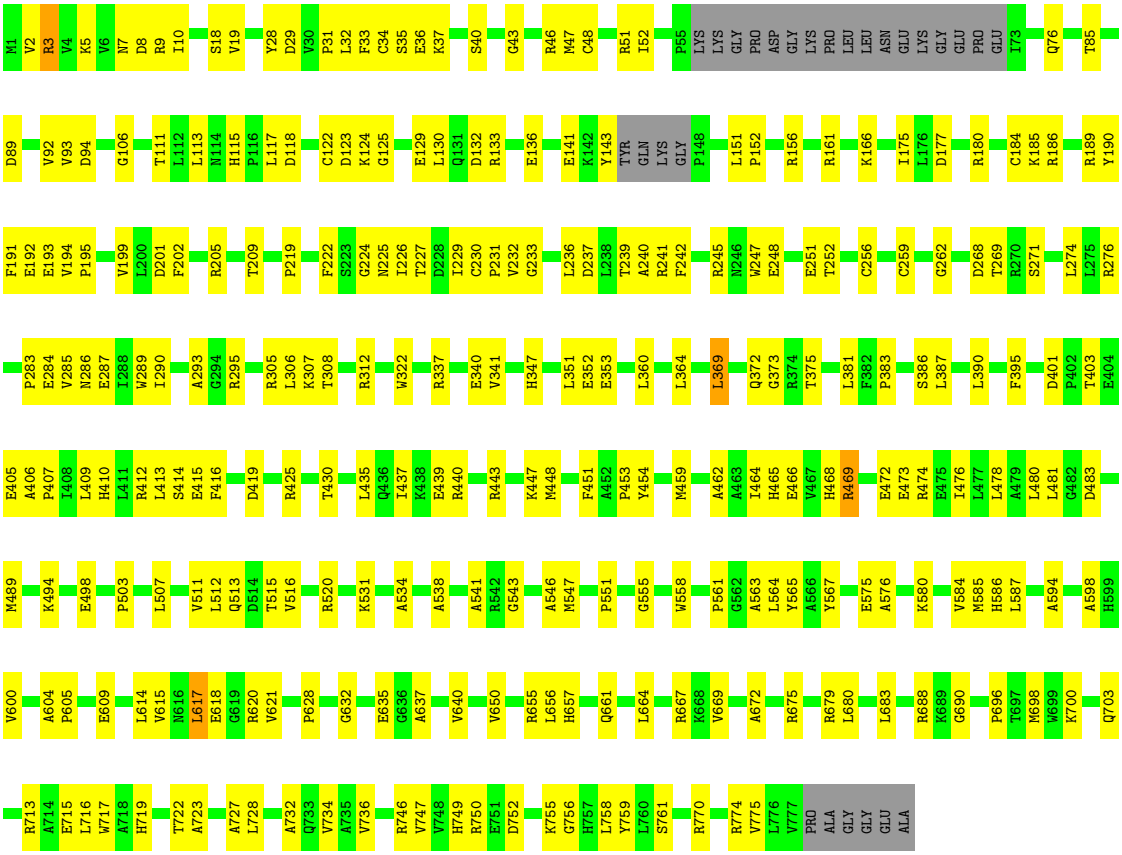






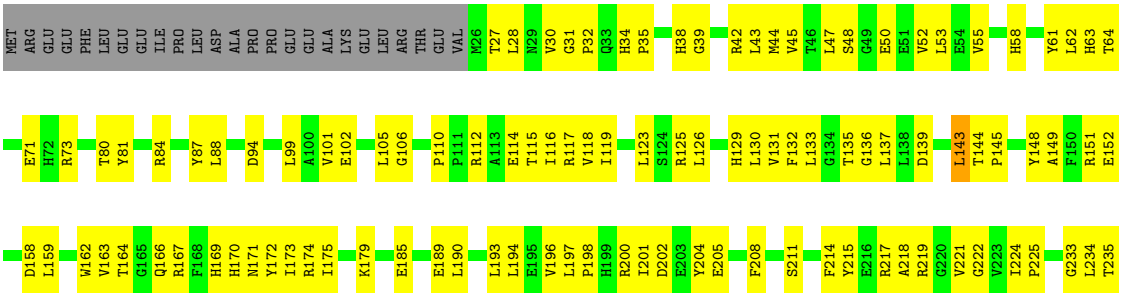
• Molecule 3: NADH-quinone oxidoreductase subunit 3

Chain D:



• Molecule 4: NADH-quinone oxidoreductase subunit 4

Chain 4:



G236 G237 S238 L239 R240 V244 V248 T261 F262 P265 G270 D271 V272 R275 M276 L277 V278 R279 I280 R281 E282 M283 R284 E285 K288 I289 Q292 L297 E298 P299 G300 P301 D304 P305 N306 I309 T310 P311 P312 P313 R314 E318 M321 E322 A323 V324 I325

Y326 H330 E333 G334 F335 H336 P337 P338 E341 E347 E352 Y356 G361 G362 S363 R367 P373 N377 L378 Q379 S380 L381 P382 Y383 A384 C385 K386 Q389 V390 P391 I396 I397 A398 S399 L400 M404 D408 R409

- Molecule 4: NADH-quinone oxidoreductase subunit 4

Chain E: 50% 42% • 6%

MET ARG GLU GLU PHE LEU GLU GLU ILE PRO LEU ASP ALA PRO PRO GLU GLU ALA LYS GLU LEU ARG THR GLU VAL M26 T27 L28 N29 V30 G31 P32 G33 H34 P35 S36 T37 H38 R42 V45 T46 L47 S48 G49 E50 E51 V52 L53 E54 V55 H58 L62 K68 E71

H72 R73 T74 Y75 L76 Q77 T80 Y81 R84 M85 D86 Y87 H93 A98 L99 E102 K103 L104 L105 A113 E114 T115 V118 E122 L123 S124 R125 H129 L130 V131 F132 G136 L137 L138 D139 L140 L143 T144 P145 F146 F147 Y148 R151 E152 R153 E154 T155 I156

L157 D158 L159 F160 E161 W162 V163 T164 R167 F168 H169 H170 N171 Y172 I173 R174 E180 E185 L193 L194 E195 V196 R200 I201 D202 E203 Y204 L207 F208 S211 Y215 E216 R217 A218 R219 G222 V223 I224 P225 P226 E227 V228 D231 L234 T235 G236 G237 S238 L239

R240 N245 Y246 D247 V248 R249 T259 Y260 T261 F262 D263 V264 P265 L266 G267 D271 V272 R275 M276 L277 V278 R279 I280 R281 E282 M283 R284 E285 S286 I289 I290 K291 Q292 R296 V302 R303 D304 P305 N306 I309 T310 P311 M321 H330 E333 G334 F335 H336 P337

P338 E341 E347 R350 G351 E352 L353 G354 Y355 V358 S359 D360 S363 M364 P365 Y366 R367 V368 K369 V370 R371 A372 P373 S374 F375 V376 N377 S380 L381 P382 Y383 A384 C385 Q389 V390 P391 D392 I396 I397 A398 S399 D406 R409

- Molecule 5: NADH-quinone oxidoreductase subunit 5

Chain 5: 57% 36% • 5%

M1 R2 L3 E4 R5 V6 L7 E18 W26 R31 E32 R33 E36 E37 M38 Y41 R42 N47 F48 D51 I52 V53 G54 L55 D56 Y57 E66 R67 F68 V71 Y72 E73 L74 V75 W80 K81 D82 R87 F88 F89 V90 R91 V92 Y93 E96 R100 L101

P102 T103 L107 W108 G109 S110 R116 E117 V118 Y119 D120 L121 I124 V125 F126 E127 L132 R133 K134 I135 L136 T137 P138 L141 H144 P145 L146 R147 K148 D149 Y150 T155 R160 Y164 A168 E169 F170 R171 L174 T175 D178 K185 G186 G187 S188 R189

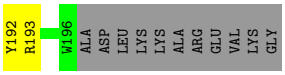
Y192 R193 W196 ALA ASP LEU LYS LYS ALA ARG GLU VAL LYS GLY

- Molecule 5: NADH-quinone oxidoreductase subunit 5

Chain F: 60% 33% • 5%

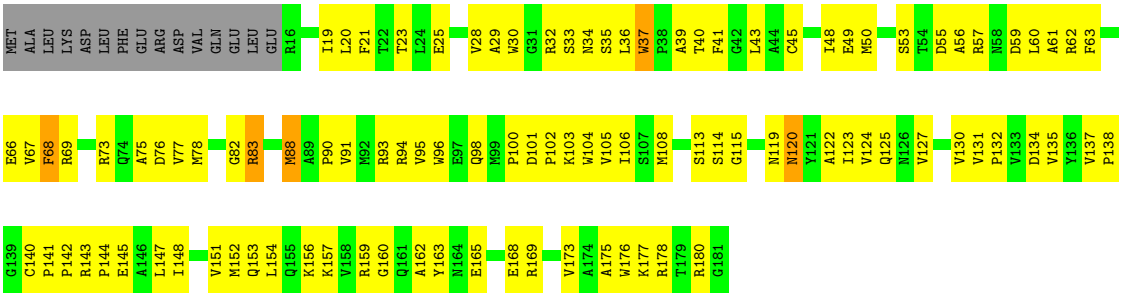
M1 R2 L3 V6 L7 A10 Y15 P16 I17 E18 L22 W26 Y27 V28 R31 E37 M38 A39 H40 Y41 F46 L49 I52 V53 G54 L55 D56 Y57 P61 R64 R67 F68 A69 V70 V71 L74 W80 D84 R87 V90 R91

E96 E97 D98 P99 R100 L101 P102 T103 V104 L107 S110 F113 R116 E117 L121 I124 V125 F126 H129 L132 H144 P145 L146 R147 K148 D149 Y150 P151 T155 F159 R160 R163 P167 F170 R171 A172 T175 D178 G186 G187 S188 R189



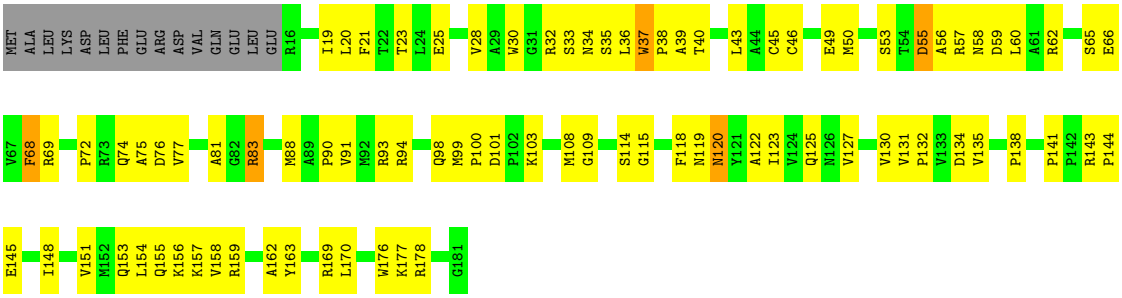
• Molecule 6: NADH-quinone oxidoreductase subunit 6

Chain 6:



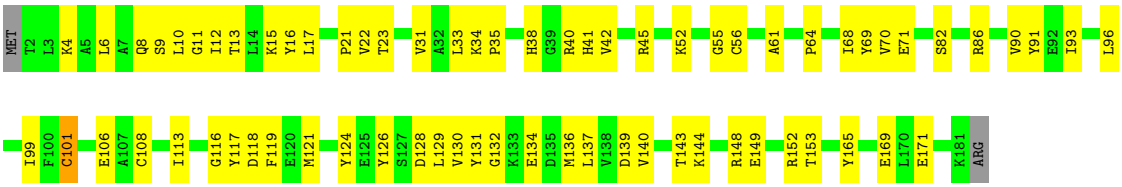
• Molecule 6: NADH-quinone oxidoreductase subunit 6

Chain G:



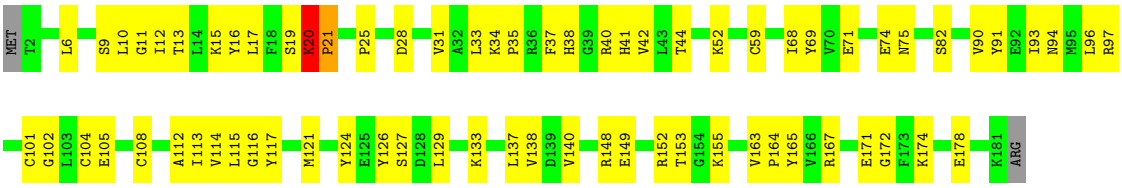
• Molecule 7: NADH-quinone oxidoreductase subunit 9

Chain 9:



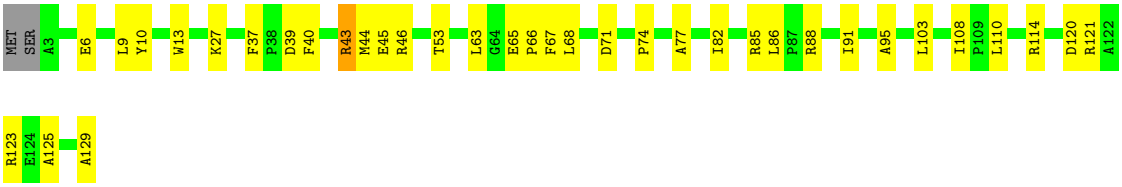
• Molecule 7: NADH-quinone oxidoreductase subunit 9

Chain O:



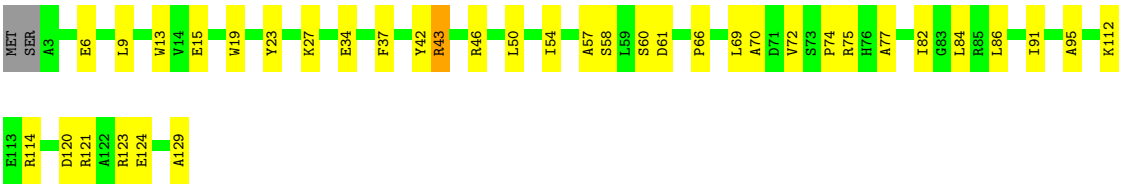
• Molecule 8: NADH-quinone oxidoreductase subunit 15

Chain 7:



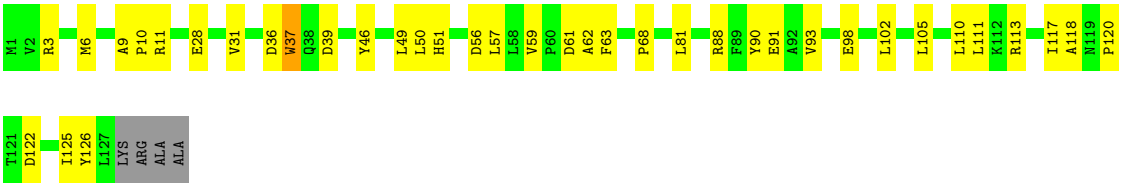
• Molecule 8: NADH-quinone oxidoreductase subunit 15

Chain I:



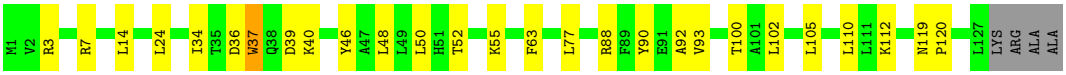
• Molecule 9: Uncharacterized protein

Chain W:



• Molecule 9: Uncharacterized protein

Chain X:

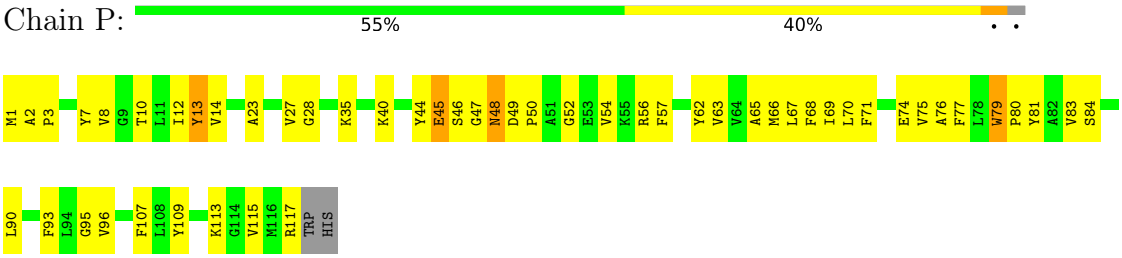


• Molecule 10: NADH-quinone oxidoreductase subunit 7

Chain A:

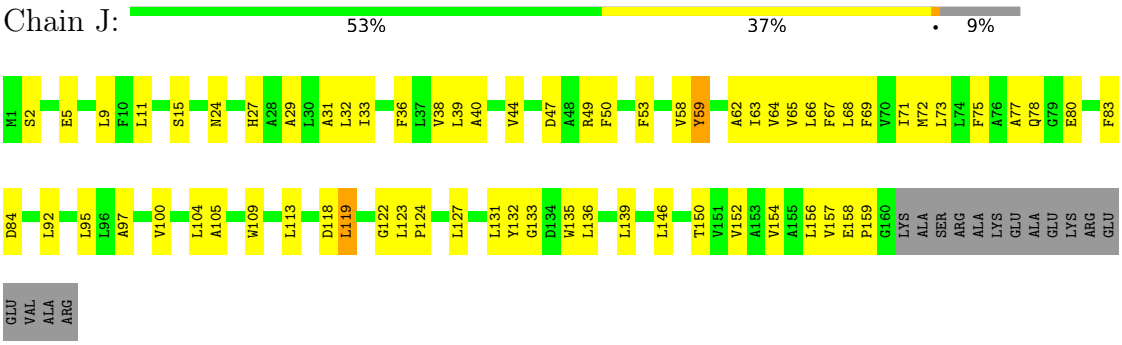
• Molecule 10: NADH-quinone oxidoreductase subunit 7

Chain P:



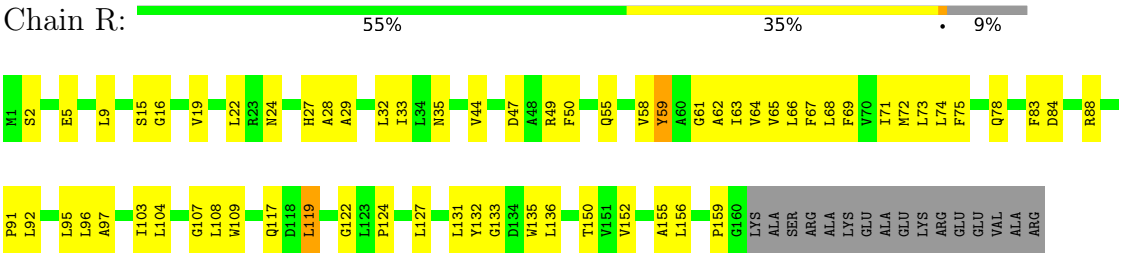
- Molecule 11: NADH-quinone oxidoreductase subunit 10

Chain J:



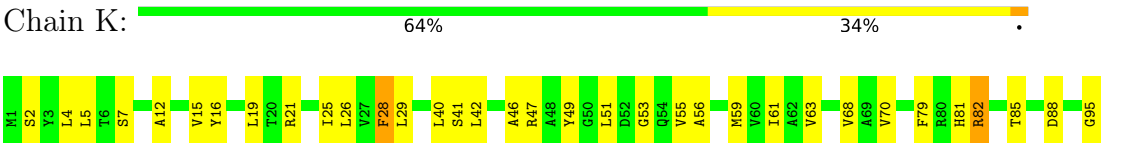
- Molecule 11: NADH-quinone oxidoreductase subunit 10

Chain R:



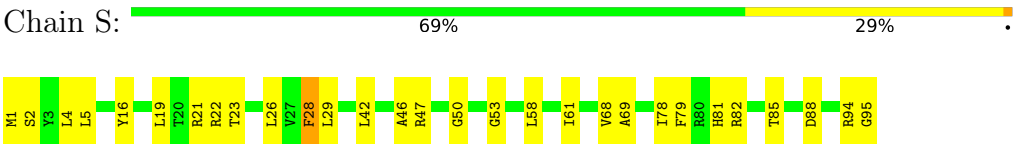
- Molecule 12: NADH-quinone oxidoreductase subunit 11

Chain K:



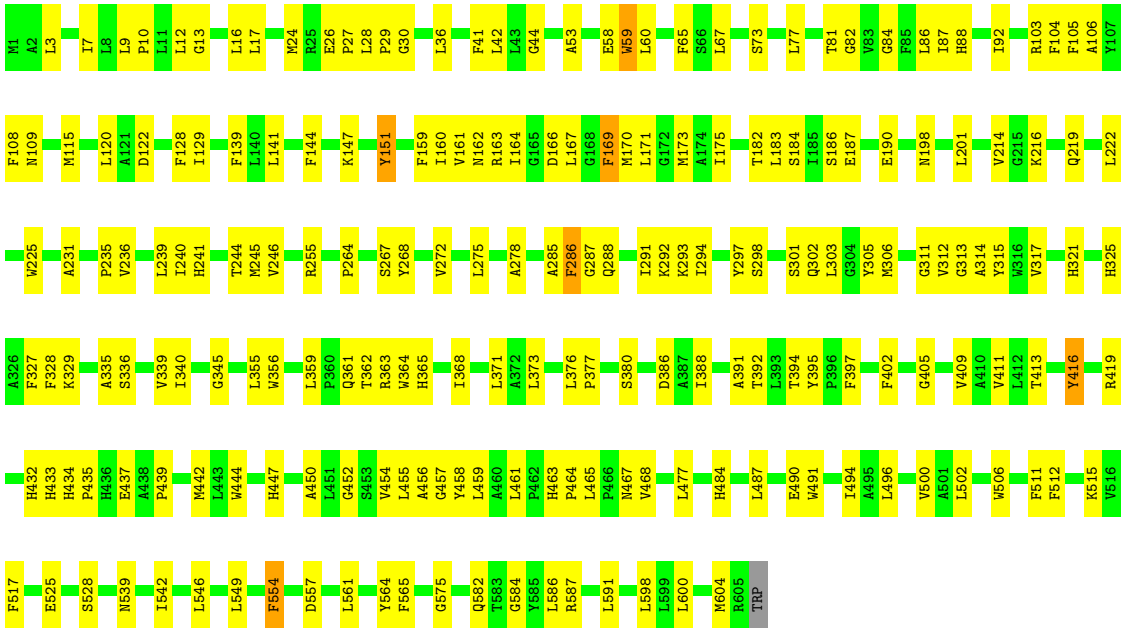
- Molecule 12: NADH-quinone oxidoreductase subunit 11

Chain S:



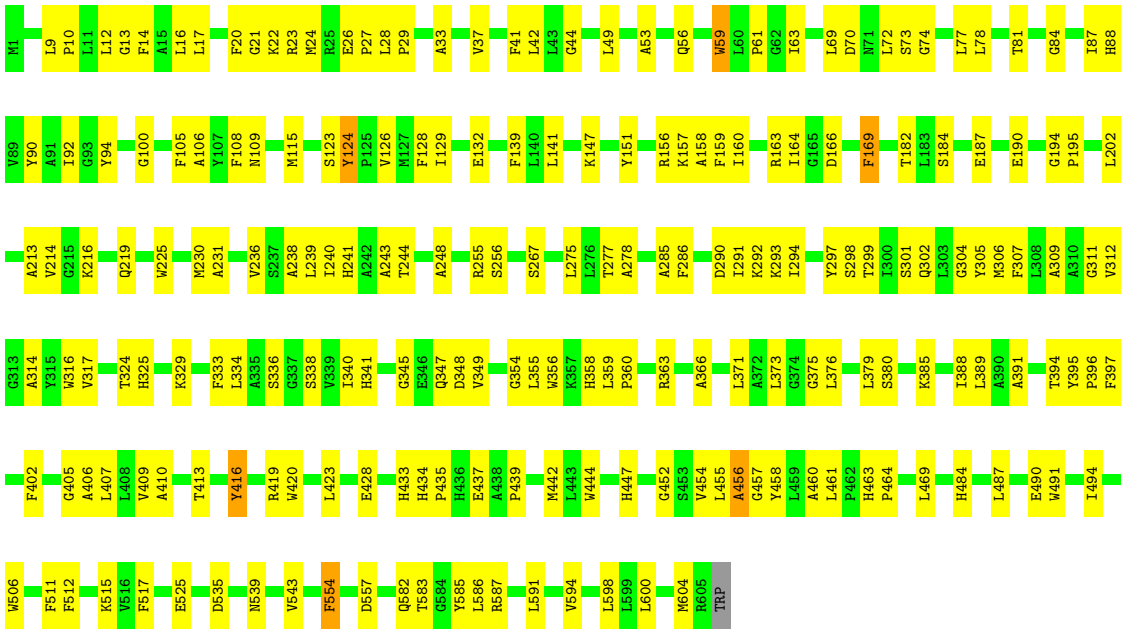
- Molecule 13: NADH-quinone oxidoreductase subunit 12

Chain L:



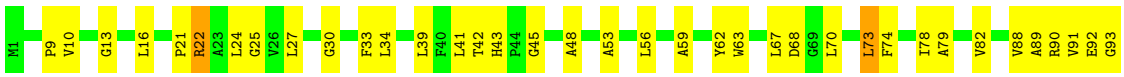
- Molecule 13: NADH-quinone oxidoreductase subunit 12

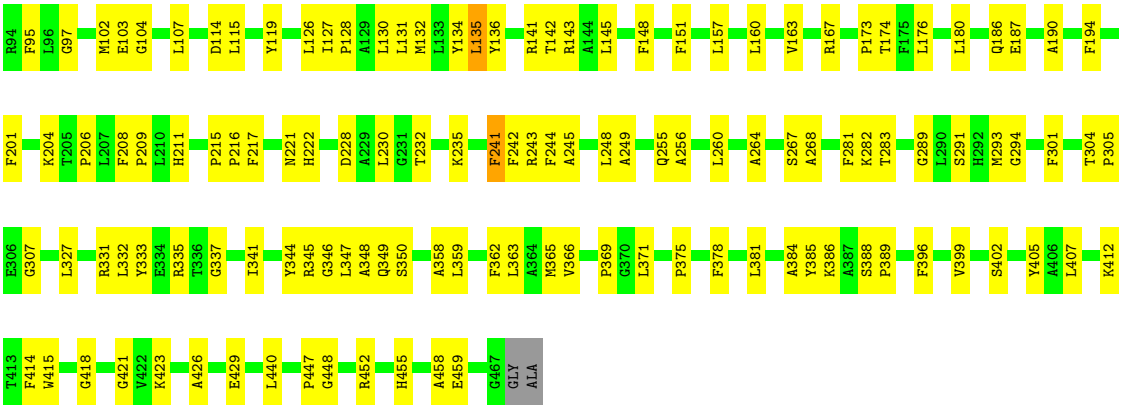
Chain T: 66% 33%



- Molecule 14: NADH-quinone oxidoreductase subunit 13

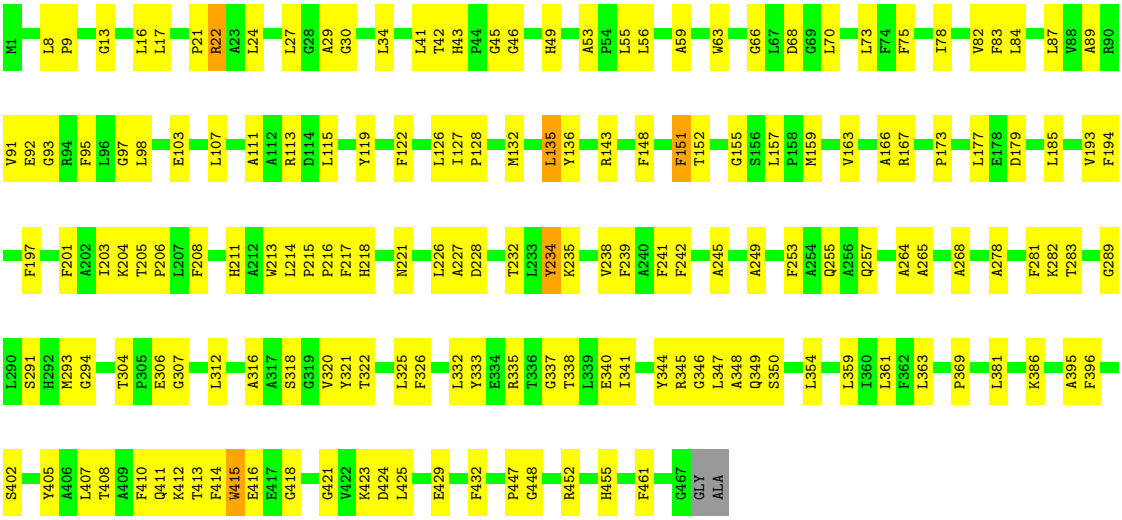
Chain M: 65% 34%





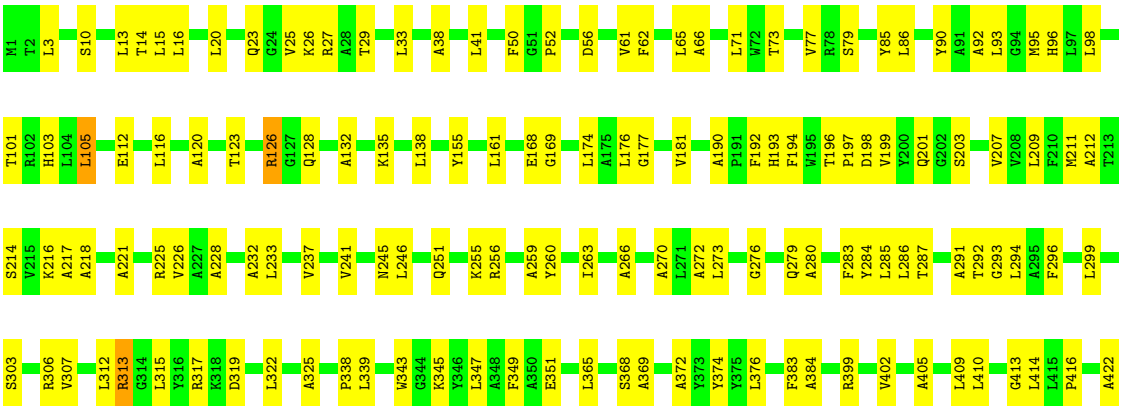
- Molecule 14: NADH-quinone oxidoreductase subunit 13

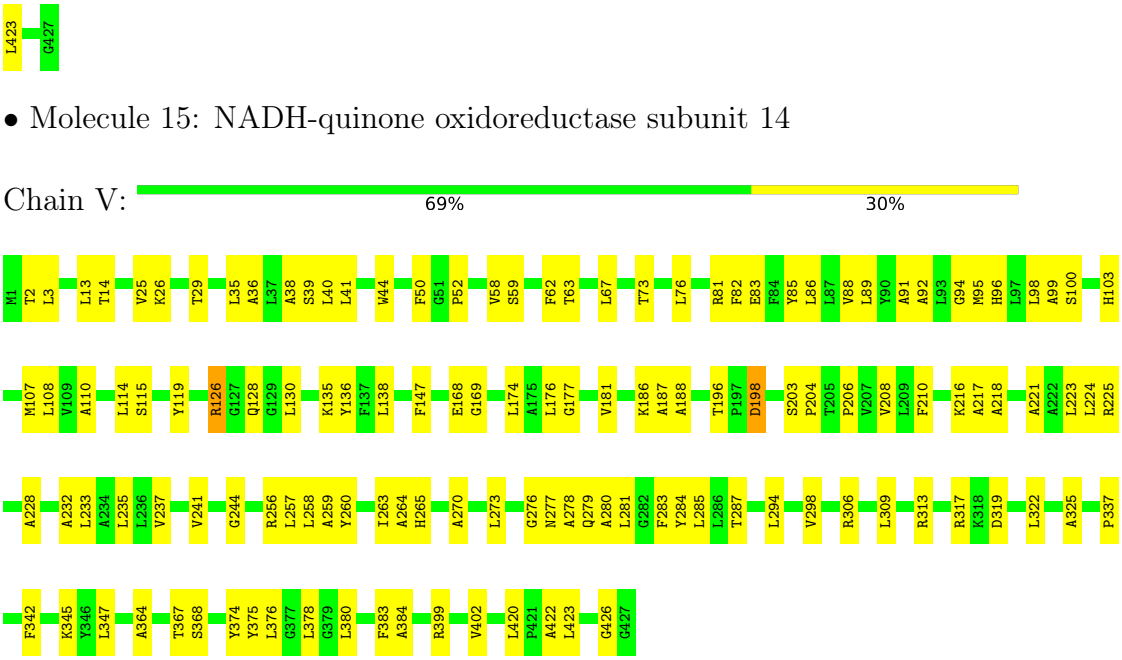
Chain U: 64% 35%

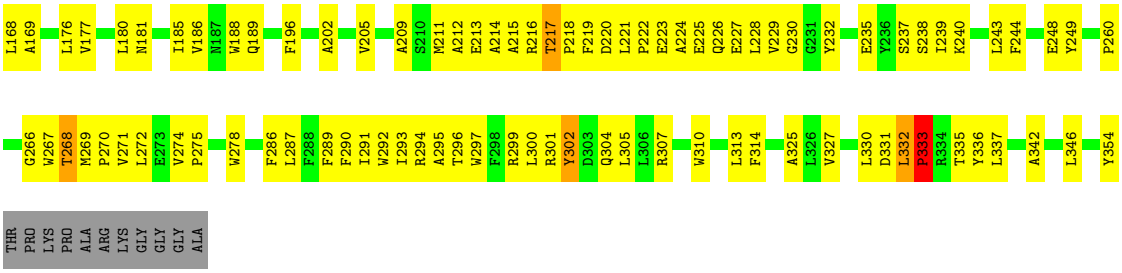


- Molecule 15: NADH-quinone oxidoreductase subunit 14

Chain N: 67% 32%




L423 G427
• Molecule 15: NADH-quinone oxidoreductase subunit 14
Chain V:
69%
30%
M1 T2 L3 L13 T14 V25 K26 T29 L35 A36 L37 A38 S39 L40 L41 W44 F50 G51 P52 V58 S59 F62 T63 L67 T73 L76 R81 F82 E83 F84 Y85 L86 L87 V88 L89 Y90 A91 A92 L93 G94 M95 H96 L97 L98 A99 S100 H103
M107 L108 V109 A110 L114 S115 Y119 R126 G127 Q128 G129 L130 K135 Y136 F137 L138 F147 E168 G169 L174 A175 L176 G177 V181 K186 A187 A188 T196 P197 D198 S203 P204 T205 P206 V207 V208 L209 F210 K216 A217 A218 A221 A222 L223 L224 R225
A228 A232 L233 A234 L235 L236 V237 V241 G244 R256 L257 L258 A259 Y260 I263 A264 H265 A270 L273 G276 N277 A278 Q279 A280 L281 G282 F283 Y284 L285 L286 T287 L294 V298 R306 L309 R313 R317 K318 D319 L322 A325 P337
F342 K345 Y346 L347 A364 T367 S368 Y374 Y375 L376 G377 L378 G379 L380 F383 A384 R399 V402 L420 P421 A422 L423 G426 G427
• Molecule 16: NADH-quinone oxidoreductase subunit 8
Chain H:
50%
43%
MET T2 Y5 P6 P9 Y10 W11 K16 F28 A29 T32 L33 R36 R37 L38 L39 A40 R41 F42 Q43 V44 R45 M46 G47 P48 N49 R50 V51 G52 P53 F54 G55 P59 L60 I64 K65 S66 I67 F68 K69 E70 D71 I72 P86 V90 L95 A96 F97 G98
L99 G103 Q112 P113 W114 V115 I116 N117 L118 D119 L120 G121 I122 L123 A127 V128 L131 A132 V133 Y134 G135 I136 F137 L138 S139 S143 K146 Y147 S148 L149 L150 G151 S152 L153 R154 S155 S156 A157 S158 L159 I160 S161 Y162 E163 L164 A169 L180 N181 D184 I185
Q189 K190 G193 W194 L195 F196 L197 Y198 P201 A202 F203 L204 V205 Y206 E213 A214 A215 R216 T217 P218 F219 D220 L221 P222 E223 A224 E225 Q226 E227 L228 V229 G230 G231 Y232 H233 T234 E235 Y236 S237 S238 L243 F244 A247 E248 Y249 A255 S256 A257 L258 I259 P260 G265 G266
W267 T268 M269 P270 V274 P275 W278 K282 F286 L287 F290 I291 W292 I293 R294 A295 T296 W297 F298 R299 L300 R301 Y302 L305 L306 R307 F308 G309 W310 G311 F312 L313 F314 A317 L326 V327 L330 D331 L332 P333 Y336 L337 S341 A342 F345 L346 L349
Y354 THR PRO LYS PRO ALA ARG LYS GLY GLY GLY GLY ALA
• Molecule 16: NADH-quinone oxidoreductase subunit 8
Chain Q:
50%
43%
MET T2 P6 M12 L15 K16 A17 V21 F28 A29 T32 E35 R36 R37 L38 L39 A40 R41 F42 Q43 V44 R45 M46 G47 P48 N49 R50 V51 G52 P53 F54 G55 Q58 D62 K65 S66 K69 E70 D71 I72 V73 V74 V83 P86 V90 V91
L94 L95 G98 L99 S107 F108 Y111 Q112 P113 W114 V115 I116 N117 L118 D119 L120 G121 I122 L123 Y124 L125 F126 A127 L131 A132 Y133 Y134 G135 I136 F137 W141 A142 S143 K146 Y147 S148 L149 L150 L153 R154 S155 S156 L159 I160 S161 Y162 E163 L164 G165 L166 G167


L168
A169
L176
V177
L180
N181
I185
V186
N187
W188
Q189
F196
A202
V205
A209
S210
M211
A212
E213
A214
A215
R216
T217
P218
F219
D220
L221
P222
E223
A224
E225
Q226
E227
L228
V229
G230
G231
Y232
E235
Y236
S237
S238
I239
K240
L243
F244
E248
Y249
P260
G266
W267
T268
M269
P270
V271
L272
E273
V274
P275
W278
F286
L287
F288
F289
F290
I291
W292
I293
R294
A295
T296
W297
F298
R299
L300
R301
Y302
D303
Q304
L305
L306
R307
W310
L313
F314
A325
L326
V327
L330
D331
L332
P333
R334
T335
Y336
L337
A342
L346
Y354
THR
PRO
LYS
PRO
ALA
ARG
LYS
GLY
GLY
GLY
ALA

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	95.98Å 340.50Å 264.27Å 90.00° 100.44° 90.00°	Depositor
Resolution (Å)	49.71 – 3.40	Depositor
% Data completeness (in resolution range)	84.1 (49.71-3.40)	Depositor
R_{merge}	0.23	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.40 (at 3.40Å)	Xtriage
Refinement program	PHENIX (dev_3026: ???)	Depositor
R, R_{free}	0.213 , 0.234	Depositor
Wilson B-factor (Å^2)	62.4	Xtriage
Anisotropy	0.027	Xtriage
L-test for twinning[2]	$< \|L\| > = 0.34$, $< L^2 > = 0.17$	Xtriage
Estimated twinning fraction	0.379 for h,-k,-h-l	Xtriage
Reported twinning fraction	0.490 for -H,-K,H+L	Depositor
Outliers	0 of 191608 reflections	Xtriage
Total number of atoms	74144	wwPDB-VP
Average B, all atoms (Å^2)	63.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.17% 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, HQW

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	0.36	0/3506	0.54	0/4745
1	B	0.29	0/3506	0.49	0/4745
2	2	0.33	0/1439	0.50	0/1953
2	C	0.29	0/1439	0.47	0/1953
3	3	0.43	0/6035	0.66	0/8185
3	D	0.41	0/6035	0.62	1/8185 (0.0%)
4	4	0.39	0/3150	0.60	1/4284 (0.0%)
4	E	0.32	0/3150	0.52	0/4284
5	5	0.40	0/1656	0.60	1/2246 (0.0%)
5	F	0.36	0/1656	0.57	0/2246
6	6	0.46	0/1319	0.66	0/1786
6	G	0.40	0/1319	0.63	1/1786 (0.1%)
7	9	0.51	1/1423 (0.1%)	0.64	0/1933
7	O	0.38	0/1423	0.71	1/1933 (0.1%)
8	7	0.34	0/1059	0.56	1/1429 (0.1%)
8	I	0.31	0/1059	0.53	0/1429
9	W	0.41	0/985	0.68	1/1335 (0.1%)
9	X	0.38	0/985	0.57	0/1335
10	A	0.34	0/940	0.53	0/1280
10	P	0.33	0/940	0.53	0/1280
11	J	0.33	0/1206	0.54	0/1649
11	R	0.29	0/1206	0.49	0/1649
12	K	0.31	0/710	0.51	0/962
12	S	0.30	0/710	0.50	0/962
13	L	0.31	0/4741	0.49	0/6460
13	T	0.28	0/4741	0.46	0/6460
14	M	0.33	0/3591	0.53	0/4896
14	U	0.28	0/3591	0.47	0/4896
15	N	0.34	0/3238	0.50	0/4434
15	V	0.31	0/3238	0.47	0/4434
16	H	0.33	0/2935	0.55	0/4014
16	Q	0.33	0/2935	0.57	1/4014 (0.0%)

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#|Z| >5	RMSZ	#|Z| >5
All	All	0.35	1/75866 (0.0%)	0.55	8/103182 (0.0%)

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
10	A	0	1
10	P	0	1
13	T	0	2
16	H	0	2
16	Q	0	3
All	All	0	10

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	9	101	CYS	CB-SG	-5.81	1.72	1.81

All (8) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
7	O	20	LYS	C-N-CD	-16.21	84.94	120.60
4	4	133	LEU	CA-CB-CG	6.46	130.16	115.30
6	G	169	ARG	C-N-CA	-6.21	106.17	121.70
5	5	189	ARG	NE-CZ-NH1	5.99	123.29	120.30
16	Q	332	LEU	CA-CB-CG	5.45	127.83	115.30
3	D	369	LEU	CA-CB-CG	5.21	127.28	115.30
9	W	105	LEU	CA-CB-CG	5.18	127.22	115.30
8	7	68	LEU	CA-CB-CG	5.11	127.05	115.30

There are no chirality outliers.

All (10) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
7	9	21	PRO	Peptide
10	A	45	GLU	Peptide
16	H	217	THR	Peptide
16	H	266	GLY	Peptide

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Mol	Chain	Res	Type	Group
10	P	45	GLU	Peptide
16	Q	217	THR	Peptide
16	Q	266	GLY	Peptide
16	Q	333	PRO	Peptide
13	T	434	HIS	Peptide
13	T	456	ALA	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	3389	122	0
1	B	3417	0	3389	155	0
2	2	1406	0	1373	63	0
2	C	1406	0	1373	58	0
3	3	5895	0	5931	235	0
3	D	5895	0	5930	196	0
4	4	3067	0	3049	166	0
4	E	3067	0	3049	166	0
5	5	1607	0	1574	81	0
5	F	1607	0	1574	65	0
6	6	1289	0	1299	104	0
6	G	1289	0	1298	99	0
7	9	1388	0	1383	70	0
7	O	1388	0	1383	65	0
8	7	1031	0	1029	35	0
8	I	1031	0	1029	30	0
9	W	967	0	1010	32	0
9	X	967	0	1010	20	0
10	A	910	0	939	59	0
10	P	910	0	939	56	0
11	J	1183	0	1286	55	0
11	R	1183	0	1286	61	0
12	K	703	0	747	34	0
12	S	703	0	747	29	0
13	L	4604	0	4734	170	0
13	T	4604	0	4734	169	0
14	M	3489	0	3606	127	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
14	U	3489	0	3606	125	0
15	N	3154	0	3343	109	0
15	V	3154	0	3343	104	0
16	H	2838	0	2903	173	0
16	Q	2838	0	2903	179	0
17	1	8	0	0	2	0
17	3	24	0	0	1	0
17	6	8	0	0	1	0
17	9	16	0	0	2	0
17	B	8	0	0	3	0
17	D	24	0	0	2	0
17	G	8	0	0	1	0
17	O	16	0	0	2	0
18	1	31	0	19	1	0
18	B	31	0	19	2	0
19	2	4	0	0	1	0
19	3	4	0	0	2	0
19	C	4	0	0	2	0
19	D	4	0	0	2	0
20	4	29	0	0	0	0
20	E	29	0	0	0	0
All	All	74144	0	75226	2779	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 19.

All (2779) 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)
9:W:102:LEU:O	9:W:110:LEU:HD13	1.16	1.26
3:D:283:PRO:HG3	3:D:425:ARG:HH21	1.00	1.13
7:O:20:LYS:N	7:O:21:PRO:HD3	1.64	1.08
3:D:283:PRO:CG	3:D:425:ARG:HH21	1.68	1.04
6:6:56:ALA:HB1	16:H:44:VAL:CG1	1.87	1.02
2:2:3:PHE:HB2	2:2:45:ARG:NH1	1.75	1.01
6:6:144:PRO:O	6:6:148:ILE:HD12	1.59	1.01
3:D:283:PRO:HG3	3:D:425:ARG:NH2	1.74	1.00
7:O:20:LYS:N	7:O:21:PRO:CD	2.24	1.00
6:G:56:ALA:CB	16:Q:44:VAL:CG1	2.38	1.00
3:3:34:CYS:N	3:3:45:CYS:SG	2.36	0.99
9:W:102:LEU:HG	9:W:110:LEU:HD12	1.40	0.98

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:W:102:LEU:O	9:W:110:LEU:CD1	2.12	0.97
16:Q:37:ARG:HH11	16:Q:41:ARG:HH22	1.12	0.96
16:Q:332:LEU:HB2	16:Q:333:PRO:HD3	1.47	0.95
6:G:56:ALA:HB1	16:Q:44:VAL:CG1	1.95	0.94
2:2:49:ILE:O	2:2:53:VAL:HG12	1.67	0.94
4:4:318:GLU:HB2	8:7:39:ASP:HA	1.49	0.93
5:F:38:MET:CE	5:F:104:VAL:HG11	1.99	0.92
6:6:56:ALA:CB	16:H:44:VAL:CG1	2.47	0.92
3:3:286:ASN:ND2	3:3:289:TRP:O	2.02	0.91
16:H:332:LEU:HB2	16:H:333:PRO:HD3	1.52	0.90
5:F:38:MET:HE3	5:F:104:VAL:HG11	1.51	0.90
3:D:283:PRO:CG	3:D:425:ARG:NH2	2.31	0.90
7:O:172:GLY:O	7:O:174:LYS:NZ	2.05	0.90
13:L:17:LEU:HB2	13:L:106:ALA:HB2	1.55	0.89
16:H:16:LYS:NZ	16:H:114:TRP:O	2.06	0.89
6:G:114:SER:OG	7:O:96:LEU:O	1.91	0.89
13:L:104:PHE:CE2	13:L:108:PHE:CE2	2.61	0.88
16:Q:274:VAL:HG12	16:Q:278:TRP:CD1	2.09	0.88
3:3:34:CYS:HG	19:3:804:FES:FE1	0.58	0.88
1:B:366:PHE:CE2	1:B:390:LEU:HD11	2.08	0.88
6:G:120:ASN:HD22	6:G:122:ALA:H	1.21	0.87
3:D:584:VAL:HG12	3:D:600:VAL:HB	1.55	0.87
6:6:56:ALA:CB	16:H:44:VAL:HG12	2.04	0.86
6:6:120:ASN:HD22	6:6:122:ALA:H	1.22	0.86
13:L:278:ALA:HA	13:L:301:SER:HA	1.58	0.86
14:U:22:ARG:NH1	14:U:92:GLU:OE1	2.09	0.85
5:5:31:ARG:HH21	5:5:100:ARG:HB2	1.38	0.85
6:6:160:GLY:O	6:6:169:ARG:NH1	2.10	0.85
16:Q:215:ALA:O	16:Q:294:ARG:NH1	2.09	0.85
13:T:557:ASP:OD1	14:U:211:HIS:NE2	2.10	0.84
14:U:21:PRO:HD2	14:U:24:LEU:HG	1.56	0.84
7:O:59:CYS:SG	7:O:91:TYR:OH	2.33	0.84
16:H:219:PHE:HB3	16:H:299:ARG:HG2	1.59	0.83
7:9:96:LEU:HD21	7:9:129:LEU:HD13	1.61	0.83
13:L:557:ASP:OD1	14:M:211:HIS:NE2	2.12	0.82
6:G:56:ALA:HB1	16:Q:44:VAL:HG13	1.61	0.82
3:D:286:ASN:ND2	3:D:289:TRP:O	2.12	0.82
5:5:185:LYS:HB2	5:5:189:ARG:HG3	1.61	0.82
13:L:584:GLY:O	15:N:135:LYS:NZ	2.13	0.82
1:1:273:ARG:O	1:1:277:TYR:HB2	1.80	0.81
2:2:61:MET:HB2	3:3:214:MET:HE3	1.62	0.81

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:1:350:HIS:O	3:3:205:ARG:NH1	2.13	0.81
9:W:102:LEU:HG	9:W:110:LEU:CD1	2.10	0.81
6:G:134:ASP:OD1	6:G:157:LYS:NZ	2.12	0.81
1:B:400:CYS:HG	17:B:501:SF4:FE3	0.92	0.81
4:4:234:LEU:HD21	4:4:238:SER:HB2	1.63	0.81
16:H:274:VAL:HG12	16:H:278:TRP:CD1	2.15	0.80
16:H:154:ARG:NH2	16:H:227:GLU:OE2	2.15	0.80
10:P:14:VAL:HG22	16:Q:95:LEU:HD22	1.62	0.80
6:G:30:TRP:CE3	6:G:34:ASN:ND2	2.50	0.80
6:6:56:ALA:HB1	16:H:44:VAL:HG13	1.64	0.80
1:B:312:SER:HG	1:B:315:HIS:HD1	0.83	0.80
3:3:349:ALA:O	3:3:540:ASN:ND2	2.11	0.79
1:B:366:PHE:CD2	1:B:390:LEU:HD11	2.17	0.79
2:C:110:GLU:HA	8:I:121:ARG:HH12	1.45	0.79
14:M:89:ALA:HB1	14:M:91:VAL:HG22	1.64	0.79
13:T:291:ILE:HD12	13:T:336:SER:HB3	1.63	0.79
10:A:65:ALA:HB3	11:J:66:LEU:HD13	1.65	0.79
15:V:309:LEU:HD22	15:V:378:LEU:HD11	1.63	0.79
16:Q:44:VAL:CG1	16:Q:45:ARG:N	2.45	0.79
16:H:50:ARG:O	16:H:52:GLY:N	2.15	0.79
1:B:359:CYS:HB2	1:B:403:ALA:HB2	1.65	0.79
14:M:217:PHE:O	14:M:221:ASN:ND2	2.15	0.79
1:B:246:SER:HB3	1:B:268:MET:HG2	1.64	0.79
16:Q:219:PHE:HB3	16:Q:299:ARG:HG2	1.65	0.78
1:B:288:GLN:NE2	1:B:335:VAL:O	2.16	0.78
16:Q:50:ARG:O	16:Q:52:GLY:N	2.16	0.78
4:4:314:ARG:HB3	8:7:44:MET:HE1	1.66	0.78
6:6:144:PRO:O	6:6:148:ILE:CD1	2.31	0.78
10:P:117:ARG:HD2	11:R:159:PRO:HD2	1.66	0.78
1:1:196:ARG:NH2	3:3:204:GLU:O	2.17	0.78
1:1:75:LYS:NZ	1:1:218:ILE:O	2.16	0.78
6:G:132:PRO:HG3	6:G:178:ARG:HD2	1.66	0.78
13:T:59:TRP:O	14:U:452:ARG:NH2	2.18	0.77
4:4:205:GLU:OE1	4:4:284:ARG:NH2	2.10	0.77
16:H:274:VAL:HG12	16:H:278:TRP:HD1	1.49	0.77
3:D:115:HIS:HB3	4:E:321:MET:HE3	1.65	0.77
3:D:401:ASP:OD2	3:D:454:TYR:OH	2.03	0.77
1:1:88:TYR:HB2	1:1:216:THR:HG22	1.67	0.77
2:2:110:GLU:HA	8:7:121:ARG:HH12	1.48	0.77
3:3:34:CYS:SG	19:3:804:FES:FE1	1.75	0.77
4:E:200:ARG:NH1	7:O:16:TYR:OH	2.18	0.77

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:1:190:ASN:ND2	1:1:198:ASN:O	2.17	0.77
1:B:90:ILE:HD11	1:B:211:LEU:HD22	1.64	0.77
13:L:458:TYR:HB3	13:L:461:LEU:HD11	1.66	0.77
14:U:228:ASP:OD2	14:U:282:LYS:NZ	2.16	0.77
4:4:30:VAL:HG13	4:4:35:PRO:HD2	1.66	0.76
7:9:55:GLY:O	7:9:86:ARG:NE	2.17	0.76
1:1:14:GLU:OE1	1:1:237:TRP:NE1	2.19	0.76
4:4:125:ARG:NH2	4:4:347:GLU:O	2.18	0.76
10:P:113:LYS:NZ	15:V:83:GLU:OE2	2.19	0.76
13:L:288:GLN:NE2	13:L:528:SER:O	2.19	0.76
3:D:186:ARG:HD3	3:D:229:ILE:HG22	1.67	0.76
6:G:56:ALA:CB	16:Q:44:VAL:HG12	2.16	0.76
10:P:35:LYS:O	10:P:40:LYS:NZ	2.19	0.76
3:D:615:VAL:HG22	3:D:621:VAL:HG12	1.68	0.76
4:E:26:MET:N	4:E:48:SER:HG	1.84	0.76
16:Q:36:ARG:HH12	16:Q:58:GLN:HG2	1.49	0.76
7:9:52:LYS:NZ	8:7:44:MET:O	2.19	0.76
4:E:84:ARG:O	6:G:83:ARG:NH2	2.19	0.76
14:M:22:ARG:NH1	14:M:92:GLU:OE1	2.19	0.76
4:4:373:PRO:O	4:4:377:ASN:ND2	2.19	0.76
8:7:120:ASP:OD1	8:7:123:ARG:NH1	2.19	0.76
3:3:507:LEU:HD22	3:3:511:VAL:HG11	1.66	0.75
3:3:710:GLU:O	3:3:713:ARG:NH1	2.18	0.75
10:A:35:LYS:O	10:A:40:LYS:NZ	2.19	0.75
15:N:279:GLN:HG3	15:N:423:LEU:HB2	1.67	0.75
6:G:34:ASN:O	16:Q:58:GLN:NE2	2.19	0.75
11:J:133:GLY:H	11:J:136:LEU:HB2	1.51	0.75
3:D:412:ARG:NH1	3:D:415:GLU:OE1	2.20	0.75
13:T:582:GLN:NE2	15:V:198:ASP:OD1	2.19	0.75
14:U:122:PHE:O	14:U:234:TYR:OH	2.05	0.75
4:E:392:ASP:OD2	16:Q:301:ARG:NH1	2.18	0.75
2:2:171:LYS:NZ	2:2:178:GLU:O	2.20	0.75
3:3:31:PRO:HB2	3:3:47:MET:HB3	1.68	0.75
13:T:147:LYS:NZ	14:U:349:GLN:OE1	2.20	0.75
6:6:119:ASN:HA	6:6:125:GLN:HE22	1.52	0.75
3:D:7:ASN:ND2	3:D:94:ASP:OD1	2.20	0.75
10:P:57:PHE:HE2	16:Q:149:LEU:HD13	1.52	0.75
16:H:302:TYR:HA	16:H:305:LEU:HB3	1.68	0.74
3:3:21:ASP:OD1	3:3:432:PHE:N	2.21	0.74
3:D:31:PRO:HB2	3:D:47:MET:HB3	1.67	0.74
4:4:47:LEU:HD21	4:4:390:VAL:HG22	1.68	0.74

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:3:154:TYR:HB3	4:4:322:GLU:HB2	1.67	0.74
1:B:190:ASN:ND2	1:B:198:ASN:O	2.19	0.74
1:B:254:ILE:HD11	1:B:330:LEU:HD11	1.69	0.74
13:T:182:THR:HB	13:T:187:GLU:HG3	1.69	0.74
15:V:136:TYR:OH	15:V:186:LYS:NZ	2.20	0.74
4:E:85:MET:HE1	4:E:370:VAL:HG21	1.69	0.74
13:T:84:GLY:O	13:T:88:HIS:ND1	2.18	0.74
16:Q:44:VAL:HG12	16:Q:45:ARG:H	1.52	0.74
3:3:538:ALA:HB3	3:3:541:ALA:HB2	1.69	0.74
15:N:280:ALA:HB1	15:N:347:LEU:HB3	1.70	0.74
13:T:275:LEU:HD11	13:T:405:GLY:HA3	1.68	0.74
4:4:152:GLU:OE2	4:4:204:TYR:OH	2.04	0.74
1:1:372:ALA:O	1:1:376:THR:OG1	2.05	0.73
6:6:114:SER:OG	7:9:96:LEU:O	2.05	0.73
9:W:98:GLU:OE2	9:W:113:ARG:NH1	2.14	0.73
14:U:217:PHE:O	14:U:221:ASN:ND2	2.21	0.73
16:Q:302:TYR:HA	16:Q:305:LEU:HB3	1.68	0.73
3:D:125:GLY:HA2	3:D:245:ARG:HH21	1.53	0.73
2:C:77:LYS:H	2:C:116:LEU:HA	1.53	0.73
5:5:18:GLU:HB2	5:5:26:TRP:HB2	1.69	0.73
4:E:50:GLU:O	4:E:389:GLN:NE2	2.22	0.73
3:3:185:LYS:HB3	3:3:189:ARG:HH11	1.54	0.73
16:H:44:VAL:CG1	16:H:45:ARG:N	2.52	0.73
11:R:2:SER:HA	11:R:5:GLU:HB3	1.68	0.73
15:V:59:SER:HG	15:V:100:SER:HG	1.25	0.73
10:A:109:TYR:OH	10:A:113:LYS:NZ	2.20	0.73
6:6:19:ILE:HG23	6:6:20:LEU:HG	1.68	0.73
13:L:163:ARG:NH2	14:M:366:VAL:O	2.21	0.73
14:M:21:PRO:HD2	14:M:24:LEU:HG	1.69	0.73
4:E:333:GLU:O	4:E:363:SER:OG	2.06	0.73
7:O:96:LEU:HD21	7:O:129:LEU:HD13	1.70	0.73
13:T:305:TYR:OH	13:T:406:ALA:O	2.04	0.73
7:9:41:HIS:HB3	7:9:113:ILE:HD11	1.70	0.72
3:D:621:VAL:HG23	3:D:672:ALA:HA	1.68	0.72
4:E:38:HIS:ND1	4:E:139:ASP:OD2	2.21	0.72
14:U:268:ALA:HA	14:U:291:SER:HA	1.71	0.72
14:U:346:GLY:HA3	14:U:418:GLY:HA2	1.71	0.72
7:O:115:LEU:O	7:O:167:ARG:NH2	2.22	0.72
16:H:158:SER:HA	16:H:306:LEU:HD21	1.70	0.72
3:3:185:LYS:HB3	3:3:189:ARG:NH1	2.03	0.72
16:H:117:ASN:O	16:H:181:ASN:ND2	2.21	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:287:ILE:HA	1:B:332:PRO:HA	1.72	0.72
8:I:54:ILE:HD11	8:I:57:ALA:HB2	1.70	0.72
16:H:29:ALA:HB1	16:H:59:PRO:HB3	1.72	0.72
3:D:512:LEU:HD21	3:D:534:ALA:HB1	1.72	0.72
14:M:114:ASP:HB3	14:M:176:LEU:HD23	1.72	0.72
2:C:71:GLN:NE2	2:C:120:GLN:OE1	2.22	0.72
16:H:146:LYS:HA	16:H:149:LEU:HB2	1.72	0.71
13:T:158:ALA:HA	13:T:225:TRP:HB2	1.71	0.71
16:Q:146:LYS:HA	16:Q:149:LEU:HB2	1.70	0.71
3:D:129:GLU:O	3:D:133:ARG:HG2	1.89	0.71
5:F:10:ALA:HB1	5:F:15:TYR:HB2	1.71	0.71
4:E:222:GLY:HA3	4:E:275:ARG:HH22	1.54	0.71
16:Q:39:LEU:O	16:Q:43:GLN:HG2	1.90	0.71
16:Q:332:LEU:HB2	16:Q:333:PRO:CD	2.20	0.71
3:D:414:SER:OG	3:D:443:ARG:NH2	2.23	0.71
5:F:55:LEU:HD23	5:F:57:TYR:CZ	2.25	0.71
7:O:68:ILE:HG12	7:O:93:ILE:HG12	1.71	0.71
3:3:576:ALA:O	3:3:580:LYS:NZ	2.22	0.71
1:B:425:ALA:O	1:B:428:LYS:NZ	2.21	0.71
4:E:171:ASN:ND2	4:E:174:ARG:HH22	1.89	0.71
13:T:70:ASP:H	13:T:73:SER:HB2	1.56	0.71
3:3:716:LEU:HD21	3:3:758:LEU:HD23	1.73	0.71
3:D:352:GLU:OE2	3:D:661:GLN:NE2	2.23	0.71
4:E:341:GLU:OE2	5:F:57:TYR:OH	2.09	0.71
8:I:23:TYR:HH	8:I:123:ARG:HH11	1.39	0.71
16:Q:225:GLU:HB3	16:Q:226:GLN:HG2	1.72	0.71
2:2:61:MET:SD	3:3:214:MET:HE2	2.31	0.71
3:3:300:TRP:CD1	3:3:703:GLN:HA	2.26	0.71
4:4:144:THR:HG22	4:4:148:TYR:HE1	1.56	0.71
3:D:383:PRO:HD3	3:D:679:ARG:HH21	1.56	0.71
4:4:341:GLU:OE1	4:4:356:TYR:OH	2.08	0.70
1:B:88:TYR:HB2	1:B:216:THR:HG22	1.71	0.70
1:B:92:ASN:ND2	18:B:502:FMN:O3'	2.24	0.70
6:6:145:GLU:HG2	7:9:31:VAL:HG21	1.72	0.70
4:E:261:THR:H	4:E:292:GLN:HE22	1.35	0.70
13:L:104:PHE:HE2	13:L:108:PHE:CE2	2.09	0.70
3:D:387:LEU:HD13	3:D:412:ARG:HG3	1.74	0.70
13:T:373:LEU:HD21	13:T:416:TYR:HE1	1.55	0.70
16:Q:291:ILE:HA	16:Q:294:ARG:HG3	1.73	0.70
6:G:145:GLU:HG2	7:O:31:VAL:HG21	1.72	0.70
16:H:147:TYR:CD1	16:H:229:VAL:HG22	2.26	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:1:365:GLY:O	1:1:369:ASN:ND2	2.25	0.70
11:J:68:LEU:HD23	11:J:71:ILE:HD11	1.74	0.70
3:3:701:ALA:N	3:3:763:LEU:O	2.25	0.69
9:W:91:GLU:OE1	9:W:126:TYR:OH	2.10	0.69
11:J:50:PHE:HB2	11:J:124:PRO:HD3	1.74	0.69
2:C:132:PRO:HG2	2:C:145:VAL:HB	1.73	0.69
3:D:113:LEU:O	3:D:161:ARG:NH1	2.25	0.69
7:O:19:SER:C	7:O:21:PRO:HD2	2.12	0.69
15:V:2:THR:HG23	15:V:36:ALA:HB1	1.73	0.69
11:R:92:LEU:HD23	13:T:591:LEU:HD23	1.74	0.69
1:1:14:GLU:HB2	1:1:237:TRP:HZ2	1.57	0.69
10:A:69:ILE:HG22	11:J:62:ALA:HB1	1.74	0.69
4:E:30:VAL:HG13	4:E:35:PRO:HD2	1.74	0.69
6:G:19:ILE:HG23	6:G:20:LEU:HG	1.73	0.69
16:Q:117:ASN:O	16:Q:181:ASN:ND2	2.26	0.69
16:Q:205:VAL:HG12	16:Q:313:LEU:HD22	1.73	0.69
13:L:575:GLY:HA2	15:N:246:LEU:HB3	1.75	0.69
3:D:166:LYS:NZ	3:D:177:ASP:OD2	2.23	0.69
4:E:148:TYR:O	4:E:151:ARG:HB3	1.93	0.69
4:E:265:PRO:HB2	4:E:278:VAL:HG13	1.74	0.69
7:O:28:ASP:OD2	16:Q:50:ARG:NH1	2.25	0.69
10:P:65:ALA:HB3	11:R:66:LEU:HD13	1.73	0.69
4:4:105:LEU:HD13	4:4:309:ILE:HD13	1.74	0.69
14:M:68:ASP:OD2	14:M:243:ARG:NH2	2.26	0.69
14:U:151:PHE:HD2	14:U:213:TRP:HB3	1.57	0.69
1:1:246:SER:HB3	1:1:268:MET:HG2	1.73	0.69
6:6:37:TRP:HE1	6:6:67:VAL:HB	1.58	0.69
1:B:400:CYS:SG	17:B:501:SF4:FE3	1.85	0.69
1:B:433:ARG:HH12	2:C:89:LYS:HE2	1.57	0.69
4:E:147:PHE:CZ	16:Q:43:GLN:NE2	2.61	0.69
7:O:127:SER:OG	9:X:39:ASP:OD2	2.04	0.69
4:4:136:GLY:HA2	4:4:398:ALA:HB1	1.74	0.69
11:R:83:PHE:O	12:S:22:ARG:NH1	2.26	0.69
16:Q:52:GLY:HA3	16:Q:55:GLY:H	1.57	0.69
3:3:115:HIS:HB3	4:4:321:MET:HE3	1.75	0.68
15:N:196:THR:HG22	15:N:259:ALA:HB1	1.75	0.68
3:D:271:SER:HG	7:O:69:TYR:HH	1.34	0.68
1:B:18:TYR:OH	1:B:102:LYS:O	2.10	0.68
4:E:272:VAL:HG13	4:E:399:SER:HB3	1.75	0.68
13:T:278:ALA:HB1	13:T:409:VAL:HG11	1.74	0.68
14:U:208:PHE:O	14:U:211:HIS:ND1	2.27	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:W:11:ARG:NH1	9:W:68:PRO:O	2.27	0.68
12:K:2:SER:HA	12:K:5:LEU:HD12	1.75	0.68
11:R:68:LEU:HD23	11:R:71:ILE:HD11	1.74	0.68
13:T:20:PHE:HB3	13:T:23:ARG:HE	1.59	0.68
13:T:156:ARG:NH1	14:U:408:THR:OG1	2.26	0.68
13:T:340:ILE:O	13:T:345:GLY:N	2.19	0.68
4:E:259:THR:O	4:E:296:ARG:NH2	2.27	0.68
15:V:228:ALA:HB1	15:V:233:LEU:CD1	2.24	0.68
15:V:294:LEU:HD11	15:V:325:ALA:HB1	1.73	0.68
15:N:128:GLN:OE1	15:N:306:ARG:NH2	2.27	0.68
1:B:438:ARG:OXT	2:C:146:THR:OG1	2.12	0.68
14:U:115:LEU:HD13	14:U:163:VAL:HG23	1.74	0.68
1:1:79:MET:SD	1:1:217:THR:OG1	2.52	0.68
1:1:361:GLU:OE2	3:3:162:ARG:NH2	2.26	0.68
11:J:15:SER:OG	11:J:31:ALA:O	2.12	0.68
10:A:65:ALA:O	10:A:69:ILE:HG23	1.94	0.68
6:G:21:PHE:HD1	6:G:23:THR:H	1.39	0.68
16:Q:143:SER:HB2	16:Q:235:GLU:HG3	1.74	0.68
4:4:341:GLU:OE1	5:5:91:ARG:NH2	2.27	0.68
15:V:317:ARG:NH1	15:V:384:ALA:O	2.26	0.68
3:3:384:PRO:HG3	3:3:542:ARG:NH1	2.08	0.68
4:4:338:PRO:HG2	5:5:193:ARG:HH11	1.58	0.68
8:I:37:PHE:HE1	8:I:74:PRO:HA	1.59	0.68
3:3:605:PRO:HB2	3:3:609:GLU:HG3	1.76	0.67
13:L:105:PHE:O	13:L:109:ASN:ND2	2.25	0.67
16:H:44:VAL:O	16:H:45:ARG:O	2.13	0.67
14:M:208:PHE:O	14:M:211:HIS:ND1	2.28	0.67
1:B:253:GLN:HG2	1:B:327:GLY:HA2	1.76	0.67
8:I:23:TYR:OH	8:I:123:ARG:NH1	2.23	0.67
13:T:487:LEU:HA	13:T:490:GLU:HG2	1.75	0.67
14:U:89:ALA:HB1	14:U:91:VAL:HG22	1.76	0.67
13:L:371:LEU:HD22	13:L:376:LEU:HD13	1.77	0.67
16:H:265:GLY:O	16:H:282:LYS:NZ	2.20	0.67
3:3:383:PRO:HB3	3:3:679:ARG:HH21	1.59	0.67
7:O:171:GLU:OE2	8:I:43:ARG:NH2	2.28	0.67
1:1:338:VAL:O	1:1:342:TRP:HB2	1.95	0.67
6:6:91:VAL:HG22	10:A:46:SER:HB3	1.77	0.67
4:E:148:TYR:OH	16:Q:42:PHE:O	2.12	0.67
16:Q:327:VAL:O	16:Q:331:ASP:N	2.28	0.67
4:4:409:ARG:NH2	5:5:117:GLU:OE2	2.28	0.67
16:H:159:LEU:O	16:H:163:GLU:HB2	1.94	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:G:30:TRP:CZ3	6:G:34:ASN:ND2	2.63	0.67
15:V:280:ALA:HB1	15:V:347:LEU:HB3	1.76	0.67
5:5:101:LEU:O	5:5:127:GLU:N	2.23	0.67
4:E:80:THR:O	4:E:84:ARG:NH1	2.28	0.67
3:3:305:ARG:NH1	3:3:609:GLU:OE1	2.27	0.67
3:3:208:HIS:O	8:7:85:ARG:NH2	2.24	0.67
3:3:557:SER:OG	3:3:559:ASP:OD1	2.11	0.67
1:B:63:ARG:NE	1:B:69:GLY:O	2.28	0.67
4:E:333:GLU:OE2	4:E:336:HIS:NE2	2.27	0.67
3:3:494:LYS:O	3:3:498:GLU:HG2	1.94	0.67
1:B:350:HIS:O	3:D:205:ARG:NH1	2.28	0.67
15:V:2:THR:OG1	15:V:39:SER:OG	2.12	0.67
4:4:218:ALA:HA	4:4:221:VAL:HG22	1.77	0.66
16:H:292:TRP:O	16:H:296:THR:OG1	2.07	0.66
4:4:144:THR:OG1	16:H:295:ALA:O	2.14	0.66
13:L:84:GLY:O	13:L:88:HIS:ND1	2.23	0.66
3:D:40:SER:O	3:D:189:ARG:NE	2.25	0.66
6:G:50:MET:O	6:G:53:SER:OG	2.11	0.66
6:G:56:ALA:CB	16:Q:44:VAL:HG11	2.24	0.66
6:G:93:ARG:NH1	6:G:130:VAL:O	2.28	0.66
11:R:22:LEU:O	12:S:21:ARG:NH2	2.29	0.66
2:2:24:ARG:HA	2:2:53:VAL:CG2	2.25	0.66
3:3:113:LEU:O	3:3:161:ARG:NH1	2.27	0.66
3:3:186:ARG:HD3	3:3:229:ILE:HG22	1.76	0.66
16:Q:211:MET:HG3	16:Q:218:PRO:HD3	1.78	0.66
6:6:53:SER:O	6:6:60:LEU:N	2.24	0.66
6:6:140:CYS:SG	7:9:99:ILE:HG13	2.36	0.66
4:4:265:PRO:HB2	4:4:278:VAL:HG13	1.78	0.66
4:E:171:ASN:OD1	4:E:174:ARG:NH1	2.24	0.66
10:A:6:GLU:OE1	16:H:117:ASN:N	2.25	0.66
6:6:76:ASP:OD1	16:H:65:LYS:NZ	2.28	0.66
10:P:63:VAL:HG11	10:P:115:VAL:HG11	1.77	0.66
13:T:159:PHE:HD2	14:U:407:LEU:HD11	1.60	0.66
16:Q:86:PRO:HG3	16:Q:244:PHE:CE2	2.31	0.66
3:3:149:LEU:O	3:3:149:LEU:HD23	1.95	0.66
4:E:77:GLN:O	4:E:80:THR:OG1	2.12	0.66
16:Q:227:GLU:HG2	16:Q:228:LEU:H	1.60	0.66
6:6:163:TYR:CD1	7:9:152:ARG:HD2	2.31	0.66
1:B:8:GLY:HA2	1:B:270:THR:HG22	1.78	0.66
1:1:437:TRP:HB3	2:2:92:GLY:HA3	1.78	0.66
3:3:34:CYS:HB3	3:3:45:CYS:H	1.60	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:K:7:SER:HB3	12:K:40:LEU:HD23	1.79	0.65
4:E:151:ARG:HH22	4:E:196:VAL:HG21	1.61	0.65
1:1:185:GLU:HB2	1:1:218:ILE:HD13	1.78	0.65
1:1:382:LYS:O	1:1:386:ASN:ND2	2.30	0.65
3:D:722:THR:HG21	3:D:756:GLY:H	1.61	0.65
5:F:149:ASP:O	9:X:112:LYS:NZ	2.22	0.65
14:M:346:GLY:HA3	14:M:418:GLY:HA2	1.77	0.65
15:N:315:LEU:HD21	15:N:322:LEU:HB3	1.78	0.65
4:E:409:ARG:NH2	5:F:117:GLU:OE2	2.30	0.65
16:Q:16:LYS:NZ	16:Q:114:TRP:O	2.25	0.65
1:1:195:LEU:HD23	2:2:24:ARG:HH12	1.61	0.65
3:D:8:ASP:OD2	3:D:28:TYR:OH	2.15	0.65
7:O:75:ASN:ND2	7:O:82:SER:OG	2.28	0.65
7:O:101:CYS:N	17:O:201:SF4:S4	2.69	0.65
1:1:400:CYS:SG	17:1:501:SF4:FE3	1.89	0.65
4:4:333:GLU:OE2	4:4:336:HIS:NE2	2.29	0.65
6:6:178:ARG:NH1	9:W:122:ASP:OD2	2.29	0.65
9:W:59:VAL:HG11	9:W:63:PHE:HE2	1.61	0.65
1:B:366:PHE:CD2	1:B:390:LEU:CD1	2.79	0.65
7:O:13:THR:HG21	16:Q:296:THR:HG23	1.79	0.65
4:4:173:ILE:O	4:4:174:ARG:NH1	2.29	0.65
12:K:19:LEU:HD22	13:L:591:LEU:HD12	1.78	0.65
13:L:30:GLY:HA3	13:L:92:ILE:HG12	1.79	0.65
6:G:37:TRP:HE1	6:G:69:ARG:HG3	1.62	0.65
8:I:23:TYR:HH	8:I:123:ARG:NH1	1.93	0.65
4:4:314:ARG:NH2	8:7:44:MET:SD	2.70	0.65
7:9:35:PRO:O	7:9:117:TYR:OH	2.10	0.65
4:E:103:LYS:NZ	5:F:22:LEU:O	2.27	0.65
4:E:171:ASN:HD21	4:E:174:ARG:HH22	1.44	0.65
7:O:20:LYS:N	7:O:21:PRO:HD2	2.12	0.65
10:P:69:ILE:HG22	11:R:62:ALA:HB1	1.77	0.65
13:T:241:HIS:HB3	13:T:299:THR:HG21	1.77	0.65
16:H:44:VAL:HG12	16:H:45:ARG:H	1.62	0.65
1:B:192:LEU:HD22	1:B:211:LEU:HD21	1.78	0.65
4:E:47:LEU:HD21	4:E:390:VAL:HG22	1.78	0.65
13:L:151:TYR:HB3	13:L:231:ALA:HB1	1.79	0.65
15:N:126:ARG:HD2	15:N:128:GLN:HG2	1.79	0.65
1:B:194:GLY:O	2:C:24:ARG:NH1	2.30	0.65
5:F:38:MET:CE	5:F:104:VAL:CG1	2.75	0.65
16:Q:29:ALA:O	16:Q:32:THR:OG1	2.10	0.65
6:6:105:VAL:N	6:6:134:ASP:OD2	2.27	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:E:27:THR:HA	4:E:46:THR:HA	1.77	0.65
4:E:185:GLU:OE2	7:O:165:TYR:OH	2.13	0.65
1:1:6:LEU:HD11	1:1:240:GLN:HE21	1.62	0.64
2:2:61:MET:SD	3:3:214:MET:CE	2.85	0.64
11:J:119:LEU:HD23	12:K:51:LEU:HD12	1.79	0.64
16:Q:74:VAL:HG21	16:Q:235:GLU:HB3	1.79	0.64
1:1:312:SER:OG	1:1:315:HIS:ND1	2.25	0.64
16:H:29:ALA:O	16:H:32:THR:OG1	2.16	0.64
5:5:126:PHE:H	5:5:132:LEU:HD11	1.63	0.64
8:7:74:PRO:HG2	8:7:77:ALA:HB2	1.79	0.64
13:L:115:MET:HG2	13:L:244:THR:HG22	1.79	0.64
4:E:201:ILE:HA	4:E:204:TYR:HD2	1.61	0.64
13:T:94:TYR:HE1	13:T:341:HIS:HB2	1.63	0.64
4:4:336:HIS:ND1	5:5:189:ARG:O	2.31	0.64
11:J:119:LEU:HD11	12:K:47:ARG:HA	1.78	0.64
15:N:92:ALA:HA	15:N:95:MET:HE2	1.79	0.64
1:B:75:LYS:NZ	1:B:218:ILE:O	2.27	0.64
1:B:437:TRP:HB3	2:C:92:GLY:HA3	1.78	0.64
7:O:20:LYS:H	7:O:21:PRO:HD3	1.58	0.64
16:Q:43:GLN:O	16:Q:45:ARG:N	2.31	0.64
14:U:348:ALA:HB2	14:U:414:PHE:HB3	1.79	0.64
3:3:694:LEU:HB3	3:3:762:ALA:HB2	1.78	0.64
16:H:267:TRP:CG	16:H:268:THR:N	2.63	0.64
1:1:337:MET:O	1:1:341:MET:HG2	1.96	0.64
10:A:67:LEU:HB3	16:H:310:TRP:CZ2	2.32	0.64
16:H:96:ALA:HB2	16:H:128:VAL:HG21	1.80	0.64
16:H:332:LEU:HB2	16:H:333:PRO:CD	2.27	0.64
5:F:151:PRO:HD3	9:X:112:LYS:HE2	1.80	0.64
3:3:51:ARG:HB3	3:3:94:ASP:HB3	1.79	0.64
11:J:69:PHE:O	11:J:73:LEU:HG	1.98	0.64
1:B:366:PHE:HE2	1:B:390:LEU:HD21	1.61	0.64
4:E:169:HIS:NE2	6:G:45:CYS:SG	2.69	0.64
6:G:56:ALA:HB2	16:Q:44:VAL:HG12	1.79	0.64
13:T:458:TYR:HB3	13:T:461:LEU:HD11	1.80	0.64
1:1:393:LEU:HD23	1:1:397:ARG:NH2	2.12	0.64
3:3:31:PRO:HG3	3:3:137:TYR:CD2	2.33	0.64
14:M:115:LEU:HD13	14:M:163:VAL:HG23	1.80	0.64
7:O:41:HIS:HB3	7:O:113:ILE:HD11	1.79	0.64
16:Q:232:TYR:OH	16:Q:248:GLU:OE1	2.13	0.64
4:4:306:ASN:ND2	5:5:192:TYR:OH	2.23	0.64
16:H:37:ARG:NH2	16:H:49:ASN:OD1	2.31	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:199:VAL:HG11	3:D:219:PRO:HD2	1.80	0.64
3:D:546:ALA:O	3:D:667:ARG:NH1	2.31	0.64
5:F:67:ARG:NH1	5:F:96:GLU:OE2	2.31	0.64
4:4:261:THR:H	4:4:292:GLN:HE22	1.46	0.63
10:A:1:MET:O	16:H:2:THR:N	2.31	0.63
13:L:159:PHE:HD2	14:M:407:LEU:HD11	1.62	0.63
16:H:291:ILE:HA	16:H:294:ARG:HG3	1.79	0.63
3:D:175:ILE:HG22	3:D:236:LEU:HB2	1.78	0.63
13:T:586:LEU:HD13	15:V:138:LEU:HD12	1.81	0.63
4:4:80:THR:O	4:4:84:ARG:NH1	2.31	0.63
3:D:364:LEU:HB2	3:D:650:VAL:HG21	1.79	0.63
16:Q:274:VAL:HG12	16:Q:278:TRP:HD1	1.60	0.63
3:3:405:GLU:OE1	3:3:509:ALA:N	2.27	0.63
3:3:621:VAL:HG23	3:3:672:ALA:HA	1.79	0.63
5:5:66:GLU:HB2	5:5:93:TYR:HB3	1.79	0.63
1:B:30:ASP:OD2	1:B:155:ARG:NH2	2.24	0.63
1:B:131:TYR:OH	2:C:17:LYS:O	2.12	0.63
2:C:110:GLU:OE2	8:I:114:ARG:NE	2.31	0.63
3:D:605:PRO:HB2	3:D:609:GLU:HG3	1.80	0.63
4:E:201:ILE:HG21	4:E:284:ARG:HG3	1.79	0.63
3:3:551:PRO:HB2	3:3:555:GLY:HA2	1.80	0.63
9:W:90:TYR:HB3	9:W:118:ALA:HB1	1.79	0.63
10:P:90:LEU:HD12	16:Q:330:LEU:HD21	1.79	0.63
12:S:88:ASP:OD2	13:T:587:ARG:NH1	2.32	0.63
13:T:419:ARG:NH2	13:T:525:GLU:OE2	2.32	0.63
1:B:243:THR:HG22	1:B:244:GLU:H	1.64	0.63
2:C:6:ASP:HB3	2:C:7:LYS:HE3	1.81	0.63
6:6:63:PHE:HA	16:H:50:ARG:HG2	1.81	0.63
16:H:151:GLY:HA2	16:H:154:ARG:HD3	1.81	0.63
1:B:6:LEU:HB2	1:B:241:MET:HA	1.79	0.63
1:B:38:TYR:HH	1:B:112:HIS:HD1	0.68	0.63
2:C:146:THR:HG23	2:C:149:ARG:H	1.64	0.63
6:G:59:ASP:OD1	6:G:62:ARG:NH2	2.30	0.63
6:G:62:ARG:HB3	16:Q:50:ARG:HB2	1.81	0.63
4:E:26:MET:HG2	10:P:54:VAL:HB	1.81	0.63
1:1:287:ILE:HG12	1:1:330:LEU:HB3	1.81	0.62
4:4:110:PRO:HB3	4:4:301:PRO:HG2	1.81	0.62
14:M:115:LEU:HD12	14:M:180:LEU:HD13	1.82	0.62
14:M:167:ARG:NH2	14:M:173:PRO:O	2.32	0.62
15:N:299:LEU:HD22	15:N:307:VAL:HG11	1.81	0.62
1:B:288:GLN:HE21	1:B:331:ILE:HG22	1.62	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:E:373:PRO:O	4:E:377:ASN:ND2	2.32	0.62
8:I:120:ASP:OD1	8:I:123:ARG:NH1	2.31	0.62
14:U:166:ALA:HA	14:U:185:LEU:HD21	1.81	0.62
4:4:201:ILE:HA	4:4:204:TYR:HD2	1.64	0.62
4:4:379:GLN:HE22	5:5:110:SER:HA	1.64	0.62
8:7:37:PHE:HE1	8:7:74:PRO:HA	1.64	0.62
12:S:95:GLY:HA2	15:V:256:ARG:HE	1.63	0.62
3:3:8:ASP:OD2	3:3:28:TYR:OH	2.16	0.62
14:M:130:LEU:HD12	14:M:131:LEU:N	2.14	0.62
7:O:164:PRO:HA	7:O:178:GLU:HB2	1.80	0.62
6:6:90:PRO:O	6:6:93:ARG:HB3	1.99	0.62
15:N:73:THR:HB	15:N:209:LEU:HD22	1.81	0.62
4:E:261:THR:H	4:E:292:GLN:NE2	1.96	0.62
7:9:10:LEU:HA	16:H:296:THR:HG21	1.81	0.62
10:A:63:VAL:HG11	10:A:115:VAL:HG21	1.82	0.62
13:L:380:SER:HB3	13:L:457:GLY:H	1.64	0.62
3:3:199:VAL:HG11	3:3:219:PRO:HD2	1.81	0.62
3:D:35:SER:O	3:D:186:ARG:NH2	2.32	0.62
15:V:44:TRP:CD1	15:V:426:GLY:HA3	2.34	0.62
15:V:187:ALA:O	15:V:216:LYS:NZ	2.32	0.62
16:H:143:SER:HB2	16:H:235:GLU:HG3	1.81	0.62
13:T:87:ILE:HD12	13:T:239:LEU:HD13	1.82	0.62
14:U:333:TYR:O	14:U:337:GLY:N	2.33	0.62
3:3:556:ALA:HB2	3:3:562:GLY:HA3	1.82	0.62
15:N:38:ALA:HA	15:N:41:LEU:HD12	1.82	0.62
4:E:352:GLU:O	4:E:371:ARG:NE	2.24	0.62
11:R:59:TYR:CD1	11:R:63:ILE:HD12	2.35	0.62
13:L:44:GLY:HA3	13:L:77:LEU:HD21	1.81	0.62
14:M:70:LEU:O	14:M:73:LEU:HD23	2.00	0.62
1:B:259:LYS:NZ	2:C:180:GLU:HG2	2.15	0.62
1:B:366:PHE:CE2	1:B:390:LEU:HD21	2.34	0.62
14:U:75:PHE:HZ	14:U:111:ALA:HB2	1.65	0.62
3:3:445:THR:HB	3:3:463:ALA:HB2	1.81	0.62
3:3:468:HIS:ND1	3:3:469:ARG:O	2.33	0.62
13:T:325:HIS:NE2	13:T:329:LYS:HG3	2.15	0.62
1:1:220:ASN:N	18:1:502:FMN:O3P	2.26	0.61
13:L:60:LEU:HD21	14:M:375:PRO:HB3	1.82	0.61
16:H:218:PRO:HB3	16:H:305:LEU:HD13	1.82	0.61
1:B:111:PRO:HB3	1:B:145:LEU:HD23	1.81	0.61
13:T:278:ALA:HA	13:T:301:SER:HA	1.82	0.61
1:B:293:GLY:HA3	1:B:297:THR:HG21	1.82	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:T:439:PRO:HG2	13:T:442:MET:HE3	1.83	0.61
2:2:146:THR:HG23	2:2:149:ARG:H	1.65	0.61
3:3:584:VAL:HG12	3:3:600:VAL:HB	1.82	0.61
5:5:170:PHE:HE2	7:9:61:ALA:HA	1.65	0.61
6:6:102:PRO:O	16:H:69:LYS:NZ	2.33	0.61
4:E:154:GLU:OE1	6:G:57:ARG:NH1	2.33	0.61
2:2:132:PRO:HG2	2:2:145:VAL:HB	1.82	0.61
6:G:28:VAL:O	6:G:32:ARG:HG3	2.01	0.61
14:U:402:SER:HA	14:U:405:TYR:CE2	2.35	0.61
16:Q:65:LYS:O	16:Q:69:LYS:HB2	2.00	0.61
4:4:312:PRO:HG3	4:4:323:ALA:O	1.99	0.61
4:4:341:GLU:OE2	5:5:57:TYR:OH	2.17	0.61
8:7:82:ILE:HG23	8:7:95:ALA:HB3	1.83	0.61
16:H:43:GLN:O	16:H:45:ARG:N	2.33	0.61
1:B:179:ALA:HB3	1:B:182:CYS:SG	2.41	0.61
5:F:31:ARG:NH2	5:F:98:ASP:OD2	2.28	0.61
11:R:50:PHE:HB2	11:R:124:PRO:HD3	1.81	0.61
4:4:211:SER:HB2	4:4:214:PHE:HB3	1.82	0.61
4:E:216:GLU:OE2	16:Q:304:GLN:NE2	2.34	0.61
14:U:87:LEU:HD11	14:U:432:PHE:HB2	1.82	0.61
10:P:62:TYR:CD2	11:R:66:LEU:HD11	2.36	0.61
4:E:261:THR:N	4:E:292:GLN:HE22	1.98	0.61
6:6:30:TRP:O	6:6:34:ASN:ND2	2.34	0.60
6:6:93:ARG:NH1	6:6:130:VAL:O	2.33	0.60
1:B:257:PRO:HD3	2:C:90:LEU:HD23	1.83	0.60
13:T:157:LYS:NZ	13:T:535:ASP:OD2	2.33	0.60
3:3:414:SER:OG	3:3:443:ARG:NH2	2.34	0.60
6:6:163:TYR:OH	6:6:169:ARG:NH2	2.34	0.60
12:K:79:PHE:CD2	12:K:85:THR:HA	2.36	0.60
15:N:62:PHE:HE2	15:N:285:LEU:HD22	1.65	0.60
1:B:438:ARG:HA	2:C:147:ARG:HH21	1.65	0.60
7:O:35:PRO:O	7:O:117:TYR:OH	2.18	0.60
10:P:57:PHE:CE2	16:Q:149:LEU:HD13	2.33	0.60
11:R:108:LEU:HD22	12:S:4:LEU:HB3	1.82	0.60
1:1:358:PRO:HB3	3:3:107:MET:SD	2.40	0.60
3:3:9:ARG:NH1	3:3:26:ALA:O	2.29	0.60
3:3:129:GLU:O	3:3:133:ARG:HG2	2.00	0.60
11:J:71:ILE:HG22	12:K:25:ILE:HD13	1.82	0.60
3:D:34:CYS:O	3:D:189:ARG:NH2	2.28	0.60
6:6:115:GLY:HA3	6:6:125:GLN:OE1	2.01	0.60
7:9:169:GLU:HA	8:7:45:GLU:HB3	1.83	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:356:CYS:HB3	1:B:358:PRO:HD2	1.84	0.60
6:G:83:ARG:HB2	6:G:123:ILE:HD12	1.83	0.60
1:1:184:GLU:OE1	1:1:186:THR:OG1	2.12	0.60
3:3:656:LEU:HD11	9:W:3:ARG:HD3	1.84	0.60
4:4:385:CYS:HB3	4:4:396:ILE:HG21	1.83	0.60
5:5:103:THR:HG22	5:5:126:PHE:HB3	1.81	0.60
8:I:6:GLU:O	8:I:9:LEU:HB3	2.01	0.60
1:1:95:GLU:O	1:1:135:ARG:NH1	2.31	0.60
3:3:149:LEU:HD21	4:4:301:PRO:HG3	1.83	0.60
1:B:91:CYS:HB3	1:B:132:ILE:HA	1.83	0.60
3:D:614:LEU:O	3:D:621:VAL:HA	2.02	0.60
6:G:40:THR:H	6:G:68:PHE:HE1	1.48	0.60
16:Q:48:PRO:C	16:Q:50:ARG:H	2.04	0.60
4:4:185:GLU:OE2	7:9:165:TYR:OH	2.10	0.60
5:5:137:THR:HB	5:5:141:LEU:HD22	1.83	0.60
7:9:171:GLU:OE2	8:7:43:ARG:NH2	2.34	0.60
14:M:10:VAL:HG23	14:M:104:GLY:HA3	1.83	0.60
14:M:91:VAL:HG12	14:M:222:HIS:CE1	2.36	0.60
5:F:41:TYR:HD1	5:F:46:PHE:HE2	1.49	0.60
16:Q:162:TYR:HD2	16:Q:209:ALA:HA	1.67	0.60
5:5:175:THR:HG22	5:5:178:ASP:HB2	1.83	0.60
13:L:432:HIS:HE1	13:L:434:HIS:HB2	1.66	0.60
1:B:32:TYR:OH	1:B:116:GLU:OE1	2.15	0.60
16:Q:99:LEU:HD12	16:Q:116:ILE:HG13	1.84	0.60
3:D:52:ILE:HB	3:D:76:GLN:HG3	1.84	0.60
3:D:190:TYR:OH	3:D:222:PHE:O	2.16	0.60
1:1:72:THR:HG21	1:1:223:THR:HG21	1.83	0.60
4:4:50:GLU:O	4:4:389:GLN:NE2	2.35	0.60
13:L:371:LEU:HD13	13:L:376:LEU:HD22	1.82	0.60
15:V:217:ALA:HA	15:V:285:LEU:HD23	1.83	0.60
10:A:105:VAL:HG13	15:N:15:LEU:HD21	1.84	0.59
16:Q:44:VAL:HG13	16:Q:45:ARG:N	2.16	0.59
16:H:120:LEU:HD22	16:H:180:LEU:HD12	1.84	0.59
11:R:152:VAL:O	11:R:156:LEU:HB2	2.02	0.59
14:U:206:PRO:HD2	14:U:293:MET:HG3	1.84	0.59
4:4:367:ARG:HH12	5:5:53:VAL:HG23	1.67	0.59
14:M:268:ALA:HA	14:M:291:SER:HA	1.84	0.59
4:E:352:GLU:C	4:E:371:ARG:HE	2.05	0.59
10:P:70:LEU:HD13	11:R:150:THR:HG22	1.84	0.59
11:R:97:ALA:HB2	12:S:16:TYR:HB2	1.84	0.59
3:3:326:PHE:CZ	3:3:330:LYS:HE3	2.38	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:6:124:VAL:HG22	9:W:120:PRO:HD2	1.85	0.59
3:D:425:ARG:NH2	3:D:430:THR:OG1	2.34	0.59
3:D:507:LEU:HD22	3:D:511:VAL:HG11	1.84	0.59
16:Q:41:ARG:HH12	16:Q:47:GLY:H	1.49	0.59
1:1:104:ARG:NH2	1:1:105:TYR:OH	2.35	0.59
13:L:452:GLY:O	13:L:456:ALA:N	2.35	0.59
13:L:487:LEU:HA	13:L:490:GLU:HG2	1.83	0.59
5:F:145:PRO:HA	5:F:150:TYR:CD1	2.37	0.59
15:V:38:ALA:HA	15:V:41:LEU:HD12	1.83	0.59
1:1:425:ALA:O	1:1:428:LYS:NZ	2.23	0.59
5:5:174:LEU:HD11	5:5:189:ARG:HH21	1.66	0.59
11:J:2:SER:HA	11:J:5:GLU:HB3	1.83	0.59
1:B:134:VAL:O	1:B:176:GLY:N	2.34	0.59
1:B:372:ALA:O	1:B:376:THR:OG1	2.10	0.59
5:F:18:GLU:HB2	5:F:26:TRP:HB2	1.82	0.59
6:G:101:ASP:OD2	10:P:35:LYS:HB2	2.03	0.59
10:P:65:ALA:O	10:P:69:ILE:HG23	2.02	0.59
14:U:448:GLY:O	14:U:452:ARG:HG2	2.03	0.59
1:1:293:GLY:HA3	1:1:324:GLY:H	1.67	0.59
4:4:169:HIS:CD2	6:6:141:PRO:HD3	2.38	0.59
3:D:375:THR:HA	3:D:513:GLN:OE1	2.03	0.59
4:E:225:PRO:HG2	4:E:228:VAL:HB	1.83	0.59
6:G:19:ILE:HG12	6:G:20:LEU:H	1.67	0.59
6:G:76:ASP:OD1	16:Q:65:LYS:NZ	2.34	0.59
13:T:105:PHE:O	13:T:109:ASN:ND2	2.34	0.59
2:2:146:THR:HG22	2:2:149:ARG:HB2	1.85	0.59
4:E:45:VAL:HG13	4:E:55:VAL:HG22	1.83	0.59
11:J:152:VAL:O	11:J:156:LEU:HB2	2.03	0.59
5:F:188:SER:HB3	5:F:192:TYR:HB2	1.84	0.59
3:3:611:ARG:HA	3:3:624:LEU:O	2.03	0.59
4:4:34:HIS:HE1	6:6:41:PHE:HE1	1.51	0.59
4:4:169:HIS:HD2	6:6:141:PRO:HD3	1.68	0.59
13:L:9:LEU:HB3	13:L:36:LEU:HD22	1.85	0.59
3:D:269:THR:HG22	3:D:274:LEU:HA	1.85	0.59
4:E:71:GLU:HG2	4:E:367:ARG:HA	1.85	0.59
14:U:126:LEU:O	14:U:126:LEU:HD13	2.03	0.59
15:V:62:PHE:HE2	15:V:285:LEU:HD22	1.68	0.59
3:D:469:ARG:NE	3:D:472:GLU:OE2	2.35	0.58
15:V:265:HIS:NE2	15:V:375:TYR:OH	2.36	0.58
16:H:39:LEU:O	16:H:43:GLN:HG2	2.03	0.58
3:D:750:ARG:NH2	3:D:752:ASP:OD2	2.36	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:6:134:ASP:HB3	6:6:154:LEU:HD13	1.85	0.58
16:H:162:TYR:OH	16:H:305:LEU:O	2.12	0.58
13:T:290:ASP:OD1	13:T:347:GLN:HG2	2.02	0.58
13:T:340:ILE:HB	13:T:345:GLY:HA2	1.84	0.58
15:V:319:ASP:OD2	15:V:399:ARG:NH2	2.37	0.58
3:3:193:GLU:O	3:3:443:ARG:NH2	2.33	0.58
15:N:343:TRP:CE2	15:N:416:PRO:HG3	2.39	0.58
16:H:2:THR:HA	16:H:5:TYR:HD2	1.67	0.58
15:V:92:ALA:HA	15:V:95:MET:HE2	1.85	0.58
15:V:168:GLU:HG2	15:V:169:GLY:H	1.67	0.58
16:Q:216:ARG:HB2	16:Q:294:ARG:HD2	1.86	0.58
2:2:74:PRO:O	8:7:121:ARG:NH2	2.36	0.58
4:4:190:LEU:O	4:4:194:LEU:HD13	2.03	0.58
13:L:312:VAL:HA	13:L:397:PHE:CD2	2.39	0.58
1:B:54:ILE:HG12	1:B:76:TRP:HE3	1.67	0.58
15:V:25:VAL:HG11	15:V:82:PHE:HB2	1.85	0.58
4:4:159:LEU:O	4:4:162:TRP:HB2	2.03	0.58
1:B:176:GLY:O	2:C:32:ARG:NH2	2.35	0.58
3:D:563:ALA:HB3	3:D:580:LYS:HE3	1.85	0.58
6:G:90:PRO:O	6:G:93:ARG:HB3	2.02	0.58
8:I:50:LEU:HD11	8:I:75:ARG:HB2	1.84	0.58
3:3:697:THR:OG1	3:3:762:ALA:O	2.21	0.58
6:6:39:ALA:HB2	6:6:75:ALA:HB3	1.83	0.58
9:W:102:LEU:C	9:W:110:LEU:HD13	2.14	0.58
4:E:263:ASP:HB2	4:E:285:GLU:CD	2.24	0.58
6:G:60:LEU:HG	6:G:65:SER:HB2	1.85	0.58
15:N:294:LEU:HG	15:N:402:VAL:HG13	1.86	0.58
1:B:109:ASP:OD2	2:C:174:HIS:NE2	2.33	0.58
3:3:224:GLY:O	3:3:227:THR:HB	2.03	0.58
4:4:193:LEU:HD23	4:4:194:LEU:HD12	1.84	0.58
13:L:564:TYR:OH	14:M:209:PRO:O	2.14	0.58
7:O:133:LYS:O	7:O:137:LEU:HD13	2.04	0.58
14:U:205:THR:HG23	14:U:238:VAL:HG23	1.84	0.58
4:4:31:GLY:HA3	10:A:45:GLU:OE2	2.04	0.58
7:9:13:THR:HG21	16:H:296:THR:HG23	1.86	0.58
16:H:260:PRO:HG3	16:H:286:PHE:CD2	2.39	0.58
1:B:338:VAL:O	1:B:342:TRP:HB2	2.02	0.58
4:E:374:SER:HA	4:E:377:ASN:HB2	1.86	0.58
10:P:13:TYR:CZ	16:Q:95:LEU:HA	2.39	0.58
4:E:87:TYR:CG	6:G:45:CYS:HB3	2.39	0.57
10:P:109:TYR:OH	10:P:113:LYS:NZ	2.31	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
15:V:14:THR:HA	15:V:86:LEU:HD21	1.85	0.57
15:V:196:THR:HG22	15:V:259:ALA:HB1	1.84	0.57
16:Q:72:ILE:HG22	16:Q:237:SER:HB3	1.86	0.57
4:4:132:PHE:CE2	4:4:279:ARG:HD2	2.40	0.57
5:5:75:VAL:HG13	5:5:87:ARG:HB2	1.86	0.57
6:6:19:ILE:HG12	6:6:20:LEU:H	1.69	0.57
3:D:403:THR:OG1	3:D:410:HIS:ND1	2.31	0.57
10:P:81:TYR:HB2	11:R:132:TYR:CZ	2.39	0.57
11:R:104:LEU:HD23	15:V:174:LEU:HD21	1.86	0.57
15:V:128:GLN:OE1	15:V:306:ARG:NH2	2.37	0.57
4:4:62:LEU:HD11	6:6:43:LEU:O	2.04	0.57
7:9:11:GLY:O	7:9:15:LYS:HG3	2.05	0.57
16:H:44:VAL:HG12	16:H:45:ARG:N	2.18	0.57
13:T:9:LEU:HB2	13:T:10:PRO:HD3	1.84	0.57
1:1:343:ASN:HB2	2:2:89:LYS:HZ2	1.68	0.57
10:A:81:TYR:HB2	11:J:132:TYR:CE1	2.39	0.57
1:B:17:LEU:HD22	1:B:113:LEU:HD21	1.85	0.57
1:B:249:MET:HA	1:B:267:PRO:HA	1.86	0.57
1:B:312:SER:HG	1:B:315:HIS:CE1	2.19	0.57
2:C:107:GLY:H	2:C:110:GLU:HG3	1.69	0.57
6:G:58:ASN:ND2	6:G:145:GLU:OE2	2.37	0.57
13:T:216:LYS:HD2	13:T:248:ALA:HB3	1.86	0.57
16:Q:222:PRO:HD2	16:Q:230:GLY:HA2	1.85	0.57
4:4:162:TRP:CE2	7:9:34:LYS:HD2	2.39	0.57
13:L:433:HIS:ND1	13:L:437:GLU:OE2	2.27	0.57
15:N:168:GLU:HG2	15:N:169:GLY:H	1.70	0.57
16:H:290:PHE:O	16:H:294:ARG:HG2	2.04	0.57
13:T:490:GLU:HG3	13:T:491:TRP:N	2.19	0.57
1:1:4:PRO:HA	1:1:12:ARG:HH22	1.69	0.57
4:E:129:HIS:NE2	4:E:282:GLU:OE1	2.34	0.57
4:4:45:VAL:HG13	4:4:55:VAL:HG22	1.86	0.57
5:5:42:LYS:HB2	5:5:108:TRP:CH2	2.39	0.57
6:6:56:ALA:HB2	16:H:44:VAL:HG12	1.85	0.57
10:A:108:LEU:HD23	15:N:15:LEU:HD22	1.85	0.57
16:H:161:SER:HA	16:H:310:TRP:HZ3	1.70	0.57
16:H:216:ARG:HD2	16:H:294:ARG:HA	1.87	0.57
16:H:333:PRO:HG2	16:H:336:TYR:CG	2.39	0.57
16:Q:37:ARG:O	16:Q:41:ARG:HG2	2.05	0.57
16:Q:114:TRP:NE1	16:Q:117:ASN:HB2	2.20	0.57
1:1:293:GLY:HA3	1:1:297:THR:HG21	1.85	0.57
3:3:29:ASP:OD2	5:5:187:GLY:N	2.25	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:6:50:MET:O	6:6:53:SER:OG	2.22	0.57
13:L:267:SER:HB3	13:L:311:GLY:O	2.04	0.57
1:B:195:LEU:HD23	2:C:24:ARG:NH1	2.20	0.57
5:F:103:THR:HG22	5:F:126:PHE:HB3	1.86	0.57
10:P:44:TYR:O	10:P:50:PRO:HG3	2.05	0.57
11:R:64:VAL:HG13	16:Q:134:TYR:OH	2.04	0.57
13:T:419:ARG:HB2	13:T:512:PHE:CE2	2.40	0.57
13:T:490:GLU:O	13:T:494:ILE:HG12	2.05	0.57
14:U:16:LEU:HD22	14:U:97:GLY:H	1.69	0.57
3:3:245:ARG:NH1	7:9:56:CYS:O	2.38	0.57
14:U:166:ALA:HB2	14:U:193:VAL:HG11	1.86	0.57
16:Q:290:PHE:O	16:Q:294:ARG:HG2	2.04	0.57
3:3:170:LEU:HD11	3:3:176:LEU:HD22	1.87	0.57
3:3:268:ASP:HB2	3:3:276:ARG:O	2.05	0.57
7:9:4:LYS:O	7:9:8:GLN:HG3	2.05	0.57
9:W:51:HIS:CE1	9:W:111:LEU:HD21	2.40	0.57
3:D:224:GLY:O	3:D:227:THR:HB	2.05	0.57
14:U:350:SER:OG	14:U:421:GLY:HA2	2.05	0.57
15:V:108:LEU:HB2	15:V:147:PHE:HE2	1.70	0.57
3:3:715:GLU:H	3:3:761:SER:HB2	1.69	0.56
4:4:28:LEU:HD11	16:H:147:TYR:CD2	2.41	0.56
5:5:38:MET:HA	5:5:41:TYR:HD2	1.70	0.56
12:K:28:PHE:CE2	12:K:68:VAL:HA	2.40	0.56
12:K:79:PHE:HA	12:K:82:ARG:HB3	1.85	0.56
13:L:312:VAL:HA	13:L:397:PHE:HD2	1.70	0.56
3:D:347:HIS:HB2	3:D:538:ALA:HB1	1.86	0.56
7:O:6:LEU:HB3	16:Q:297:TRP:CZ2	2.40	0.56
9:X:24:LEU:HD21	9:X:52:THR:HG21	1.85	0.56
10:A:62:TYR:CD2	11:J:66:LEU:HD11	2.39	0.56
12:K:4:LEU:HD12	12:K:41:SER:HA	1.86	0.56
13:L:162:ASN:OD1	13:L:216:LYS:NZ	2.38	0.56
16:H:190:LYS:HB2	16:H:268:THR:HG21	1.86	0.56
1:B:259:LYS:HZ3	2:C:180:GLU:HG2	1.70	0.56
3:D:185:LYS:HB3	3:D:189:ARG:HD3	1.86	0.56
10:P:77:PHE:CZ	12:S:58:LEU:HD22	2.41	0.56
14:U:221:ASN:ND2	14:U:228:ASP:OD1	2.38	0.56
1:1:243:THR:HG22	1:1:244:GLU:H	1.71	0.56
3:3:230:CYS:SG	3:3:234:ALA:HB3	2.46	0.56
13:L:214:VAL:HG13	13:L:219:GLN:HB2	1.87	0.56
14:M:62:TYR:HE2	14:M:174:THR:HG21	1.69	0.56
3:D:515:THR:HG23	3:D:683:LEU:HD13	1.87	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:R:96:LEU:HD22	13:T:594:VAL:HG12	1.86	0.56
13:T:124:TYR:HH	13:T:256:SER:HG	1.39	0.56
2:2:162:ARG:NE	2:2:164:GLU:OE2	2.36	0.56
4:4:71:GLU:OE1	5:5:148:LYS:NZ	2.29	0.56
6:6:21:PHE:HD1	6:6:23:THR:H	1.53	0.56
13:L:161:VAL:HG13	13:L:222:LEU:HD13	1.86	0.56
14:M:232:THR:HA	14:M:235:LYS:HZ2	1.69	0.56
1:B:95:GLU:O	1:B:135:ARG:NH1	2.37	0.56
3:D:227:THR:HG21	3:D:237:ASP:HB2	1.88	0.56
4:E:93:HIS:ND1	4:E:355:TYR:OH	2.24	0.56
14:U:59:ALA:O	14:U:167:ARG:NH2	2.38	0.56
3:3:194:VAL:HG12	3:3:411:LEU:HD22	1.88	0.56
5:5:67:ARG:HD3	5:5:96:GLU:HG3	1.87	0.56
11:J:92:LEU:O	11:J:95:LEU:HB3	2.06	0.56
5:F:71:VAL:HA	5:F:90:VAL:O	2.05	0.56
6:G:57:ARG:NH2	6:G:143:ARG:HH22	2.04	0.56
13:T:17:LEU:HA	13:T:21:GLY:HA2	1.86	0.56
1:1:352:SER:HB3	3:3:206:GLY:HA2	1.87	0.56
3:3:367:PRO:O	3:3:552:GLY:N	2.22	0.56
4:4:84:ARG:HG3	4:4:169:HIS:ND1	2.21	0.56
10:A:57:PHE:HE2	16:H:149:LEU:HD13	1.70	0.56
4:E:140:LEU:HD21	4:E:217:ARG:NH1	2.20	0.56
4:E:201:ILE:HA	4:E:204:TYR:CD2	2.40	0.56
1:1:54:ILE:HG12	1:1:76:TRP:HE3	1.70	0.56
13:L:314:ALA:HB1	13:L:317:VAL:HB	1.88	0.56
4:E:87:TYR:CB	6:G:45:CYS:HB3	2.36	0.56
13:T:286:PHE:HD2	13:T:416:TYR:HB3	1.69	0.56
15:V:270:ALA:HA	15:V:273:LEU:HD23	1.88	0.56
1:1:253:GLN:HG2	1:1:327:GLY:HA2	1.87	0.56
3:3:112:LEU:HD23	3:3:130:LEU:HD21	1.88	0.56
5:5:53:VAL:HG22	5:5:55:LEU:CD1	2.36	0.56
13:L:286:PHE:O	13:L:419:ARG:NH1	2.39	0.56
15:N:201:GLN:OE1	15:N:256:ARG:NH1	2.39	0.56
8:I:42:TYR:O	8:I:46:ARG:NH2	2.39	0.56
13:T:151:TYR:HB3	13:T:231:ALA:HB1	1.88	0.56
7:9:101:CYS:N	17:9:201:SF4:S4	2.75	0.56
14:M:157:LEU:HB3	15:N:365:LEU:HB3	1.88	0.56
14:M:304:THR:O	14:M:307:GLY:N	2.39	0.56
16:H:190:LYS:HD3	16:H:268:THR:HG22	1.87	0.56
3:D:351:LEU:HD11	3:D:615:VAL:HG23	1.88	0.56
3:D:494:LYS:O	3:D:498:GLU:HG2	2.06	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:G:127:VAL:HG12	6:G:131:VAL:HG22	1.88	0.56
13:T:391:ALA:O	13:T:395:TYR:HB2	2.06	0.56
14:U:304:THR:O	14:U:307:GLY:N	2.38	0.56
14:U:318:SER:HA	14:U:321:TYR:CZ	2.41	0.56
16:Q:212:ALA:HA	16:Q:218:PRO:HG3	1.86	0.56
1:1:404:ASP:HA	1:1:407:VAL:HG22	1.88	0.55
3:3:300:TRP:HD1	3:3:703:GLN:HA	1.72	0.55
13:L:444:TRP:HE3	13:L:447:HIS:HD2	1.54	0.55
4:4:201:ILE:HG21	4:4:284:ARG:HG3	1.89	0.55
16:H:225:GLU:HB3	16:H:226:GLN:HG2	1.88	0.55
10:P:7:TYR:CD2	11:R:44:VAL:HG11	2.41	0.55
13:T:230:MET:O	13:T:292:LYS:NZ	2.39	0.55
13:T:413:THR:HA	13:T:416:TYR:CE2	2.41	0.55
4:4:84:ARG:O	6:6:83:ARG:NH2	2.39	0.55
4:4:304:ASP:O	4:4:310:THR:OG1	2.09	0.55
5:5:160:ARG:HH12	7:9:132:GLY:HA3	1.70	0.55
16:H:227:GLU:HG2	16:H:228:LEU:H	1.71	0.55
1:B:122:GLY:HA2	1:B:127:ALA:HB3	1.89	0.55
1:B:238:PHE:CZ	1:B:248:GLY:HA3	2.41	0.55
7:O:44:THR:HA	7:O:138:VAL:HG13	1.89	0.55
14:U:22:ARG:HH12	14:U:92:GLU:HG3	1.71	0.55
3:3:587:LEU:O	3:3:604:ALA:N	2.40	0.55
11:R:19:VAL:HG21	11:R:32:LEU:HB2	1.87	0.55
5:5:42:LYS:NZ	5:5:107:LEU:O	2.39	0.55
6:6:145:GLU:HA	6:6:148:ILE:HD13	1.88	0.55
12:K:88:ASP:OD2	13:L:587:ARG:NH1	2.39	0.55
13:L:12:LEU:O	13:L:16:LEU:HG	2.06	0.55
14:M:215:PRO:HG2	14:M:216:PRO:HD3	1.89	0.55
3:3:271:SER:OG	7:9:69:TYR:OH	2.22	0.55
3:3:373:GLY:HA3	3:3:538:ALA:HB2	1.88	0.55
4:4:162:TRP:CD2	7:9:34:LYS:HD2	2.41	0.55
15:N:217:ALA:HA	15:N:285:LEU:HD23	1.89	0.55
3:D:576:ALA:O	3:D:580:LYS:NZ	2.33	0.55
15:V:98:LEU:HD23	15:V:218:ALA:HB1	1.88	0.55
16:Q:131:LEU:HA	16:Q:134:TYR:HB2	1.89	0.55
1:1:118:MET:HG2	1:1:224:LEU:HD13	1.88	0.55
1:1:437:TRP:O	2:2:147:ARG:NH2	2.40	0.55
4:4:47:LEU:HD13	4:4:52:VAL:HA	1.89	0.55
5:F:144:HIS:HB2	5:F:147:ARG:HD3	1.87	0.55
15:V:94:GLY:O	15:V:110:ALA:HB1	2.05	0.55
16:Q:70:GLU:O	16:Q:237:SER:OG	2.14	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:1:32:TYR:OH	1:1:116:GLU:OE1	2.20	0.55
2:2:108:PRO:HA	2:2:119:VAL:HG23	1.89	0.55
3:3:243:ARG:HH11	3:3:275:LEU:HD23	1.72	0.55
3:D:247:TRP:CD1	5:F:172:ALA:HB2	2.42	0.55
4:E:389:GLN:HG3	4:E:391:PRO:HD2	1.89	0.55
5:F:167:PRO:HA	5:F:170:PHE:HB3	1.88	0.55
13:T:214:VAL:HG13	13:T:219:GLN:HB2	1.88	0.55
16:Q:120:LEU:HD22	16:Q:180:LEU:HD12	1.88	0.55
6:6:59:ASP:OD1	6:6:62:ARG:NH2	2.40	0.55
8:7:10:TYR:O	8:7:13:TRP:HB3	2.07	0.55
14:M:157:LEU:HD12	15:N:369:ALA:HB2	1.88	0.55
15:N:52:PRO:HB3	15:N:103:HIS:HB2	1.88	0.55
1:B:342:TRP:CD1	1:B:371:PHE:HB3	2.42	0.55
1:B:358:PRO:HG3	3:D:46:ARG:HD3	1.88	0.55
3:D:117:LEU:HA	4:E:321:MET:HE2	1.89	0.55
4:E:75:TYR:CZ	4:E:337:PRO:HG2	2.41	0.55
4:E:275:ARG:HD2	4:E:399:SER:HB2	1.87	0.55
7:O:71:GLU:HB2	7:O:90:VAL:HB	1.88	0.55
13:T:88:HIS:NE2	13:T:108:PHE:HB3	2.22	0.55
5:5:33:ARG:NH1	5:5:36:GLU:OE2	2.40	0.55
5:5:174:LEU:HD11	5:5:189:ARG:NH2	2.21	0.55
7:9:6:LEU:HB3	16:H:297:TRP:CZ2	2.41	0.55
9:W:31:VAL:HG11	9:W:81:LEU:HD13	1.88	0.55
9:W:59:VAL:HG11	9:W:63:PHE:CE2	2.40	0.55
13:L:187:GLU:HA	13:L:190:GLU:HG2	1.89	0.55
13:L:361:GLN:O	13:L:365:HIS:ND1	2.40	0.55
14:M:333:TYR:O	14:M:337:GLY:N	2.40	0.55
1:B:16:THR:OG1	1:B:233:ARG:NH2	2.40	0.55
4:E:222:GLY:HA3	4:E:275:ARG:NH2	2.21	0.55
13:T:213:ALA:HB1	13:T:307:PHE:HZ	1.72	0.55
13:T:554:PHE:CZ	14:U:283:THR:HG21	2.42	0.55
15:V:224:LEU:HD11	15:V:281:LEU:HD23	1.88	0.55
15:N:319:ASP:HB3	15:N:322:LEU:HB2	1.89	0.54
2:C:9:ASP:OD1	2:C:9:ASP:N	2.40	0.54
3:D:373:GLY:HA3	3:D:538:ALA:HB2	1.88	0.54
4:E:131:VAL:HG23	4:E:153:ARG:HD2	1.90	0.54
14:U:41:LEU:O	14:U:42:THR:HG22	2.07	0.54
16:Q:267:TRP:CG	16:Q:268:THR:N	2.73	0.54
1:1:170:ASP:OD1	1:1:171:LEU:N	2.40	0.54
2:2:7:LYS:HD3	2:2:33:ARG:NH1	2.23	0.54
5:5:121:LEU:HA	5:5:145:PRO:HD2	1.89	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:J:104:LEU:HD23	15:N:174:LEU:HD21	1.89	0.54
13:L:59:TRP:O	14:M:452:ARG:NH2	2.39	0.54
13:L:160:ILE:O	13:L:164:ILE:HG13	2.07	0.54
5:F:38:MET:HE3	5:F:104:VAL:CG1	2.32	0.54
3:3:33:PHE:HB2	3:3:45:CYS:SG	2.48	0.54
3:3:715:GLU:OE1	3:3:717:TRP:NE1	2.31	0.54
13:L:255:ARG:HD2	13:L:477:LEU:HD23	1.90	0.54
14:M:448:GLY:O	14:M:452:ARG:HG2	2.07	0.54
15:N:79:SER:O	15:N:85:TYR:OH	2.12	0.54
13:T:359:LEU:O	13:T:363:ARG:NH1	2.39	0.54
15:V:233:LEU:HD21	15:V:273:LEU:HB3	1.90	0.54
3:3:351:LEU:HD11	3:3:615:VAL:HG23	1.89	0.54
3:3:583:VAL:HG23	3:3:598:ALA:HA	1.89	0.54
4:4:163:VAL:HG13	4:4:164:THR:HG23	1.89	0.54
13:L:373:LEU:HD21	13:L:416:TYR:HE1	1.73	0.54
8:I:60:SER:HA	8:I:66:PRO:HA	1.89	0.54
10:P:3:PRO:HD2	16:Q:2:THR:HB	1.89	0.54
13:T:94:TYR:CE1	13:T:341:HIS:HB2	2.41	0.54
16:Q:117:ASN:ND2	16:Q:181:ASN:OD1	2.41	0.54
13:L:246:VAL:HB	13:L:303:LEU:HD21	1.87	0.54
14:M:13:GLY:HA2	14:M:97:GLY:HA2	1.90	0.54
4:E:338:PRO:HG3	5:F:193:ARG:HB2	1.89	0.54
8:I:34:GLU:OE1	8:I:58:SER:OG	2.18	0.54
16:Q:90:VAL:HG21	16:Q:243:LEU:HB3	1.88	0.54
2:2:76:GLY:H	2:2:118:SER:HG	1.52	0.54
3:3:512:LEU:HD21	3:3:534:ALA:HB1	1.88	0.54
4:4:48:SER:HB3	10:A:55:LYS:HE3	1.88	0.54
11:J:47:ASP:O	11:J:122:GLY:N	2.41	0.54
3:D:201:ASP:OD1	3:D:202:PHE:N	2.38	0.54
4:E:84:ARG:HG2	17:G:201:SF4:S2	2.48	0.54
5:F:155:THR:HG23	9:X:93:VAL:HB	1.88	0.54
13:T:128:PHE:HD1	13:T:169:PHE:CD2	2.26	0.54
13:T:285:ALA:HA	13:T:297:TYR:HB2	1.90	0.54
1:1:193:GLU:OE1	1:1:200:ARG:NH2	2.41	0.54
4:4:102:GLU:OE2	4:4:117:ARG:NH2	2.40	0.54
4:4:123:LEU:HD12	4:4:126:LEU:HD12	1.90	0.54
4:4:130:LEU:HD22	4:4:149:ALA:HB1	1.89	0.54
5:5:103:THR:HG23	5:5:127:GLU:O	2.08	0.54
11:J:59:TYR:CE2	12:K:61:ILE:HG12	2.42	0.54
13:L:87:ILE:HD12	13:L:239:LEU:HD13	1.89	0.54
13:L:286:PHE:HD2	13:L:416:TYR:HB3	1.71	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
14:M:126:LEU:HD13	14:M:130:LEU:HD23	1.89	0.54
3:D:33:PHE:HZ	3:D:130:LEU:HA	1.72	0.54
3:D:736:VAL:HG22	3:D:775:VAL:HG22	1.90	0.54
14:U:84:LEU:HB3	14:U:432:PHE:CE1	2.43	0.54
14:U:345:ARG:HG2	14:U:412:LYS:O	2.08	0.54
16:Q:12:MET:HE1	16:Q:15:LEU:HD22	1.88	0.54
16:Q:202:ALA:HA	16:Q:205:VAL:HG22	1.90	0.54
3:3:370:ASP:OD1	3:3:374:ARG:HD3	2.08	0.54
4:4:42:ARG:HB3	4:4:58:HIS:HB2	1.90	0.54
15:N:299:LEU:HD21	15:N:312:LEU:HD21	1.90	0.54
1:B:250:LYS:NZ	1:B:325:THR:O	2.37	0.54
4:E:50:GLU:CD	16:Q:154:ARG:HH12	2.11	0.54
3:3:378:PRO:HG2	3:3:680:LEU:HD23	1.89	0.54
4:4:143:LEU:H	4:4:143:LEU:HD23	1.73	0.54
1:B:193:GLU:OE1	1:B:200:ARG:NH2	2.26	0.54
3:D:690:GLY:HA3	3:D:770:ARG:NH2	2.23	0.54
13:T:214:VAL:HG22	13:T:219:GLN:HB2	1.90	0.54
1:1:160:LYS:O	1:1:168:SER:OG	2.16	0.54
3:3:693:TYR:O	3:3:760:LEU:N	2.37	0.54
4:4:99:LEU:HD23	4:4:102:GLU:OE1	2.08	0.54
4:4:137:LEU:HD23	4:4:145:PRO:HG2	1.90	0.54
14:M:305:PRO:HB3	14:M:459:GLU:HA	1.89	0.54
16:H:52:GLY:HA3	16:H:55:GLY:H	1.72	0.54
5:F:39:ALA:HA	5:F:107:LEU:HD21	1.91	0.54
13:T:61:PRO:HD3	14:U:452:ARG:HE	1.72	0.54
13:T:324:THR:HG22	13:T:380:SER:HB2	1.90	0.54
14:U:206:PRO:HD3	14:U:235:LYS:HG2	1.88	0.54
1:1:185:GLU:O	1:1:189:MET:HG3	2.08	0.53
1:1:259:LYS:HA	1:1:284:LEU:HD21	1.90	0.53
4:4:34:HIS:HE1	6:6:41:PHE:CE1	2.26	0.53
6:6:101:ASP:OD1	6:6:180:ARG:NH2	2.40	0.53
7:9:121:MET:HB2	7:9:131:TYR:OH	2.09	0.53
7:9:128:ASP:O	7:9:144:LYS:NZ	2.38	0.53
13:L:104:PHE:CE2	13:L:108:PHE:CZ	2.96	0.53
14:M:130:LEU:HD12	14:M:130:LEU:C	2.29	0.53
16:H:150:LEU:O	16:H:154:ARG:HG3	2.07	0.53
10:P:62:TYR:HD2	11:R:66:LEU:HD11	1.73	0.53
13:T:90:TYR:OH	13:T:338:SER:OG	2.22	0.53
13:T:115:MET:HG2	13:T:244:THR:HG22	1.89	0.53
4:4:285:GLU:O	4:4:289:ILE:HG12	2.07	0.53
14:M:335:ARG:NH1	14:M:423:LYS:O	2.40	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:51:ARG:HB3	3:D:94:ASP:HB3	1.90	0.53
3:D:283:PRO:HG2	3:D:425:ARG:NH2	2.23	0.53
14:U:215:PRO:HG2	14:U:216:PRO:HD3	1.90	0.53
3:3:397:LEU:HD21	3:3:480:LEU:HD13	1.89	0.53
3:3:401:ASP:O	3:3:405:GLU:HG3	2.09	0.53
3:3:594:ALA:O	3:3:598:ALA:HB3	2.08	0.53
15:N:343:TRP:NE1	15:N:413:GLY:O	2.41	0.53
16:H:147:TYR:HE1	16:H:228:LEU:HA	1.74	0.53
14:U:346:GLY:O	14:U:349:GLN:HG2	2.08	0.53
2:2:3:PHE:CB	2:2:45:ARG:NH1	2.61	0.53
2:2:27:ILE:HG13	2:2:53:VAL:HG21	1.90	0.53
4:4:224:ILE:HB	4:4:270:GLY:HA3	1.91	0.53
10:A:81:TYR:CE2	10:A:96:VAL:HG11	2.43	0.53
16:H:50:ARG:C	16:H:52:GLY:H	2.11	0.53
3:D:248:GLU:HG2	5:F:170:PHE:CE1	2.44	0.53
6:6:168:GLU:OE1	3:D:520:ARG:NH2	2.42	0.53
13:L:413:THR:HA	13:L:416:TYR:CE2	2.43	0.53
14:M:402:SER:HA	14:M:405:TYR:CE2	2.44	0.53
15:N:62:PHE:CE2	15:N:285:LEU:HD22	2.43	0.53
16:H:232:TYR:HB2	16:H:244:PHE:CE1	2.42	0.53
3:D:340:GLU:HB3	3:D:564:LEU:HB2	1.89	0.53
3:D:586:HIS:NE2	3:D:640:VAL:HG21	2.23	0.53
8:I:13:TRP:CD2	8:I:72:VAL:HB	2.43	0.53
8:I:74:PRO:HG2	8:I:77:ALA:HB2	1.91	0.53
14:U:43:HIS:NE2	14:U:45:GLY:O	2.42	0.53
14:M:206:PRO:HD2	14:M:293:MET:HG3	1.88	0.53
1:B:275:LEU:HA	1:B:279:TRP:HD1	1.73	0.53
2:C:85:THR:HG22	2:C:86:LEU:H	1.73	0.53
3:D:453:PRO:HA	3:D:468:HIS:O	2.09	0.53
3:D:713:ARG:NE	3:D:746:ARG:HH21	2.07	0.53
14:U:70:LEU:HD13	14:U:312:LEU:HD13	1.89	0.53
16:Q:150:LEU:HD21	16:Q:154:ARG:HH11	1.73	0.53
3:3:728:LEU:HB3	3:3:747:VAL:HG11	1.91	0.53
2:C:134:ILE:O	2:C:142:VAL:N	2.41	0.53
6:G:118:PHE:O	6:G:125:GLN:NE2	2.37	0.53
7:O:52:LYS:HB2	7:O:112:ALA:HB2	1.89	0.53
10:P:56:ARG:HD3	11:R:74:LEU:HA	1.91	0.53
16:Q:35:GLU:OE1	16:Q:249:TYR:OH	2.15	0.53
1:1:192:LEU:HD22	1:1:211:LEU:HD21	1.89	0.53
3:3:256:CYS:HB2	3:3:265:ILE:HD13	1.90	0.53
5:5:80:TRP:HA	5:5:80:TRP:CE3	2.44	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:7:6:GLU:O	8:7:9:LEU:HB3	2.09	0.53
15:N:345:LYS:NZ	15:N:368:SER:OG	2.41	0.53
16:H:45:ARG:HG2	16:H:46:MET:N	2.24	0.53
1:B:293:GLY:O	1:B:327:GLY:N	2.40	0.53
14:U:75:PHE:CZ	14:U:111:ALA:HB2	2.43	0.53
3:3:285:VAL:HG13	3:3:286:ASN:H	1.74	0.53
16:H:44:VAL:O	16:H:45:ARG:C	2.47	0.53
16:H:287:LEU:O	16:H:291:ILE:HG13	2.09	0.53
1:B:386:ASN:OD1	3:D:156:ARG:NE	2.41	0.53
3:D:48:CYS:HB3	19:D:804:FES:S2	2.48	0.53
13:T:286:PHE:O	13:T:419:ARG:NH1	2.42	0.53
13:T:586:LEU:HD11	15:V:135:LYS:HA	1.91	0.53
5:5:82:ASP:OD1	5:5:82:ASP:N	2.41	0.53
6:6:66:GLU:HG2	16:H:36:ARG:HD3	1.91	0.53
6:6:94:ARG:O	6:6:98:GLN:N	2.41	0.53
16:H:147:TYR:HD1	16:H:229:VAL:HG22	1.71	0.53
4:E:160:PHE:O	4:E:164:THR:N	2.38	0.53
6:G:59:ASP:OD2	16:Q:45:ARG:HG3	2.09	0.53
16:Q:274:VAL:HG22	16:Q:275:PRO:HD2	1.90	0.53
3:3:476:ILE:HG23	3:3:490:VAL:HG13	1.91	0.52
4:4:201:ILE:HA	4:4:204:TYR:CD2	2.45	0.52
5:5:55:LEU:O	5:5:68:PHE:HA	2.10	0.52
1:B:242:GLY:HA2	1:B:268:MET:O	2.08	0.52
3:D:185:LYS:HB3	3:D:189:ARG:HH11	1.74	0.52
16:Q:150:LEU:O	16:Q:154:ARG:HG3	2.09	0.52
1:1:288:GLN:HE21	1:1:331:ILE:HG22	1.75	0.52
3:3:32:LEU:HD11	3:3:35:SER:HB2	1.91	0.52
3:3:664:LEU:HD22	3:3:669:VAL:HG11	1.91	0.52
4:4:224:ILE:HD11	4:4:275:ARG:CZ	2.40	0.52
10:A:93:PHE:CD2	10:A:94:LEU:HD12	2.44	0.52
1:B:18:TYR:N	1:B:265:GLU:OE1	2.37	0.52
2:C:146:THR:HG22	2:C:149:ARG:HB2	1.91	0.52
4:E:285:GLU:O	4:E:289:ILE:HG12	2.08	0.52
13:T:433:HIS:ND1	13:T:433:HIS:O	2.42	0.52
14:U:91:VAL:HG23	14:U:92:GLU:H	1.74	0.52
3:3:301:ALA:O	3:3:305:ARG:HD2	2.09	0.52
13:L:463:HIS:HE1	13:L:487:LEU:HD22	1.73	0.52
14:M:256:ALA:O	14:M:260:LEU:HG	2.09	0.52
4:E:200:ARG:NH1	4:E:203:GLU:OE1	2.42	0.52
4:E:281:ARG:HD3	4:E:284:ARG:HH12	1.75	0.52
12:S:2:SER:HA	12:S:5:LEU:HD12	1.92	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
15:V:228:ALA:CB	15:V:233:LEU:HD11	2.40	0.52
3:3:614:LEU:O	3:3:621:VAL:HA	2.10	0.52
6:6:127:VAL:HG12	6:6:131:VAL:HG22	1.92	0.52
10:A:13:TYR:CZ	16:H:95:LEU:HA	2.43	0.52
13:L:386:ASP:OD2	13:L:494:ILE:HA	2.09	0.52
3:D:242:PHE:HD2	7:O:74:GLU:HB2	1.74	0.52
3:D:407:PRO:O	3:D:410:HIS:HB3	2.10	0.52
12:S:28:PHE:CZ	12:S:68:VAL:HA	2.44	0.52
1:1:206:PRO:HA	1:1:209:SER:O	2.10	0.52
3:3:309:PRO:HG2	3:3:320:ALA:O	2.09	0.52
7:9:10:LEU:HD12	16:H:296:THR:HG21	1.92	0.52
11:J:65:VAL:HG23	16:H:134:TYR:CZ	2.45	0.52
13:L:325:HIS:NE2	13:L:329:LYS:HG3	2.24	0.52
1:B:393:LEU:HD22	3:D:106:GLY:HA3	1.91	0.52
1:B:424:LEU:HG	1:B:429:ARG:O	2.10	0.52
3:D:124:LYS:HG2	3:D:236:LEU:HD21	1.90	0.52
4:E:370:VAL:HB	4:E:409:ARG:HD2	1.92	0.52
11:R:29:ALA:O	11:R:33:ILE:HG13	2.09	0.52
11:R:131:LEU:HA	11:R:135:TRP:HB2	1.92	0.52
15:V:63:THR:HG22	15:V:96:HIS:HA	1.90	0.52
15:V:91:ALA:HA	15:V:114:LEU:HA	1.92	0.52
16:Q:36:ARG:NH1	16:Q:58:GLN:HG2	2.23	0.52
16:Q:224:ALA:HA	16:Q:229:VAL:HA	1.91	0.52
2:2:24:ARG:HA	2:2:53:VAL:HG21	1.91	0.52
10:A:67:LEU:HD23	16:H:310:TRP:CE2	2.45	0.52
13:L:88:HIS:O	13:L:92:ILE:HG13	2.10	0.52
13:L:129:ILE:HG12	14:M:369:PRO:HB2	1.92	0.52
13:L:600:LEU:HD11	15:N:232:ALA:HB1	1.91	0.52
14:U:30:GLY:O	14:U:34:LEU:HG	2.10	0.52
2:2:87:SER:HB2	19:2:201:FES:S2	2.50	0.52
3:3:115:HIS:HB3	4:4:321:MET:CE	2.39	0.52
4:4:281:ARG:HD3	4:4:284:ARG:HH12	1.73	0.52
9:W:6:MET:O	9:W:62:ALA:HB2	2.10	0.52
15:N:65:LEU:HD22	15:N:286:LEU:HD23	1.91	0.52
15:N:216:LYS:NZ	15:N:266:ALA:HB2	2.24	0.52
16:H:131:LEU:HA	16:H:134:TYR:HB2	1.91	0.52
1:B:362:GLY:HA3	1:B:394:ILE:HD11	1.91	0.52
2:C:31:LEU:HD22	2:C:41:ILE:HD13	1.91	0.52
3:D:225:ASN:O	3:D:229:ILE:HG13	2.09	0.52
3:D:233:GLY:N	17:D:801:SF4:S2	2.79	0.52
6:G:163:TYR:O	7:O:148:ARG:NE	2.43	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:R:32:LEU:HD13	12:S:29:LEU:HG	1.90	0.52
15:V:13:LEU:HD22	15:V:25:VAL:HG13	1.92	0.52
15:V:99:ALA:O	15:V:225:ARG:NH1	2.43	0.52
3:3:131:GLN:HG2	4:4:325:ILE:HG23	1.92	0.52
3:3:178:ARG:HH22	8:7:65:GLU:CD	2.13	0.52
4:4:47:LEU:HD12	4:4:48:SER:N	2.24	0.52
7:9:45:ARG:NH2	7:9:139:ASP:OD2	2.41	0.52
14:M:102:MET:HB3	14:M:230:LEU:HD23	1.91	0.52
14:M:350:SER:OG	14:M:421:GLY:HA2	2.10	0.52
15:N:313:ARG:HB2	15:N:384:ALA:HB3	1.91	0.52
16:H:147:TYR:CE1	16:H:228:LEU:HD13	2.45	0.52
3:D:285:VAL:HG13	3:D:286:ASN:H	1.75	0.52
4:E:350:ARG:O	4:E:373:PRO:HB2	2.10	0.52
8:I:43:ARG:HA	8:I:46:ARG:HH21	1.74	0.52
9:X:37:TRP:HE1	9:X:40:LYS:NZ	2.08	0.52
3:3:734:VAL:HG13	3:3:775:VAL:HG13	1.92	0.52
6:6:119:ASN:HA	6:6:125:GLN:NE2	2.23	0.52
12:K:4:LEU:CD1	12:K:41:SER:HA	2.40	0.52
13:L:285:ALA:O	13:L:294:ILE:HG13	2.10	0.52
13:L:405:GLY:O	13:L:409:VAL:HG23	2.10	0.52
4:E:26:MET:HB2	4:E:47:LEU:O	2.10	0.52
10:P:95:GLY:HA3	11:R:136:LEU:HD21	1.92	0.52
13:T:129:ILE:HG12	14:U:369:PRO:HB2	1.90	0.52
15:V:270:ALA:O	15:V:273:LEU:HB2	2.10	0.52
8:7:86:LEU:HB2	8:7:91:ILE:HB	1.92	0.52
11:J:131:LEU:HD21	11:J:139:LEU:HD13	1.91	0.52
4:E:132:PHE:CE2	4:E:279:ARG:HD2	2.45	0.52
6:G:143:ARG:NE	6:G:145:GLU:OE1	2.42	0.52
11:R:47:ASP:O	11:R:122:GLY:N	2.39	0.52
14:U:206:PRO:HG3	14:U:214:LEU:HD22	1.91	0.52
13:L:293:LYS:O	13:L:297:TYR:HD1	1.92	0.51
13:L:458:TYR:HD1	13:L:461:LEU:HD21	1.73	0.51
1:B:186:THR:O	1:B:200:ARG:HG3	2.09	0.51
4:E:271:ASP:O	4:E:275:ARG:NE	2.36	0.51
7:O:59:CYS:HB2	7:O:104:CYS:HB2	1.91	0.51
10:P:77:PHE:O	10:P:80:PRO:HD2	2.10	0.51
11:R:75:PHE:HZ	11:R:78:GLN:HE21	1.57	0.51
12:S:46:ALA:HB2	12:S:53:GLY:HA3	1.91	0.51
16:Q:122:ILE:HA	16:Q:125:LEU:HD12	1.91	0.51
1:1:131:TYR:OH	2:2:17:LYS:O	2.24	0.51
5:5:67:ARG:NH1	5:5:96:GLU:OE2	2.44	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:9:68:ILE:HG12	7:9:93:ILE:HG12	1.91	0.51
11:J:124:PRO:HA	11:J:127:LEU:HB2	1.93	0.51
14:M:119:TYR:CE1	14:M:160:LEU:HD13	2.45	0.51
16:H:150:LEU:HD23	16:H:154:ARG:HD2	1.92	0.51
11:R:119:LEU:HD11	12:S:47:ARG:HA	1.92	0.51
13:T:160:ILE:O	13:T:164:ILE:HG13	2.10	0.51
15:V:188:ALA:HB3	15:V:216:LYS:HZ1	1.74	0.51
1:1:113:LEU:HD12	1:1:228:VAL:HG21	1.92	0.51
1:1:162:LEU:O	1:1:165:THR:HG22	2.11	0.51
2:2:74:PRO:HD3	8:7:125:ALA:HB2	1.91	0.51
14:M:43:HIS:NE2	14:M:45:GLY:O	2.43	0.51
15:N:203:SER:O	15:N:255:LYS:NZ	2.43	0.51
1:B:165:THR:HG23	1:B:167:PHE:H	1.75	0.51
4:E:163:VAL:HG13	4:E:164:THR:HG23	1.93	0.51
6:G:72:PRO:O	6:G:99:MET:HG3	2.10	0.51
13:T:17:LEU:HD22	13:T:29:PRO:HB3	1.92	0.51
16:Q:136:ILE:HG23	16:Q:232:TYR:HD2	1.76	0.51
6:6:153:GLN:HG3	7:9:124:TYR:CZ	2.46	0.51
11:J:157:VAL:HG12	11:J:159:PRO:HD3	1.90	0.51
14:M:228:ASP:OD2	14:M:282:LYS:NZ	2.34	0.51
16:H:293:ILE:HG23	16:H:297:TRP:CE3	2.45	0.51
1:B:243:THR:HG21	1:B:315:HIS:CE1	2.46	0.51
14:U:24:LEU:HD22	14:U:27:LEU:HD21	1.92	0.51
14:U:347:LEU:HB2	14:U:413:THR:O	2.10	0.51
3:3:127:ALA:HB3	3:3:246:ASN:ND2	2.25	0.51
13:L:171:LEU:O	13:L:175:ILE:HG13	2.10	0.51
13:L:433:HIS:ND1	13:L:433:HIS:O	2.42	0.51
15:N:319:ASP:CG	15:N:399:ARG:HH21	2.14	0.51
16:H:86:PRO:HG3	16:H:244:PHE:CE2	2.46	0.51
16:H:217:THR:O	16:H:217:THR:HG22	2.11	0.51
1:B:283:PRO:HB3	1:B:287:ILE:HD13	1.92	0.51
3:D:237:ASP:OD1	3:D:239:THR:HG22	2.11	0.51
3:D:419:ASP:HA	3:D:447:LYS:NZ	2.26	0.51
15:V:228:ALA:CB	15:V:233:LEU:CD1	2.89	0.51
1:1:46:LYS:HE2	1:1:163:PHE:HB3	1.92	0.51
1:1:249:MET:HA	1:1:267:PRO:HA	1.93	0.51
2:2:49:ILE:O	2:2:53:VAL:CG1	2.51	0.51
2:2:85:THR:HG22	2:2:86:LEU:H	1.76	0.51
4:4:233:GLY:HA2	5:5:48:PHE:HE1	1.75	0.51
4:4:333:GLU:O	4:4:363:SER:OG	2.25	0.51
13:L:104:PHE:HZ	13:L:235:PRO:HG2	1.76	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:L:391:ALA:O	13:L:395:TYR:HB2	2.11	0.51
15:N:56:ASP:OD1	15:N:225:ARG:NH1	2.44	0.51
15:N:294:LEU:HD12	15:N:405:ALA:HB3	1.92	0.51
15:N:347:LEU:O	15:N:351:GLU:HG2	2.11	0.51
16:H:227:GLU:HB2	16:H:299:ARG:HH12	1.76	0.51
1:B:422:LEU:O	1:B:426:ARG:N	2.26	0.51
3:D:713:ARG:NH2	3:D:715:GLU:OE2	2.44	0.51
3:D:716:LEU:HD21	3:D:758:LEU:HD23	1.93	0.51
11:R:69:PHE:O	11:R:73:LEU:HG	2.11	0.51
14:U:155:GLY:HA3	14:U:203:ILE:HG21	1.93	0.51
15:V:279:GLN:HG3	15:V:423:LEU:HB2	1.93	0.51
1:1:132:ILE:HD11	1:1:171:LEU:HD13	1.92	0.51
5:5:155:THR:O	6:6:119:ASN:ND2	2.42	0.51
6:6:113:SER:HB3	7:9:96:LEU:HD13	1.92	0.51
16:H:44:VAL:HG13	16:H:45:ARG:N	2.26	0.51
4:E:42:ARG:HB3	4:E:58:HIS:HB2	1.93	0.51
8:I:61:ASP:HB2	8:I:129:ALA:OXT	2.10	0.51
14:U:264:ALA:HB1	14:U:294:GLY:O	2.10	0.51
15:V:177:GLY:O	15:V:181:VAL:HG23	2.11	0.51
15:V:237:VAL:HG22	15:V:270:ALA:HB3	1.93	0.51
1:1:395:GLU:OE2	1:1:408:TRP:NE1	2.43	0.51
10:A:44:TYR:O	10:A:50:PRO:HG3	2.11	0.51
15:N:372:ALA:O	15:N:376:LEU:HB2	2.10	0.51
16:H:224:ALA:HA	16:H:229:VAL:HA	1.92	0.51
3:D:3:ARG:HE	3:D:10:ILE:HG21	1.76	0.51
11:R:155:ALA:O	15:V:81:ARG:NH1	2.43	0.51
15:V:29:THR:HG21	15:V:85:TYR:HB3	1.92	0.51
10:A:88:LEU:HB3	10:A:92:GLY:HA3	1.93	0.51
3:D:224:GLY:HA3	3:D:295:ARG:HD2	1.92	0.51
3:D:717:TRP:HB2	3:D:759:TYR:HB2	1.92	0.51
4:E:99:LEU:HD23	4:E:102:GLU:OE1	2.11	0.51
6:G:37:TRP:HB3	6:G:75:ALA:HA	1.92	0.51
7:O:17:LEU:HA	16:Q:41:ARG:O	2.11	0.51
13:T:13:GLY:O	13:T:17:LEU:HG	2.10	0.51
1:1:357:THR:HG23	1:1:360:ARG:NH2	2.26	0.51
2:2:61:MET:CE	3:3:214:MET:HG3	2.41	0.51
3:3:237:ASP:OD1	3:3:239:THR:HG22	2.11	0.51
3:3:243:ARG:HB3	3:3:275:LEU:HD22	1.91	0.51
13:L:287:GLY:HA3	13:L:528:SER:HB2	1.93	0.51
15:N:228:ALA:HB1	15:N:233:LEU:CD1	2.40	0.51
16:H:48:PRO:C	16:H:50:ARG:H	2.14	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
16:H:139:SER:OG	16:H:232:TYR:HA	2.11	0.51
1:B:270:THR:O	1:B:311:MET:HG3	2.11	0.51
13:T:298:SER:O	13:T:302:GLN:HG2	2.11	0.51
13:T:458:TYR:HD1	13:T:461:LEU:HD21	1.76	0.51
1:1:241:MET:SD	1:1:249:MET:HB3	2.51	0.50
3:3:135:VAL:O	5:5:188:SER:HB2	2.10	0.50
14:M:426:ALA:N	14:M:429:GLU:OE1	2.37	0.50
16:H:169:ALA:HB1	16:H:206:TYR:HB2	1.91	0.50
3:D:190:TYR:O	3:D:195:PRO:HD2	2.11	0.50
3:D:322:TRP:CH2	3:D:635:GLU:HB2	2.46	0.50
4:E:224:ILE:HD11	4:E:275:ARG:CZ	2.41	0.50
5:F:16:PRO:HD2	5:F:28:VAL:HG13	1.92	0.50
5:F:160:ARG:HB2	5:F:163:ARG:HH21	1.76	0.50
13:T:12:LEU:O	13:T:16:LEU:HG	2.11	0.50
16:Q:221:LEU:N	16:Q:222:PRO:HA	2.26	0.50
1:1:74:LEU:HD12	1:1:77:SER:OG	2.11	0.50
3:3:370:ASP:OD2	3:3:558:TRP:HD1	1.94	0.50
4:4:42:ARG:HD2	4:4:61:TYR:OH	2.11	0.50
6:6:157:LYS:HA	6:6:162:ALA:HB2	1.93	0.50
14:M:91:VAL:HG23	14:M:92:GLU:H	1.76	0.50
1:B:90:ILE:HB	1:B:218:ILE:HG12	1.92	0.50
3:D:2:VAL:HG13	3:D:89:ASP:HA	1.92	0.50
3:D:688:ARG:HB3	3:D:770:ARG:HB2	1.92	0.50
6:G:119:ASN:HA	6:G:125:GLN:NE2	2.26	0.50
6:G:135:VAL:HG21	6:G:154:LEU:HB2	1.93	0.50
1:1:201:LEU:HD21	3:3:84:VAL:HB	1.93	0.50
5:5:53:VAL:HG13	5:5:71:VAL:HB	1.92	0.50
13:L:411:VAL:HG23	13:L:500:VAL:HG13	1.91	0.50
15:N:10:SER:HB3	15:N:90:TYR:HE1	1.75	0.50
15:N:23:GLN:HB3	15:N:27:ARG:NH2	2.27	0.50
15:N:93:LEU:O	15:N:96:HIS:HB3	2.11	0.50
3:D:192:GLU:HG3	3:D:440:ARG:HH11	1.76	0.50
3:D:305:ARG:HH22	3:D:605:PRO:HA	1.74	0.50
3:D:690:GLY:HA3	3:D:770:ARG:HH21	1.76	0.50
6:G:35:SER:OG	16:Q:62:ASP:HA	2.11	0.50
16:Q:227:GLU:HG2	16:Q:228:LEU:N	2.26	0.50
3:3:136:GLU:HG2	5:5:186:GLY:O	2.10	0.50
3:3:501:LYS:H	3:3:501:LYS:HD2	1.76	0.50
4:4:32:PRO:HB2	6:6:88:MET:HE1	1.92	0.50
4:4:239:LEU:HG	4:4:244:VAL:HB	1.93	0.50
10:A:81:TYR:HB2	11:J:132:TYR:CZ	2.46	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:K:21:ARG:CZ	12:K:26:LEU:HD23	2.41	0.50
14:M:241:PHE:HA	14:M:245:ALA:HB3	1.93	0.50
16:H:308:PHE:O	16:H:312:PHE:HB3	2.11	0.50
3:D:283:PRO:HA	3:D:287:GLU:HA	1.92	0.50
3:D:416:PHE:HE2	3:D:448:MET:HB3	1.77	0.50
4:E:46:THR:O	4:E:53:LEU:HB2	2.12	0.50
11:R:19:VAL:HG23	11:R:28:ALA:O	2.12	0.50
13:T:380:SER:HB3	13:T:457:GLY:H	1.76	0.50
15:V:63:THR:HG21	15:V:96:HIS:ND1	2.25	0.50
3:3:34:CYS:HB3	3:3:45:CYS:SG	2.51	0.50
4:4:211:SER:OG	4:4:215:TYR:HB2	2.12	0.50
5:5:155:THR:HG23	9:W:93:VAL:HB	1.93	0.50
5:5:170:PHE:CE2	7:9:61:ALA:HA	2.45	0.50
3:D:18:SER:HB2	3:D:435:LEU:HG	1.94	0.50
6:G:59:ASP:OD1	6:G:59:ASP:N	2.44	0.50
6:G:154:LEU:O	6:G:158:VAL:HG13	2.12	0.50
12:S:1:MET:HG3	12:S:5:LEU:HD11	1.93	0.50
13:T:433:HIS:ND1	13:T:437:GLU:OE2	2.38	0.50
3:3:439:GLU:HG2	3:3:440:ARG:HG2	1.93	0.50
4:4:225:PRO:HG3	4:4:383:TYR:OH	2.12	0.50
7:9:42:VAL:HA	7:9:136:MET:O	2.11	0.50
14:M:56:LEU:HB3	14:M:59:ALA:HB3	1.94	0.50
14:M:381:LEU:HB2	14:M:396:PHE:CZ	2.46	0.50
16:H:205:VAL:HG21	16:H:317:ALA:HB2	1.94	0.50
3:D:561:PRO:HB3	3:D:575:GLU:O	2.12	0.50
3:D:586:HIS:CE1	3:D:640:VAL:HG21	2.46	0.50
4:E:211:SER:HB2	4:E:215:TYR:N	2.27	0.50
11:R:44:VAL:HG22	11:R:49:ARG:HA	1.93	0.50
13:T:291:ILE:HA	13:T:294:ILE:HG22	1.92	0.50
15:V:76:LEU:HD12	15:V:206:PRO:HB3	1.94	0.50
1:1:201:LEU:HA	1:1:399:PHE:HZ	1.77	0.50
1:1:395:GLU:HB2	1:1:407:VAL:HG21	1.94	0.50
11:J:39:LEU:HD11	12:K:40:LEU:HD13	1.93	0.50
14:M:53:ALA:HB3	14:M:63:TRP:HB2	1.94	0.50
1:B:97:GLU:OE2	1:B:296:SER:N	2.42	0.50
11:R:124:PRO:HA	11:R:127:LEU:HB2	1.94	0.50
14:U:95:PHE:HB3	14:U:136:TYR:CE2	2.47	0.50
15:V:422:ALA:O	15:V:423:LEU:HD23	2.12	0.50
16:Q:6:PRO:HG2	16:Q:112:GLN:NE2	2.27	0.50
2:2:85:THR:OG1	2:2:124:CYS:N	2.45	0.50
3:3:29:ASP:OD1	3:3:29:ASP:N	2.45	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:4:158:ASP:OD2	6:6:57:ARG:NH1	2.36	0.50
16:H:6:PRO:HG2	16:H:112:GLN:NE2	2.27	0.50
3:D:538:ALA:HB3	3:D:541:ALA:HB2	1.94	0.50
3:D:700:LYS:N	3:D:703:GLN:OE1	2.31	0.50
5:F:175:THR:HG22	5:F:178:ASP:HB2	1.94	0.50
13:T:238:ALA:HB2	13:T:333:PHE:HB3	1.94	0.50
13:T:356:TRP:CE3	13:T:363:ARG:HD2	2.47	0.50
13:T:366:ALA:HB1	13:T:420:TRP:CZ3	2.46	0.50
15:V:203:SER:HB2	15:V:208:VAL:HG22	1.93	0.50
15:V:317:ARG:HH12	15:V:383:PHE:C	2.15	0.50
16:Q:35:GLU:OE2	16:Q:294:ARG:NE	2.37	0.50
16:Q:274:VAL:CG2	16:Q:275:PRO:HD2	2.41	0.50
4:4:84:ARG:HG3	4:4:169:HIS:CE1	2.46	0.50
6:6:37:TRP:NE1	6:6:67:VAL:HB	2.25	0.50
1:B:91:CYS:SG	1:B:221:VAL:HG22	2.51	0.50
8:I:82:ILE:HG23	8:I:95:ALA:HB3	1.93	0.50
1:1:223:THR:O	1:1:227:VAL:HG23	2.11	0.49
10:A:68:PHE:CD2	16:H:164:LEU:HB2	2.47	0.49
11:J:40:ALA:O	11:J:44:VAL:HG23	2.12	0.49
13:L:59:TRP:HE1	14:M:447:PRO:HD2	1.76	0.49
13:L:163:ARG:HE	14:M:399:VAL:HB	1.77	0.49
16:H:327:VAL:HG21	16:H:337:LEU:HD21	1.94	0.49
2:C:87:SER:HB2	19:C:201:FES:S2	2.51	0.49
3:D:451:PHE:CD1	3:D:466:GLU:HB3	2.47	0.49
4:E:341:GLU:HG2	4:E:358:VAL:HG22	1.94	0.49
6:G:69:ARG:HD3	6:G:74:GLN:OE1	2.12	0.49
13:T:285:ALA:O	13:T:294:ILE:HG13	2.12	0.49
13:T:554:PHE:HE2	14:U:278:ALA:HA	1.77	0.49
3:3:125:GLY:HA2	3:3:245:ARG:HH21	1.77	0.49
3:3:410:HIS:CD2	3:3:411:LEU:HD23	2.46	0.49
4:4:200:ARG:NH1	7:9:16:TYR:OH	2.45	0.49
10:A:111:TRP:CH2	16:H:307:ARG:HG2	2.47	0.49
13:L:104:PHE:HE2	13:L:108:PHE:HE2	1.59	0.49
13:L:139:PHE:CE2	14:M:407:LEU:HD13	2.47	0.49
15:N:14:THR:HA	15:N:86:LEU:HD21	1.95	0.49
3:D:185:LYS:O	3:D:189:ARG:HB2	2.12	0.49
6:G:76:ASP:CG	16:Q:65:LYS:HZ3	2.15	0.49
13:T:437:GLU:O	13:T:439:PRO:HD3	2.12	0.49
16:Q:159:LEU:O	16:Q:163:GLU:HB2	2.12	0.49
16:Q:342:ALA:O	16:Q:346:LEU:HG	2.12	0.49
1:1:275:LEU:HA	1:1:279:TRP:HD1	1.77	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:2:101:THR:HG23	2:2:106:ILE:O	2.12	0.49
13:L:41:PHE:HB2	13:L:81:THR:HB	1.95	0.49
16:Q:83:VAL:O	16:Q:86:PRO:HD2	2.12	0.49
1:1:438:ARG:OXT	2:2:146:THR:OG1	2.30	0.49
3:3:375:THR:HB	3:3:512:LEU:O	2.13	0.49
3:3:405:GLU:HG2	3:3:696:PRO:HB2	1.94	0.49
3:3:694:LEU:HD12	3:3:769:LEU:HB2	1.95	0.49
10:A:107:PHE:HA	10:A:110:GLU:HG2	1.93	0.49
13:L:163:ARG:HD3	14:M:399:VAL:O	2.11	0.49
15:N:272:ALA:O	15:N:276:GLY:N	2.44	0.49
16:H:137:PHE:HA	16:H:152:SER:HB2	1.94	0.49
4:E:248:VAL:HB	4:E:347:GLU:HB2	1.94	0.49
6:G:62:ARG:CZ	7:O:25:PRO:HA	2.43	0.49
10:P:66:MET:HG3	12:S:69:ALA:HB1	1.94	0.49
10:P:76:ALA:HA	10:P:79:TRP:CE3	2.48	0.49
10:P:76:ALA:HA	10:P:79:TRP:HE3	1.77	0.49
11:R:69:PHE:HZ	16:Q:156:SER:HG	1.59	0.49
12:S:46:ALA:O	12:S:50:GLY:N	2.44	0.49
14:U:194:PHE:CZ	14:U:253:PHE:HB2	2.47	0.49
15:V:52:PRO:HB3	15:V:103:HIS:HB2	1.95	0.49
3:3:48:CYS:SG	3:3:83:CYS:N	2.85	0.49
11:J:75:PHE:CZ	11:J:78:GLN:HG2	2.47	0.49
12:K:55:VAL:O	12:K:59:MET:HG2	2.12	0.49
14:M:16:LEU:HD12	14:M:25:GLY:HA3	1.94	0.49
16:H:99:LEU:HD12	16:H:116:ILE:HG13	1.93	0.49
1:B:106:ILE:HD11	1:B:251:LEU:HD21	1.94	0.49
2:C:109:GLY:O	8:I:121:ARG:NH2	2.46	0.49
3:D:29:ASP:OD2	5:F:187:GLY:N	2.25	0.49
16:Q:45:ARG:HG2	16:Q:46:MET:N	2.26	0.49
2:2:9:ASP:N	2:2:9:ASP:OD1	2.44	0.49
3:3:290:ILE:HG23	17:3:803:SF4:S4	2.53	0.49
4:4:211:SER:O	4:4:215:TYR:HB2	2.12	0.49
6:6:138:PRO:O	6:6:142:PRO:HB3	2.12	0.49
13:L:335:ALA:O	13:L:339:VAL:HG23	2.13	0.49
2:C:24:ARG:HH21	2:C:59:GLU:HB3	1.77	0.49
2:C:97:TRP:CH2	2:C:119:VAL:HB	2.48	0.49
3:D:5:LYS:O	3:D:93:VAL:N	2.28	0.49
3:D:225:ASN:HD21	3:D:289:TRP:HB3	1.77	0.49
14:U:93:GLY:O	14:U:136:TYR:OH	2.21	0.49
2:2:79:HIS:N	2:2:137:ASN:OD1	2.43	0.49
4:4:84:ARG:NE	4:4:169:HIS:HB3	2.28	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:6:101:ASP:OD2	10:A:35:LYS:HB2	2.12	0.49
13:L:7:ILE:O	13:L:10:PRO:HD2	2.13	0.49
15:N:343:TRP:NE1	15:N:416:PRO:HG3	2.28	0.49
1:B:50:PRO:HA	1:B:53:VAL:HG12	1.94	0.49
3:D:34:CYS:SG	3:D:35:SER:N	2.85	0.49
11:R:59:TYR:CE2	12:S:61:ILE:HG12	2.47	0.49
14:U:316:ALA:O	14:U:320:VAL:HG23	2.12	0.49
3:3:717:TRP:HB3	3:3:753:VAL:HG21	1.95	0.49
13:L:173:MET:HB3	14:M:378:PHE:HZ	1.77	0.49
4:E:98:ALA:O	4:E:102:GLU:HG3	2.12	0.49
6:G:69:ARG:NH2	16:Q:223:GLU:OE2	2.45	0.49
13:T:354:GLY:HA3	13:T:428:GLU:O	2.13	0.49
14:U:335:ARG:NH1	14:U:423:LYS:O	2.45	0.49
15:V:257:LEU:HD23	15:V:258:LEU:HD23	1.94	0.49
3:3:118:ASP:OD2	3:3:166:LYS:NZ	2.26	0.49
5:5:145:PRO:HA	5:5:150:TYR:CD1	2.48	0.49
13:L:24:MET:SD	13:L:28:LEU:HD23	2.52	0.49
13:L:59:TRP:NE1	14:M:447:PRO:HD2	2.28	0.49
14:M:359:LEU:O	14:M:363:LEU:HG	2.13	0.49
5:F:55:LEU:HB2	5:F:69:ALA:O	2.13	0.49
13:T:141:LEU:HB3	13:T:236:VAL:HG11	1.94	0.49
14:U:46:GLY:HA2	14:U:68:ASP:HA	1.95	0.49
2:2:161:LYS:HB3	2:2:166:ILE:HG12	1.94	0.49
12:K:28:PHE:CZ	12:K:68:VAL:HA	2.48	0.49
1:B:259:LYS:HG3	2:C:179:VAL:O	2.12	0.49
3:D:405:GLU:HG2	3:D:696:PRO:HB2	1.95	0.49
4:E:87:TYR:HB3	6:G:45:CYS:HB3	1.94	0.49
5:F:15:TYR:OH	5:F:37:GLU:HG3	2.13	0.49
6:G:30:TRP:CH2	16:Q:51:VAL:CG1	2.96	0.49
6:G:60:LEU:O	6:G:65:SER:HB2	2.13	0.49
6:G:91:VAL:HG13	10:P:46:SER:HB3	1.95	0.49
11:R:61:GLY:O	11:R:65:VAL:HG21	2.13	0.49
16:Q:71:ASP:HB2	16:Q:238:SER:HB3	1.94	0.49
3:3:42:ILE:HD12	3:3:42:ILE:O	2.12	0.48
3:3:290:ILE:HB	3:3:295:ARG:HH21	1.78	0.48
11:J:53:PHE:CE2	16:H:120:LEU:HB2	2.48	0.48
13:L:490:GLU:HG3	13:L:491:TRP:N	2.26	0.48
16:H:237:SER:OG	16:H:238:SER:N	2.44	0.48
3:D:360:LEU:O	3:D:364:LEU:N	2.40	0.48
13:T:187:GLU:O	13:T:190:GLU:HG2	2.13	0.48
14:U:232:THR:HA	14:U:235:LYS:NZ	2.28	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
15:V:283:PHE:O	15:V:287:THR:HG23	2.13	0.48
16:Q:118:LEU:O	16:Q:181:ASN:ND2	2.45	0.48
16:Q:218:PRO:C	16:Q:220:ASP:H	2.17	0.48
1:1:357:THR:HA	1:1:360:ARG:NH1	2.28	0.48
3:3:557:SER:H	3:3:560:GLU:HB2	1.78	0.48
6:6:35:SER:O	16:H:65:LYS:HD2	2.14	0.48
6:6:91:VAL:O	6:6:95:VAL:HG23	2.13	0.48
6:6:163:TYR:HD1	7:9:152:ARG:HD2	1.75	0.48
11:J:24:ASN:HB3	11:J:27:HIS:HB2	1.94	0.48
14:M:115:LEU:HD11	14:M:248:LEU:CD2	2.44	0.48
3:D:413:LEU:HA	3:D:416:PHE:HB3	1.95	0.48
6:G:163:TYR:CD1	7:O:152:ARG:HD2	2.48	0.48
8:I:86:LEU:HB2	8:I:91:ILE:HB	1.95	0.48
16:Q:41:ARG:NH1	16:Q:47:GLY:H	2.10	0.48
3:3:465:HIS:N	3:3:489:MET:SD	2.82	0.48
4:4:53:LEU:O	4:4:386:LYS:HG3	2.13	0.48
4:4:87:TYR:CB	6:6:45:CYS:HB3	2.44	0.48
7:9:149:GLU:O	7:9:153:THR:OG1	2.17	0.48
14:M:93:GLY:O	14:M:136:TYR:OH	2.16	0.48
15:N:233:LEU:HD21	15:N:273:LEU:HB3	1.94	0.48
16:H:40:ALA:HB2	16:H:45:ARG:HH21	1.77	0.48
16:H:224:ALA:HB2	16:H:233:HIS:CE1	2.48	0.48
3:D:476:ILE:O	3:D:480:LEU:HG	2.13	0.48
6:G:120:ASN:ND2	6:G:122:ALA:H	2.02	0.48
6:G:130:VAL:HG13	9:X:120:PRO:O	2.13	0.48
13:T:267:SER:HB3	13:T:311:GLY:O	2.14	0.48
1:1:394:ILE:HG22	1:1:403:ALA:HB1	1.95	0.48
5:5:68:PHE:HB3	5:5:124:ILE:HD11	1.95	0.48
10:A:22:VAL:O	10:A:26:LEU:HG	2.12	0.48
13:L:58:GLU:HG3	14:M:452:ARG:HH22	1.78	0.48
13:L:264:PRO:HA	13:L:397:PHE:HE1	1.78	0.48
14:M:327:LEU:O	14:M:331:ARG:HG2	2.13	0.48
1:B:292:PRO:HA	1:B:328:VAL:HG13	1.95	0.48
3:D:125:GLY:HA2	3:D:245:ARG:NH2	2.26	0.48
3:D:353:GLU:CD	3:D:637:ALA:HB3	2.34	0.48
13:T:515:LYS:HA	13:T:517:PHE:CE2	2.48	0.48
3:3:165:ASP:HB2	8:7:66:PRO:HG2	1.93	0.48
3:3:688:ARG:HD3	3:3:688:ARG:HA	1.52	0.48
4:4:131:VAL:O	4:4:135:THR:HG23	2.14	0.48
5:5:121:LEU:O	5:5:144:HIS:HB3	2.13	0.48
5:5:138:PRO:HG2	5:5:141:LEU:HD13	1.96	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:A:71:PHE:O	10:A:75:VAL:HG23	2.13	0.48
13:L:291:ILE:HG13	13:L:292:LYS:N	2.29	0.48
15:N:95:MET:SD	15:N:214:SER:HB3	2.54	0.48
15:N:216:LYS:HZ3	15:N:266:ALA:HB2	1.79	0.48
15:N:245:ASN:OD1	15:N:374:TYR:OH	2.31	0.48
16:H:70:GLU:HG3	16:H:70:GLU:O	2.14	0.48
4:E:144:THR:HG22	4:E:148:TYR:HE1	1.78	0.48
13:T:240:ILE:HG22	13:T:241:HIS:HD2	1.78	0.48
13:T:463:HIS:CG	13:T:464:PRO:HD3	2.47	0.48
14:U:91:VAL:HB	14:U:95:PHE:CE1	2.48	0.48
16:Q:300:LEU:O	16:Q:301:ARG:HG2	2.13	0.48
1:1:290:ILE:HD12	1:1:292:PRO:HD3	1.95	0.48
6:6:28:VAL:O	6:6:32:ARG:HG3	2.14	0.48
6:6:115:GLY:HA2	6:6:125:GLN:HA	1.95	0.48
9:W:6:MET:HG3	9:W:9:ALA:HB3	1.94	0.48
3:D:386:SER:HB2	3:D:675:ARG:NH1	2.28	0.48
3:D:732:ALA:O	3:D:747:VAL:HG23	2.14	0.48
4:E:118:VAL:O	4:E:122:GLU:HG2	2.13	0.48
4:E:152:GLU:OE2	4:E:204:TYR:OH	2.31	0.48
4:E:162:TRP:NE1	7:O:34:LYS:HD2	2.28	0.48
10:P:23:ALA:O	10:P:27:VAL:HG23	2.14	0.48
12:S:19:LEU:HD22	13:T:591:LEU:HD12	1.95	0.48
12:S:95:GLY:HA2	15:V:256:ARG:NE	2.29	0.48
15:V:224:LEU:HD22	15:V:276:GLY:HA2	1.94	0.48
4:4:185:GLU:O	4:4:189:GLU:HG2	2.13	0.48
4:4:379:GLN:O	4:4:382:PRO:HD2	2.13	0.48
6:6:62:ARG:O	16:H:48:PRO:HB3	2.12	0.48
8:7:86:LEU:HD12	8:7:91:ILE:HD12	1.96	0.48
9:W:28:GLU:O	9:W:88:ARG:NH2	2.42	0.48
13:L:298:SER:O	13:L:302:GLN:HG2	2.14	0.48
13:L:437:GLU:O	13:L:439:PRO:HD3	2.13	0.48
14:M:345:ARG:HG2	14:M:412:LYS:O	2.13	0.48
1:B:81:LYS:HE3	1:B:126:ARG:HH12	1.78	0.48
6:G:40:THR:HB	6:G:68:PHE:HZ	1.77	0.48
14:U:53:ALA:HB3	14:U:63:TRP:HB2	1.95	0.48
14:U:411:GLN:HA	14:U:415:TRP:HB2	1.95	0.48
16:Q:274:VAL:CG1	16:Q:278:TRP:CD1	2.90	0.48
1:1:400:CYS:HG	17:1:501:SF4:FE3	1.29	0.48
3:3:368:HIS:HB3	3:3:556:ALA:H	1.79	0.48
3:3:504:VAL:HG12	3:3:506:ILE:HG13	1.95	0.48
6:6:73:ARG:NH1	10:A:40:LYS:O	2.44	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:L:167:LEU:HD21	14:M:396:PHE:HB3	1.95	0.48
14:M:190:ALA:HB1	14:M:249:ALA:HB1	1.96	0.48
16:H:181:ASN:O	16:H:185:ILE:HG13	2.14	0.48
1:B:6:LEU:HD11	1:B:240:GLN:HE21	1.78	0.48
1:B:223:THR:O	1:B:227:VAL:HG23	2.14	0.48
10:P:48:ASN:OD1	10:P:49:ASP:HB2	2.13	0.48
13:T:604:MET:HG2	15:V:232:ALA:HB2	1.95	0.48
14:U:194:PHE:HB2	14:U:249:ALA:HB3	1.94	0.48
14:U:335:ARG:HH12	14:U:424:ASP:C	2.16	0.48
1:1:189:MET:O	1:1:193:GLU:HB2	2.14	0.48
15:N:280:ALA:CB	15:N:347:LEU:HB3	2.43	0.48
1:B:251:LEU:HD12	1:B:265:GLU:HG3	1.95	0.48
6:G:55:ASP:O	6:G:59:ASP:HB3	2.13	0.48
13:T:314:ALA:HB1	13:T:317:VAL:HB	1.96	0.48
14:U:84:LEU:HB3	14:U:432:PHE:CD1	2.49	0.48
6:6:60:LEU:HD21	6:6:151:VAL:HG11	1.96	0.48
15:N:77:VAL:HG12	15:N:85:TYR:HE1	1.78	0.48
15:N:283:PHE:O	15:N:287:THR:HG23	2.14	0.48
16:H:310:TRP:CE3	16:H:314:PHE:HE2	2.32	0.48
7:O:6:LEU:HB3	16:Q:297:TRP:HZ2	1.79	0.48
9:X:24:LEU:HD22	9:X:55:LYS:HE3	1.96	0.48
13:T:72:LEU:HB3	13:T:255:ARG:NH1	2.29	0.48
2:2:61:MET:HE1	3:3:214:MET:HG3	1.96	0.47
3:3:223:SER:O	3:3:226:ILE:HG12	2.14	0.47
4:4:171:ASN:OD1	4:4:174:ARG:NH1	2.38	0.47
4:4:265:PRO:HG2	4:4:282:GLU:HG2	1.96	0.47
4:4:311:PRO:HD3	4:4:330:HIS:CE1	2.49	0.47
13:L:128:PHE:CE1	13:L:166:ASP:HB3	2.48	0.47
13:L:302:GLN:O	13:L:306:MET:HG3	2.14	0.47
13:L:313:GLY:HA2	13:L:315:TYR:CZ	2.49	0.47
13:L:394:THR:HB	13:L:484:HIS:O	2.13	0.47
13:L:490:GLU:O	13:L:494:ILE:HG12	2.13	0.47
1:B:189:MET:HB3	1:B:211:LEU:HD13	1.95	0.47
3:D:33:PHE:CZ	3:D:130:LEU:HA	2.49	0.47
11:R:22:LEU:HD13	11:R:27:HIS:HB3	1.94	0.47
13:T:90:TYR:CG	13:T:334:LEU:HD13	2.48	0.47
14:U:232:THR:HA	14:U:235:LYS:HZ2	1.79	0.47
16:Q:70:GLU:O	16:Q:70:GLU:HG3	2.13	0.47
3:3:175:ILE:O	3:3:235:LEU:HA	2.14	0.47
3:3:476:ILE:O	3:3:480:LEU:HG	2.15	0.47
3:3:616:ASN:ND2	3:3:622:LEU:HD11	2.28	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:A:83:VAL:HG23	10:A:84:SER:H	1.79	0.47
1:B:365:GLY:O	1:B:369:ASN:ND2	2.47	0.47
3:D:594:ALA:O	3:D:598:ALA:HB3	2.14	0.47
3:D:688:ARG:HD3	3:D:688:ARG:HA	1.52	0.47
6:G:39:ALA:N	6:G:77:VAL:O	2.34	0.47
6:G:148:ILE:O	6:G:151:VAL:HG22	2.13	0.47
3:3:47:MET:HE1	3:3:108:VAL:N	2.30	0.47
3:3:550:LEU:HD22	3:3:684:ARG:HH21	1.79	0.47
3:3:585:MET:HB3	3:3:587:LEU:HD13	1.95	0.47
5:5:102:PRO:HA	5:5:127:GLU:HB2	1.95	0.47
13:L:166:ASP:O	13:L:170:MET:HG3	2.14	0.47
15:N:61:VAL:O	15:N:65:LEU:HG	2.14	0.47
3:D:406:ALA:O	3:D:409:LEU:HB2	2.14	0.47
3:D:587:LEU:O	3:D:604:ALA:N	2.44	0.47
4:E:156:ILE:O	4:E:159:LEU:HB2	2.15	0.47
7:O:94:ASN:OD1	7:O:97:ARG:N	2.47	0.47
13:T:349:VAL:HG13	13:T:423:LEU:HB3	1.97	0.47
15:V:198:ASP:OD1	15:V:256:ARG:NH2	2.47	0.47
1:1:4:PRO:O	1:1:5:ILE:HG13	2.15	0.47
2:2:79:HIS:H	2:2:137:ASN:CG	2.17	0.47
4:4:337:PRO:O	4:4:361:GLY:HA2	2.14	0.47
9:W:122:ASP:O	9:W:125:ILE:HG12	2.14	0.47
11:J:80:GLU:HB2	11:J:83:PHE:CE2	2.49	0.47
13:L:444:TRP:O	13:L:447:HIS:HB2	2.14	0.47
14:M:186:GLN:HG2	14:M:187:GLU:H	1.79	0.47
15:N:194:PHE:O	15:N:197:PRO:HD2	2.14	0.47
3:D:32:LEU:HD11	3:D:35:SER:HB2	1.96	0.47
3:D:307:LYS:HE3	3:D:632:GLY:HA2	1.96	0.47
4:E:84:ARG:CZ	4:E:169:HIS:HB3	2.44	0.47
4:E:86:ASP:HB2	4:E:406:ASP:OD2	2.15	0.47
14:U:232:THR:HG21	14:U:322:THR:HG21	1.96	0.47
16:Q:133:VAL:HG11	16:Q:160:ILE:HG13	1.96	0.47
3:3:193:GLU:HB3	3:3:418:ARG:HH12	1.79	0.47
3:3:347:HIS:HB2	3:3:538:ALA:HB1	1.97	0.47
3:3:505:LEU:O	3:3:532:VAL:HA	2.14	0.47
11:J:63:ILE:HG23	12:K:68:VAL:HG11	1.95	0.47
13:L:26:GLU:O	13:L:29:PRO:HD2	2.13	0.47
13:L:461:LEU:N	13:L:467:ASN:OD1	2.47	0.47
14:M:91:VAL:HB	14:M:95:PHE:HE1	1.79	0.47
14:M:232:THR:HA	14:M:235:LYS:NZ	2.30	0.47
14:M:281:PHE:CE1	14:M:341:ILE:HG22	2.48	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
16:H:39:LEU:O	16:H:43:GLN:CG	2.62	0.47
3:D:734:VAL:HG13	3:D:775:VAL:HG13	1.96	0.47
6:G:153:GLN:HG3	7:O:124:TYR:CZ	2.49	0.47
13:T:41:PHE:HD2	13:T:42:LEU:HD12	1.79	0.47
13:T:302:GLN:O	13:T:306:MET:HG3	2.14	0.47
13:T:355:LEU:HB3	13:T:359:LEU:HD12	1.96	0.47
16:Q:40:ALA:HB2	16:Q:45:ARG:HH21	1.79	0.47
16:Q:44:VAL:O	16:Q:45:ARG:O	2.32	0.47
16:Q:169:ALA:HB2	16:Q:205:VAL:HG23	1.97	0.47
3:3:190:TYR:O	3:3:195:PRO:HD2	2.15	0.47
4:4:115:THR:O	4:4:119:ILE:HG13	2.14	0.47
16:H:189:GLN:O	16:H:193:GLY:HA2	2.14	0.47
16:H:255:ALA:O	16:H:259:ILE:HG13	2.14	0.47
4:E:310:THR:HG22	4:E:311:PRO:O	2.15	0.47
6:G:163:TYR:H	7:O:152:ARG:NH1	2.13	0.47
8:I:58:SER:HB3	8:I:69:LEU:HD23	1.96	0.47
11:R:68:LEU:HD13	16:Q:137:PHE:HZ	1.78	0.47
12:S:28:PHE:CE2	12:S:68:VAL:HA	2.50	0.47
14:U:332:LEU:HA	14:U:335:ARG:HG2	1.96	0.47
1:1:26:SER:HA	1:1:31:TYR:CG	2.49	0.47
3:3:165:ASP:OD2	3:3:168:HIS:HB2	2.14	0.47
3:3:375:THR:HG21	3:3:512:LEU:HB3	1.96	0.47
3:3:689:LYS:H	3:3:689:LYS:HG2	1.52	0.47
4:4:62:LEU:HB2	4:4:408:ASP:OD2	2.15	0.47
4:4:87:TYR:CG	6:6:45:CYS:HB3	2.50	0.47
6:6:96:TRP:HZ2	6:6:175:ALA:HB1	1.79	0.47
9:W:49:LEU:HD12	9:W:57:LEU:O	2.15	0.47
13:L:9:LEU:HB2	13:L:10:PRO:HD3	1.97	0.47
13:L:355:LEU:HB3	13:L:359:LEU:HD12	1.97	0.47
14:M:119:TYR:OH	14:M:160:LEU:HB2	2.14	0.47
15:N:259:ALA:O	15:N:263:ILE:HG13	2.14	0.47
1:B:195:LEU:HD23	2:C:24:ARG:HH12	1.80	0.47
1:B:250:LYS:HB3	1:B:252:TYR:CE1	2.50	0.47
2:C:24:ARG:NH2	2:C:59:GLU:HB3	2.29	0.47
3:D:191:PHE:HE2	3:D:226:ILE:HD13	1.79	0.47
4:E:38:HIS:CE1	4:E:397:ILE:HG22	2.50	0.47
4:E:47:LEU:HD22	4:E:52:VAL:HA	1.95	0.47
4:E:372:ALA:HB3	4:E:375:PHE:HB2	1.95	0.47
5:F:38:MET:HA	5:F:41:TYR:HD2	1.80	0.47
6:G:56:ALA:HB3	16:Q:44:VAL:HG11	1.95	0.47
10:P:7:TYR:HD2	11:R:44:VAL:HG11	1.79	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:R:88:ARG:O	11:R:91:PRO:HD2	2.15	0.47
13:T:53:ALA:HB3	13:T:69:LEU:HB3	1.97	0.47
13:T:312:VAL:HA	13:T:397:PHE:CD2	2.50	0.47
13:T:413:THR:HA	13:T:416:TYR:CZ	2.50	0.47
15:V:376:LEU:O	15:V:380:LEU:N	2.37	0.47
16:Q:260:PRO:HG3	16:Q:286:PHE:CD2	2.50	0.47
1:1:157:TYR:O	1:1:158:LEU:HD23	2.15	0.47
3:3:259:CYS:SG	3:3:261:VAL:HG22	2.55	0.47
13:L:10:PRO:HB2	13:L:109:ASN:O	2.15	0.47
13:L:291:ILE:HD12	13:L:336:SER:HB3	1.97	0.47
14:M:33:PHE:HA	14:M:79:ALA:HB1	1.97	0.47
14:M:127:ILE:O	14:M:130:LEU:HG	2.15	0.47
14:M:371:LEU:HD12	14:M:440:LEU:HB3	1.96	0.47
15:N:120:ALA:O	15:N:123:THR:OG1	2.25	0.47
3:D:481:LEU:HD11	3:D:520:ARG:HB3	1.97	0.47
3:D:723:ALA:O	3:D:727:ALA:N	2.47	0.47
16:Q:333:PRO:HB2	16:Q:335:THR:H	1.79	0.47
4:4:148:TYR:HE2	7:9:16:TYR:CG	2.33	0.47
4:4:379:GLN:NE2	5:5:110:SER:HA	2.29	0.47
7:9:108:CYS:HA	17:9:202:SF4:S3	2.55	0.47
16:H:326:LEU:HD12	16:H:330:LEU:HD23	1.97	0.47
1:B:167:PHE:CE2	1:B:169:PHE:HB2	2.50	0.47
3:D:115:HIS:HB3	4:E:321:MET:CE	2.41	0.47
16:Q:107:SER:OG	16:Q:113:PRO:HG3	2.15	0.47
1:1:343:ASN:HA	1:1:346:ARG:HG2	1.97	0.47
8:7:44:MET:HE2	8:7:46:ARG:HH22	1.80	0.47
10:A:71:PHE:O	10:A:74:GLU:HB3	2.15	0.47
11:J:59:TYR:HE2	12:K:61:ILE:HG12	1.77	0.47
12:K:56:ALA:HA	15:N:105:LEU:HD13	1.96	0.47
14:M:148:PHE:HE1	14:M:204:LYS:HZ3	1.62	0.47
16:H:71:ASP:HB2	16:H:238:SER:HB3	1.97	0.47
1:B:272:PHE:CZ	1:B:316:LEU:HD21	2.50	0.47
1:B:373:LYS:NZ	1:B:383:ASP:OD1	2.46	0.47
4:E:385:CYS:HB3	4:E:396:ILE:HG21	1.96	0.47
9:X:36:ASP:OD1	9:X:36:ASP:N	2.48	0.47
14:U:127:ILE:HB	14:U:128:PRO:HD3	1.96	0.47
14:U:159:MET:HG3	14:U:197:PHE:CD1	2.50	0.47
15:V:98:LEU:HD12	15:V:107:MET:HG2	1.96	0.47
15:V:319:ASP:HB3	15:V:322:LEU:HB2	1.97	0.47
3:3:616:ASN:HD22	3:3:622:LEU:HD11	1.80	0.46
11:J:113:LEU:HD21	12:K:49:TYR:OH	2.15	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:K:70:VAL:HG21	15:N:116:LEU:HD22	1.97	0.46
13:L:515:LYS:HA	13:L:517:PHE:CZ	2.49	0.46
1:B:380:GLU:N	1:B:383:ASP:OD2	2.40	0.46
3:D:728:LEU:O	3:D:749:HIS:NE2	2.35	0.46
4:E:306:ASN:ND2	5:F:192:TYR:OH	2.48	0.46
13:T:20:PHE:HD1	13:T:23:ARG:HH21	1.62	0.46
13:T:24:MET:HB3	13:T:28:LEU:HD23	1.97	0.46
13:T:405:GLY:O	13:T:409:VAL:HG23	2.14	0.46
1:1:6:LEU:HD21	1:1:12:ARG:HG3	1.97	0.46
1:1:356:CYS:HB3	1:1:358:PRO:HD2	1.96	0.46
2:2:130:THR:HB	2:2:143:GLU:HB3	1.96	0.46
5:5:103:THR:N	5:5:127:GLU:O	2.43	0.46
6:6:102:PRO:HD3	10:A:33:PRO:HG2	1.98	0.46
10:A:41:LEU:HD23	16:H:72:ILE:HD11	1.97	0.46
15:N:10:SER:HB3	15:N:90:TYR:CE1	2.50	0.46
1:B:135:ARG:NE	1:B:137:GLU:HB2	2.29	0.46
3:D:656:LEU:HD21	9:X:3:ARG:HD3	1.95	0.46
4:E:138:LEU:HD13	4:E:143:LEU:HA	1.97	0.46
7:O:108:CYS:HA	17:O:202:SF4:S3	2.55	0.46
11:R:64:VAL:HA	11:R:67:PHE:HB2	1.96	0.46
13:T:70:ASP:OD2	13:T:255:ARG:NH2	2.44	0.46
14:U:70:LEU:O	14:U:73:LEU:HD23	2.15	0.46
1:1:352:SER:O	3:3:205:ARG:HD2	2.15	0.46
3:3:260:PRO:HB2	3:3:617:LEU:HB3	1.96	0.46
5:5:71:VAL:HA	5:5:90:VAL:O	2.15	0.46
10:A:68:PHE:HD2	16:H:164:LEU:HB2	1.79	0.46
13:L:377:PRO:HG2	13:L:502:LEU:HD11	1.97	0.46
1:B:18:TYR:OH	1:B:105:TYR:HB2	2.15	0.46
1:B:186:THR:HB	1:B:200:ARG:H	1.81	0.46
3:D:191:PHE:CE2	3:D:226:ILE:HD13	2.50	0.46
4:E:31:GLY:HA3	10:P:45:GLU:OE2	2.16	0.46
4:E:360:ASP:HB2	5:F:61:PRO:CD	2.45	0.46
6:G:163:TYR:H	7:O:152:ARG:HH12	1.63	0.46
14:U:242:PHE:CZ	14:U:461:PHE:HD2	2.34	0.46
16:Q:6:PRO:HG2	16:Q:112:GLN:HE21	1.80	0.46
16:Q:186:VAL:HG11	16:Q:267:TRP:CZ3	2.50	0.46
1:1:49:THR:OG1	1:1:52:GLU:HG3	2.16	0.46
2:2:40:TRP:CD1	2:2:74:PRO:HA	2.51	0.46
3:3:413:LEU:HA	3:3:416:PHE:HB3	1.97	0.46
4:4:352:GLU:CD	5:5:87:ARG:HH22	2.19	0.46
13:L:286:PHE:HA	13:L:294:ILE:HD11	1.98	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:L:586:LEU:HD13	15:N:138:LEU:HD12	1.97	0.46
15:N:317:ARG:HH12	15:N:383:PHE:C	2.17	0.46
4:E:125:ARG:HD2	4:E:286:SER:OG	2.15	0.46
7:O:149:GLU:O	7:O:153:THR:CB	2.63	0.46
11:R:50:PHE:HB3	11:R:122:GLY:O	2.16	0.46
14:U:201:PHE:CD2	14:U:245:ALA:HB2	2.51	0.46
14:U:218:HIS:HA	14:U:228:ASP:OD1	2.15	0.46
15:V:85:TYR:O	15:V:88:VAL:HB	2.15	0.46
3:3:270:ARG:HB3	3:3:275:LEU:HD11	1.98	0.46
3:3:723:ALA:O	3:3:727:ALA:N	2.49	0.46
4:4:318:GLU:HB2	8:7:39:ASP:CA	2.34	0.46
13:L:41:PHE:HD2	13:L:42:LEU:HD12	1.78	0.46
13:L:554:PHE:HZ	14:M:283:THR:HG21	1.79	0.46
15:N:3:LEU:HD13	15:N:96:HIS:HD2	1.80	0.46
1:B:18:TYR:CZ	1:B:105:TYR:HB2	2.50	0.46
1:B:103:ASP:OD1	1:B:222:GLU:HB2	2.15	0.46
4:E:226:PRO:HB2	5:F:80:TRP:CH2	2.51	0.46
13:T:366:ALA:HB1	13:T:420:TRP:HZ3	1.80	0.46
14:U:148:PHE:O	14:U:152:THR:HG23	2.15	0.46
14:U:253:PHE:CZ	14:U:257:GLN:HG3	2.51	0.46
15:V:345:LYS:NZ	15:V:368:SER:OG	2.41	0.46
16:Q:176:LEU:HD21	16:Q:337:LEU:HD12	1.97	0.46
2:2:34:VAL:HG11	2:2:45:ARG:HG3	1.97	0.46
2:2:45:ARG:O	2:2:49:ILE:HG13	2.15	0.46
2:2:61:MET:SD	3:3:214:MET:HE3	2.55	0.46
3:3:248:GLU:HG2	5:5:170:PHE:CE1	2.50	0.46
7:9:40:ARG:O	7:9:116:GLY:N	2.47	0.46
10:A:23:ALA:O	10:A:27:VAL:HG23	2.16	0.46
14:M:41:LEU:O	14:M:42:THR:HG22	2.16	0.46
14:M:128:PRO:O	14:M:132:MET:HG2	2.16	0.46
14:M:167:ARG:HA	14:M:180:LEU:HD21	1.98	0.46
16:H:221:LEU:N	16:H:222:PRO:HA	2.31	0.46
3:D:439:GLU:HG2	3:D:440:ARG:HG2	1.98	0.46
4:E:36:SER:HB2	16:Q:226:GLN:HA	1.98	0.46
8:I:19:TRP:CD1	8:I:112:LYS:HE3	2.51	0.46
13:T:20:PHE:O	13:T:22:LYS:N	2.48	0.46
14:U:55:LEU:O	14:U:56:LEU:HD12	2.15	0.46
4:4:28:LEU:HD12	10:A:51:ALA:HA	1.98	0.46
4:4:381:LEU:HB3	4:4:382:PRO:HD3	1.96	0.46
6:6:108:MET:HA	6:6:137:VAL:HG13	1.98	0.46
10:A:70:LEU:HD13	11:J:150:THR:HG22	1.98	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:L:419:ARG:HB2	13:L:512:PHE:CD2	2.50	0.46
13:L:459:LEU:O	13:L:468:VAL:N	2.39	0.46
14:M:344:TYR:O	14:M:347:LEU:HD23	2.15	0.46
15:N:62:PHE:CG	15:N:221:ALA:HB2	2.50	0.46
1:B:135:ARG:HH21	1:B:137:GLU:CD	2.19	0.46
1:B:211:LEU:CB	1:B:216:THR:HG21	2.46	0.46
1:B:211:LEU:HB2	1:B:216:THR:HG21	1.98	0.46
2:C:15:PHE:HE1	2:C:53:VAL:HG23	1.80	0.46
4:E:384:ALA:HB1	4:E:396:ILE:HD11	1.98	0.46
13:T:463:HIS:CE1	13:T:487:LEU:HD22	2.51	0.46
14:U:238:VAL:O	14:U:241:PHE:HB2	2.16	0.46
2:2:61:MET:O	2:2:65:SER:OG	2.26	0.46
3:3:83:CYS:SG	3:3:84:VAL:HG13	2.56	0.46
3:3:267:ALA:HA	3:3:277:ILE:HD13	1.98	0.46
5:5:116:ARG:NH2	5:5:135:ILE:HG12	2.31	0.46
8:7:37:PHE:N	8:7:53:THR:O	2.43	0.46
11:J:105:ALA:O	11:J:109:TRP:HB2	2.16	0.46
12:K:46:ALA:HA	15:N:155:TYR:HE2	1.80	0.46
14:M:332:LEU:HA	14:M:335:ARG:HG2	1.98	0.46
15:N:181:VAL:HA	15:N:192:PHE:CE2	2.51	0.46
15:N:339:LEU:HD23	15:N:410:LEU:HA	1.97	0.46
1:B:162:LEU:O	1:B:165:THR:HG22	2.16	0.46
3:D:459:MET:HG2	3:D:465:HIS:HB2	1.98	0.46
5:F:2:ARG:HG3	5:F:84:ASP:OD2	2.16	0.46
6:G:53:SER:O	6:G:60:LEU:N	2.43	0.46
7:O:11:GLY:O	7:O:15:LYS:HG3	2.15	0.46
7:O:105:GLU:CD	7:O:114:VAL:HG13	2.36	0.46
13:T:299:THR:HG23	13:T:325:HIS:HE1	1.81	0.46
14:U:70:LEU:HD11	14:U:312:LEU:HD22	1.98	0.46
14:U:281:PHE:HE2	14:U:332:LEU:HD21	1.81	0.46
14:U:289:GLY:O	14:U:293:MET:HG2	2.16	0.46
14:U:306:GLU:OE2	14:U:386:LYS:NZ	2.48	0.46
16:Q:134:TYR:HA	16:Q:137:PHE:CE2	2.50	0.46
3:3:310:LEU:HB3	3:3:317:LEU:HB3	1.98	0.46
4:4:115:THR:O	4:4:118:VAL:HG22	2.16	0.46
14:M:131:LEU:O	14:M:135:LEU:HD23	2.15	0.46
15:N:101:THR:O	15:N:225:ARG:NH2	2.49	0.46
15:N:270:ALA:O	15:N:273:LEU:HB2	2.16	0.46
16:H:32:THR:O	16:H:36:ARG:HG3	2.16	0.46
16:H:134:TYR:HA	16:H:137:PHE:CE2	2.51	0.46
16:H:185:ILE:HG22	16:H:189:GLN:OE1	2.15	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
16:H:300:LEU:O	16:H:301:ARG:HG2	2.16	0.46
1:B:39:GLU:O	1:B:43:ARG:HG2	2.16	0.46
3:D:462:ALA:O	3:D:465:HIS:ND1	2.49	0.46
5:F:3:LEU:O	5:F:7:LEU:HG	2.16	0.46
5:F:6:VAL:HG13	5:F:41:TYR:HE1	1.81	0.46
6:G:46:CYS:SG	6:G:109:GLY:HA3	2.55	0.46
6:G:138:PRO:HG2	7:O:121:MET:HG3	1.98	0.46
12:S:78:ILE:HG12	15:V:130:LEU:HB3	1.98	0.46
13:T:291:ILE:HG13	13:T:292:LYS:N	2.31	0.46
13:T:409:VAL:O	13:T:413:THR:HG23	2.16	0.46
14:U:281:PHE:CE1	14:U:341:ILE:HG22	2.51	0.46
16:Q:269:MET:HG3	16:Q:270:PRO:HD2	1.98	0.46
1:1:357:THR:HG23	1:1:360:ARG:HH22	1.81	0.46
3:3:136:GLU:HG2	5:5:189:ARG:HG2	1.98	0.46
3:3:225:ASN:O	3:3:229:ILE:HG13	2.16	0.46
3:3:300:TRP:HZ3	3:3:606:THR:HG21	1.81	0.46
3:3:559:ASP:OD2	3:3:686:LYS:NZ	2.48	0.46
4:4:390:VAL:HB	4:4:391:PRO:HD3	1.98	0.46
11:J:59:TYR:O	11:J:64:VAL:HG12	2.16	0.46
16:H:222:PRO:O	16:H:230:GLY:HA3	2.16	0.46
2:C:135:GLN:HB2	2:C:141:TYR:HD1	1.81	0.46
3:D:151:LEU:HD12	3:D:152:PRO:HD2	1.98	0.46
3:D:664:LEU:O	3:D:669:VAL:HG12	2.15	0.46
4:E:381:LEU:HB3	4:E:382:PRO:HD3	1.98	0.46
7:O:149:GLU:O	7:O:153:THR:OG1	2.27	0.46
10:P:93:PHE:O	10:P:96:VAL:HG12	2.16	0.46
11:R:133:GLY:H	11:R:136:LEU:HB2	1.81	0.46
12:S:94:ARG:NH1	13:T:583:THR:O	2.49	0.46
14:U:335:ARG:NH2	14:U:429:GLU:OE1	2.49	0.46
15:V:244:GLY:O	15:V:260:TYR:HB3	2.16	0.46
3:3:8:ASP:OD1	3:3:9:ARG:HG3	2.14	0.45
3:3:163:HIS:ND1	8:7:71:ASP:HB2	2.32	0.45
3:3:410:HIS:HD2	3:3:411:LEU:HD23	1.81	0.45
11:J:69:PHE:HZ	16:H:156:SER:HB3	1.81	0.45
13:L:163:ARG:NE	14:M:399:VAL:HB	2.31	0.45
13:L:198:ASN:ND2	13:L:201:LEU:HB2	2.31	0.45
16:H:227:GLU:HG2	16:H:228:LEU:N	2.30	0.45
3:D:136:GLU:HG2	5:F:189:ARG:HG2	1.98	0.45
4:E:236:GLY:C	4:E:238:SER:H	2.20	0.45
13:T:348:ASP:OD1	13:T:349:VAL:N	2.45	0.45
15:V:58:VAL:HB	15:V:225:ARG:HH11	1.81	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
16:Q:127:ALA:O	16:Q:131:LEU:HG	2.16	0.45
2:2:110:GLU:OE2	8:7:114:ARG:NE	2.38	0.45
3:3:115:HIS:CG	3:3:116:PRO:HD2	2.50	0.45
3:3:506:ILE:HG12	3:3:533:LEU:HB2	1.99	0.45
4:4:84:ARG:CZ	4:4:169:HIS:HB3	2.46	0.45
6:6:147:LEU:O	6:6:151:VAL:HG13	2.16	0.45
10:A:1:MET:HG3	11:J:123:LEU:HD11	1.97	0.45
13:L:388:ILE:O	13:L:392:THR:OG1	2.34	0.45
16:H:215:ALA:O	16:H:294:ARG:NH1	2.47	0.45
1:B:203:PRO:HB2	1:B:204:PRO:HD3	1.98	0.45
3:D:516:VAL:O	3:D:520:ARG:HG3	2.16	0.45
4:E:341:GLU:OE1	5:F:91:ARG:NH2	2.49	0.45
10:P:67:LEU:HB3	16:Q:310:TRP:HZ2	1.82	0.45
13:T:325:HIS:CD2	13:T:329:LYS:HG3	2.51	0.45
16:Q:149:LEU:O	16:Q:153:LEU:HG	2.16	0.45
1:1:76:TRP:O	1:1:81:LYS:NZ	2.48	0.45
7:9:82:SER:OG	7:9:86:ARG:O	2.23	0.45
11:J:100:VAL:HA	13:L:598:LEU:HD21	1.96	0.45
15:N:176:LEU:HD22	15:N:226:VAL:HG13	1.98	0.45
1:B:6:LEU:HD21	1:B:12:ARG:HG3	1.98	0.45
1:B:298:PRO:HD2	1:B:321:SER:HA	1.98	0.45
3:D:43:GLY:HA2	19:D:804:FES:S1	2.57	0.45
5:F:28:VAL:HA	5:F:91:ARG:O	2.16	0.45
5:F:99:PRO:HB2	5:F:124:ILE:HA	1.98	0.45
13:T:90:TYR:CD2	13:T:334:LEU:HD13	2.51	0.45
13:T:380:SER:HB3	13:T:456:ALA:HB3	1.99	0.45
13:T:463:HIS:CD2	13:T:464:PRO:HD3	2.51	0.45
16:Q:17:ALA:O	16:Q:21:VAL:HG23	2.16	0.45
1:1:195:LEU:CD2	2:2:24:ARG:HH12	2.28	0.45
1:1:259:LYS:NZ	2:2:180:GLU:HG2	2.30	0.45
3:3:417:VAL:HA	3:3:447:LYS:HD3	1.99	0.45
4:4:39:GLY:O	4:4:404:MET:HG3	2.16	0.45
6:6:148:ILE:O	6:6:152:MET:HG3	2.15	0.45
13:L:240:ILE:HG22	13:L:241:HIS:HD2	1.81	0.45
14:M:260:LEU:HB3	14:M:301:PHE:CE2	2.52	0.45
1:B:201:LEU:HG	1:B:203:PRO:HD2	1.99	0.45
4:E:105:LEU:HD13	4:E:309:ILE:HD13	1.98	0.45
4:E:172:TYR:OH	4:E:180:GLU:O	2.24	0.45
5:F:49:LEU:HD21	5:F:52:ILE:HD11	1.99	0.45
13:T:219:GLN:OE1	13:T:304:GLY:HA2	2.17	0.45
13:T:600:LEU:O	13:T:604:MET:HG3	2.16	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
16:Q:150:LEU:HD23	16:Q:154:ARG:HD2	1.99	0.45
3:3:6:VAL:HG21	3:3:23:VAL:HA	1.99	0.45
4:4:38:HIS:ND1	4:4:139:ASP:OD2	2.48	0.45
6:6:32:ARG:HB3	6:6:104:TRP:HH2	1.82	0.45
7:9:126:TYR:HB3	9:W:39:ASP:CG	2.36	0.45
7:9:126:TYR:HB3	9:W:39:ASP:OD2	2.17	0.45
10:A:66:MET:O	10:A:69:ILE:HG12	2.16	0.45
16:H:67:ILE:HG13	16:H:68:PHE:HD1	1.82	0.45
16:H:218:PRO:C	16:H:220:ASP:H	2.20	0.45
16:H:218:PRO:HA	16:H:300:LEU:HB2	1.99	0.45
1:B:98:PRO:HA	2:C:124:CYS:SG	2.57	0.45
4:E:47:LEU:HD12	4:E:48:SER:N	2.31	0.45
4:E:140:LEU:HD11	4:E:217:ARG:HH22	1.82	0.45
6:G:37:TRP:NE1	6:G:69:ARG:HG3	2.30	0.45
6:G:53:SER:HB3	6:G:144:PRO:HB3	1.97	0.45
6:G:162:ALA:O	6:G:170:LEU:N	2.27	0.45
10:P:71:PHE:O	10:P:74:GLU:HB3	2.16	0.45
4:4:114:GLU:O	4:4:118:VAL:HG13	2.16	0.45
4:4:288:LYS:HD3	4:4:288:LYS:HA	1.72	0.45
6:6:73:ARG:NH2	10:A:40:LYS:O	2.47	0.45
13:L:317:VAL:HG12	13:L:388:ILE:HG12	1.98	0.45
14:M:260:LEU:HB3	14:M:301:PHE:CD2	2.51	0.45
1:B:297:THR:HG22	1:B:322:MET:HG3	1.98	0.45
3:D:468:HIS:CE1	3:D:473:GLU:HG3	2.51	0.45
4:E:32:PRO:HD3	4:E:42:ARG:HG3	1.98	0.45
4:E:281:ARG:HD3	4:E:284:ARG:NH1	2.30	0.45
5:F:55:LEU:HD23	5:F:57:TYR:CE2	2.52	0.45
7:O:137:LEU:O	7:O:140:VAL:HG12	2.16	0.45
8:I:70:ALA:HA	8:I:84:LEU:HD23	1.99	0.45
10:P:1:MET:HG2	10:P:2:ALA:H	1.82	0.45
11:R:96:LEU:HD23	13:T:598:LEU:HD12	1.97	0.45
11:R:109:TRP:HA	11:R:109:TRP:CE3	2.52	0.45
13:T:26:GLU:HB3	13:T:27:PRO:HD3	1.97	0.45
13:T:239:LEU:HD12	13:T:239:LEU:HA	1.79	0.45
13:T:358:HIS:O	13:T:360:PRO:HD3	2.16	0.45
3:3:11:VAL:HG11	3:3:25:HIS:CD2	2.52	0.45
3:3:300:TRP:HE1	3:3:703:GLN:HG2	1.81	0.45
3:3:327:LEU:HD23	3:3:327:LEU:HA	1.78	0.45
3:3:557:SER:N	3:3:560:GLU:HB2	2.32	0.45
4:4:265:PRO:CB	4:4:278:VAL:HG13	2.46	0.45
11:J:135:TRP:HZ3	15:N:105:LEU:HD22	1.82	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:K:81:HIS:CD2	12:K:81:HIS:H	2.35	0.45
13:L:13:GLY:O	13:L:17:LEU:HG	2.16	0.45
13:L:554:PHE:CZ	14:M:283:THR:HG21	2.51	0.45
16:H:98:GLY:O	16:H:114:TRP:HB2	2.17	0.45
2:C:15:PHE:CE1	2:C:53:VAL:HG23	2.51	0.45
3:D:722:THR:CG2	3:D:756:GLY:H	2.30	0.45
4:E:115:THR:O	4:E:118:VAL:HG22	2.16	0.45
5:F:80:TRP:CE3	5:F:80:TRP:HA	2.52	0.45
6:G:99:MET:HB3	6:G:103:LYS:HD3	1.97	0.45
6:G:125:GLN:HB2	9:X:119:ASN:HD21	1.81	0.45
15:V:294:LEU:HG	15:V:402:VAL:HG13	1.98	0.45
16:Q:185:ILE:HG22	16:Q:189:GLN:OE1	2.17	0.45
16:Q:333:PRO:HG2	16:Q:336:TYR:CG	2.52	0.45
3:3:697:THR:HG21	3:3:761:SER:OG	2.16	0.45
3:3:735:ALA:HA	3:3:744:GLU:HA	1.97	0.45
4:4:211:SER:OG	4:4:215:TYR:CB	2.65	0.45
12:K:63:VAL:HG13	15:N:112:GLU:HG3	1.98	0.45
13:L:73:SER:HB3	13:L:120:LEU:HD23	1.97	0.45
13:L:305:TYR:HB3	13:L:321:HIS:CD2	2.52	0.45
13:L:371:LEU:HB3	13:L:376:LEU:HB2	1.99	0.45
14:M:130:LEU:HB2	14:M:145:LEU:HD11	1.99	0.45
15:N:207:VAL:O	15:N:211:MET:HG3	2.17	0.45
2:C:79:HIS:ND1	2:C:118:SER:HB2	2.31	0.45
5:F:64:ARG:HD3	5:F:64:ARG:HA	1.64	0.45
10:P:10:THR:OG1	16:Q:118:LEU:HD21	2.17	0.45
10:P:66:MET:O	10:P:69:ILE:HG12	2.17	0.45
13:T:139:PHE:CE2	14:U:407:LEU:HD13	2.52	0.45
13:T:371:LEU:HB3	13:T:376:LEU:HB2	1.98	0.45
4:4:73:ARG:NH2	4:4:81:TYR:OH	2.50	0.45
4:4:236:GLY:C	4:4:238:SER:H	2.19	0.45
5:5:33:ARG:O	5:5:37:GLU:HB2	2.17	0.45
11:J:64:VAL:HA	11:J:67:PHE:HB2	1.99	0.45
13:L:325:HIS:HA	13:L:328:PHE:CE2	2.52	0.45
15:N:345:LYS:HB3	15:N:349:PHE:CE2	2.51	0.45
16:H:202:ALA:O	16:H:205:VAL:HG22	2.17	0.45
1:B:97:GLU:OE1	1:B:180:TYR:OH	2.35	0.45
1:B:193:GLU:OE1	1:B:211:LEU:HD12	2.16	0.45
18:B:502:FMN:H9	18:B:502:FMN:H1'1	1.73	0.45
4:E:144:THR:HG23	16:Q:43:GLN:HB3	1.99	0.45
15:V:13:LEU:HB3	15:V:86:LEU:HD11	1.98	0.45
15:V:364:ALA:O	15:V:367:THR:OG1	2.29	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:1:115:ILE:O	1:1:119:ILE:HG13	2.16	0.45
1:1:211:LEU:HB2	1:1:216:THR:HG21	1.98	0.45
3:3:139:LEU:HD12	4:4:326:TYR:CZ	2.52	0.45
3:3:399:LEU:O	3:3:508:GLY:N	2.48	0.45
3:3:503:PRO:HG3	3:3:528:LYS:HD3	1.98	0.45
5:5:1:MET:HB3	5:5:5:ARG:NH2	2.32	0.45
6:6:21:PHE:O	6:6:25:GLU:HG2	2.16	0.45
7:9:137:LEU:O	7:9:140:VAL:HG12	2.17	0.45
10:A:74:GLU:O	10:A:78:LEU:HG	2.17	0.45
11:J:5:GLU:O	11:J:9:LEU:HG	2.17	0.45
13:L:463:HIS:CG	13:L:464:PRO:HD3	2.52	0.45
15:N:228:ALA:HB1	15:N:233:LEU:HD13	1.99	0.45
2:C:4:PHE:HB3	2:C:11:LEU:HD11	1.99	0.45
3:D:474:ARG:NH2	3:D:516:VAL:HG21	2.32	0.45
13:T:88:HIS:O	13:T:92:ILE:HG13	2.16	0.45
13:T:219:GLN:NE2	13:T:277:THR:HG21	2.31	0.45
13:T:312:VAL:HA	13:T:397:PHE:HD2	1.82	0.45
13:T:394:THR:HB	13:T:484:HIS:O	2.16	0.45
16:Q:147:TYR:CD1	16:Q:229:VAL:HG22	2.52	0.45
1:1:6:LEU:HB2	1:1:241:MET:HA	1.99	0.44
3:3:269:THR:HG21	3:3:629:ILE:HG12	1.99	0.44
4:4:219:ARG:HD3	4:4:271:ASP:OD2	2.17	0.44
10:A:76:ALA:HA	10:A:79:TRP:CE3	2.52	0.44
14:M:384:ALA:O	14:M:388:SER:N	2.47	0.44
2:C:29:PRO:O	2:C:32:ARG:HB3	2.17	0.44
3:D:381:LEU:HD22	3:D:680:LEU:O	2.17	0.44
4:E:87:TYR:HB3	4:E:169:HIS:HE1	1.82	0.44
7:O:33:LEU:HB2	7:O:163:VAL:HG12	1.99	0.44
7:O:59:CYS:HB2	7:O:104:CYS:CB	2.47	0.44
14:U:22:ARG:NH1	14:U:92:GLU:CD	2.69	0.44
3:3:46:ARG:NH2	3:3:81:ALA:HB2	2.33	0.44
4:4:101:VAL:O	4:4:105:LEU:HG	2.17	0.44
4:4:169:HIS:HE2	6:6:45:CYS:HB2	1.83	0.44
5:5:103:THR:CG2	5:5:126:PHE:HB3	2.47	0.44
10:A:33:PRO:HD2	16:H:70:GLU:HB2	2.00	0.44
13:L:26:GLU:HB3	13:L:27:PRO:HD3	1.99	0.44
13:L:264:PRO:HA	13:L:397:PHE:CE1	2.52	0.44
4:E:168:PHE:CE1	6:G:141:PRO:HG3	2.52	0.44
4:E:249:ARG:HB2	4:E:262:PHE:HE2	1.81	0.44
6:G:119:ASN:HA	6:G:125:GLN:HE22	1.82	0.44
14:U:13:GLY:HA2	14:U:97:GLY:HA2	1.99	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
16:Q:39:LEU:HD22	16:Q:295:ALA:HB2	1.99	0.44
16:Q:289:PHE:O	16:Q:293:ILE:HG12	2.17	0.44
3:3:293:ALA:HB2	3:3:698:MET:HG2	2.00	0.44
4:4:55:VAL:O	4:4:382:PRO:HG3	2.17	0.44
4:4:276:MET:O	4:4:280:ILE:HG13	2.17	0.44
7:9:9:SER:OG	16:H:296:THR:HG22	2.18	0.44
13:L:439:PRO:HB2	13:L:442:MET:HB2	1.98	0.44
14:M:30:GLY:O	14:M:34:LEU:HG	2.17	0.44
14:M:95:PHE:HB3	14:M:136:TYR:CZ	2.52	0.44
15:N:14:THR:OG1	15:N:90:TYR:OH	2.31	0.44
16:H:310:TRP:HA	16:H:314:PHE:CD2	2.51	0.44
1:B:275:LEU:HA	1:B:279:TRP:CD1	2.52	0.44
2:C:78:TYR:CZ	2:C:157:LEU:HD22	2.51	0.44
6:G:36:LEU:O	6:G:38:PRO:HD3	2.17	0.44
6:G:115:GLY:N	6:G:125:GLN:O	2.50	0.44
14:U:119:TYR:OH	14:U:157:LEU:HD23	2.18	0.44
3:3:34:CYS:CB	3:3:45:CYS:SG	3.05	0.44
13:L:128:PHE:HD1	13:L:169:PHE:CD2	2.36	0.44
14:M:346:GLY:O	14:M:349:GLN:HG2	2.17	0.44
3:D:657:HIS:O	3:D:661:GLN:HG2	2.17	0.44
4:E:47:LEU:HD13	4:E:52:VAL:HA	2.00	0.44
4:E:154:GLU:OE1	4:E:167:ARG:NH1	2.50	0.44
6:G:40:THR:HB	6:G:68:PHE:CZ	2.53	0.44
13:T:202:LEU:HD12	13:T:202:LEU:HA	1.87	0.44
15:V:228:ALA:HB1	15:V:233:LEU:HD13	1.99	0.44
2:2:46:ILE:HD12	3:3:214:MET:HE1	1.99	0.44
3:3:717:TRP:HB2	3:3:759:TYR:HB2	1.99	0.44
4:4:338:PRO:HG2	5:5:193:ARG:NH1	2.28	0.44
13:L:214:VAL:HG22	13:L:219:GLN:HB2	2.00	0.44
13:L:222:LEU:O	13:L:225:TRP:HD1	2.01	0.44
1:B:386:ASN:O	1:B:390:LEU:HG	2.18	0.44
3:D:252:THR:OG1	3:D:628:PRO:HD3	2.18	0.44
4:E:114:GLU:O	4:E:118:VAL:HG13	2.18	0.44
5:F:38:MET:HE1	5:F:104:VAL:HG11	1.92	0.44
6:G:37:TRP:HE1	6:G:69:ARG:CG	2.30	0.44
13:T:128:PHE:CE1	13:T:166:ASP:HB3	2.53	0.44
14:U:335:ARG:NH1	14:U:424:ASP:O	2.43	0.44
15:V:257:LEU:HD11	15:V:374:TYR:HB2	1.98	0.44
3:3:9:ARG:HD2	3:3:26:ALA:O	2.18	0.44
5:5:74:LEU:HD12	5:5:88:PHE:CZ	2.52	0.44
5:5:80:TRP:HA	5:5:80:TRP:HE3	1.82	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:5:160:ARG:NH2	7:9:130:VAL:O	2.51	0.44
8:7:103:LEU:O	8:7:110:LEU:N	2.28	0.44
9:W:10:PRO:HG3	9:W:62:ALA:O	2.18	0.44
13:L:461:LEU:HB3	13:L:465:LEU:HB2	1.99	0.44
13:L:463:HIS:CE1	13:L:487:LEU:HD22	2.52	0.44
16:H:9:PRO:HB2	16:H:11:TRP:CD1	2.52	0.44
3:D:372:GLN:O	3:D:558:TRP:CD2	2.71	0.44
3:D:451:PHE:CE1	3:D:466:GLU:HB3	2.53	0.44
5:F:103:THR:CG2	5:F:126:PHE:HB3	2.47	0.44
6:G:25:GLU:HA	6:G:28:VAL:HG12	1.99	0.44
9:X:102:LEU:HD12	9:X:105:LEU:HD11	1.98	0.44
11:R:155:ALA:HB1	15:V:81:ARG:HH11	1.83	0.44
13:T:275:LEU:HD13	13:T:402:PHE:HA	2.00	0.44
15:V:3:LEU:HD13	15:V:96:HIS:HD2	1.83	0.44
15:V:259:ALA:O	15:V:263:ILE:HG13	2.18	0.44
16:Q:108:PHE:CG	16:Q:108:PHE:O	2.71	0.44
4:4:112:ARG:HG3	4:4:297:LEU:HD11	1.99	0.44
6:6:33:SER:O	6:6:36:LEU:HG	2.18	0.44
6:6:41:PHE:HZ	6:6:88:MET:HE3	1.82	0.44
7:9:17:LEU:HD12	16:H:42:PHE:CZ	2.52	0.44
15:N:338:PRO:HB2	15:N:414:LEU:HD23	2.00	0.44
16:H:162:TYR:OH	16:H:308:PHE:HD1	2.00	0.44
1:B:157:TYR:O	1:B:158:LEU:HD23	2.18	0.44
3:D:40:SER:HB3	3:D:437:ILE:HG22	2.00	0.44
3:D:585:MET:HB3	3:D:587:LEU:HD13	2.00	0.44
4:E:73:ARG:HG3	4:E:77:GLN:OE1	2.18	0.44
6:G:81:ALA:HA	6:G:108:MET:HB3	1.99	0.44
6:G:143:ARG:HH21	7:O:31:VAL:CG1	2.31	0.44
6:G:155:GLN:O	6:G:159:ARG:HG3	2.17	0.44
13:T:286:PHE:HB2	13:T:419:ARG:HD3	1.99	0.44
15:V:62:PHE:CG	15:V:221:ALA:HB2	2.53	0.44
16:Q:44:VAL:O	16:Q:45:ARG:C	2.55	0.44
3:3:36:GLU:HB3	3:3:39:LEU:HD12	2.00	0.44
4:4:63:HIS:O	6:6:122:ALA:HB1	2.18	0.44
6:6:138:PRO:HG2	7:9:121:MET:HG3	1.99	0.44
10:A:34:LYS:N	16:H:70:GLU:OE1	2.46	0.44
14:M:157:LEU:O	15:N:365:LEU:HD13	2.17	0.44
1:B:323:LEU:HD11	1:B:326:GLY:HA2	1.98	0.44
5:F:155:THR:O	6:G:119:ASN:ND2	2.45	0.44
6:G:100:PRO:HA	16:Q:70:GLU:HG2	2.00	0.44
9:X:7:ARG:NH2	9:X:100:THR:HG23	2.33	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:R:5:GLU:O	11:R:9:LEU:HG	2.17	0.44
13:T:126:VAL:HA	13:T:129:ILE:HD12	2.00	0.44
14:U:204:LYS:HE3	14:U:234:TYR:O	2.18	0.44
14:U:325:LEU:HG	14:U:361:LEU:HB3	2.00	0.44
2:2:40:TRP:CH2	8:7:125:ALA:HA	2.53	0.44
3:3:117:LEU:HA	4:4:321:MET:HE2	2.00	0.44
3:3:722:THR:HG21	3:3:755:LYS:HA	1.98	0.44
4:4:314:ARG:NH1	7:9:106:GLU:O	2.51	0.44
11:J:32:LEU:HD13	12:K:29:LEU:HG	2.00	0.44
13:L:3:LEU:HD22	13:L:53:ALA:HB3	1.99	0.44
13:L:82:GLY:O	13:L:86:LEU:HG	2.17	0.44
3:D:618:GLU:OE2	3:D:620:ARG:NE	2.42	0.44
4:E:352:GLU:HB3	4:E:371:ARG:CZ	2.48	0.44
4:E:367:ARG:NH1	4:E:369:LYS:HB2	2.32	0.44
10:P:44:TYR:CD2	10:P:45:GLU:HB2	2.53	0.44
10:P:71:PHE:O	10:P:75:VAL:HG23	2.17	0.44
13:T:72:LEU:HD23	13:T:255:ARG:HD3	2.00	0.44
13:T:290:ASP:OD1	13:T:291:ILE:N	2.50	0.44
13:T:539:ASN:HA	13:T:543:VAL:HB	1.99	0.44
1:1:111:PRO:HB3	1:1:145:LEU:HD23	1.99	0.43
1:1:214:LYS:O	1:1:216:THR:HG23	2.18	0.43
1:1:410:VAL:HG12	1:1:414:LEU:HD13	2.00	0.43
7:9:10:LEU:HD12	16:H:296:THR:CG2	2.47	0.43
16:H:122:ILE:HG13	16:H:123:LEU:HD12	1.99	0.43
16:H:332:LEU:HD12	16:H:332:LEU:H	1.83	0.43
1:B:137:GLU:HB3	2:C:141:TYR:OH	2.18	0.43
7:O:19:SER:C	7:O:21:PRO:CD	2.73	0.43
9:X:46:TYR:N	9:X:63:PHE:O	2.50	0.43
12:S:79:PHE:CD2	12:S:85:THR:HA	2.53	0.43
13:T:469:LEU:HD12	13:T:469:LEU:HA	1.82	0.43
14:U:113:ARG:O	14:U:177:LEU:HB2	2.19	0.43
15:V:237:VAL:O	15:V:241:VAL:HG23	2.18	0.43
16:Q:168:LEU:HD12	16:Q:314:PHE:HB3	1.99	0.43
1:1:50:PRO:HA	1:1:53:VAL:HG12	2.00	0.43
1:1:361:GLU:HB3	3:3:113:LEU:HD22	1.99	0.43
2:2:3:PHE:HB2	2:2:45:ARG:HH11	1.75	0.43
2:2:171:LYS:O	2:2:177:HIS:HE1	2.01	0.43
4:4:222:GLY:O	4:4:224:ILE:HG13	2.18	0.43
6:6:39:ALA:HB2	6:6:75:ALA:CB	2.48	0.43
13:L:65:PHE:CZ	13:L:67:LEU:HD21	2.53	0.43
13:L:182:THR:HB	13:L:187:GLU:HG3	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:L:463:HIS:NE2	13:L:487:LEU:HD13	2.32	0.43
15:N:190:ALA:HA	15:N:192:PHE:H	1.83	0.43
1:B:301:PRO:O	1:B:306:VAL:HG11	2.18	0.43
2:C:85:THR:HB	19:C:201:FES:S2	2.59	0.43
3:D:19:VAL:HG23	3:D:85:THR:O	2.18	0.43
3:D:242:PHE:CD2	7:O:74:GLU:HB2	2.53	0.43
3:D:534:ALA:O	3:D:617:LEU:HD12	2.17	0.43
13:T:312:VAL:O	13:T:396:PRO:HD2	2.18	0.43
15:V:420:LEU:HA	15:V:423:LEU:HG	1.99	0.43
16:Q:177:VAL:HG22	16:Q:188:TRP:CG	2.54	0.43
1:1:424:LEU:HG	1:1:429:ARG:O	2.18	0.43
4:4:166:GLN:OE1	4:4:170:HIS:HA	2.18	0.43
6:6:82:GLY:HA2	17:6:201:SF4:S4	2.58	0.43
11:J:104:LEU:HA	15:N:174:LEU:HD21	1.99	0.43
13:L:340:ILE:HB	13:L:345:GLY:HA2	1.99	0.43
14:M:9:PRO:HG2	14:M:107:LEU:HD12	2.00	0.43
15:N:13:LEU:HD22	15:N:25:VAL:HG13	2.00	0.43
15:N:198:ASP:OD1	15:N:256:ARG:NH2	2.51	0.43
1:B:83:ASP:CG	1:B:87:HIS:HE2	2.20	0.43
3:D:312:ARG:NH2	3:D:598:ALA:O	2.51	0.43
4:E:123:LEU:HG	4:E:156:ILE:HG23	2.00	0.43
4:E:208:PHE:CE2	4:E:276:MET:HG2	2.54	0.43
4:E:231:ASP:O	5:F:110:SER:OG	2.35	0.43
6:G:91:VAL:HG22	10:P:46:SER:HB3	2.00	0.43
12:S:81:HIS:CD2	12:S:81:HIS:H	2.36	0.43
13:T:33:ALA:O	13:T:37:VAL:HG23	2.19	0.43
14:U:29:ALA:HB1	14:U:83:PHE:HA	1.99	0.43
16:Q:271:VAL:HG12	16:Q:272:LEU:HG	2.00	0.43
3:3:382:PHE:HB3	3:3:532:VAL:HB	2.00	0.43
3:3:409:LEU:HD23	3:3:409:LEU:HA	1.76	0.43
4:4:42:ARG:O	4:4:43:LEU:HD23	2.19	0.43
8:7:27:LYS:HD3	8:7:27:LYS:HA	1.86	0.43
11:J:36:PHE:CD2	11:J:59:TYR:HB3	2.54	0.43
13:L:103:ARG:NH2	13:L:144:PHE:O	2.45	0.43
14:M:289:GLY:O	14:M:293:MET:HG2	2.18	0.43
15:N:26:LYS:O	15:N:29:THR:OG1	2.30	0.43
15:N:193:HIS:CD2	15:N:263:ILE:HD13	2.52	0.43
16:H:136:ILE:HG23	16:H:232:TYR:HD2	1.83	0.43
2:C:82:VAL:HG22	2:C:134:ILE:HG12	2.01	0.43
3:D:36:GLU:OE1	3:D:37:LYS:N	2.51	0.43
4:E:26:MET:HE1	10:P:57:PHE:HA	2.01	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:E:352:GLU:CD	5:F:87:ARG:HH22	2.21	0.43
7:O:40:ARG:O	7:O:116:GLY:N	2.52	0.43
11:R:58:VAL:O	11:R:62:ALA:HB3	2.18	0.43
13:T:316:TRP:HZ3	13:T:460:ALA:HB1	1.82	0.43
14:U:159:MET:HG3	14:U:197:PHE:HD1	1.83	0.43
14:U:338:THR:HG22	14:U:340:GLU:H	1.82	0.43
15:V:188:ALA:HB3	15:V:216:LYS:NZ	2.32	0.43
2:2:147:ARG:HE	2:2:147:ARG:HB2	1.72	0.43
3:3:136:GLU:HB3	5:5:187:GLY:HA3	2.01	0.43
4:4:73:ARG:NH2	7:9:64:PRO:O	2.50	0.43
4:4:167:ARG:HD3	6:6:143:ARG:HH12	1.83	0.43
8:7:40:PHE:CZ	8:7:53:THR:HG21	2.54	0.43
9:W:31:VAL:HG22	9:W:50:LEU:HD13	2.00	0.43
14:M:90:ARG:HD2	14:M:90:ARG:HA	1.79	0.43
16:H:345:PHE:CZ	16:H:349:LEU:HD22	2.53	0.43
1:B:3:GLY:HA2	1:B:4:PRO:HD3	1.89	0.43
1:B:274:GLU:HG2	1:B:279:TRP:CD1	2.54	0.43
4:E:34:HIS:HA	4:E:35:PRO:HA	1.83	0.43
4:E:99:LEU:HA	4:E:102:GLU:OE1	2.18	0.43
4:E:207:LEU:HD21	7:O:12:ILE:HD11	2.00	0.43
8:I:43:ARG:HA	8:I:46:ARG:NH2	2.33	0.43
10:P:71:PHE:CE2	10:P:107:PHE:HB2	2.54	0.43
11:R:44:VAL:HG13	11:R:49:ARG:HG2	1.99	0.43
14:U:359:LEU:HB2	14:U:410:PHE:CE1	2.53	0.43
15:V:58:VAL:HG22	15:V:278:ALA:HB1	2.01	0.43
16:Q:214:ALA:HB1	16:Q:248:GLU:HG3	1.99	0.43
16:Q:224:ALA:HA	16:Q:230:GLY:H	1.84	0.43
1:1:272:PHE:HE1	1:1:309:THR:HB	1.83	0.43
4:4:148:TYR:O	4:4:151:ARG:HB3	2.18	0.43
6:6:104:TRP:HE1	6:6:173:VAL:HG22	1.83	0.43
7:9:6:LEU:HD23	16:H:297:TRP:CE2	2.53	0.43
8:7:63:LEU:HD13	8:7:129:ALA:HB3	2.00	0.43
12:K:46:ALA:HB2	12:K:53:GLY:HA3	2.00	0.43
13:L:268:TYR:O	13:L:272:VAL:HG23	2.17	0.43
13:L:359:LEU:HB3	13:L:362:THR:HB	2.01	0.43
14:M:201:PHE:CE2	14:M:245:ALA:HB2	2.54	0.43
16:H:257:ALA:O	16:H:260:PRO:HD2	2.19	0.43
1:B:79:MET:SD	1:B:217:THR:OG1	2.77	0.43
1:B:303:THR:H	1:B:306:VAL:HB	1.84	0.43
4:E:62:LEU:HD11	6:G:43:LEU:O	2.18	0.43
9:X:14:LEU:HD13	9:X:77:LEU:HB2	2.01	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:T:385:LYS:NZ	13:T:413:THR:OG1	2.52	0.43
14:U:143:ARG:HD3	14:U:143:ARG:HA	1.69	0.43
16:Q:181:ASN:O	16:Q:185:ILE:HG13	2.18	0.43
16:Q:232:TYR:HB2	16:Q:244:PHE:CE1	2.53	0.43
1:1:45:LEU:HD12	1:1:163:PHE:CE2	2.54	0.43
4:4:240:ARG:HA	4:4:244:VAL:H	1.82	0.43
11:J:29:ALA:O	11:J:33:ILE:HG13	2.18	0.43
12:K:95:GLY:N	13:L:582:GLN:O	2.40	0.43
13:L:104:PHE:CZ	13:L:108:PHE:CZ	3.06	0.43
16:H:90:VAL:HG21	16:H:243:LEU:HB3	2.00	0.43
16:H:90:VAL:HA	16:H:247:ALA:HB2	2.00	0.43
16:H:216:ARG:NH1	16:H:294:ARG:O	2.50	0.43
16:H:267:TRP:CD1	16:H:275:PRO:HA	2.53	0.43
3:D:141:GLU:HG2	3:D:143:TYR:CZ	2.54	0.43
3:D:351:LEU:HB3	3:D:664:LEU:HD21	2.00	0.43
3:D:719:HIS:NE2	3:D:755:LYS:HE2	2.34	0.43
4:E:38:HIS:CE1	4:E:398:ALA:HA	2.53	0.43
13:T:41:PHE:HB2	13:T:81:THR:HB	2.00	0.43
13:T:583:THR:HG1	13:T:585:TYR:HD2	1.65	0.43
14:U:91:VAL:HG21	14:U:226:LEU:HD22	2.00	0.43
14:U:173:PRO:HG2	14:U:179:ASP:OD2	2.19	0.43
15:V:98:LEU:HD23	15:V:218:ALA:CB	2.47	0.43
16:Q:52:GLY:HA3	16:Q:55:GLY:N	2.31	0.43
16:Q:310:TRP:CE3	16:Q:314:PHE:HE2	2.37	0.43
1:1:145:LEU:O	1:1:149:ILE:HG13	2.18	0.43
1:1:357:THR:N	1:1:358:PRO:HD2	2.34	0.43
5:5:164:TYR:HB3	9:W:37:TRP:HZ3	1.84	0.43
6:6:69:ARG:HB2	6:6:75:ALA:HB2	2.00	0.43
6:6:163:TYR:HB2	7:9:152:ARG:HH11	1.83	0.43
7:9:71:GLU:HB2	7:9:90:VAL:HB	2.01	0.43
10:A:57:PHE:HB3	10:A:58:PRO:HD2	2.01	0.43
13:L:586:LEU:HD11	15:N:135:LYS:HA	2.00	0.43
16:H:127:ALA:O	16:H:131:LEU:HG	2.17	0.43
16:H:155:SER:OG	16:H:156:SER:N	2.52	0.43
16:H:330:LEU:HD13	16:H:330:LEU:HA	1.89	0.43
1:B:288:GLN:NE2	1:B:332:PRO:O	2.52	0.43
2:C:130:THR:HB	2:C:143:GLU:HB3	2.00	0.43
3:D:124:LYS:HG3	3:D:233:GLY:HA2	2.01	0.43
3:D:136:GLU:OE1	5:F:186:GLY:N	2.32	0.43
4:E:372:ALA:HB2	4:E:409:ARG:HD3	2.01	0.43
5:F:155:THR:N	6:G:119:ASN:OD1	2.36	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:P:7:TYR:CD1	16:Q:118:LEU:HD22	2.54	0.43
14:U:347:LEU:HB2	14:U:414:PHE:HA	2.01	0.43
16:Q:132:ALA:O	16:Q:136:ILE:HG13	2.17	0.43
2:2:40:TRP:CE2	2:2:74:PRO:HG3	2.54	0.43
3:3:468:HIS:ND1	3:3:472:GLU:HB3	2.34	0.43
6:6:78:MET:O	6:6:105:VAL:HA	2.19	0.43
7:9:33:LEU:HD11	7:9:119:PHE:HE2	1.84	0.43
9:W:36:ASP:OD1	9:W:36:ASP:N	2.51	0.43
12:K:15:VAL:O	12:K:19:LEU:HG	2.18	0.43
14:M:103:GLU:O	14:M:107:LEU:HG	2.19	0.43
15:N:294:LEU:HD21	15:N:325:ALA:HB1	1.99	0.43
1:B:101:PHE:CE1	1:B:253:GLN:HB2	2.54	0.43
2:C:28:MET:O	2:C:70:TYR:OH	2.34	0.43
3:D:8:ASP:OD1	3:D:9:ARG:HG3	2.18	0.43
3:D:543:GLY:O	3:D:547:MET:HG2	2.19	0.43
5:F:53:VAL:HG13	5:F:71:VAL:HB	1.99	0.43
10:P:49:ASP:CG	10:P:52:GLY:HA3	2.39	0.43
11:R:15:SER:HB3	11:R:35:ASN:OD1	2.19	0.43
13:T:293:LYS:O	13:T:297:TYR:HD1	2.02	0.43
14:U:281:PHE:CE2	14:U:332:LEU:HD21	2.54	0.43
15:V:217:ALA:HA	15:V:285:LEU:CD2	2.49	0.43
1:1:20:HIS:HB3	1:1:31:TYR:HE1	1.84	0.43
3:3:347:HIS:HB2	3:3:538:ALA:CB	2.48	0.43
3:3:603:PRO:HG2	3:3:634:ALA:HA	2.01	0.43
3:3:732:ALA:O	3:3:747:VAL:HG23	2.18	0.43
5:5:132:LEU:HD23	5:5:132:LEU:HA	1.82	0.43
5:5:134:LYS:NZ	5:5:141:LEU:O	2.52	0.43
6:6:40:THR:HB	6:6:68:PHE:CZ	2.54	0.43
6:6:163:TYR:H	7:9:152:ARG:NH1	2.17	0.43
7:9:41:HIS:HB2	7:9:136:MET:SD	2.59	0.43
10:A:1:MET:HG2	11:J:49:ARG:HH12	1.84	0.43
10:A:7:TYR:N	10:A:7:TYR:CD1	2.86	0.43
15:N:73:THR:O	15:N:77:VAL:HG23	2.18	0.43
15:N:303:SER:HB3	15:N:307:VAL:HG22	1.99	0.43
16:H:342:ALA:O	16:H:346:LEU:HG	2.19	0.43
3:D:230:CYS:HA	3:D:231:PRO:HD2	1.93	0.43
4:E:154:GLU:OE2	4:E:157:LEU:HD12	2.19	0.43
4:E:367:ARG:HH12	4:E:369:LYS:HB2	1.83	0.43
6:G:115:GLY:HA2	6:G:125:GLN:HA	2.00	0.43
7:O:155:LYS:HA	7:O:155:LYS:HD2	1.88	0.43
10:P:28:GLY:HA3	16:Q:239:ILE:HB	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:R:72:MET:HG2	16:Q:141:TRP:CE3	2.53	0.43
12:S:23:THR:OG1	12:S:26:LEU:HD13	2.18	0.43
15:V:26:LYS:O	15:V:29:THR:OG1	2.30	0.43
15:V:73:THR:HG21	15:V:210:PHE:HB2	1.99	0.43
15:V:277:ASN:C	15:V:279:GLN:H	2.22	0.43
16:Q:39:LEU:CD2	16:Q:295:ALA:HB2	2.48	0.43
16:Q:237:SER:OG	16:Q:238:SER:N	2.51	0.43
3:3:33:PHE:HB2	3:3:45:CYS:CB	2.50	0.42
3:3:54:LEU:HD13	3:3:91:MET:HB2	2.00	0.42
4:4:169:HIS:NE2	6:6:45:CYS:SG	2.92	0.42
4:4:172:TYR:O	4:4:179:LYS:HB2	2.19	0.42
7:9:134:GLU:CD	7:9:134:GLU:H	2.23	0.42
11:J:146:LEU:O	11:J:150:THR:HG23	2.19	0.42
12:K:46:ALA:HB2	12:K:53:GLY:CA	2.49	0.42
13:L:450:ALA:O	13:L:454:VAL:HG23	2.18	0.42
13:L:549:LEU:HD23	13:L:549:LEU:HA	1.89	0.42
13:L:600:LEU:O	13:L:604:MET:HG3	2.19	0.42
1:B:135:ARG:HE	1:B:137:GLU:HB2	1.83	0.42
2:C:42:ARG:HB2	2:C:45:ARG:HG2	2.01	0.42
3:D:118:ASP:O	3:D:122:CYS:HB2	2.19	0.42
3:D:189:ARG:O	3:D:193:GLU:HB2	2.19	0.42
5:F:121:LEU:O	5:F:144:HIS:HB3	2.18	0.42
8:I:13:TRP:CE3	8:I:72:VAL:HB	2.53	0.42
13:T:340:ILE:HG22	13:T:347:GLN:H	1.84	0.42
14:U:135:LEU:HG	14:U:136:TYR:CD2	2.54	0.42
14:U:359:LEU:O	14:U:363:LEU:HG	2.19	0.42
15:V:115:SER:HB2	15:V:119:TYR:CZ	2.54	0.42
15:V:224:LEU:HD13	15:V:278:ALA:HB2	2.01	0.42
16:Q:71:ASP:OD1	16:Q:240:LYS:NZ	2.31	0.42
1:1:22:GLY:HA2	2:2:174:HIS:CD2	2.55	0.42
1:1:63:ARG:NH1	1:1:313:TYR:HD2	2.18	0.42
1:1:434:PRO:HG2	1:1:436:LEU:CD1	2.49	0.42
4:4:158:ASP:CG	6:6:57:ARG:HH12	2.18	0.42
4:4:190:LEU:HD12	4:4:194:LEU:HD13	2.00	0.42
6:6:61:ALA:HB1	6:6:66:GLU:OE1	2.18	0.42
13:L:147:LYS:NZ	14:M:349:GLN:OE1	2.43	0.42
13:L:162:ASN:ND2	13:L:166:ASP:OD2	2.52	0.42
15:N:33:LEU:HB2	15:N:71:LEU:HD21	2.01	0.42
3:D:227:THR:CG2	3:D:237:ASP:HB2	2.48	0.42
3:D:395:PHE:HB3	3:D:503:PRO:HB3	2.00	0.42
3:D:567:TYR:HA	3:D:584:VAL:HG23	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:728:LEU:HD22	3:D:734:VAL:HG21	2.00	0.42
4:E:194:LEU:HD21	4:E:290:ILE:HG22	2.01	0.42
13:T:44:GLY:HA3	13:T:77:LEU:HD21	2.01	0.42
15:V:108:LEU:HB2	15:V:147:PHE:CE2	2.51	0.42
3:3:28:TYR:CE2	3:3:96:LEU:HD11	2.54	0.42
4:4:214:PHE:HA	4:4:217:ARG:HB2	2.00	0.42
7:9:9:SER:O	7:9:12:ILE:HG13	2.18	0.42
8:7:67:PHE:O	8:7:86:LEU:HD22	2.19	0.42
11:J:53:PHE:HE2	16:H:120:LEU:O	2.02	0.42
13:L:275:LEU:HD13	13:L:402:PHE:HD1	1.84	0.42
14:M:43:HIS:HD2	14:M:48:ALA:HB2	1.84	0.42
15:N:237:VAL:O	15:N:241:VAL:HG23	2.20	0.42
16:H:132:ALA:O	16:H:136:ILE:HG13	2.19	0.42
16:H:216:ARG:NH1	16:H:294:ARG:HB3	2.34	0.42
1:B:201:LEU:O	1:B:204:PRO:HD2	2.19	0.42
3:D:152:PRO:HD3	4:E:305:PRO:HB2	2.01	0.42
6:G:60:LEU:HG	6:G:65:SER:CB	2.50	0.42
11:R:103:ILE:O	11:R:107:GLY:N	2.47	0.42
13:T:59:TRP:HE1	14:U:447:PRO:HD2	1.85	0.42
16:Q:217:THR:OG1	16:Q:293:ILE:HG22	2.19	0.42
3:3:307:LYS:HB3	3:3:307:LYS:HE2	1.76	0.42
4:4:48:SER:CB	10:A:55:LYS:HE3	2.50	0.42
4:4:389:GLN:HG3	4:4:391:PRO:HD2	2.02	0.42
4:4:400:LEU:HD23	4:4:400:LEU:HA	1.90	0.42
13:L:419:ARG:NH2	13:L:525:GLU:OE2	2.53	0.42
14:M:160:LEU:O	14:M:163:VAL:HG12	2.19	0.42
15:N:251:GLN:OE1	15:N:256:ARG:HD3	2.19	0.42
16:H:60:LEU:O	16:H:64:ILE:HG13	2.20	0.42
16:H:233:HIS:ND1	16:H:234:THR:OG1	2.46	0.42
1:B:290:ILE:HG22	1:B:330:LEU:HD22	2.01	0.42
2:C:89:LYS:HA	2:C:93:ALA:H	1.84	0.42
4:E:219:ARG:HD3	4:E:271:ASP:OD2	2.19	0.42
4:E:236:GLY:O	4:E:238:SER:N	2.52	0.42
3:3:451:PHE:CE1	3:3:466:GLU:HB3	2.55	0.42
4:4:144:THR:HG22	4:4:148:TYR:CE1	2.46	0.42
4:4:248:VAL:HB	4:4:347:GLU:HB2	2.01	0.42
5:5:3:LEU:O	5:5:7:LEU:HG	2.20	0.42
6:6:105:VAL:HB	6:6:132:PRO:O	2.19	0.42
10:A:111:TRP:HH2	16:H:307:ARG:HG2	1.85	0.42
13:L:461:LEU:HD13	13:L:465:LEU:HB3	2.02	0.42
14:M:134:TYR:O	14:M:141:ARG:HD3	2.19	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	2.01	0.42
15:N:422:ALA:O	15:N:423:LEU:HD23	2.19	0.42
16:H:189:GLN:HG2	16:H:195:LEU:H	1.85	0.42
16:H:198:TYR:O	16:H:341:SER:OG	2.31	0.42
1:B:342:TRP:CE3	1:B:346:ARG:HD2	2.55	0.42
2:C:100:LEU:HD13	2:C:150:LEU:HD21	2.01	0.42
3:D:719:HIS:CD2	3:D:755:LYS:HG2	2.54	0.42
8:I:120:ASP:O	8:I:124:GLU:HG3	2.19	0.42
10:P:81:TYR:HE2	16:Q:325:ALA:HB1	1.85	0.42
14:U:17:LEU:HD11	14:U:98:LEU:HD23	2.01	0.42
15:V:204:PRO:O	15:V:208:VAL:HG23	2.19	0.42
15:V:241:VAL:HA	15:V:264:ALA:HA	2.00	0.42
4:4:272:VAL:HG13	4:4:399:SER:HB3	2.00	0.42
4:4:314:ARG:HB3	8:7:44:MET:CE	2.44	0.42
5:5:51:ASP:O	5:5:72:TYR:HA	2.19	0.42
5:5:160:ARG:HH12	7:9:132:GLY:CA	2.31	0.42
9:W:125:ILE:HD13	9:W:125:ILE:HG21	1.76	0.42
14:M:148:PHE:HE1	14:M:204:LYS:NZ	2.18	0.42
15:N:66:ALA:HB1	15:N:95:MET:HE3	2.01	0.42
16:H:151:GLY:HA2	16:H:154:ARG:CD	2.47	0.42
16:H:201:PRO:O	16:H:204:LEU:HB2	2.19	0.42
2:C:88:CYS:HA	2:C:131:ALA:HB1	2.01	0.42
3:D:32:LEU:CD1	3:D:35:SER:HB2	2.49	0.42
5:F:38:MET:HA	5:F:41:TYR:HB2	2.02	0.42
9:X:102:LEU:HG	9:X:110:LEU:HD13	2.01	0.42
11:R:24:ASN:HB3	11:R:27:HIS:HB2	2.01	0.42
11:R:55:GLN:NE2	11:R:59:TYR:CD2	2.87	0.42
14:U:268:ALA:HA	14:U:291:SER:CA	2.46	0.42
3:3:213:THR:OG1	3:3:215:ASP:N	2.49	0.42
3:3:243:ARG:NH1	3:3:275:LEU:HA	2.34	0.42
3:3:470:PRO:HB3	3:3:770:ARG:HD2	2.02	0.42
4:4:94:ASP:HB3	4:4:173:ILE:HG21	2.01	0.42
4:4:112:ARG:O	4:4:116:ILE:HG13	2.20	0.42
4:4:175:ILE:HG13	4:4:335:PHE:HZ	1.84	0.42
4:4:356:TYR:HE1	5:5:26:TRP:HZ2	1.68	0.42
6:6:100:PRO:O	6:6:103:LYS:HD3	2.18	0.42
10:A:49:ASP:CG	10:A:52:GLY:HA3	2.40	0.42
14:M:16:LEU:HD22	14:M:97:GLY:H	1.85	0.42
1:B:433:ARG:NH2	2:C:94:GLU:HG3	2.35	0.42
2:C:83:CYS:HA	2:C:122:VAL:O	2.19	0.42
3:D:240:ALA:HB1	3:D:276:ARG:HB2	2.02	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:383:PRO:HG2	3:D:531:LYS:HA	2.02	0.42
4:E:136:GLY:HA2	4:E:398:ALA:HB1	2.01	0.42
4:E:234:LEU:HD12	4:E:380:SER:HB2	2.02	0.42
4:E:271:ASP:C	4:E:275:ARG:HH21	2.23	0.42
5:F:129:HIS:HB3	5:F:132:LEU:HG	2.02	0.42
7:O:40:ARG:HH12	7:O:42:VAL:HG12	1.85	0.42
9:X:48:LEU:HD21	9:X:50:LEU:HB2	2.02	0.42
11:R:16:GLY:HA2	11:R:19:VAL:HG12	2.02	0.42
13:T:194:GLY:HA3	13:T:195:PRO:HD3	1.87	0.42
16:Q:163:GLU:O	16:Q:166:LEU:HB2	2.19	0.42
1:1:203:PRO:HB2	1:1:204:PRO:HD3	2.01	0.42
2:2:26:ALA:O	2:2:30:LEU:HG	2.19	0.42
3:3:203:ILE:HG21	8:7:88:ARG:HG2	2.01	0.42
4:4:88:LEU:HD21	6:6:48:ILE:HD13	2.01	0.42
5:5:74:LEU:HD12	5:5:88:PHE:CE1	2.54	0.42
6:6:29:ALA:HB1	6:6:159:ARG:HA	2.01	0.42
6:6:57:ARG:HA	7:9:23:THR:HA	2.01	0.42
7:9:52:LYS:NZ	7:9:171:GLU:OE2	2.33	0.42
11:J:97:ALA:HB2	12:K:16:TYR:HB2	2.01	0.42
13:L:239:LEU:HD12	13:L:239:LEU:HA	1.84	0.42
14:M:194:PHE:HB2	14:M:249:ALA:HB3	2.01	0.42
14:M:215:PRO:CG	14:M:216:PRO:HD3	2.49	0.42
15:N:212:ALA:HB1	15:N:292:THR:HG21	2.01	0.42
16:H:147:TYR:HE1	16:H:229:VAL:H	1.68	0.42
1:B:404:ASP:N	1:B:404:ASP:OD1	2.51	0.42
16:Q:213:GLU:N	16:Q:213:GLU:OE1	2.53	0.42
1:1:90:ILE:HB	1:1:218:ILE:HG12	2.01	0.42
1:1:273:ARG:HA	1:1:277:TYR:HD2	1.85	0.42
3:3:238:LEU:HG	3:3:707:LYS:HE2	2.02	0.42
6:6:36:LEU:HA	6:6:76:ASP:OD2	2.20	0.42
7:9:6:LEU:O	7:9:10:LEU:HD13	2.20	0.42
13:L:268:TYR:HD1	13:L:397:PHE:HB3	1.84	0.42
13:L:454:VAL:HB	13:L:455:LEU:HD22	2.02	0.42
14:M:24:LEU:HD22	14:M:27:LEU:HD21	2.02	0.42
14:M:119:TYR:CZ	14:M:160:LEU:HD13	2.55	0.42
16:H:149:LEU:HD23	16:H:149:LEU:HA	1.82	0.42
1:B:118:MET:HG2	1:B:224:LEU:HD13	2.00	0.42
3:D:194:VAL:HB	3:D:195:PRO:HD3	2.01	0.42
3:D:387:LEU:O	3:D:390:LEU:HB3	2.20	0.42
3:D:469:ARG:H	3:D:469:ARG:HG2	1.54	0.42
3:D:584:VAL:HA	3:D:600:VAL:O	2.20	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:E:238:SER:HA	4:E:275:ARG:HG2	2.00	0.42
6:G:66:GLU:OE2	16:Q:45:ARG:NH2	2.53	0.42
8:I:27:LYS:HA	8:I:27:LYS:HD3	1.87	0.42
11:R:92:LEU:O	11:R:95:LEU:HB3	2.20	0.42
13:T:444:TRP:O	13:T:447:HIS:HB2	2.20	0.42
16:Q:287:LEU:O	16:Q:291:ILE:HG13	2.19	0.42
1:1:342:TRP:NE1	1:1:372:ALA:HA	2.34	0.42
2:2:79:HIS:H	2:2:137:ASN:ND2	2.18	0.42
3:3:170:LEU:HD23	3:3:170:LEU:HA	1.75	0.42
4:4:149:ALA:HA	4:4:204:TYR:OH	2.20	0.42
4:4:235:THR:HG21	4:4:352:GLU:HB2	2.00	0.42
5:5:101:LEU:HD12	5:5:101:LEU:HA	1.93	0.42
14:M:371:LEU:HD13	14:M:371:LEU:HA	1.91	0.42
15:N:209:LEU:HG	15:N:293:GLY:HA2	2.02	0.42
1:B:214:LYS:O	1:B:216:THR:HG23	2.20	0.42
1:B:289:ALA:HB3	1:B:337:MET:HE3	2.02	0.42
2:C:85:THR:OG1	2:C:124:CYS:N	2.52	0.42
3:D:480:LEU:HD23	3:D:480:LEU:HA	1.83	0.42
4:E:260:TYR:HA	4:E:292:GLN:NE2	2.35	0.42
7:O:9:SER:O	7:O:12:ILE:HG13	2.20	0.42
7:O:178:GLU:HG3	7:O:178:GLU:O	2.20	0.42
11:R:117:GLN:HB2	12:S:47:ARG:O	2.19	0.42
13:T:454:VAL:HB	13:T:455:LEU:HD22	2.02	0.42
14:U:304:THR:HG21	14:U:386:LYS:HB2	2.01	0.42
14:U:344:TYR:O	14:U:347:LEU:HD23	2.20	0.42
16:Q:98:GLY:O	16:Q:114:TRP:HB2	2.19	0.42
1:1:393:LEU:HD23	1:1:397:ARG:HH22	1.81	0.41
2:2:77:LYS:O	2:2:137:ASN:ND2	2.53	0.41
3:3:290:ILE:HB	3:3:295:ARG:NH2	2.35	0.41
3:3:356:LEU:HD22	3:3:654:PHE:HB2	2.02	0.41
3:3:371:PHE:CE1	3:3:374:ARG:HG3	2.55	0.41
5:5:6:VAL:HG13	5:5:41:TYR:HE1	1.85	0.41
7:9:41:HIS:HB3	7:9:113:ILE:CD1	2.42	0.41
10:A:7:TYR:N	10:A:7:TYR:HD1	2.18	0.41
10:A:93:PHE:O	10:A:96:VAL:HG12	2.20	0.41
12:K:42:LEU:HD23	12:K:42:LEU:HA	1.86	0.41
13:L:496:LEU:HD12	13:L:496:LEU:HA	1.93	0.41
13:L:604:MET:HG2	15:N:232:ALA:HB2	2.02	0.41
14:M:385:TYR:CE1	14:M:389:PRO:HB3	2.55	0.41
15:N:209:LEU:HB2	15:N:296:PHE:HB3	2.01	0.41
3:D:5:LYS:HB3	3:D:92:VAL:HA	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:551:PRO:HB2	3:D:555:GLY:HA2	2.02	0.41
4:E:132:PHE:HE1	4:E:398:ALA:O	2.03	0.41
4:E:276:MET:O	4:E:280:ILE:HG13	2.20	0.41
12:S:42:LEU:HD23	12:S:42:LEU:HA	1.94	0.41
12:S:47:ARG:HE	12:S:47:ARG:HB3	1.61	0.41
13:T:309:ALA:HB2	13:T:388:ILE:HD13	2.01	0.41
14:U:452:ARG:HD3	14:U:452:ARG:HA	1.80	0.41
15:V:25:VAL:O	15:V:29:THR:HG23	2.19	0.41
15:V:176:LEU:HD23	15:V:176:LEU:HA	1.91	0.41
1:1:4:PRO:HA	1:1:12:ARG:HH12	1.85	0.41
1:1:149:ILE:HG22	1:1:153:ARG:HE	1.85	0.41
4:4:102:GLU:O	4:4:106:GLY:N	2.53	0.41
4:4:185:GLU:OE1	4:4:185:GLU:N	2.54	0.41
5:5:52:ILE:HG22	5:5:118:VAL:HG21	2.02	0.41
7:9:149:GLU:O	7:9:153:THR:CB	2.67	0.41
15:N:177:GLY:O	15:N:181:VAL:HG23	2.19	0.41
1:B:272:PHE:CE2	1:B:292:PRO:HB3	2.55	0.41
1:B:272:PHE:HZ	1:B:316:LEU:HD11	1.85	0.41
1:B:272:PHE:HZ	1:B:316:LEU:HD21	1.85	0.41
3:D:307:LYS:HB3	3:D:307:LYS:HE2	1.84	0.41
7:O:25:PRO:HB2	16:Q:50:ARG:HH22	1.84	0.41
9:X:88:ARG:HB3	9:X:90:TYR:CE1	2.56	0.41
10:P:47:GLY:O	10:P:48:ASN:HB3	2.21	0.41
13:T:14:PHE:HB2	13:T:109:ASN:HB2	2.02	0.41
13:T:239:LEU:HD12	13:T:243:ALA:HB3	2.02	0.41
14:U:215:PRO:CG	14:U:216:PRO:HD3	2.50	0.41
14:U:354:LEU:HD13	14:U:425:LEU:HG	2.02	0.41
16:Q:108:PHE:HB2	16:Q:112:GLN:O	2.20	0.41
1:1:393:LEU:HA	1:1:397:ARG:CZ	2.50	0.41
2:2:41:ILE:HD12	2:2:70:TYR:HB3	2.02	0.41
3:3:115:HIS:CD2	3:3:116:PRO:HD2	2.55	0.41
12:K:47:ARG:HE	12:K:47:ARG:HB3	1.67	0.41
14:M:78:ILE:O	14:M:82:VAL:HG23	2.20	0.41
14:M:93:GLY:HA3	14:M:136:TYR:CE1	2.55	0.41
1:B:356:CYS:N	17:B:501:SF4:S3	2.83	0.41
1:B:400:CYS:HA	1:B:401:PRO:HD3	1.89	0.41
4:E:28:LEU:HD12	10:P:50:PRO:O	2.19	0.41
4:E:137:LEU:HD23	4:E:145:PRO:HB2	2.02	0.41
4:E:302:VAL:HG23	4:E:303:ARG:HG2	2.03	0.41
7:O:102:GLY:HA2	7:O:115:LEU:HD11	2.01	0.41
10:P:8:VAL:O	10:P:12:ILE:HG13	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:T:14:PHE:CD1	13:T:106:ALA:HB1	2.54	0.41
13:T:123:SER:HA	13:T:184:SER:HA	2.01	0.41
13:T:132:GLU:OE2	13:T:163:ARG:NH1	2.54	0.41
16:Q:66:SER:O	16:Q:238:SER:OG	2.31	0.41
4:4:224:ILE:HD12	4:4:270:GLY:C	2.40	0.41
6:6:143:ARG:NE	6:6:145:GLU:OE1	2.54	0.41
13:L:30:GLY:HA2	13:L:105:PHE:CE1	2.56	0.41
13:L:364:TRP:O	13:L:368:ILE:HG13	2.20	0.41
13:L:433:HIS:O	13:L:433:HIS:CG	2.73	0.41
14:M:130:LEU:HD12	14:M:131:LEU:HD23	2.01	0.41
14:M:208:PHE:N	14:M:267:SER:OG	2.53	0.41
16:H:274:VAL:CG1	16:H:278:TRP:CD1	2.98	0.41
1:B:74:LEU:HD12	1:B:77:SER:OG	2.20	0.41
3:D:728:LEU:HB3	3:D:747:VAL:HG11	2.01	0.41
4:E:113:ALA:HB2	4:E:302:VAL:O	2.20	0.41
4:E:222:GLY:O	4:E:224:ILE:HG13	2.21	0.41
6:G:94:ARG:O	6:G:98:GLN:N	2.46	0.41
6:G:115:GLY:HA3	6:G:125:GLN:OE1	2.21	0.41
7:O:10:LEU:HB3	16:Q:292:TRP:CZ2	2.55	0.41
8:I:15:GLU:HG3	8:I:19:TRP:NE1	2.36	0.41
13:T:452:GLY:O	13:T:456:ALA:N	2.53	0.41
15:V:223:LEU:HB3	15:V:273:LEU:HD11	2.01	0.41
15:V:281:LEU:HD12	15:V:281:LEU:HA	1.78	0.41
16:Q:12:MET:HG2	16:Q:111:TYR:CD2	2.55	0.41
1:1:53:VAL:O	1:1:57:VAL:HG23	2.20	0.41
1:1:62:LEU:HD13	1:1:238:PHE:CZ	2.55	0.41
1:1:118:MET:CG	1:1:224:LEU:HD13	2.49	0.41
1:1:404:ASP:OD1	1:1:404:ASP:N	2.53	0.41
3:3:40:SER:HG	3:3:189:ARG:HD2	1.86	0.41
3:3:254:THR:OG1	3:3:624:LEU:HD23	2.19	0.41
3:3:460:LYS:HD3	3:3:460:LYS:HA	1.88	0.41
13:L:122:ASP:OD2	13:L:184:SER:OG	2.38	0.41
13:L:356:TRP:CE3	13:L:363:ARG:HD2	2.56	0.41
13:L:413:THR:HA	13:L:416:TYR:CZ	2.56	0.41
4:E:68:LYS:HB2	5:F:146:LEU:HD23	2.03	0.41
11:R:75:PHE:CE2	11:R:78:GLN:HG2	2.56	0.41
14:U:221:ASN:HB3	14:U:227:ALA:HB3	2.02	0.41
15:V:126:ARG:HD2	15:V:128:GLN:HG2	2.02	0.41
2:2:112:THR:HG22	2:2:117:PHE:H	1.85	0.41
3:3:112:LEU:CD2	3:3:130:LEU:HD21	2.49	0.41
3:3:118:ASP:O	3:3:122:CYS:HB2	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:3:368:HIS:HB3	3:3:556:ALA:N	2.35	0.41
4:4:62:LEU:HA	4:4:62:LEU:HD23	1.68	0.41
4:4:112:ARG:NH1	4:4:299:PRO:HA	2.35	0.41
13:L:561:LEU:HG	13:L:565:PHE:CE2	2.56	0.41
15:N:181:VAL:HA	15:N:192:PHE:HE2	1.84	0.41
1:B:149:ILE:CG2	1:B:153:ARG:HH21	2.34	0.41
1:B:291:ILE:O	1:B:328:VAL:HA	2.20	0.41
1:B:317:GLN:HA	1:B:321:SER:O	2.21	0.41
3:D:123:ASP:OD2	3:D:241:ARG:HA	2.20	0.41
5:F:159:PHE:HB2	5:F:163:ARG:O	2.20	0.41
9:X:34:ILE:HG23	9:X:92:ALA:HB3	2.02	0.41
13:T:433:HIS:O	13:T:433:HIS:CG	2.73	0.41
14:U:265:ALA:HA	14:U:395:ALA:HB2	2.01	0.41
14:U:346:GLY:HA2	14:U:416:GLU:O	2.20	0.41
16:Q:162:TYR:CD2	16:Q:209:ALA:HA	2.51	0.41
1:1:394:ILE:HB	1:1:407:VAL:HG11	2.03	0.41
11:J:72:MET:HE2	16:H:153:LEU:HD21	2.03	0.41
11:J:97:ALA:O	12:K:12:ALA:HB1	2.20	0.41
13:L:542:ILE:O	13:L:546:LEU:HG	2.20	0.41
14:M:39:LEU:HB3	14:M:67:LEU:HD21	2.02	0.41
14:M:95:PHE:HB3	14:M:136:TYR:CE2	2.56	0.41
15:N:291:ALA:HB2	15:N:409:LEU:HD11	2.02	0.41
16:H:327:VAL:O	16:H:331:ASP:N	2.49	0.41
3:D:306:LEU:HD11	3:D:308:THR:O	2.20	0.41
7:O:126:TYR:HB3	9:X:39:ASP:CG	2.41	0.41
2:2:101:THR:HG22	8:7:108:ILE:HG12	2.02	0.41
3:3:201:ASP:OD1	3:3:202:PHE:N	2.49	0.41
3:3:387:LEU:O	3:3:390:LEU:HB3	2.20	0.41
3:3:694:LEU:HA	3:3:760:LEU:O	2.21	0.41
10:A:67:LEU:HD21	10:A:110:GLU:OE2	2.21	0.41
11:J:58:VAL:O	11:J:62:ALA:HB3	2.20	0.41
13:L:582:GLN:OE1	15:N:260:TYR:OH	2.36	0.41
14:M:143:ARG:HA	14:M:143:ARG:HD3	1.68	0.41
1:B:245:GLN:HB2	1:B:314:GLU:CD	2.41	0.41
1:B:246:SER:HG	1:B:313:TYR:H	1.65	0.41
1:B:357:THR:HG21	3:D:111:THR:OG1	2.21	0.41
4:E:38:HIS:HE1	4:E:398:ALA:HA	1.85	0.41
4:E:73:ARG:NE	4:E:81:TYR:OH	2.54	0.41
10:P:67:LEU:HD23	16:Q:310:TRP:CZ2	2.56	0.41
16:Q:293:ILE:HD12	16:Q:297:TRP:CZ3	2.56	0.41
1:1:342:TRP:CZ2	1:1:372:ALA:HA	2.56	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:2:154:LEU:HD23	2:2:154:LEU:HA	1.78	0.41
3:3:116:PRO:O	3:3:117:LEU:HB2	2.21	0.41
3:3:168:HIS:O	3:3:176:LEU:N	2.51	0.41
3:3:355:LEU:HB2	3:3:547:MET:SD	2.61	0.41
3:3:473:GLU:O	3:3:476:ILE:N	2.53	0.41
4:4:27:THR:HG22	4:4:44:MET:HE3	2.03	0.41
4:4:202:ASP:OD1	4:4:284:ARG:NE	2.54	0.41
5:5:47:ASN:O	5:5:108:TRP:NE1	2.43	0.41
5:5:53:VAL:HG22	5:5:55:LEU:HD11	2.03	0.41
5:5:120:ASP:OD1	5:5:137:THR:OG1	2.29	0.41
6:6:165:GLU:OE2	7:9:148:ARG:NH1	2.53	0.41
7:9:41:HIS:O	7:9:136:MET:HB3	2.20	0.41
7:9:70:VAL:HG22	7:9:91:TYR:CD2	2.56	0.41
7:9:118:ASP:HB3	7:9:143:THR:CG2	2.51	0.41
10:A:48:ASN:OD1	10:A:49:ASP:HB2	2.20	0.41
11:J:154:VAL:O	11:J:158:GLU:HB2	2.21	0.41
13:L:327:PHE:CE1	13:L:452:GLY:HA3	2.56	0.41
13:L:587:ARG:O	13:L:591:LEU:HD13	2.21	0.41
14:M:141:ARG:HG3	14:M:142:THR:H	1.85	0.41
15:N:155:TYR:HB2	15:N:161:LEU:HD21	2.03	0.41
1:B:63:ARG:HD3	1:B:313:TYR:CD2	2.56	0.41
1:B:352:SER:OG	1:B:359:CYS:SG	2.72	0.41
2:C:78:TYR:HD2	2:C:116:LEU:HD12	1.86	0.41
3:D:256:CYS:O	3:D:262:GLY:HA2	2.21	0.41
3:D:284:GLU:H	3:D:284:GLU:HG2	1.68	0.41
3:D:341:VAL:HG22	3:D:565:TYR:HB2	2.03	0.41
4:E:34:HIS:HB2	10:P:45:GLU:OE2	2.21	0.41
4:E:185:GLU:OE1	4:E:185:GLU:N	2.52	0.41
4:E:330:HIS:O	4:E:334:GLY:HA2	2.20	0.41
4:E:353:LEU:HD12	4:E:354:GLY:H	1.86	0.41
6:G:177:LYS:HE3	6:G:177:LYS:HB2	1.78	0.41
7:O:37:PHE:HB3	7:O:117:TYR:HD1	1.86	0.41
12:S:94:ARG:HG2	13:T:583:THR:O	2.21	0.41
13:T:59:TRP:HB3	13:T:63:ILE:O	2.20	0.41
13:T:379:LEU:HD23	13:T:379:LEU:HA	1.88	0.41
14:U:8:LEU:HB3	14:U:9:PRO:HD3	2.03	0.41
14:U:381:LEU:HB2	14:U:396:PHE:CZ	2.55	0.41
15:V:280:ALA:HA	15:V:347:LEU:HD13	2.03	0.41
16:Q:65:LYS:NZ	16:Q:69:LYS:HE2	2.35	0.41
16:Q:122:ILE:HG13	16:Q:123:LEU:HD12	2.03	0.41
1:1:100:SER:HA	1:1:253:GLN:HE21	1.86	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:3:180:ARG:O	3:3:232:VAL:HG21	2.20	0.41
7:9:22:VAL:HB	16:H:44:VAL:CG2	2.51	0.41
13:L:491:TRP:HA	13:L:494:ILE:HG12	2.01	0.41
14:M:73:LEU:HD23	14:M:74:PHE:N	2.36	0.41
14:M:264:ALA:HB1	14:M:294:GLY:O	2.20	0.41
16:H:269:MET:HG3	16:H:270:PRO:HD2	2.02	0.41
1:B:102:LYS:HB3	1:B:253:GLN:OE1	2.21	0.41
1:B:197:ALA:HB3	2:C:66:PHE:CE2	2.56	0.41
1:B:433:ARG:HH12	2:C:89:LYS:CE	2.30	0.41
2:C:47:GLU:HB3	2:C:51:ARG:HH12	1.86	0.41
3:D:251:GLU:HG2	3:D:268:ASP:OD1	2.21	0.41
6:G:33:SER:O	6:G:36:LEU:HG	2.21	0.41
6:G:37:TRP:HB2	16:Q:65:LYS:HE2	2.03	0.41
13:T:49:LEU:HD23	13:T:49:LEU:HA	1.94	0.41
13:T:90:TYR:CE1	13:T:334:LEU:HD22	2.56	0.41
13:T:293:LYS:HE2	13:T:297:TYR:HE1	1.86	0.41
14:U:49:HIS:O	14:U:66:GLY:HA2	2.21	0.41
14:U:78:ILE:O	14:U:82:VAL:HG23	2.21	0.41
16:Q:91:VAL:O	16:Q:95:LEU:HG	2.20	0.41
2:2:7:LYS:O	2:2:11:LEU:HG	2.22	0.40
3:3:192:GLU:O	3:3:443:ARG:NH1	2.54	0.40
3:3:256:CYS:O	3:3:262:GLY:HA2	2.21	0.40
3:3:349:ALA:HB3	3:3:544:LEU:HD21	2.04	0.40
3:3:455:ARG:NH2	3:3:750:ARG:NH2	2.69	0.40
4:4:64:THR:OG1	6:6:123:ILE:HD11	2.20	0.40
4:4:193:LEU:HA	4:4:196:VAL:HG12	2.02	0.40
4:4:197:LEU:N	4:4:198:PRO:HD2	2.36	0.40
5:5:168:ALA:HA	5:5:171:ARG:HH11	1.86	0.40
6:6:39:ALA:N	6:6:77:VAL:O	2.35	0.40
6:6:78:MET:HB3	6:6:105:VAL:HG22	2.03	0.40
9:W:46:TYR:O	9:W:61:ASP:HA	2.21	0.40
13:L:216:LYS:HD3	13:L:245:MET:SD	2.61	0.40
14:M:141:ARG:HG3	14:M:142:THR:N	2.36	0.40
14:M:242:PHE:HZ	14:M:458:ALA:HA	1.85	0.40
14:M:244:PHE:O	14:M:248:LEU:HB2	2.21	0.40
15:N:16:LEU:O	15:N:20:LEU:N	2.55	0.40
1:B:259:LYS:HB3	1:B:281:GLY:HA3	2.02	0.40
3:D:290:ILE:HG23	17:D:803:SF4:S4	2.61	0.40
3:D:307:LYS:HE3	3:D:632:GLY:CA	2.51	0.40
4:E:156:ILE:HG12	4:E:193:LEU:HD11	2.03	0.40
5:F:101:LEU:HD12	5:F:101:LEU:HA	1.99	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:F:113:PHE:O	5:F:116:ARG:HB2	2.21	0.40
10:P:68:PHE:CD2	16:Q:164:LEU:HB2	2.56	0.40
10:P:83:VAL:HG23	10:P:84:SER:H	1.86	0.40
13:T:385:LYS:NZ	13:T:410:ALA:HA	2.36	0.40
13:T:600:LEU:HD12	15:V:235:LEU:HD23	2.03	0.40
16:Q:216:ARG:HD2	16:Q:294:ARG:HA	2.02	0.40
1:1:211:LEU:HD12	1:1:211:LEU:HA	1.91	0.40
3:3:503:PRO:CG	3:3:528:LYS:HD3	2.51	0.40
7:9:17:LEU:HA	16:H:41:ARG:O	2.21	0.40
10:A:60:HIS:CE1	16:H:306:LEU:HD12	2.55	0.40
13:L:141:LEU:HB3	13:L:236:VAL:HG11	2.02	0.40
13:L:598:LEU:HD23	13:L:598:LEU:HA	1.90	0.40
14:M:88:VAL:HG22	14:M:331:ARG:HE	1.86	0.40
14:M:362:PHE:O	14:M:365:MET:HB3	2.20	0.40
15:N:294:LEU:CG	15:N:402:VAL:HG13	2.49	0.40
15:N:345:LYS:O	15:N:349:PHE:CD2	2.74	0.40
16:H:2:THR:HA	16:H:5:TYR:CD2	2.51	0.40
16:H:103:GLY:O	16:H:113:PRO:HG2	2.21	0.40
2:C:147:ARG:HE	2:C:147:ARG:HB2	1.72	0.40
3:D:464:ILE:HA	3:D:489:MET:SD	2.61	0.40
4:E:73:ARG:O	4:E:365:PRO:HD2	2.22	0.40
4:E:240:ARG:O	4:E:267:GLY:N	2.47	0.40
4:E:245:ASN:HA	4:E:266:LEU:HD21	2.03	0.40
4:E:352:GLU:OE2	5:F:87:ARG:NH2	2.53	0.40
7:O:20:LYS:H	7:O:20:LYS:HG3	1.74	0.40
12:S:21:ARG:NE	12:S:26:LEU:HD23	2.37	0.40
13:T:74:GLY:O	13:T:78:LEU:HG	2.21	0.40
14:U:103:GLU:O	14:U:107:LEU:HG	2.21	0.40
14:U:381:LEU:HB2	14:U:396:PHE:CE2	2.57	0.40
16:Q:21:VAL:HG13	16:Q:94:LEU:HD13	2.03	0.40
16:Q:267:TRP:O	16:Q:269:MET:N	2.54	0.40
16:Q:301:ARG:O	16:Q:302:TYR:HB3	2.21	0.40
1:1:20:HIS:HB3	1:1:31:TYR:CE1	2.55	0.40
1:1:435:SER:HA	2:2:95:GLU:OE2	2.21	0.40
3:3:133:ARG:HA	3:3:136:GLU:OE2	2.21	0.40
3:3:438:LYS:O	3:3:441:MET:HG3	2.21	0.40
3:3:715:GLU:HA	3:3:746:ARG:O	2.21	0.40
4:4:236:GLY:O	4:4:238:SER:N	2.54	0.40
4:4:396:ILE:HA	4:4:399:SER:OG	2.20	0.40
5:5:116:ARG:HB3	5:5:135:ILE:HG13	2.03	0.40
10:A:107:PHE:HE1	16:H:310:TRP:HD1	1.68	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:J:11:LEU:HB3	11:J:38:VAL:HG21	2.02	0.40
13:L:356:TRP:CZ3	13:L:363:ARG:HD2	2.55	0.40
14:M:348:ALA:HB2	14:M:414:PHE:HB3	2.02	0.40
16:H:33:LEU:HD11	16:H:55:GLY:O	2.21	0.40
4:E:246:TYR:OH	4:E:352:GLU:OE1	2.39	0.40
5:F:55:LEU:O	5:F:68:PHE:HA	2.21	0.40
13:T:22:LYS:HZ1	13:T:100:GLY:HA2	1.86	0.40
14:U:148:PHE:HA	14:U:213:TRP:HB2	2.04	0.40
16:Q:155:SER:OG	16:Q:156:SER:N	2.55	0.40
16:Q:291:ILE:HA	16:Q:294:ARG:CG	2.45	0.40
1:1:201:LEU:HD11	3:3:84:VAL:HG21	2.03	0.40
2:2:3:PHE:CE2	2:2:34:VAL:HG22	2.55	0.40
3:3:136:GLU:HA	5:5:188:SER:H	1.86	0.40
3:3:243:ARG:HD2	3:3:275:LEU:HD22	2.02	0.40
3:3:307:LYS:HE3	3:3:632:GLY:HA2	2.03	0.40
5:5:54:GLY:O	5:5:55:LEU:HD12	2.21	0.40
8:7:44:MET:CE	8:7:46:ARG:HH22	2.34	0.40
10:A:47:GLY:O	10:A:48:ASN:HB3	2.21	0.40
13:L:122:ASP:OD1	13:L:186:SER:HB3	2.22	0.40
13:L:183:LEU:HD23	13:L:183:LEU:HA	1.74	0.40
13:L:539:ASN:N	13:L:539:ASN:OD1	2.54	0.40
14:M:127:ILE:O	14:M:131:LEU:HG	2.22	0.40
15:N:255:LYS:HE2	15:N:306:ARG:HA	2.03	0.40
16:H:5:TYR:OH	16:H:184:ASP:OD1	2.25	0.40
16:H:44:VAL:C	16:H:45:ARG:O	2.59	0.40
16:H:274:VAL:CG2	16:H:275:PRO:HD2	2.52	0.40
3:D:180:ARG:O	3:D:232:VAL:HG21	2.22	0.40
3:D:202:PHE:HB3	3:D:209:THR:CG2	2.52	0.40
3:D:478:LEU:HG	3:D:483:ASP:HB2	2.03	0.40
4:E:26:MET:N	4:E:48:SER:OG	2.48	0.40
13:T:389:LEU:HD21	13:T:407:LEU:HD13	2.03	0.40
13:T:554:PHE:HZ	14:U:283:THR:HG21	1.84	0.40
15:V:35:LEU:HD23	15:V:35:LEU:HA	1.93	0.40
15:V:40:LEU:HD12	15:V:67:LEU:HD12	2.02	0.40
15:V:89:LEU:HD23	15:V:89:LEU:HA	1.87	0.40
15:V:256:ARG:HG2	15:V:260:TYR:HE2	1.86	0.40
15:V:294:LEU:O	15:V:298:VAL:HG23	2.21	0.40
15:V:337:PRO:HG3	15:V:342:PHE:CD2	2.56	0.40
1:1:45:LEU:HD12	1:1:163:PHE:CD2	2.56	0.40
1:1:135:ARG:HE	1:1:137:GLU:HB2	1.86	0.40
3:3:40:SER:HA	3:3:437:ILE:O	2.21	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:3:196:GLY:HA3	3:3:461:TRP:CZ2	2.56	0.40
3:3:451:PHE:HE1	3:3:466:GLU:HB3	1.87	0.40
6:6:106:ILE:HG12	6:6:135:VAL:HB	2.03	0.40
9:W:51:HIS:HA	9:W:56:ASP:OD1	2.22	0.40
9:W:113:ARG:O	9:W:117:ILE:HG12	2.21	0.40
11:J:75:PHE:CZ	11:J:77:ALA:HB3	2.57	0.40
14:M:304:THR:HG21	14:M:386:LYS:HB2	2.04	0.40
14:M:358:ALA:O	14:M:362:PHE:HD2	2.04	0.40
15:N:98:LEU:HD23	15:N:218:ALA:HB1	2.03	0.40
16:H:213:GLU:OE1	16:H:213:GLU:N	2.55	0.40
1:B:357:THR:N	1:B:358:PRO:HD2	2.36	0.40
2:C:110:GLU:HA	8:I:121:ARG:NH1	2.25	0.40
3:D:293:ALA:HB2	3:D:698:MET:HG2	2.04	0.40
4:E:169:HIS:HE2	6:G:45:CYS:CB	2.35	0.40
5:F:74:LEU:O	5:F:87:ARG:HA	2.20	0.40
11:R:155:ALA:HB2	15:V:83:GLU:HG2	2.03	0.40
13:T:184:SER:HB3	13:T:187:GLU:HG2	2.02	0.40
13:T:371:LEU:O	13:T:375:GLY:N	2.55	0.40
14:U:128:PRO:O	14:U:132:MET:HG2	2.21	0.40
16:Q:28:PHE:HB2	16:Q:249:TYR:HB3	2.04	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%)	403 (93%)	32 (7%)	0	100	100
1	B	435/438 (99%)	399 (92%)	36 (8%)	0	100	100
2	2	176/181 (97%)	170 (97%)	6 (3%)	0	100	100
2	C	176/181 (97%)	169 (96%)	7 (4%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
3	3	750/783 (96%)	702 (94%)	48 (6%)	0	100	100
3	D	750/783 (96%)	700 (93%)	50 (7%)	0	100	100
4	4	382/409 (93%)	361 (94%)	21 (6%)	0	100	100
4	E	382/409 (93%)	357 (94%)	25 (6%)	0	100	100
5	5	194/207 (94%)	183 (94%)	11 (6%)	0	100	100
5	F	194/207 (94%)	182 (94%)	12 (6%)	0	100	100
6	6	164/181 (91%)	144 (88%)	20 (12%)	0	100	100
6	G	164/181 (91%)	148 (90%)	16 (10%)	0	100	100
7	9	178/182 (98%)	166 (93%)	12 (7%)	0	100	100
7	O	178/182 (98%)	172 (97%)	5 (3%)	1 (1%)	25	57
8	7	125/129 (97%)	115 (92%)	10 (8%)	0	100	100
8	I	125/129 (97%)	116 (93%)	9 (7%)	0	100	100
9	W	125/131 (95%)	121 (97%)	4 (3%)	0	100	100
9	X	125/131 (95%)	121 (97%)	4 (3%)	0	100	100
10	A	115/119 (97%)	105 (91%)	10 (9%)	0	100	100
10	P	115/119 (97%)	105 (91%)	10 (9%)	0	100	100
11	J	158/176 (90%)	148 (94%)	10 (6%)	0	100	100
11	R	158/176 (90%)	146 (92%)	12 (8%)	0	100	100
12	K	93/95 (98%)	88 (95%)	5 (5%)	0	100	100
12	S	93/95 (98%)	87 (94%)	6 (6%)	0	100	100
13	L	603/606 (100%)	568 (94%)	34 (6%)	1 (0%)	47	78
13	T	603/606 (100%)	569 (94%)	33 (6%)	1 (0%)	47	78
14	M	465/469 (99%)	438 (94%)	27 (6%)	0	100	100
14	U	465/469 (99%)	437 (94%)	28 (6%)	0	100	100
15	N	425/427 (100%)	400 (94%)	25 (6%)	0	100	100
15	V	425/427 (100%)	402 (95%)	23 (5%)	0	100	100
16	H	351/365 (96%)	302 (86%)	42 (12%)	7 (2%)	7	30
16	Q	351/365 (96%)	302 (86%)	42 (12%)	7 (2%)	7	30
All	All	9478/9796 (97%)	8826 (93%)	635 (7%)	17 (0%)	47	78

All (17) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
16	H	45	ARG
16	H	51	VAL
7	O	21	PRO
16	Q	51	VAL
16	H	44	VAL
16	Q	44	VAL
16	Q	45	ARG
16	H	50	ARG
16	H	218	PRO
16	H	268	THR
16	Q	50	ARG
13	L	435	PRO
16	Q	268	THR
13	T	435	PRO
16	Q	333	PRO
16	H	53	PRO
16	Q	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%)	344 (97%)	11 (3%)	40	68
1	B	355/356 (100%)	345 (97%)	10 (3%)	43	70
2	2	150/152 (99%)	144 (96%)	6 (4%)	31	60
2	C	150/152 (99%)	144 (96%)	6 (4%)	31	60
3	3	609/628 (97%)	599 (98%)	10 (2%)	62	81
3	D	609/628 (97%)	598 (98%)	11 (2%)	59	79
4	4	332/355 (94%)	328 (99%)	4 (1%)	71	85
4	E	332/355 (94%)	326 (98%)	6 (2%)	59	79
5	5	167/175 (95%)	163 (98%)	4 (2%)	49	74
5	F	167/175 (95%)	164 (98%)	3 (2%)	59	79
6	6	135/149 (91%)	125 (93%)	10 (7%)	13	42

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
6	G	135/149 (91%)	126 (93%)	9 (7%)	16	46
7	9	148/150 (99%)	147 (99%)	1 (1%)	84	92
7	O	148/150 (99%)	146 (99%)	2 (1%)	67	83
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%)	98 (99%)	1 (1%)	76	88
10	A	90/92 (98%)	88 (98%)	2 (2%)	52	75
10	P	90/92 (98%)	87 (97%)	3 (3%)	38	66
11	J	118/130 (91%)	114 (97%)	4 (3%)	37	65
11	R	118/130 (91%)	115 (98%)	3 (2%)	47	72
12	K	71/71 (100%)	69 (97%)	2 (3%)	43	70
12	S	71/71 (100%)	69 (97%)	2 (3%)	43	70
13	L	453/454 (100%)	445 (98%)	8 (2%)	59	79
13	T	453/454 (100%)	445 (98%)	8 (2%)	59	79
14	M	332/332 (100%)	324 (98%)	8 (2%)	49	74
14	U	332/332 (100%)	323 (97%)	9 (3%)	44	70
15	N	302/302 (100%)	297 (98%)	5 (2%)	60	80
15	V	302/302 (100%)	297 (98%)	5 (2%)	60	80
16	H	293/300 (98%)	280 (96%)	13 (4%)	28	58
16	Q	293/300 (98%)	282 (96%)	11 (4%)	33	61
All	All	7516/7706 (98%)	7336 (98%)	180 (2%)	49	74

All (180) 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	337	MET
1	1	342	TRP
1	1	353	CYS
1	1	359	CYS
1	1	366	PHE
1	1	397	ARG

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Mol	Chain	Res	Type
1	1	437	TRP
1	1	438	ARG
2	2	7	LYS
2	2	33	ARG
2	2	35	GLN
2	2	45	ARG
2	2	116	LEU
2	2	147	ARG
3	3	3	ARG
3	3	184	CYS
3	3	259	CYS
3	3	260	PRO
3	3	337	ARG
3	3	616	ASN
3	3	651	ARG
3	3	655	ARG
3	3	761	SER
3	3	774	ARG
4	4	129	HIS
4	4	143	LEU
4	4	208	PHE
4	4	262	PHE
5	5	31	ARG
5	5	38	MET
5	5	147	ARG
5	5	178	ASP
6	6	37	TRP
6	6	49	GLU
6	6	55	ASP
6	6	68	PHE
6	6	83	ARG
6	6	88	MET
6	6	120	ASN
6	6	156	LYS
6	6	176	TRP
6	6	177	LYS
7	9	38	HIS
8	7	43	ARG
9	W	37	TRP
10	A	13	TYR
10	A	48	ASN
11	J	59	TYR

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Mol	Chain	Res	Type
11	J	84	ASP
11	J	118	ASP
11	J	119	LEU
12	K	28	PHE
12	K	82	ARG
13	L	59	TRP
13	L	151	TYR
13	L	169	PHE
13	L	286	PHE
13	L	416	TYR
13	L	506	TRP
13	L	511	PHE
13	L	554	PHE
14	M	22	ARG
14	M	73	LEU
14	M	135	LEU
14	M	151	PHE
14	M	241	PHE
14	M	255	GLN
14	M	415	TRP
14	M	455	HIS
15	N	50	PHE
15	N	105	LEU
15	N	126	ARG
15	N	284	TYR
15	N	313	ARG
16	H	28	PHE
16	H	37	ARG
16	H	43	GLN
16	H	44	VAL
16	H	119	ASP
16	H	134	TYR
16	H	147	TYR
16	H	149	LEU
16	H	196	PHE
16	H	249	TYR
16	H	302	TYR
16	H	307	ARG
16	H	354	TYR
1	B	81	LYS
1	B	249	MET
1	B	337	MET

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Mol	Chain	Res	Type
1	B	342	TRP
1	B	353	CYS
1	B	355	LYS
1	B	359	CYS
1	B	366	PHE
1	B	397	ARG
1	B	437	TRP
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	132	ASP
3	D	184	CYS
3	D	259	CYS
3	D	337	ARG
3	D	369	LEU
3	D	469	ARG
3	D	617	LEU
3	D	655	ARG
3	D	761	SER
3	D	774	ARG
4	E	87	TYR
4	E	129	HIS
4	E	143	LEU
4	E	152	GLU
4	E	208	PHE
4	E	262	PHE
5	F	31	ARG
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	88	MET
6	G	120	ASN
6	G	156	LYS
6	G	176	TRP

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Mol	Chain	Res	Type
7	O	20	LYS
7	O	38	HIS
8	I	43	ARG
9	X	37	TRP
10	P	13	TYR
10	P	48	ASN
10	P	79	TRP
11	R	59	TYR
11	R	84	ASP
11	R	119	LEU
12	S	28	PHE
12	S	82	ARG
13	T	56	GLN
13	T	59	TRP
13	T	124	TYR
13	T	169	PHE
13	T	416	TYR
13	T	506	TRP
13	T	511	PHE
13	T	554	PHE
14	U	22	ARG
14	U	135	LEU
14	U	151	PHE
14	U	234	TYR
14	U	239	PHE
14	U	255	GLN
14	U	326	PHE
14	U	415	TRP
14	U	455	HIS
15	V	50	PHE
15	V	126	ARG
15	V	198	ASP
15	V	284	TYR
15	V	313	ARG
16	Q	28	PHE
16	Q	44	VAL
16	Q	54	PHE
16	Q	119	ASP
16	Q	134	TYR
16	Q	147	TYR
16	Q	149	LEU
16	Q	196	PHE

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Mol	Chain	Res	Type
16	Q	302	TYR
16	Q	307	ARG
16	Q	354	TYR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (55) such sidechains are listed below:

Mol	Chain	Res	Type
1	1	92	ASN
1	1	240	GLN
1	1	288	GLN
1	1	343	ASN
2	2	174	HIS
3	3	168	HIS
3	3	661	GLN
3	3	709	GLN
4	4	34	HIS
4	4	292	GLN
4	4	330	HIS
4	4	379	GLN
5	5	112	ASN
6	6	120	ASN
6	6	153	GLN
9	W	43	GLN
10	A	60	HIS
12	K	81	HIS
13	L	288	GLN
13	L	358	HIS
13	L	432	HIS
13	L	544	ASN
14	M	221	ASN
14	M	255	GLN
15	N	245	ASN
16	H	112	GLN
16	H	117	ASN
16	H	183	ASN
1	B	92	ASN
1	B	219	ASN
1	B	240	GLN
1	B	288	GLN
1	B	350	HIS
2	C	177	HIS
3	D	104	GLN

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Mol	Chain	Res	Type
3	D	168	HIS
3	D	368	HIS
3	D	436	GLN
4	E	292	GLN
6	G	120	ASN
6	G	153	GLN
9	X	43	GLN
10	P	60	HIS
11	R	78	GLN
12	S	81	HIS
13	T	302	GLN
13	T	341	HIS
13	T	432	HIS
14	U	221	ASN
14	U	255	GLN
15	V	245	ASN
16	Q	43	GLN
16	Q	117	ASN
16	Q	183	ASN
16	Q	251	HIS

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	$\#\|Z\| > 2$
20	HQW	4	501	-	29,31,31	1.30	4 (13%)	29,44,44	1.49	6 (20%)
18	FMN	1	502	-	33,33,33	1.11	2 (6%)	48,50,50	1.29	9 (18%)
17	SF4	O	202	7	0,12,12	-	-	-		
17	SF4	9	201	7	0,12,12	-	-	-		
19	FES	3	804	3	0,4,4	-	-	-		
17	SF4	D	803	3	0,12,12	-	-	-		
17	SF4	3	803	3	0,12,12	-	-	-		
17	SF4	3	802	3	0,12,12	-	-	-		
17	SF4	9	202	7	0,12,12	-	-	-		
20	HQW	E	501	-	29,31,31	1.01	1 (3%)	29,44,44	1.58	6 (20%)
17	SF4	D	801	3	0,12,12	-	-	-		
17	SF4	B	501	1	0,12,12	-	-	-		
17	SF4	D	802	3	0,12,12	-	-	-		
18	FMN	B	502	-	33,33,33	1.08	2 (6%)	48,50,50	1.31	7 (14%)
17	SF4	6	201	6	0,12,12	-	-	-		
19	FES	D	804	3	0,4,4	-	-	-		
19	FES	2	201	2	0,4,4	-	-	-		
17	SF4	G	201	6	0,12,12	-	-	-		
17	SF4	O	201	7	0,12,12	-	-	-		
17	SF4	1	501	1	0,12,12	-	-	-		
17	SF4	3	801	3	0,12,12	-	-	-		
19	FES	C	201	2	0,4,4	-	-	-		

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
20	HQW	4	501	-	-	4/13/27/27	0/3/3/3
18	FMN	1	502	-	-	8/18/18/18	0/3/3/3
17	SF4	O	202	7	-	-	0/6/5/5
17	SF4	9	201	7	-	-	0/6/5/5
19	FES	3	804	3	-	-	0/1/1/1
17	SF4	D	803	3	-	-	0/6/5/5
17	SF4	3	803	3	-	-	0/6/5/5
20	HQW	E	501	-	-	4/13/27/27	0/3/3/3

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
17	SF4	3	802	3	-	-	0/6/5/5
17	SF4	9	202	7	-	-	0/6/5/5
17	SF4	D	801	3	-	-	0/6/5/5
17	SF4	B	501	1	-	-	0/6/5/5
17	SF4	D	802	3	-	-	0/6/5/5
18	FMN	B	502	-	-	8/18/18/18	0/3/3/3
17	SF4	6	201	6	-	-	0/6/5/5
19	FES	D	804	3	-	-	0/1/1/1
19	FES	2	201	2	-	-	0/1/1/1
17	SF4	G	201	6	-	-	0/6/5/5
17	SF4	O	201	7	-	-	0/6/5/5
17	SF4	1	501	1	-	-	0/6/5/5
17	SF4	3	801	3	-	-	0/6/5/5
19	FES	C	201	2	-	-	0/1/1/1

All (9) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
18	1	502	FMN	C4A-N5	4.23	1.39	1.30
18	B	502	FMN	C4A-N5	3.90	1.38	1.30
20	E	501	HQW	C23-N1	2.87	1.51	1.45
20	4	501	HQW	C23-N1	2.72	1.51	1.45
20	4	501	HQW	O25-C13	2.69	1.40	1.35
18	1	502	FMN	C10-N1	2.64	1.38	1.33
18	B	502	FMN	C10-N1	2.60	1.38	1.33
20	4	501	HQW	O26-C13	2.28	1.39	1.34
20	4	501	HQW	O24-C2	-2.12	1.40	1.44

All (28) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
20	E	501	HQW	C17-C14-C10	-4.13	123.70	130.74
20	E	501	HQW	O24-C5-C4	3.26	109.16	105.58
20	4	501	HQW	C17-C14-C10	-3.06	125.53	130.74
18	1	502	FMN	C4-N3-C2	-2.98	120.14	125.64
18	B	502	FMN	C4-N3-C2	-2.96	120.17	125.64
18	1	502	FMN	C4A-C4-N3	2.92	120.60	113.19
18	B	502	FMN	O4-C4-C4A	-2.85	119.03	126.60
20	4	501	HQW	O24-C5-C4	2.83	108.69	105.58
18	B	502	FMN	C5A-C9A-N10	2.78	120.83	117.95
18	B	502	FMN	C4A-C4-N3	2.68	119.98	113.19
20	E	501	HQW	O25-C13-O26	-2.65	110.75	113.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
20	4	501	HQW	O27-C9-C11	2.62	128.46	120.73
20	E	501	HQW	O25-C6-C7	2.57	124.27	121.64
18	1	502	FMN	C9A-C5A-N5	-2.56	119.65	122.43
18	B	502	FMN	C9A-C5A-N5	-2.49	119.73	122.43
18	1	502	FMN	C4A-C10-N10	2.48	120.10	116.48
20	E	501	HQW	C15-C10-C14	-2.39	119.63	124.64
18	1	502	FMN	C4A-C10-N1	-2.33	119.32	124.73
18	1	502	FMN	C10-N1-C2	2.32	121.54	116.90
18	1	502	FMN	O4-C4-C4A	-2.27	120.58	126.60
18	1	502	FMN	C10-C4A-N5	-2.26	120.06	124.86
18	1	502	FMN	C5A-C9A-N10	2.25	120.27	117.95
20	4	501	HQW	C15-C10-C14	-2.22	119.99	124.64
18	B	502	FMN	C4A-C10-N1	-2.14	119.77	124.73
20	4	501	HQW	O27-C9-C7	-2.08	114.61	120.73
18	B	502	FMN	C9-C9A-N10	-2.06	119.05	121.84
20	E	501	HQW	C14-C10-C8	2.04	122.61	116.96
20	4	501	HQW	C14-C10-C8	2.01	122.54	116.96

There are no chirality outliers.

All (24) 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	O2'-C2'-C3'-O3'
18	1	502	FMN	O2'-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	O2'-C2'-C3'-O3'
18	B	502	FMN	O2'-C2'-C3'-C4'
18	B	502	FMN	O4'-C4'-C5'-O5'
20	4	501	HQW	C14-C10-C8-C4
20	4	501	HQW	C15-C10-C8-C4
20	E	501	HQW	C14-C10-C8-C4
20	E	501	HQW	C15-C10-C8-C4
20	E	501	HQW	C10-C14-C17-C19
20	4	501	HQW	C10-C14-C17-C18

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Mol	Chain	Res	Type	Atoms
20	E	501	HQW	C10-C14-C17-C18
20	4	501	HQW	C10-C14-C17-C19
18	B	502	FMN	C3'-C4'-C5'-O5'
18	1	502	FMN	C3'-C4'-C5'-O5'

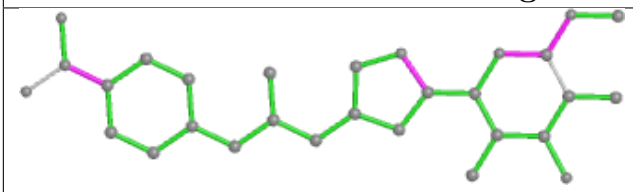
There are no ring outliers.

17 monomers are involved in 24 short contacts:

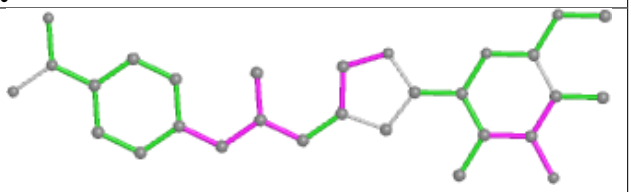
Mol	Chain	Res	Type	Clashes	Symm-Clashes
18	1	502	FMN	1	0
17	O	202	SF4	1	0
17	9	201	SF4	1	0
19	3	804	FES	2	0
17	D	803	SF4	1	0
17	3	803	SF4	1	0
17	9	202	SF4	1	0
17	D	801	SF4	1	0
17	B	501	SF4	3	0
18	B	502	FMN	2	0
17	6	201	SF4	1	0
19	D	804	FES	2	0
19	2	201	FES	1	0
17	G	201	SF4	1	0
17	O	201	SF4	1	0
17	1	501	SF4	2	0
19	C	201	FES	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.

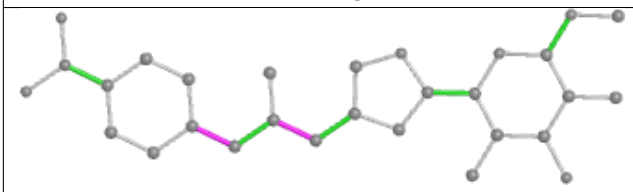
Ligand HQW 4 501



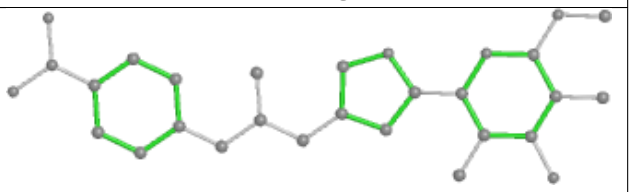
Bond lengths



Bond angles

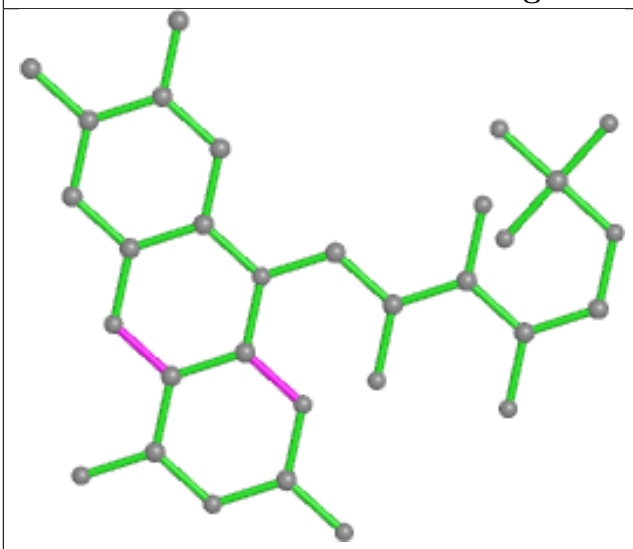


Torsions

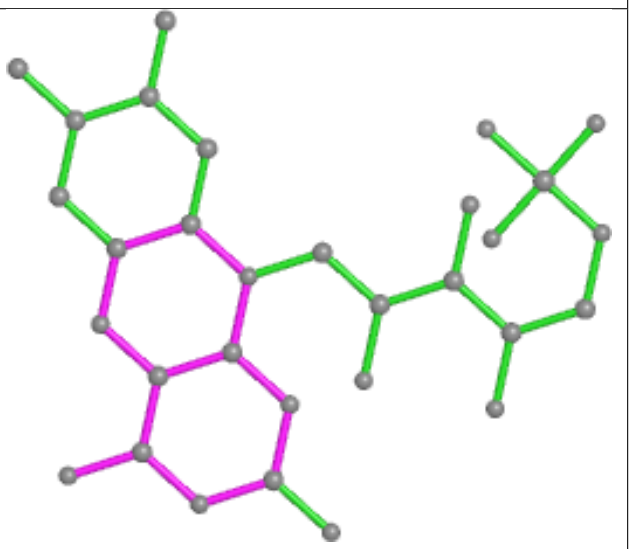


Rings

Ligand FMN 1 502



Bond lengths



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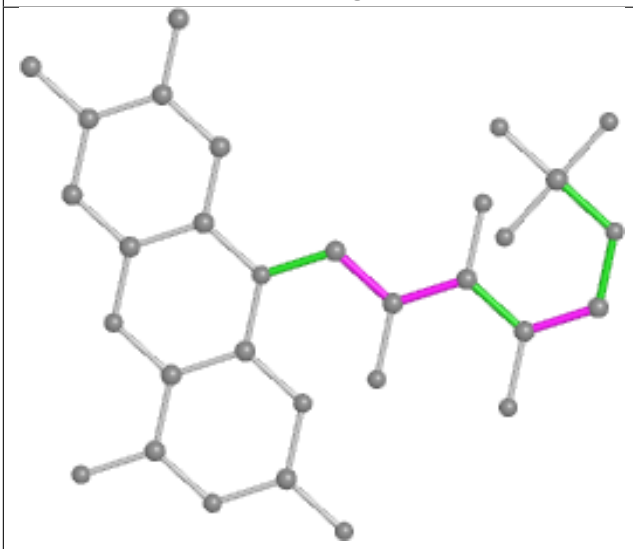

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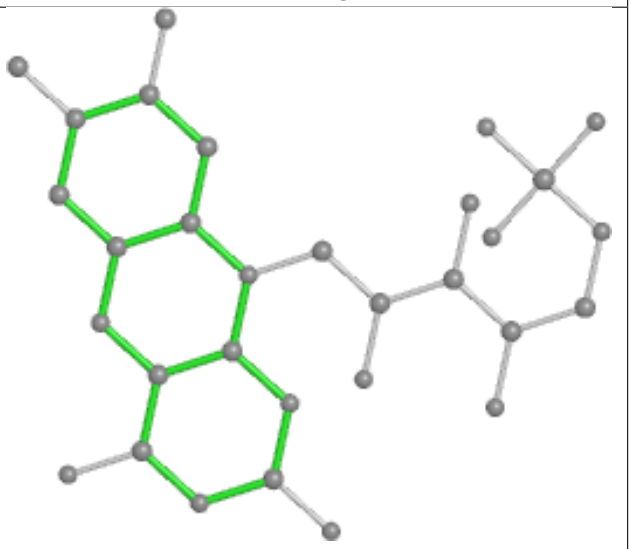
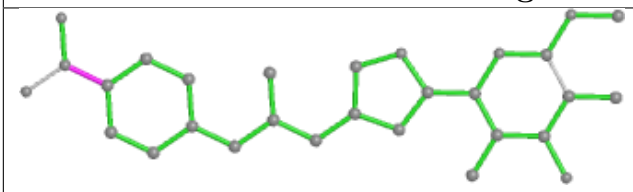
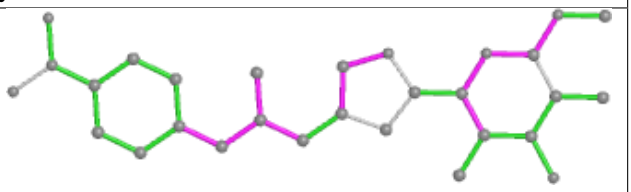


Rings

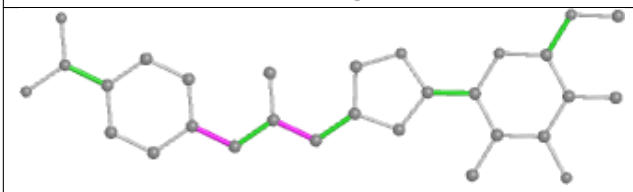
Ligand HQW E 501



Bond lengths



Bond angles



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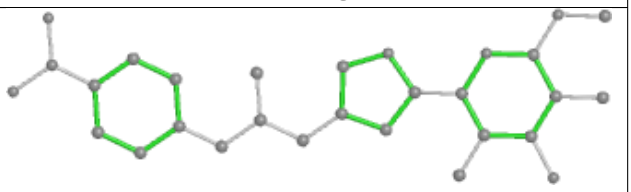
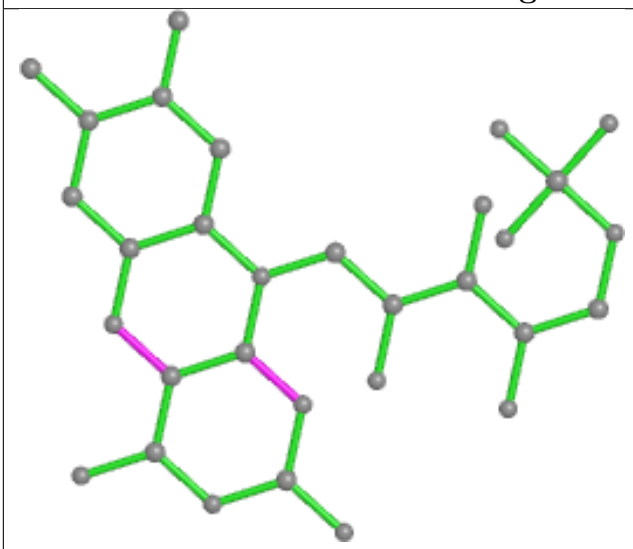


Rings

Ligand FMN B 502



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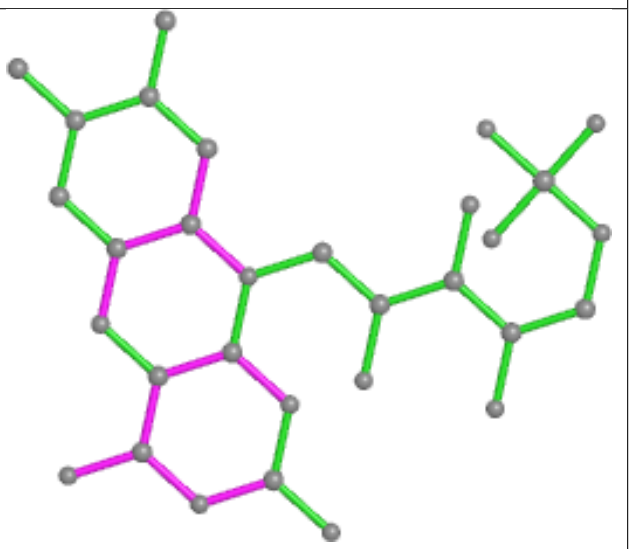
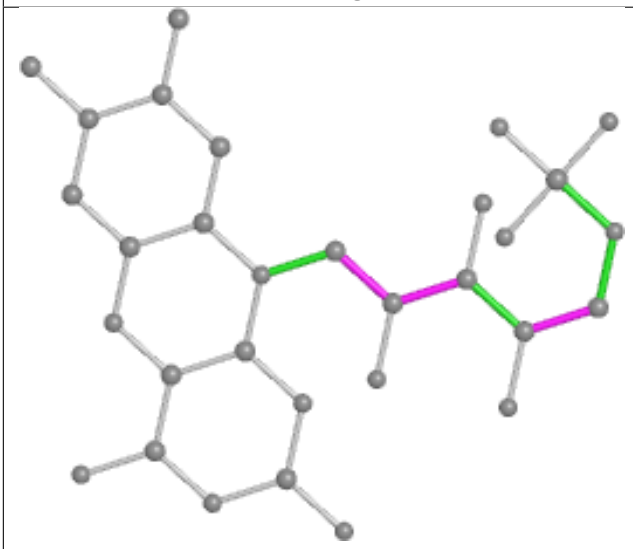
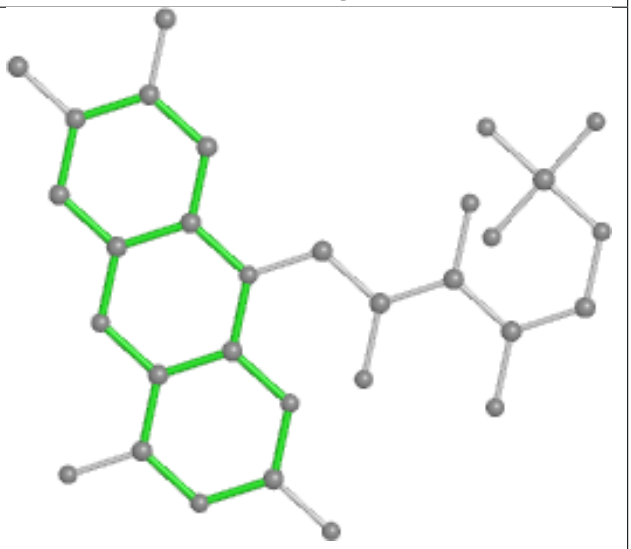


Bond angles



Torsions



Rings

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.