Full wwPDB X-ray Structure Validation Report (i)

May 27, 2024 – 08:03 PM EDT

PDB ID	:	6I1P
Title	:	Respiratory complex I from Thermus thermophilus with bound NADH
Authors	:	Gutierrez-Fernandez, J.; Minhas, G.S.; Sazanov, L.A.
Deposited on	:	2018-10-29
Resolution	:	3.21 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:

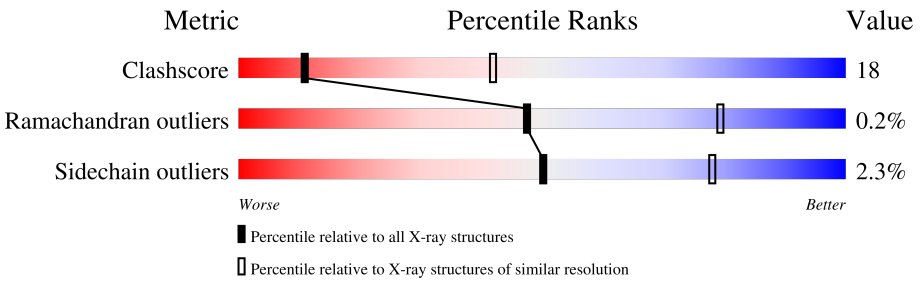
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	FAILED
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36.2

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 3.21 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	1253 (3.20-3.20)
Ramachandran outliers	138981	1234 (3.20-3.20)
Sidechain outliers	138945	1233 (3.20-3.20)

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	60% 38% •
1	B	438	55% 44% •
2	2	181	71% 25% • •
2	C	181	60% 38% • •
3	3	783	57% 38% • •
3	D	783	59% 37% •
4	4	409	49% 43% • 6%
4	E	409	51% 42% • 6%

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Mol	Chain	Length	Quality of chain
5	5	207	55% 39% • 5%
5	F	207	57% 36% • 5%
6	6	181	43% 46% • 8%
6	G	181	39% 51% • 8%
7	9	182	61% 37% ••
7	O	182	58% 39% ••
8	7	129	71% 26% ••
8	I	129	64% 33% ••
9	W	131	66% 30% ••
9	X	131	74% 23% •
10	A	119	56% 40% ••
10	P	119	61% 35% ••
11	J	176	54% 35% • 9%
11	R	176	55% 35% • 9%
12	K	95	68% 32%
12	S	95	77% 22% •
13	L	606	67% 33%
13	T	606	68% 32%
14	M	469	61% 38% •
14	U	469	65% 33% •
15	N	427	71% 29%
15	V	427	64% 36%
16	H	365	52% 43% ••
16	Q	365	49% 45% ••

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	3	803	-	-	X	-
17	SF4	9	201	-	-	X	-
17	SF4	9	202	-	-	X	-
17	SF4	G	201	-	-	X	-
17	SF4	O	202	-	-	X	-
20	FES	C	201	-	-	X	-
20	FES	D	804	-	-	X	-

2 Entry composition (i)

There are 20 unique types of molecules in this entry. The entry contains 74174 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

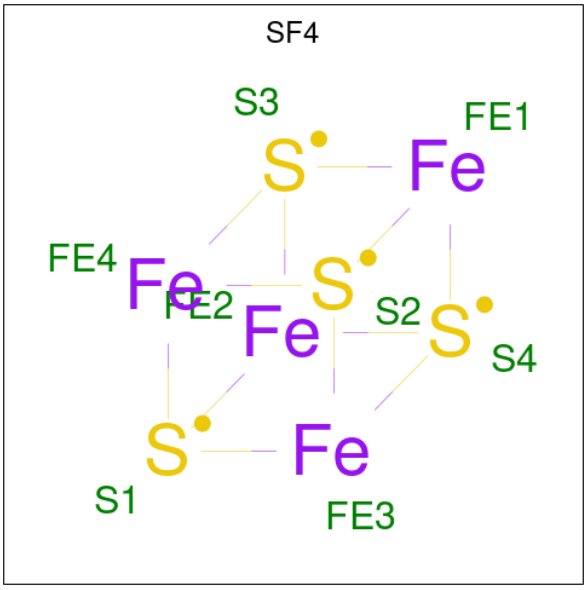
- Molecule 15 is a protein called NADH-quinone oxidoreductase subunit 14.

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

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

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

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



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

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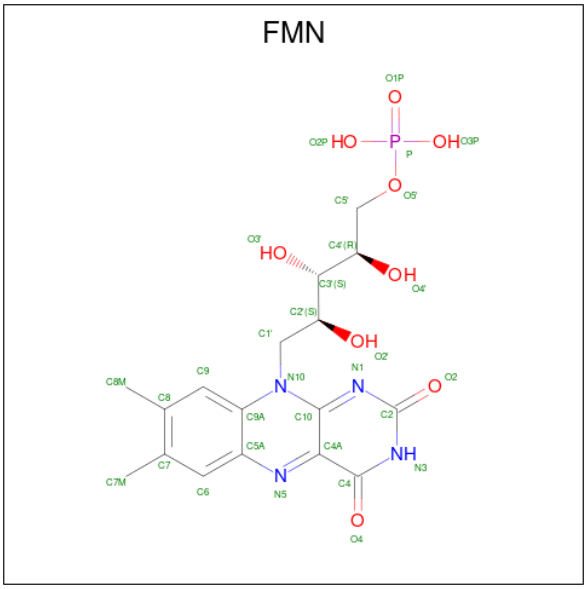
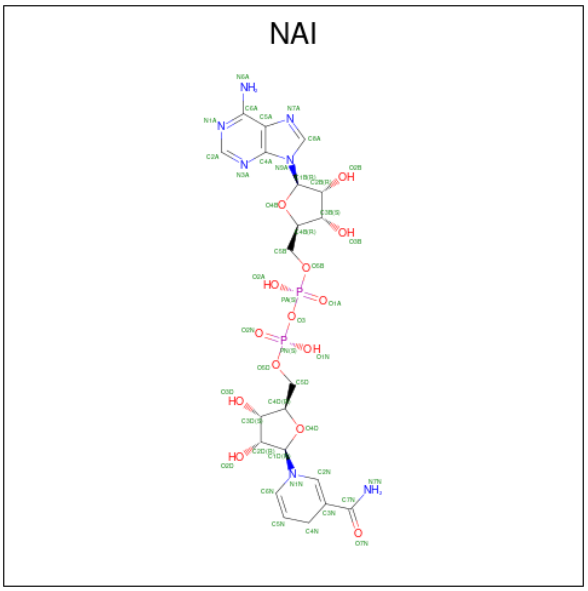
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
17	D	1	Total	Fe	S		0	0
			8	4	4			
17	D	1	Total	Fe	S		0	0
			8	4	4			
17	G	1	Total	Fe	S		0	0
			8	4	4			
17	O	1	Total	Fe	S		0	0
			8	4	4			
17	O	1	Total	Fe	S		0	0
			8	4	4			

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



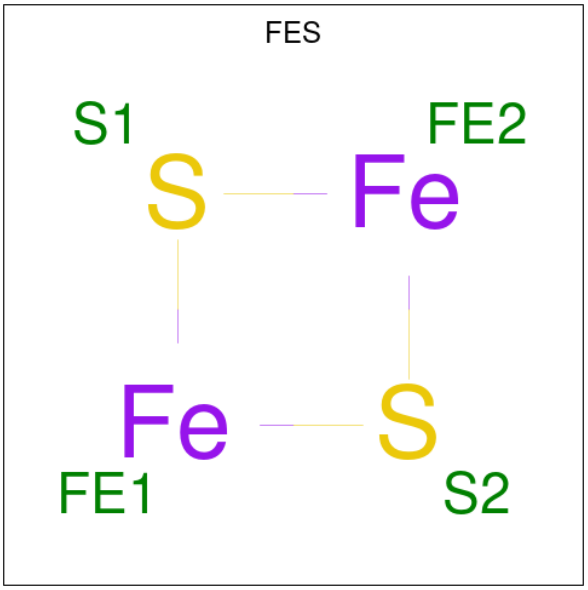
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
18	1	1	Total	C	N	O	P	0	0
			31	17	4	9	1		
18	B	1	Total	C	N	O	P	0	0
			31	17	4	9	1		

- Molecule 19 is 1,4-DIHYDRONICOTINAMIDE ADENINE DINUCLEOTIDE (three-letter code: NAI) (formula: $C_{21}H_{29}N_7O_{14}P_2$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
			Total	C	N	O	P		
19	1	1	44	21	7	14	2	0	0
			Total	C	N	O	P		
19	B	1	44	21	7	14	2	0	0

- Molecule 20 is FE2/S2 (INORGANIC) CLUSTER (three-letter code: FES) (formula: Fe_2S_2).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	Fe	S		
20	2	1	4	2	2	0	0
			Total	Fe	S		
20	3	1	4	2	2	0	0

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

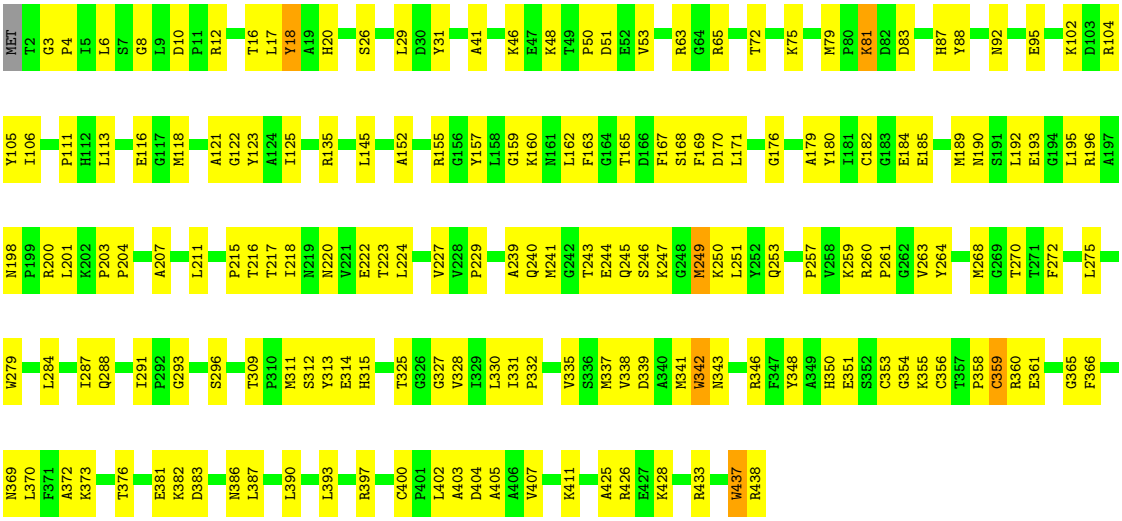
3 Residue-property plots (i)

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.

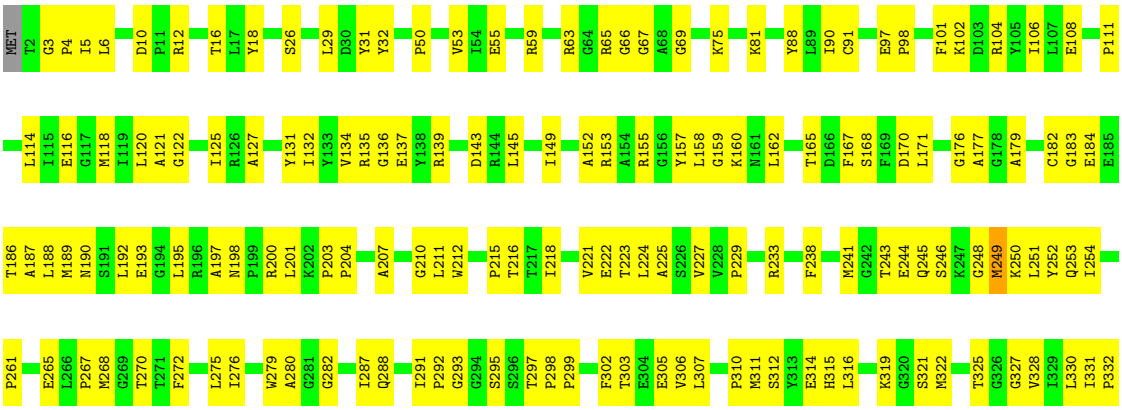
• Molecule 1: NADH-quinone oxidoreductase subunit 1

Chain 1:



• Molecule 1: NADH-quinone oxidoreductase subunit 1

Chain B:



E333 R334 V335 S336 M337 V338 D339 A340 M341 W342 N343 S352 C353 G354 K355 C356 C359 A364 G365 F366 L370 F371 A372 K373 I374 G375 T376 E381 E385 N386 L387 E395 G396 R397 S398 F399 C400 A403 D404 V407 W408 P409 S413 F417 Y421 A425 R426

E427 K428 R429 R433 P434 W437 R438

- Molecule 2: NADH-quinone oxidoreductase subunit 2

Chain 2: 71% 25% • •

MET GLY F3 F4 K7 Q8 D9 F10 L11 E12 E13 T14 F15 A16 K17 R24 A25 A26 L30 L31 R32 R33 V34 Q35 R45 I49 V53 K77 Y78 H79 T85 L86 S87 C88 K89 G92 A93 E94 D98 G107 P108 G109 E110 V111 T112 G115 L116 F117

S118 V119 A131 E143 T146 R147 A148 R149 L154 K161 R162 E165 I166 K171 H177 E178 V179 E180 VAL

- Molecule 2: NADH-quinone oxidoreductase subunit 2

Chain C: 60% 38% • •

MET GLY F3 F4 D5 D6 K7 Q8 D9 F10 L11 K17 R24 I27 L31 R32 R33 V34 Q35 I41 R45 E48 I49 A50 V53 G54 T55 M61 S65 F66 Q71 P74 T75 G76 H79 L80 Q81 V82 C83 A84 T85 L86 S87 C88 K89 G92

E95 L96 W97 I106 G107 P108 G109 E110 V111 T112 L116 F117 S118 V119 Q120 K121 V122 E123 C124 L125 H129 T130 A131 P132 Q135 V136 N137 Y141 V142 E143 C144 V145 T146 R147 A148 R149 L154 K161 R162 E165 I166 G173 V176 H177 E180 VAL

- Molecule 3: NADH-quinone oxidoreductase subunit 3

Chain 3: 57% 38% • •

M1 V2 R3 D8 R9 A26 G27 Y28 D29 V30 P31 L32 F33 C34 S35 L39 I42 G43 A44 C45 R46 M47 C48 L49 V50 R51 P55 LYS LYS GLY PRO ASP GLY LYS PRO LEU LEU ASN GLU LYS GLY GLU PRO GLU I73 Q76 P77 A81 S82 T85 A86

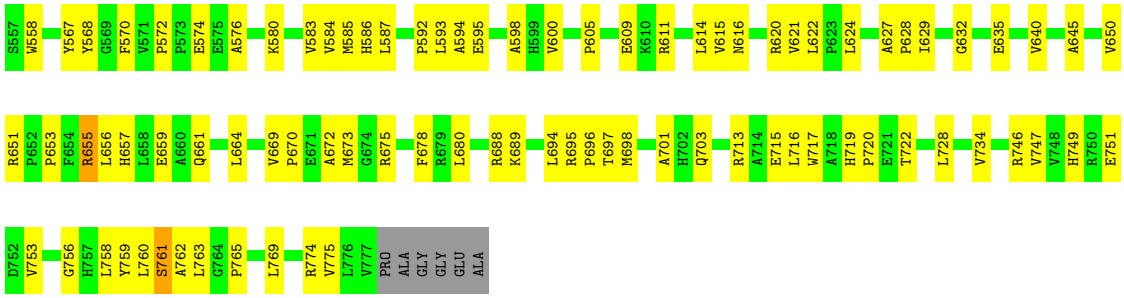
D89 D94 T95 L96 S97 D98 R101 M107 L113 N114 H115 P116 L117 D118 C119 C122 D123 K124 G125 G126 A127 C128 E129 L130 Q131 D132 R133 E136 Y137 Y143 TYR GLN LYS GLY P148 Y154 R161 R162 D165 K166 P169 L170 I175 L176 E179 R180

C184 K185 R186 R189 Y190 V194 P195 V199 L200 D201 F202 I203 E204 R205 P219 F222 S223 G224 N225 I226 T227 D228 I229 C230 P231 V232 G233 A234 L235 L236 D237 L238 T239 A240 R241 F242 R243 A244 R245 N246 W247 E248 C256 C259 P260 V261 G262 C263 G264 I265 T266 A267 D268

T269 R270 S271 L274 L275 R276 T277 R278 A279 R280 E281 V285 N286 E287 I288 W289 I290 R295 F296 G297 H298 E299 W300 A301 D302 R305 L306 K307 L317 L327 K330 R337 L343 Y344 H347 E352 L355 L356 A357 S358 E359 L360 A361 L364 P367 H368

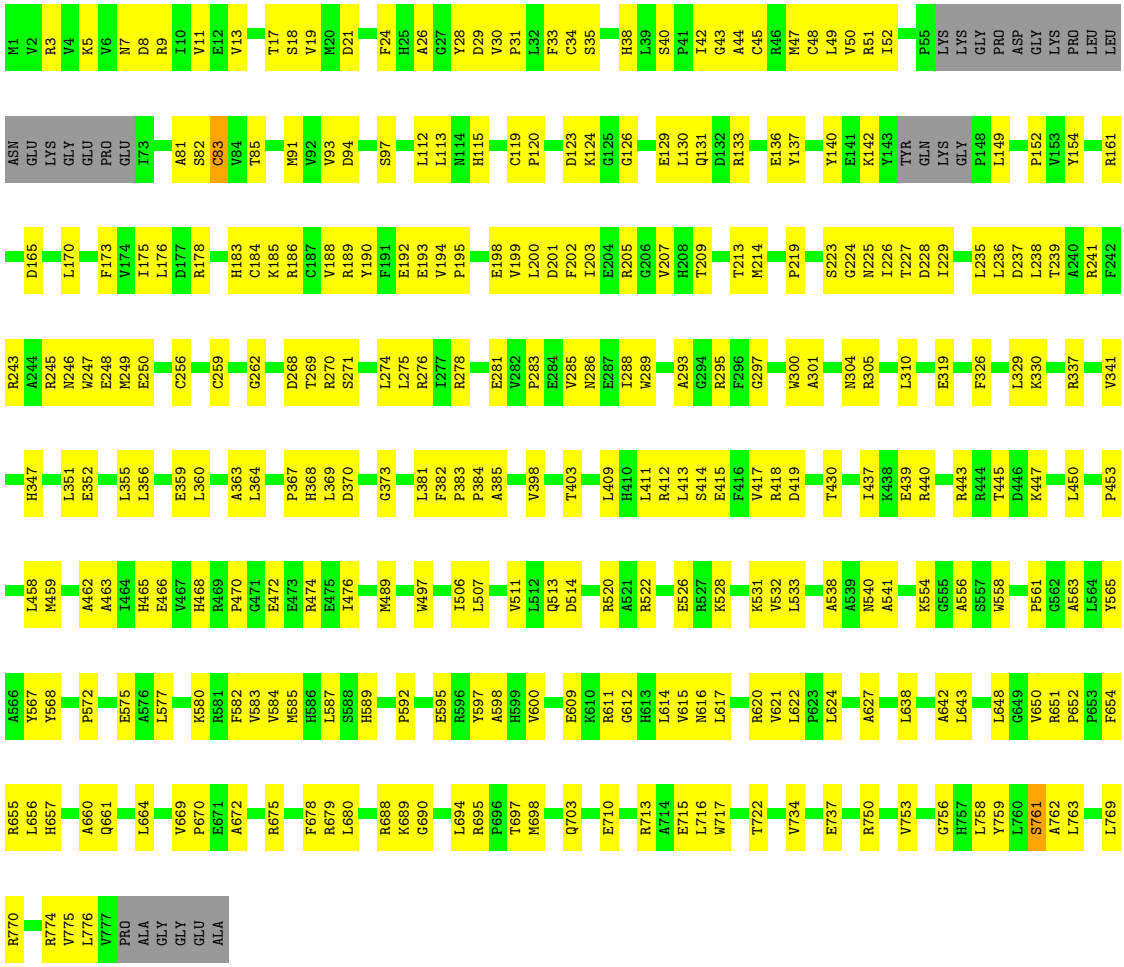
L369 D370 L381 F382 P383 P384 A385 S386 L387 L390 L391 L397 V398 E404 E405 A406 P407 I408 L409 H410 L411 S414 E415 F416 K421 P422 P423 P431 L435 Q436 I437 K438 E439 R440 M441 P442 R443 R444 T445 D446 K447 M448 F451 A452 P453 M459 K460 A463 I464

H465 E466 V467 H468 R469 P470 E473 I476 L477 L478 A479 L480 M489 K494 E498 K501 N502 P503 V504 L505 I506 L507 G508 A509 G510 V511 L512 A521 R522 L523 R527 K528 K531 V532 L533 A534 A538 A541 R542 G543 L544 M547 G548 V549 G552 A556



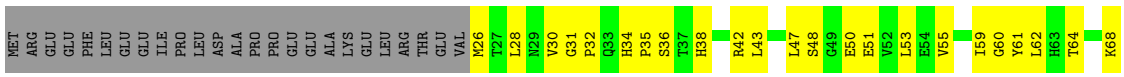
- Molecule 3: NADH-quinone oxidoreductase subunit 3

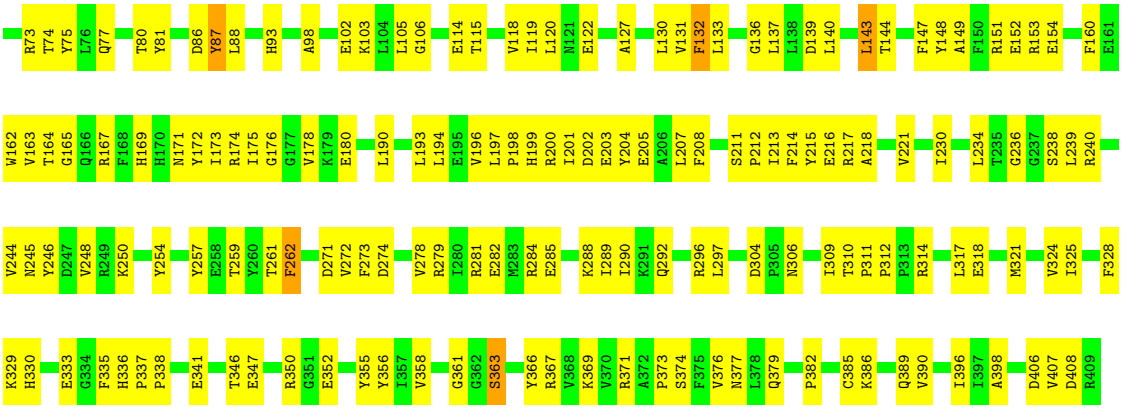
Chain D:



- Molecule 4: NADH-quinone oxidoreductase subunit 4

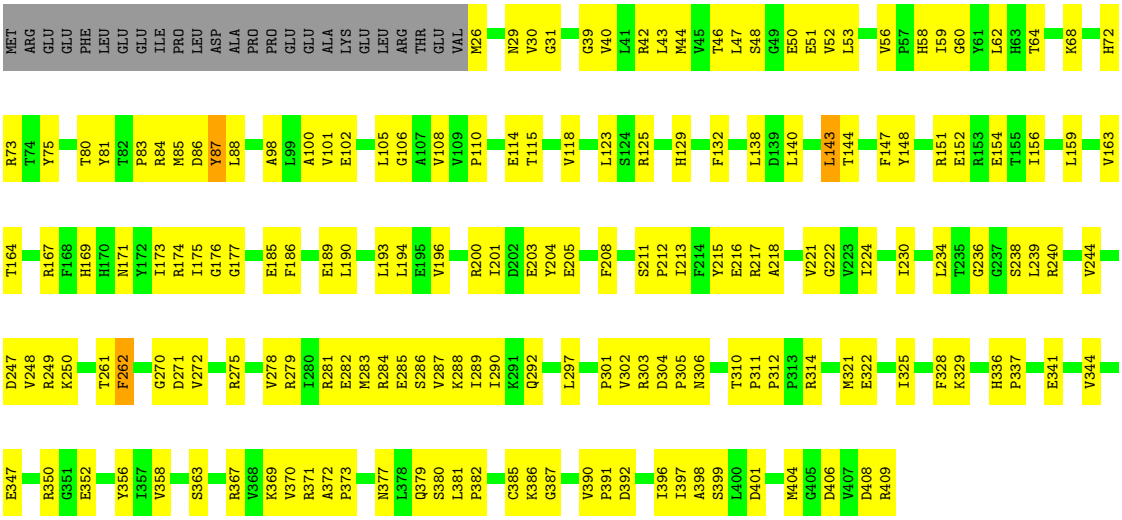
Chain 4:





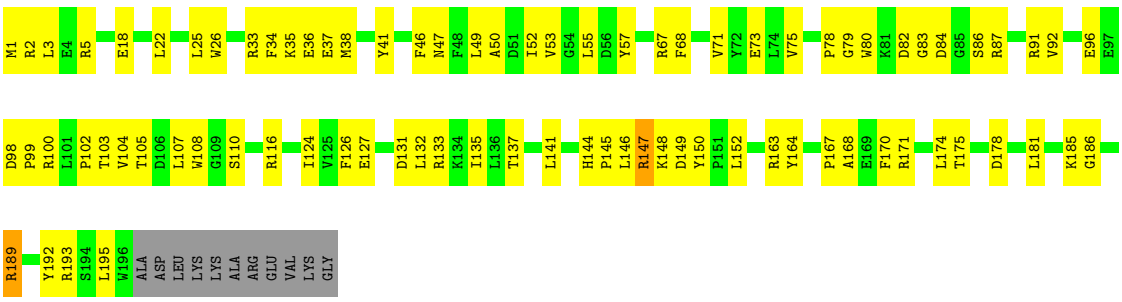
- Molecule 4: NADH-quinone oxidoreductase subunit 4

Chain E: 51% 42% • 6%



- Molecule 5: NADH-quinone oxidoreductase subunit 5

Chain 5: 55% 39% • 5%

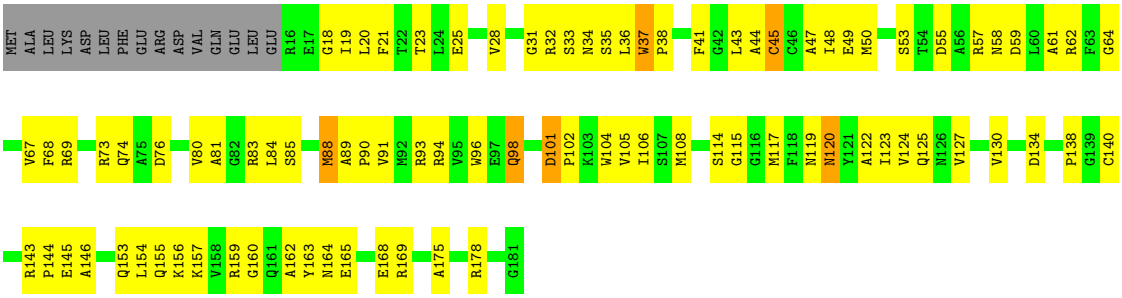


- Molecule 5: NADH-quinone oxidoreductase subunit 5

Chain F: 57% 36% • 5%

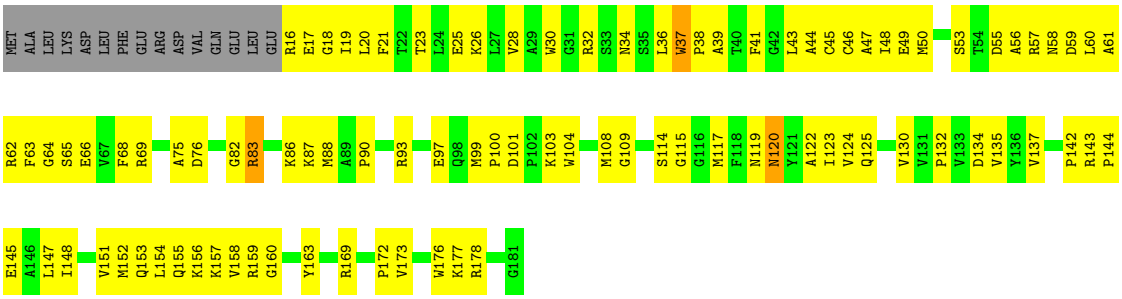
- Molecule 6: NADH-quinone oxidoreductase subunit 6

Chain 6:



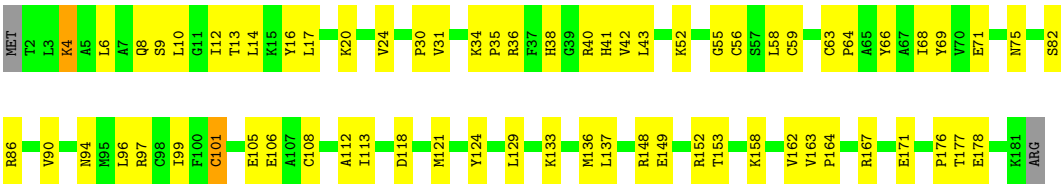
- Molecule 6: NADH-quinone oxidoreductase subunit 6

Chain G:



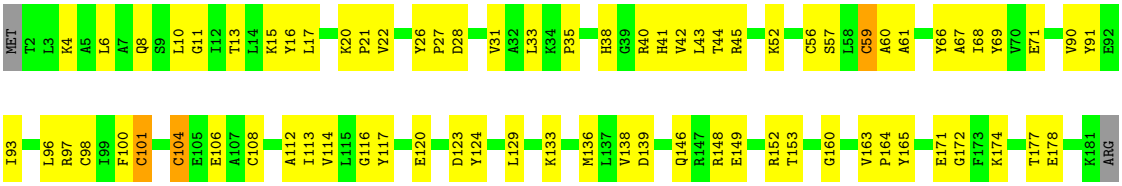
- Molecule 7: NADH-quinone oxidoreductase subunit 9

Chain 9:



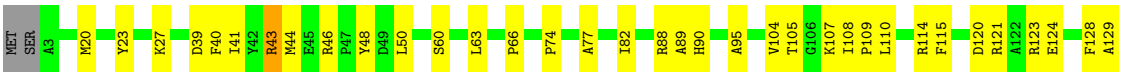
- Molecule 7: NADH-quinone oxidoreductase subunit 9

Chain O:



• Molecule 8: NADH-quinone oxidoreductase subunit 15

Chain 7:

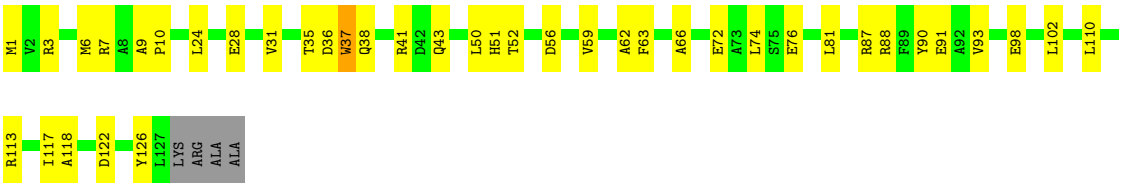


• Molecule 8: NADH-quinone oxidoreductase subunit 15

Chain I:

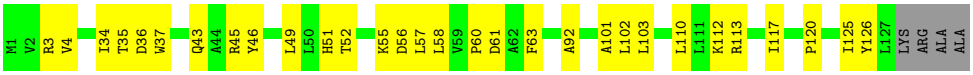
• Molecule 9: NADH-quinone oxidoreductase subunit 16

Chain W:



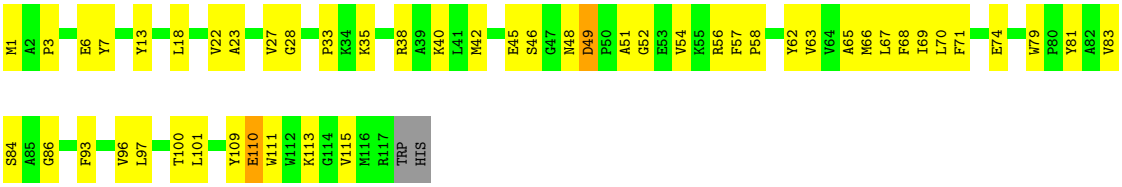
• Molecule 9: NADH-quinone oxidoreductase subunit 16

Chain X:



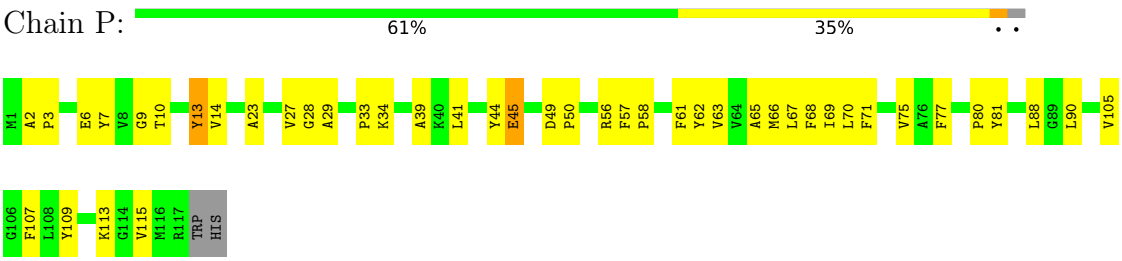
• Molecule 10: NADH-quinone oxidoreductase subunit 7

Chain A:



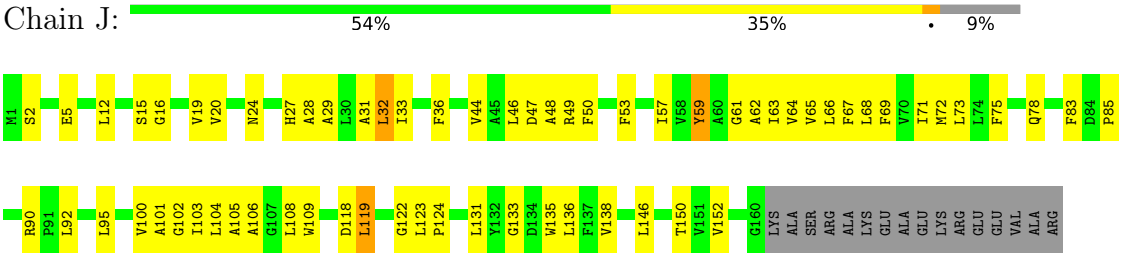
• Molecule 10: NADH-quinone oxidoreductase subunit 7

Chain P:



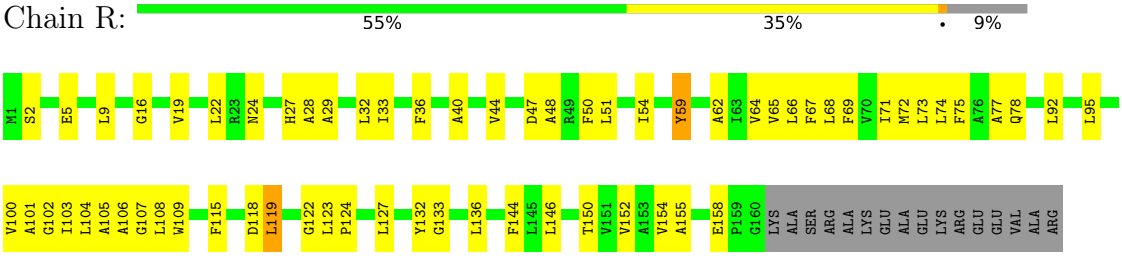
• Molecule 11: NADH-quinone oxidoreductase subunit 10

Chain J:



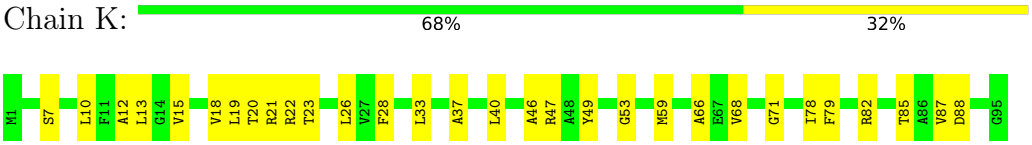
• Molecule 11: NADH-quinone oxidoreductase subunit 10

Chain R:



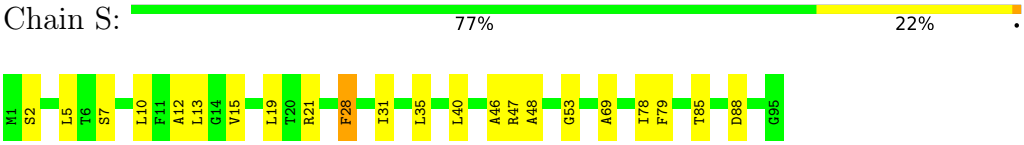
• Molecule 12: NADH-quinone oxidoreductase subunit 11

Chain K:



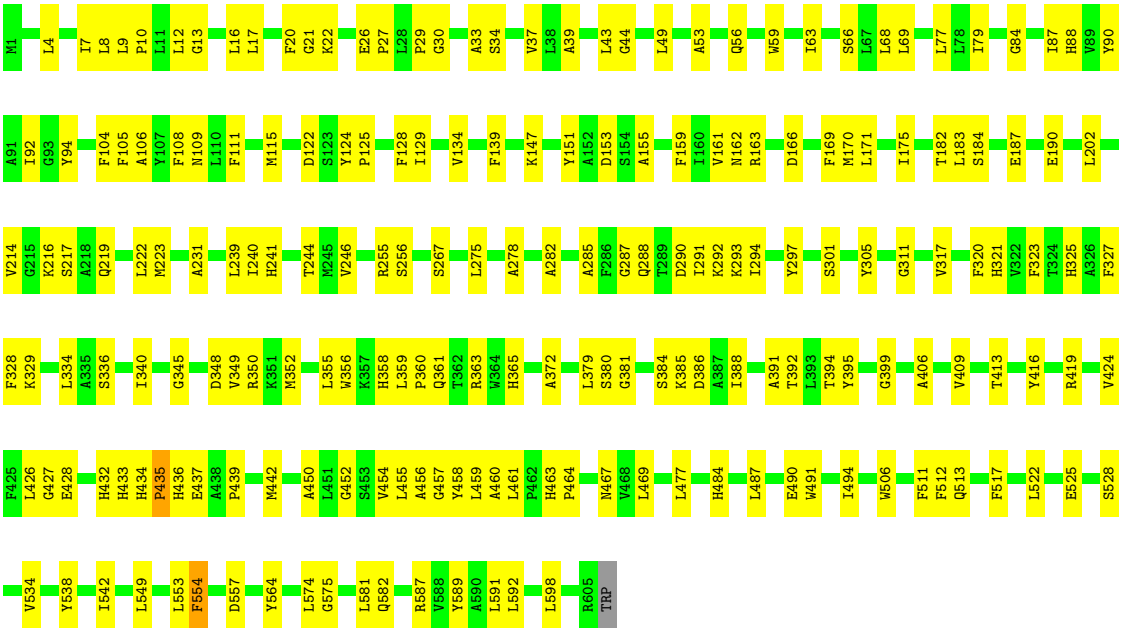
• Molecule 12: NADH-quinone oxidoreductase subunit 11

Chain S:



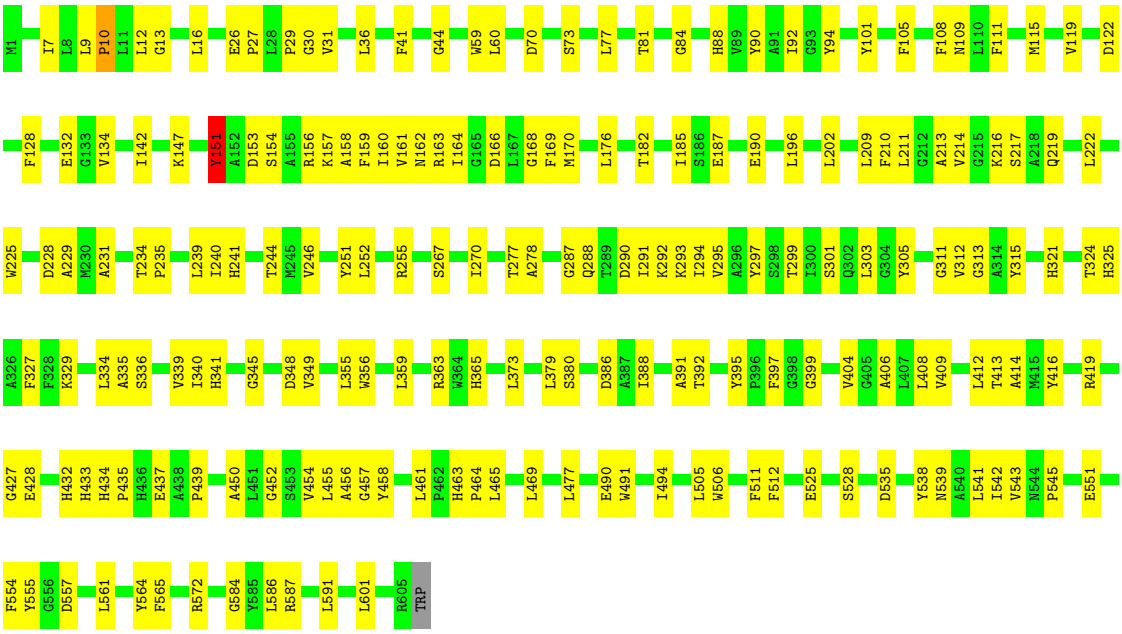
• Molecule 13: NADH-quinone oxidoreductase subunit 12

Chain L:



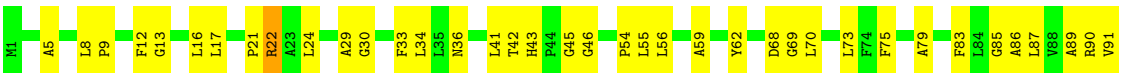
- Molecule 13: NADH-quinone oxidoreductase subunit 12

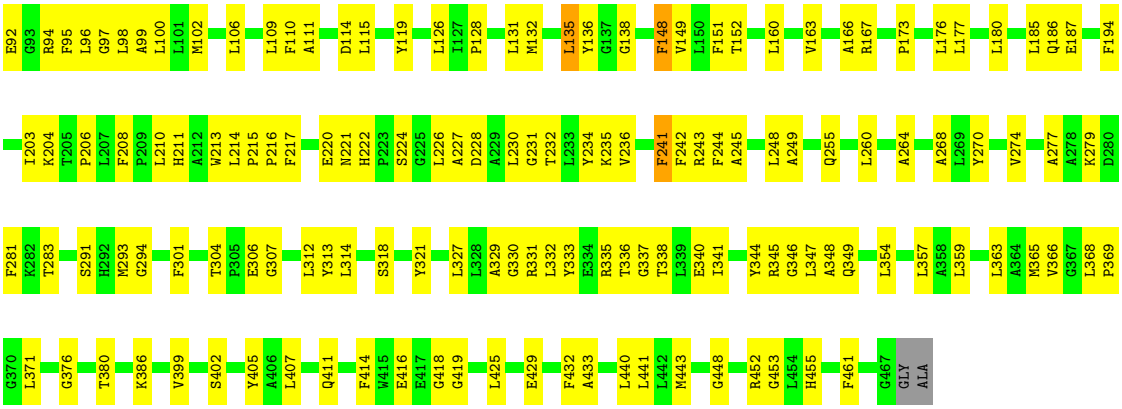
Chain T: 68% 32%



- Molecule 14: NADH-quinone oxidoreductase subunit 13

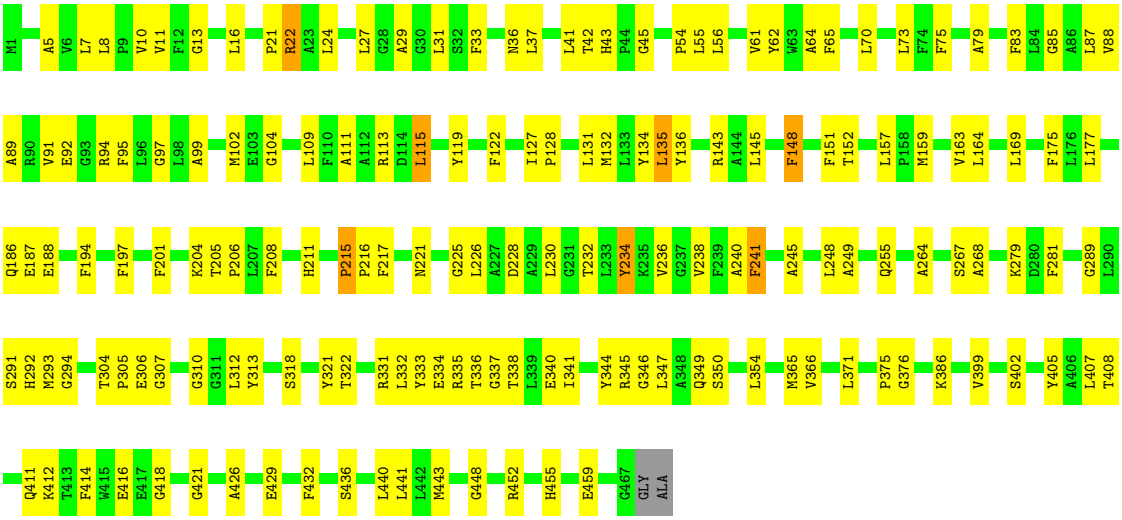
Chain M: 61% 38%





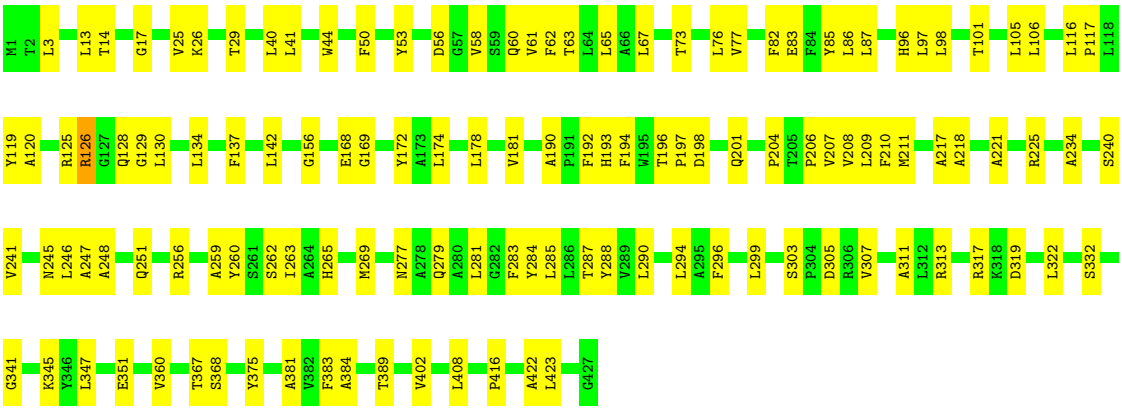
• Molecule 14: NADH-quinone oxidoreductase subunit 13

Chain U: 65% 33%



• Molecule 15: NADH-quinone oxidoreductase subunit 14

Chain N: 71% 29%



• Molecule 15: NADH-quinone oxidoreductase subunit 14

Chain V: 64% 36%

M1 T2 L3 A7 S10 V11 A12 L13 T14 L15 L16 L20 Q23 G24 V25 K26 R27 A28 T29 A36 L37 A38 S39 L40 L41 W44 F50 G51 P52 Y53 V58 S59 Q60 V61 F62 T63 L64 L65 A66 T73 V74 V77 R78 S79 F82 E83 F84 Y85 L86

L87 V88 L89 Y90 L93 G94 N95 H96 L97 L98 A99 S100 T101 R102 H103 L106 M107 L108 L114 A120 T123 W124 R125 R126 G127 Q128 A132 A133 L134 K135 Y136 F137 L138 L139 G140 F147 E168 G169 L176 G177 L178 L179 L180 V181 F185 K186 A187 A188 L189 A190

P191 F192 H193 T196 P197 D198 V199 Y200 Q201 P204 V207 V208 L209 F210 M211 A212 K216 A217 A218 A221 R225 A228 L233 Q251 K255 R256 L257 I263 A272 G276 Q279 A280 L281 G282 F283 Y284 L285 L286 T287 L294 L299 I302

D305 R306 V307 P308 L309 L312 R313 G314 L315 Y316 R317 K318 D319 L322 F326 L327 V328 L334 L339 F342 W343 G344 K345 Y346 L347 W358 S368 A369 V370 S371 A372 Y373 Y374 Y375 L378 A384 F391 V402 A405 G413 L414 L415 P416 G417 L418 V419

L420 L423 G427

- Molecule 16: NADH-quinone oxidoreductase subunit 8

Chain H: 52% 43% • •

MET T2 Y5 P6 V7 D8 K16 A17 V20 V21 L24 A29 T32 E35 L39 F42 Q43 V44 R45 M46 G47 P48 N49 R50 V51 G52 P53 F54 G55 L60 I64 K65 S66 I67 F68 K69 E70 D71 I72 V73 V74 F82 V83 A96 L99

F108 Q112 P113 W114 V115 I116 N117 L118 D119 L120 G121 I122 L125 F126 A127 V128 L131 A132 V133 Y134 G135 I136 F137 L138 S143 K146 Y147 S148 L149 L150 L153 R154 S155 S156 A157 S158 L159 I160 S161 Y162 E163 L164 L168 L171 L180 N181 V186 N187 W188 Q189

K190 G193 W194 L195 F196 F200 P201 A202 F203 L204 V205 I208 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 I239 K240 Y249 A255 I259 P260 F263 L264 G265 G266 W267 T268 V271

L272 E273 V274 P275 Y276 L277 W278 K282 F286 L287 F288 F289 F290 I291 W292 I293 R294 A295 T296 W297 F298 R299 L300 R301 Y302 D303 Q304 L305 L306 R307 F308 G309 W310 F314 P315 L316 A317 L318 F321 L322 A325 L326 A329 L332 P333 R334 T335 Y336 V352 L353 Y354 THR

PRO LYS PRO ALA ARG LYS GLY GLY GLY ALA

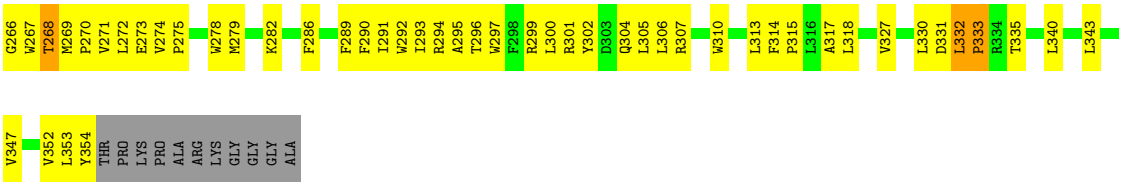
- Molecule 16: NADH-quinone oxidoreductase subunit 8

Chain Q: 49% 45% • •

MET T2 Y5 D8 V13 A14 L15 K16 A17 L18 L19 V20 V21 L24 L25 F28 A29 T32 E35 R36 L39 A40 R41 F42 Q43 V44 R45 M46 G47 P48 N49 R50 V51 G52 P53 F54 G55 L56 L57 Q58 K65 S66 I67 F68 K69 E70 D71 I72 Q76

L81 A85 P86 V90 L94 L95 A96 L99 F102 Q112 V115 I116 N117 L118 D119 L120 G121 I122 Y124 L125 F126 A127 V128 L131 A132 V133 Y134 G135 I136 F137 L138 S139 G140 W141 A142 S143 G144 Y147 S148 L149 L150 G151 S152 L153 R154 L159 E163 L164

L168 L171 V177 L180 N181 I185 Q189 F196 A202 F203 L204 V205 A212 A215 R216 T217 P218 F219 D220 L221 P222 E223 A224 E225 Q226 E227 L228 V229 G230 G231 Y232 E235 Y236 S237 S238 I239 K240 W241 A242 L243 F244 Y249 A257 P260 G265


G266
W267
T268
M269
P270
V271
L272
E273
V274
P275
W278
M279
K282
F286
F289
F290
I291
W292
I293
R294
A295
T296
W297
F298
R299
L300
R301
Y302
D303
Q304
L305
L306
R307
W310
L313
F314
P315
L316
A317
L318
V327
L330
D331
L332
P333
R334
T335
L340
L343
V347
V352
L353
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	96.11Å 341.45Å 263.89Å 90.00° 100.52° 90.00°	Depositor
Resolution (Å)	58.71 – 3.21	Depositor
% Data completeness (in resolution range)	76.1 (58.71-3.21)	Depositor
R_{merge}	0.16	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.27 (at 3.19Å)	Xtriage
Refinement program	PHENIX (1.13rc1_2961: ???)	Depositor
R, R_{free}	0.210 , 0.231	Depositor
Wilson B-factor (Å^2)	73.9	Xtriage
Anisotropy	0.034	Xtriage
L-test for twinning[2]	$< \|L\| > = 0.35$, $< L^2 > = 0.17$	Xtriage
Estimated twinning fraction	0.357 for h,-k,-h-l	Xtriage
Reported twinning fraction	0.470 for -H,-K,H+L	Depositor
Outliers	0 of 207039 reflections	Xtriage
Total number of atoms	74174	wwPDB-VP
Average B, all atoms (Å^2)	74.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.75% 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, NAI, FES

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	0.34	0/3506	0.51	0/4745
1	B	0.31	0/3506	0.49	0/4745
2	2	0.35	0/1439	0.50	0/1953
2	C	0.32	0/1439	0.50	0/1953
3	3	0.51	2/6035 (0.0%)	0.73	3/8185 (0.0%)
3	D	0.40	0/6035	0.60	0/8185
4	4	0.44	0/3150	0.62	0/4284
4	E	0.34	0/3150	0.51	0/4284
5	5	0.43	0/1656	0.66	1/2246 (0.0%)
5	F	0.37	0/1656	0.57	0/2246
6	6	0.46	0/1319	0.64	0/1786
6	G	0.46	0/1319	0.62	0/1786
7	9	0.53	1/1423 (0.1%)	0.65	0/1933
7	O	0.48	1/1423 (0.1%)	0.65	1/1933 (0.1%)
8	7	0.32	0/1059	0.53	0/1429
8	I	0.36	0/1059	0.57	0/1429
9	W	0.43	0/985	0.62	0/1335
9	X	0.37	0/985	0.57	0/1335
10	A	0.33	0/940	0.52	0/1280
10	P	0.35	0/940	0.51	0/1280
11	J	0.31	0/1206	0.50	0/1649
11	R	0.32	0/1206	0.53	0/1649
12	K	0.31	0/710	0.53	0/962
12	S	0.30	0/710	0.51	0/962
13	L	0.29	0/4741	0.47	0/6460
13	T	0.29	0/4741	0.48	1/6460 (0.0%)
14	M	0.30	0/3591	0.48	0/4896
14	U	0.32	0/3591	0.51	0/4896
15	N	0.31	0/3238	0.47	0/4434
15	V	0.34	0/3238	0.52	0/4434
16	H	0.34	0/2935	0.55	0/4014
16	Q	0.37	0/2935	0.56	0/4014

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#|Z| >5	RMSZ	#|Z| >5
All	All	0.37	4/75866 (0.0%)	0.56	6/103182 (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
7	O	0	2
10	P	0	1
16	H	0	3
16	Q	0	3
All	All	0	10

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	9	101	CYS	CB-SG	-6.08	1.72	1.82
3	3	263	CYS	CB-SG	-5.98	1.72	1.81
7	O	101	CYS	CB-SG	-5.30	1.73	1.81
3	3	381	LEU	C-N	-5.26	1.22	1.34

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
7	O	59	CYS	CA-CB-SG	7.71	127.88	114.00
3	3	276	ARG	NE-CZ-NH1	6.14	123.37	120.30
13	T	151	TYR	N-CA-CB	5.82	121.08	110.60
3	3	435	LEU	CB-CG-CD1	-5.49	101.67	111.00
5	5	189	ARG	NE-CZ-NH1	5.35	122.97	120.30
3	3	276	ARG	NE-CZ-NH2	-5.28	117.66	120.30

There are no chirality outliers.

All (10) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
7	9	20	LYS	Peptide
16	H	217	THR	Peptide
16	H	266	GLY	Peptide
16	H	43	GLN	Peptide

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Mol	Chain	Res	Type	Group
7	O	20	LYS	Peptide
7	O	21	PRO	Peptide
10	P	45	GLU	Peptide
16	Q	217	THR	Peptide
16	Q	266	GLY	Peptide
16	Q	43	GLN	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	116	0
1	B	3417	0	3388	152	0
2	2	1406	0	1373	37	0
2	C	1406	0	1373	71	0
3	3	5895	0	5929	232	0
3	D	5895	0	5930	218	0
4	4	3067	0	3049	167	0
4	E	3067	0	3049	162	0
5	5	1607	0	1574	77	0
5	F	1607	0	1574	76	0
6	6	1289	0	1298	84	0
6	G	1289	0	1298	100	0
7	9	1388	0	1383	72	0
7	O	1388	0	1383	69	0
8	7	1031	0	1029	36	0
8	I	1031	0	1029	36	0
9	W	967	0	1010	32	0
9	X	967	0	1010	23	0
10	A	910	0	939	53	0
10	P	910	0	939	53	0
11	J	1183	0	1286	63	0
11	R	1183	0	1286	56	0
12	K	703	0	747	29	0
12	S	703	0	747	17	0
13	L	4604	0	4734	162	0
13	T	4604	0	4734	136	0
14	M	3489	0	3606	131	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
14	U	3489	0	3606	124	0
15	N	3154	0	3343	98	0
15	V	3154	0	3343	113	0
16	H	2838	0	2903	154	0
16	Q	2838	0	2903	175	0
17	1	8	0	0	3	0
17	3	24	0	0	2	0
17	6	8	0	0	0	0
17	9	16	0	0	6	0
17	B	8	0	0	1	0
17	D	24	0	0	1	0
17	G	8	0	0	2	0
17	O	16	0	0	3	0
18	1	31	0	19	8	0
18	B	31	0	19	2	0
19	1	44	0	27	3	0
19	B	44	0	27	4	0
20	2	4	0	0	1	0
20	3	4	0	0	0	0
20	C	4	0	0	2	0
20	D	4	0	0	2	0
All	All	74174	0	75276	2718	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 18.

All (2718) 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)
4:4:190:LEU:O	4:4:194:LEU:HD13	1.54	1.05
7:9:133:LYS:O	7:9:137:LEU:HD13	1.57	1.04
3:D:286:ASN:ND2	3:D:289:TRP:O	1.96	0.98
4:E:47:LEU:HD13	4:E:51:GLU:O	1.62	0.97
3:3:42:ILE:HD12	3:3:42:ILE:O	1.65	0.96
4:E:47:LEU:CD1	4:E:51:GLU:O	2.16	0.94
3:3:397:LEU:HD21	3:3:480:LEU:HD13	1.49	0.92
7:9:52:LYS:NZ	8:7:44:MET:O	2.03	0.92
16:Q:274:VAL:HG12	16:Q:278:TRP:CD1	2.03	0.91
6:G:145:GLU:HG2	7:O:31:VAL:HG21	1.50	0.90
14:M:22:ARG:NH1	14:M:92:GLU:OE1	2.06	0.88
5:F:38:MET:CE	5:F:104:VAL:HG11	2.03	0.88

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:I:37:PHE:HE1	8:I:74:PRO:HA	1.40	0.87
16:Q:215:ALA:O	16:Q:294:ARG:NH1	2.07	0.87
5:5:175:THR:HG22	5:5:178:ASP:HB2	1.57	0.86
4:E:169:HIS:NE2	6:G:45:CYS:SG	2.48	0.86
3:3:115:HIS:HB3	4:4:321:MET:HE3	1.58	0.86
1:B:190:ASN:ND2	1:B:198:ASN:O	2.08	0.86
1:1:437:TRP:HB3	2:2:92:GLY:HA3	1.57	0.85
4:4:261:THR:H	4:4:292:GLN:HE22	1.23	0.85
6:6:160:GLY:O	6:6:169:ARG:NH1	2.09	0.85
16:Q:333:PRO:HB2	16:Q:335:THR:H	1.41	0.85
2:C:106:ILE:HD11	2:C:112:THR:HB	1.57	0.84
3:D:194:VAL:HG12	3:D:411:LEU:HD22	1.59	0.84
4:E:314:ARG:NH2	7:O:108:CYS:O	2.11	0.83
5:F:38:MET:HE3	5:F:104:VAL:HG11	1.60	0.83
10:P:14:VAL:HG22	16:Q:95:LEU:HD22	1.60	0.83
3:3:286:ASN:ND2	3:3:289:TRP:O	2.12	0.83
16:Q:271:VAL:HG12	16:Q:272:LEU:HG	1.61	0.82
13:L:557:ASP:OD1	14:M:211:HIS:NE2	2.12	0.82
13:T:94:TYR:HE1	13:T:341:HIS:HB2	1.44	0.82
16:Q:143:SER:HB2	16:Q:235:GLU:HG3	1.61	0.82
3:3:31:PRO:HB2	3:3:47:MET:HB3	1.60	0.82
10:A:70:LEU:HD13	11:J:150:THR:HG22	1.61	0.82
4:4:152:GLU:OE2	4:4:204:TYR:OH	1.98	0.82
7:9:75:ASN:ND2	7:9:82:SER:OG	2.13	0.82
3:3:584:VAL:HG12	3:3:600:VAL:HB	1.62	0.81
3:3:616:ASN:HD22	3:3:622:LEU:HD11	1.45	0.81
4:E:261:THR:H	4:E:292:GLN:HE22	1.28	0.81
4:4:373:PRO:O	4:4:377:ASN:ND2	2.14	0.81
1:B:437:TRP:HB3	2:C:92:GLY:HA3	1.62	0.81
3:D:584:VAL:HG12	3:D:600:VAL:HB	1.61	0.81
3:D:352:GLU:OE2	3:D:661:GLN:NE2	2.14	0.81
14:M:68:ASP:OD2	14:M:243:ARG:NH2	2.14	0.81
14:M:268:ALA:HA	14:M:291:SER:HA	1.61	0.81
3:3:305:ARG:HH22	3:3:605:PRO:HA	1.46	0.80
10:P:113:LYS:NZ	15:V:83:GLU:OE2	2.11	0.80
15:N:193:HIS:HB2	15:N:263:ILE:HD13	1.64	0.80
16:H:50:ARG:O	16:H:52:GLY:N	2.12	0.80
8:7:23:TYR:HH	8:7:123:ARG:HH11	1.29	0.80
13:L:458:TYR:HB3	13:L:461:LEU:HD11	1.64	0.80
7:O:171:GLU:OE2	8:I:43:ARG:NH2	2.14	0.80
15:V:128:GLN:OE1	15:V:306:ARG:NH2	2.14	0.80

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:115:HIS:HB3	4:E:321:MET:HE3	1.62	0.80
10:A:35:LYS:O	10:A:40:LYS:NZ	2.15	0.79
3:3:609:GLU:HA	3:3:627:ALA:H	1.47	0.79
6:G:134:ASP:OD1	6:G:157:LYS:NZ	2.15	0.79
3:3:51:ARG:HB3	3:3:94:ASP:HB3	1.65	0.79
15:V:309:LEU:HD22	15:V:378:LEU:HD11	1.62	0.79
2:C:106:ILE:HD13	2:C:112:THR:N	1.98	0.79
3:D:688:ARG:HB3	3:D:770:ARG:HB2	1.63	0.79
14:U:217:PHE:O	14:U:221:ASN:ND2	2.16	0.79
2:C:24:ARG:HA	2:C:53:VAL:HG22	1.64	0.78
13:T:584:GLY:O	15:V:135:LYS:NZ	2.14	0.78
1:1:361:GLU:OE2	3:3:162:ARG:NH2	2.17	0.78
1:B:425:ALA:O	1:B:428:LYS:NZ	2.15	0.78
2:C:106:ILE:HD11	2:C:112:THR:CB	2.14	0.78
3:D:611:ARG:HH21	9:X:101:ALA:HB1	1.47	0.78
6:G:120:ASN:HD22	6:G:122:ALA:H	1.29	0.78
4:E:306:ASN:ND2	5:F:192:TYR:OH	2.17	0.78
3:3:256:CYS:HB2	3:3:265:ILE:HD13	1.64	0.78
6:6:120:ASN:HD22	6:6:122:ALA:H	1.30	0.77
3:3:414:SER:OG	3:3:443:ARG:NH2	2.18	0.77
16:H:332:LEU:HB2	16:H:333:PRO:HD3	1.66	0.77
2:C:109:GLY:O	8:I:121:ARG:NH2	2.17	0.77
3:3:268:ASP:OD2	3:3:278:ARG:NH1	2.14	0.77
3:D:34:CYS:SG	3:D:35:SER:N	2.57	0.77
11:R:69:PHE:O	11:R:73:LEU:HG	1.85	0.77
3:3:370:ASP:OD2	3:3:558:TRP:HD1	1.68	0.77
14:M:115:LEU:HD12	14:M:180:LEU:HD13	1.64	0.77
15:V:193:HIS:HB2	15:V:263:ILE:HD13	1.67	0.77
9:X:45:ARG:NH1	9:X:61:ASP:OD2	2.17	0.77
3:3:290:ILE:HG23	17:3:803:SF4:S4	2.25	0.76
5:5:185:LYS:HB2	5:5:189:ARG:HG3	1.65	0.76
6:6:119:ASN:HA	6:6:125:GLN:HE22	1.50	0.76
11:J:68:LEU:HD23	11:J:71:ILE:HD11	1.67	0.76
1:B:65:ARG:NH1	1:B:249:MET:O	2.19	0.76
7:O:40:ARG:O	7:O:116:GLY:N	2.18	0.76
13:T:278:ALA:HA	13:T:301:SER:HA	1.65	0.76
14:U:345:ARG:NH1	14:U:416:GLU:OE1	2.19	0.76
4:4:306:ASN:ND2	5:5:192:TYR:OH	2.18	0.76
13:T:157:LYS:NZ	13:T:535:ASP:OD2	2.19	0.76
6:6:94:ARG:HD2	10:A:46:SER:HA	1.66	0.76
16:Q:50:ARG:O	16:Q:52:GLY:N	2.17	0.76

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:6:19:ILE:HG23	6:6:20:LEU:HG	1.68	0.76
3:D:717:TRP:HB2	3:D:759:TYR:HB2	1.66	0.76
4:E:200:ARG:NH1	7:O:16:TYR:OH	2.18	0.75
4:E:216:GLU:OE2	16:Q:304:GLN:NE2	2.20	0.75
13:L:575:GLY:HA2	15:N:246:LEU:HB3	1.68	0.75
3:3:635:GLU:OE2	9:W:7:ARG:NH1	2.20	0.75
1:B:359:CYS:HB2	1:B:403:ALA:HB2	1.69	0.75
4:E:144:THR:HG22	4:E:148:TYR:HE1	1.52	0.75
6:G:19:ILE:HG23	6:G:20:LEU:HG	1.66	0.75
3:3:269:THR:HG22	3:3:274:LEU:HA	1.69	0.75
3:3:616:ASN:ND2	3:3:622:LEU:HD11	2.02	0.75
7:9:96:LEU:HD21	7:9:129:LEU:HD13	1.69	0.75
14:U:89:ALA:HB1	14:U:91:VAL:HG22	1.65	0.75
14:U:208:PHE:O	14:U:211:HIS:ND1	2.20	0.75
8:7:63:LEU:HD13	8:7:129:ALA:HB3	1.69	0.74
3:3:190:TYR:OH	3:3:222:PHE:O	2.06	0.74
4:4:352:GLU:OE2	5:5:87:ARG:NH1	2.20	0.74
11:R:47:ASP:O	11:R:122:GLY:N	2.20	0.74
11:R:133:GLY:H	11:R:136:LEU:HB2	1.52	0.74
16:H:117:ASN:O	16:H:181:ASN:ND2	2.20	0.74
1:B:29:LEU:HD23	1:B:155:ARG:HD2	1.68	0.74
13:L:105:PHE:O	13:L:109:ASN:ND2	2.19	0.74
13:L:162:ASN:OD1	13:L:216:LYS:NZ	2.21	0.74
4:E:84:ARG:HG2	17:G:201:SF4:S2	2.28	0.74
3:3:203:ILE:HG21	8:7:88:ARG:HG2	1.70	0.74
3:3:344:TYR:HB3	3:3:570:PHE:HE1	1.51	0.74
15:N:294:LEU:HG	15:N:402:VAL:HG13	1.69	0.74
16:H:16:LYS:NZ	16:H:114:TRP:O	2.20	0.74
1:B:288:GLN:NE2	1:B:335:VAL:O	2.20	0.74
4:4:333:GLU:OE2	4:4:336:HIS:NE2	2.21	0.74
3:3:113:LEU:O	3:3:161:ARG:NH1	2.21	0.74
14:U:268:ALA:HA	14:U:291:SER:HA	1.68	0.74
1:B:4:PRO:HA	1:B:12:ARG:HH12	1.53	0.73
1:B:305:GLU:OE1	1:B:319:LYS:NZ	2.20	0.73
5:F:134:LYS:NZ	5:F:141:LEU:O	2.20	0.73
1:B:287:ILE:HA	1:B:332:PRO:HA	1.70	0.73
8:I:120:ASP:OD1	8:I:123:ARG:NH1	2.19	0.73
16:H:216:ARG:HD2	16:H:294:ARG:HA	1.68	0.73
13:L:163:ARG:NH2	14:M:366:VAL:O	2.22	0.73
14:M:89:ALA:HB1	14:M:91:VAL:HG22	1.68	0.73
7:O:172:GLY:O	7:O:174:LYS:NZ	2.19	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:1:400:CYS:HG	17:1:501:SF4:FE3	1.01	0.73
16:H:219:PHE:HB3	16:H:299:ARG:HG2	1.70	0.73
4:4:171:ASN:OD1	4:4:174:ARG:NH1	2.18	0.73
15:N:13:LEU:HD22	15:N:25:VAL:HG13	1.70	0.73
3:D:247:TRP:CD1	5:F:172:ALA:HB2	2.24	0.73
3:D:462:ALA:O	3:D:465:HIS:ND1	2.22	0.73
6:G:119:ASN:HA	6:G:125:GLN:HE22	1.54	0.73
7:O:96:LEU:HD21	7:O:129:LEU:HD13	1.69	0.73
10:P:3:PRO:HD2	16:Q:2:THR:HB	1.70	0.73
4:4:200:ARG:NH1	7:9:16:TYR:OH	2.21	0.73
16:Q:291:ILE:HA	16:Q:294:ARG:HG3	1.69	0.73
3:D:414:SER:OG	3:D:443:ARG:NH2	2.21	0.72
6:G:34:ASN:O	16:Q:58:GLN:NE2	2.22	0.72
8:7:23:TYR:HH	8:7:123:ARG:NH1	1.86	0.72
14:M:217:PHE:O	14:M:221:ASN:ND2	2.21	0.72
3:D:722:THR:HG21	3:D:756:GLY:H	1.53	0.72
15:V:2:THR:HG1	15:V:39:SER:HG	1.31	0.72
1:1:246:SER:HB3	1:1:268:MET:HG2	1.69	0.72
4:4:341:GLU:OE1	5:5:91:ARG:NH2	2.19	0.72
5:5:18:GLU:HB2	5:5:26:TRP:HB2	1.69	0.72
10:P:109:TYR:OH	10:P:113:LYS:NZ	2.21	0.72
13:T:557:ASP:OD1	14:U:211:HIS:NE2	2.13	0.72
13:T:458:TYR:HB3	13:T:461:LEU:HD11	1.71	0.72
5:5:168:ALA:HA	5:5:171:ARG:NH1	2.04	0.72
3:D:31:PRO:HB2	3:D:47:MET:HB3	1.70	0.72
1:1:16:THR:HG21	1:1:229:PRO:HB3	1.72	0.72
13:L:84:GLY:O	13:L:88:HIS:ND1	2.20	0.72
6:6:114:SER:OG	7:9:96:LEU:O	2.06	0.72
4:4:73:ARG:NH2	4:4:81:TYR:OH	2.23	0.72
2:C:106:ILE:CD1	2:C:112:THR:N	2.53	0.72
16:H:271:VAL:HG12	16:H:272:LEU:HG	1.70	0.71
11:R:22:LEU:O	12:S:21:ARG:NH2	2.23	0.71
5:5:38:MET:HE3	5:5:104:VAL:HG11	1.71	0.71
3:D:412:ARG:NH1	3:D:415:GLU:OE1	2.23	0.71
16:H:52:GLY:HA3	16:H:55:GLY:H	1.55	0.71
16:H:265:GLY:O	16:H:282:LYS:NZ	2.17	0.71
13:T:419:ARG:NH2	13:T:525:GLU:OE2	2.22	0.71
8:7:120:ASP:OD1	8:7:123:ARG:NH1	2.23	0.71
3:D:18:SER:OG	3:D:82:SER:O	2.07	0.71
3:D:710:GLU:O	3:D:713:ARG:NH1	2.21	0.71
3:3:538:ALA:HB3	3:3:541:ALA:HB2	1.72	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:253:GLN:HG2	1:B:327:GLY:HA2	1.72	0.71
1:B:433:ARG:HH12	2:C:89:LYS:HE2	1.55	0.71
13:T:84:GLY:O	13:T:88:HIS:ND1	2.21	0.71
14:U:128:PRO:O	14:U:132:MET:HG2	1.91	0.71
3:3:468:HIS:ND1	3:3:469:ARG:O	2.23	0.71
5:5:3:LEU:HD21	5:5:25:LEU:HD22	1.71	0.71
6:6:165:GLU:OE2	7:9:148:ARG:NH1	2.23	0.71
13:L:161:VAL:HG13	13:L:222:LEU:HD13	1.73	0.71
13:L:278:ALA:HA	13:L:301:SER:HA	1.73	0.71
5:F:103:THR:HG22	5:F:126:PHE:HB3	1.71	0.71
11:J:133:GLY:H	11:J:136:LEU:HB2	1.56	0.71
12:K:7:SER:HB3	12:K:40:LEU:HD23	1.71	0.71
14:M:345:ARG:NH1	14:M:416:GLU:OE1	2.24	0.71
3:D:694:LEU:HB3	3:D:762:ALA:HB2	1.73	0.71
6:G:93:ARG:NH1	6:G:130:VAL:O	2.24	0.71
3:3:115:HIS:CD2	3:3:116:PRO:HD2	2.26	0.70
4:E:110:PRO:HB3	4:E:301:PRO:HG2	1.70	0.70
2:C:110:GLU:HA	8:I:121:ARG:HH12	1.55	0.70
3:D:34:CYS:N	3:D:45:CYS:SG	2.61	0.70
13:T:105:PHE:O	13:T:109:ASN:ND2	2.23	0.70
2:2:85:THR:HG22	2:2:86:LEU:H	1.56	0.70
4:4:318:GLU:HB2	8:7:39:ASP:HA	1.73	0.70
16:Q:52:GLY:HA3	16:Q:55:GLY:H	1.54	0.70
1:1:287:ILE:HA	1:1:332:PRO:HA	1.74	0.70
1:1:342:TRP:HE1	1:1:372:ALA:HA	1.57	0.70
16:H:162:TYR:OH	16:H:305:LEU:O	2.07	0.70
4:4:103:LYS:NZ	5:5:22:LEU:O	2.25	0.70
13:L:305:TYR:OH	13:L:406:ALA:O	2.08	0.70
2:C:87:SER:HB2	20:C:201:FES:S2	2.31	0.70
6:G:50:MET:O	6:G:53:SER:OG	2.10	0.70
1:B:88:TYR:HB2	1:B:216:THR:HG22	1.72	0.70
3:D:621:VAL:HG23	3:D:672:ALA:HA	1.73	0.70
4:E:372:ALA:HB2	4:E:409:ARG:HD3	1.74	0.70
9:X:60:PRO:HB3	9:X:103:LEU:HD13	1.74	0.70
14:U:21:PRO:HD2	14:U:24:LEU:HG	1.73	0.70
16:H:29:ALA:O	16:H:32:THR:OG1	2.08	0.70
7:9:108:CYS:HA	17:9:202:SF4:S3	2.31	0.69
15:N:201:GLN:OE1	15:N:256:ARG:NH1	2.25	0.69
1:1:79:MET:SD	1:1:217:THR:OG1	2.50	0.69
3:3:435:LEU:O	3:3:438:LYS:NZ	2.24	0.69
4:E:154:GLU:OE2	4:E:167:ARG:NH2	2.25	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
14:M:208:PHE:O	14:M:211:HIS:ND1	2.24	0.69
1:B:370:LEU:HD12	1:B:387:LEU:HB2	1.73	0.69
3:D:34:CYS:HB3	3:D:45:CYS:H	1.57	0.69
4:E:392:ASP:OD2	16:Q:301:ARG:NH1	2.25	0.69
1:1:350:HIS:O	3:3:205:ARG:NH1	2.25	0.69
3:3:576:ALA:O	3:3:580:LYS:NZ	2.17	0.69
10:P:69:ILE:HG22	11:R:62:ALA:HB1	1.75	0.69
1:1:288:GLN:NE2	1:1:335:VAL:O	2.26	0.69
3:3:494:LYS:O	3:3:498:GLU:HG2	1.92	0.69
3:3:507:LEU:HD22	3:3:511:VAL:HG11	1.75	0.69
8:7:63:LEU:CD1	8:7:129:ALA:HB3	2.22	0.69
14:U:304:THR:O	14:U:307:GLY:N	2.24	0.69
1:B:189:MET:O	1:B:193:GLU:HB2	1.93	0.69
4:E:352:GLU:O	4:E:371:ARG:NE	2.19	0.69
13:T:432:HIS:HE1	13:T:434:HIS:HB2	1.57	0.69
1:1:425:ALA:O	1:1:428:LYS:NZ	2.17	0.69
3:3:129:GLU:O	3:3:133:ARG:HG2	1.93	0.69
14:M:166:ALA:HA	14:M:185:LEU:HD21	1.74	0.69
1:B:16:THR:HG21	1:B:229:PRO:HB3	1.74	0.69
16:Q:168:LEU:HD13	16:Q:318:LEU:HB3	1.73	0.69
16:H:218:PRO:HB3	16:H:305:LEU:HD13	1.75	0.68
1:B:246:SER:HB3	1:B:268:MET:HG2	1.73	0.68
6:G:63:PHE:HA	16:Q:50:ARG:HG2	1.74	0.68
8:I:74:PRO:HG2	8:I:77:ALA:HB2	1.74	0.68
4:4:167:ARG:HD3	6:6:143:ARG:HH12	1.59	0.68
7:O:101:CYS:N	17:O:201:SF4:S4	2.66	0.68
10:A:109:TYR:OH	10:A:113:LYS:NZ	2.25	0.68
11:J:47:ASP:O	11:J:122:GLY:N	2.27	0.68
14:M:86:ALA:HA	14:M:96:LEU:HD11	1.76	0.68
13:T:305:TYR:OH	13:T:406:ALA:O	2.10	0.68
4:4:144:THR:OG1	16:H:295:ALA:O	2.10	0.68
14:M:177:LEU:HD21	14:M:243:ARG:HD2	1.75	0.68
3:D:113:LEU:O	3:D:161:ARG:NH1	2.27	0.68
12:S:7:SER:HB3	12:S:40:LEU:HD23	1.75	0.68
3:D:48:CYS:HB3	20:D:804:FES:S2	2.33	0.68
11:R:124:PRO:HA	11:R:127:LEU:HB2	1.74	0.68
3:3:199:VAL:HG11	3:3:219:PRO:HD2	1.75	0.68
5:F:39:ALA:HA	5:F:107:LEU:HD21	1.74	0.68
4:4:240:ARG:NH1	4:4:282:GLU:OE2	2.27	0.68
14:M:371:LEU:HD12	14:M:440:LEU:HB3	1.76	0.68
4:E:314:ARG:NH2	8:I:44:MET:SD	2.66	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:3:611:ARG:HA	3:3:624:LEU:O	1.94	0.68
1:B:104:ARG:NH2	2:C:143:GLU:OE2	2.24	0.68
13:T:288:GLN:NE2	13:T:528:SER:O	2.27	0.68
6:6:69:ARG:NH2	16:H:223:GLU:OE2	2.27	0.68
14:M:55:LEU:HD11	15:N:416:PRO:HD2	1.76	0.68
3:3:701:ALA:N	3:3:763:LEU:O	2.27	0.67
11:J:24:ASN:HB3	11:J:27:HIS:HB2	1.77	0.67
13:L:288:GLN:NE2	13:L:528:SER:O	2.27	0.67
13:L:432:HIS:HE1	13:L:434:HIS:HB2	1.58	0.67
16:H:189:GLN:NE2	16:H:264:LEU:O	2.27	0.67
1:B:195:LEU:HD23	2:C:24:ARG:HH12	1.56	0.67
3:D:48:CYS:SG	3:D:83:CYS:N	2.67	0.67
1:1:4:PRO:HA	1:1:12:ARG:HH12	1.59	0.67
3:3:98:ASP:OD1	3:3:101:ARG:NH2	2.27	0.67
6:G:37:TRP:HB3	6:G:75:ALA:HA	1.77	0.67
13:L:182:THR:HB	13:L:187:GLU:HG3	1.76	0.67
16:H:43:GLN:O	16:H:45:ARG:N	2.27	0.67
3:3:186:ARG:HD3	3:3:229:ILE:HG22	1.77	0.67
1:1:18:TYR:OH	1:1:102:LYS:O	2.11	0.67
3:3:717:TRP:HB2	3:3:759:TYR:HB2	1.77	0.67
5:5:35:LYS:NZ	5:5:103:THR:O	2.28	0.67
1:B:339:ASP:OD1	1:B:433:ARG:NH2	2.28	0.67
7:O:68:ILE:HG12	7:O:93:ILE:HG12	1.77	0.67
1:1:433:ARG:HH12	2:2:89:LYS:HE2	1.58	0.67
10:A:48:ASN:OD1	10:A:49:ASP:HB2	1.94	0.67
3:3:290:ILE:HB	3:3:295:ARG:HH21	1.58	0.67
7:O:120:GLU:OE1	7:O:146:GLN:NE2	2.28	0.67
6:6:33:SER:HB2	6:6:155:GLN:HG2	1.77	0.67
13:L:159:PHE:HD2	14:M:407:LEU:HD11	1.59	0.67
1:B:139:ARG:NH1	1:B:143:ASP:OD2	2.27	0.67
6:G:125:GLN:OE1	7:O:97:ARG:NH1	2.26	0.67
6:6:50:MET:O	6:6:53:SER:OG	2.10	0.67
6:6:90:PRO:O	6:6:93:ARG:HB3	1.95	0.67
2:C:106:ILE:HD11	2:C:112:THR:CA	2.24	0.67
3:D:129:GLU:O	3:D:133:ARG:HG2	1.94	0.67
4:E:194:LEU:HD21	4:E:290:ILE:HG22	1.77	0.67
6:G:17:GLU:HG3	10:P:33:PRO:HA	1.77	0.67
13:T:163:ARG:HE	14:U:399:VAL:HB	1.58	0.67
2:2:34:VAL:HG11	2:2:45:ARG:HG3	1.75	0.66
3:3:367:PRO:O	3:3:552:GLY:N	2.29	0.66
3:D:227:THR:HG21	3:D:237:ASP:HB2	1.77	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:E:381:LEU:HD11	4:E:397:ILE:HG12	1.77	0.66
13:L:66:SER:HB3	13:L:122:ASP:HB3	1.77	0.66
13:L:582:GLN:NE2	15:N:194:PHE:O	2.29	0.66
4:E:83:PRO:HB2	4:E:169:HIS:HA	1.78	0.66
14:U:115:LEU:HD13	14:U:163:VAL:HG23	1.76	0.66
1:B:177:ALA:HA	2:C:32:ARG:HH21	1.61	0.66
16:H:218:PRO:HA	16:H:300:LEU:HB2	1.77	0.66
1:B:312:SER:OG	1:B:315:HIS:ND1	2.23	0.66
4:4:259:THR:O	4:4:296:ARG:NH2	2.28	0.66
13:L:380:SER:HB3	13:L:457:GLY:H	1.60	0.66
16:Q:65:LYS:O	16:Q:69:LYS:HB2	1.96	0.66
16:Q:274:VAL:HG12	16:Q:278:TRP:HD1	1.56	0.66
16:Q:332:LEU:HB2	16:Q:333:PRO:HD3	1.76	0.66
3:3:225:ASN:O	3:3:229:ILE:HG13	1.96	0.66
6:G:119:ASN:HA	6:G:125:GLN:NE2	2.11	0.66
13:T:151:TYR:HB3	13:T:231:ALA:HB1	1.77	0.66
1:1:104:ARG:NH2	1:1:105:TYR:OH	2.29	0.66
14:M:91:VAL:HG12	14:M:222:HIS:CE1	2.31	0.66
3:D:19:VAL:HG21	3:D:52:ILE:HD11	1.76	0.66
11:J:85:PRO:HA	12:K:22:ARG:HH12	1.61	0.66
7:9:41:HIS:HB3	7:9:113:ILE:HD11	1.77	0.65
7:O:43:LEU:HA	7:O:112:ALA:O	1.96	0.65
4:4:240:ARG:NH2	4:4:347:GLU:OE2	2.27	0.65
6:6:93:ARG:NH1	6:6:130:VAL:O	2.30	0.65
6:6:157:LYS:HB2	7:9:124:TYR:HE2	1.62	0.65
7:9:101:CYS:N	17:9:201:SF4:S4	2.68	0.65
16:H:71:ASP:OD1	16:H:240:LYS:NZ	2.19	0.65
16:H:168:LEU:HD13	16:H:318:LEU:HB3	1.78	0.65
2:C:27:ILE:HG13	2:C:53:VAL:HG21	1.77	0.65
4:E:81:TYR:OH	6:G:117:MET:O	2.13	0.65
6:G:60:LEU:HD21	6:G:151:VAL:HG11	1.78	0.65
10:P:65:ALA:HB3	11:R:66:LEU:HD13	1.79	0.65
13:T:44:GLY:HA3	13:T:77:LEU:HD21	1.78	0.65
5:5:144:HIS:HB2	5:5:147:ARG:HD3	1.77	0.65
10:A:63:VAL:HG11	10:A:115:VAL:HG21	1.77	0.65
4:E:222:GLY:HA3	4:E:275:ARG:HH22	1.60	0.65
4:E:87:TYR:CG	6:G:45:CYS:HB3	2.32	0.65
15:V:58:VAL:HB	15:V:225:ARG:HH11	1.61	0.65
1:1:88:TYR:HB2	1:1:216:THR:HG22	1.79	0.65
9:W:28:GLU:O	9:W:88:ARG:NH2	2.29	0.65
10:A:3:PRO:HD2	16:H:2:THR:HB	1.78	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:J:15:SER:OG	11:J:31:ALA:O	2.14	0.65
16:Q:117:ASN:O	16:Q:181:ASN:ND2	2.28	0.65
13:L:487:LEU:HA	13:L:490:GLU:HG2	1.77	0.65
1:B:372:ALA:O	1:B:376:THR:OG1	2.12	0.65
4:E:373:PRO:O	4:E:377:ASN:ND2	2.29	0.65
14:U:333:TYR:O	14:U:337:GLY:N	2.30	0.65
14:M:102:MET:HB3	14:M:230:LEU:HD23	1.78	0.65
16:H:333:PRO:HB2	16:H:335:THR:H	1.62	0.65
8:I:20:MET:HG2	8:I:115:PHE:CZ	2.32	0.65
10:P:28:GLY:HA2	16:Q:67:ILE:HG22	1.77	0.65
4:4:371:ARG:NH2	4:4:376:VAL:HG21	2.12	0.65
3:3:259:CYS:SG	3:3:261:VAL:HG22	2.36	0.64
4:4:102:GLU:O	4:4:106:GLY:N	2.31	0.64
4:4:132:PHE:CE2	4:4:279:ARG:HD2	2.33	0.64
13:T:162:ASN:OD1	13:T:216:LYS:NZ	2.30	0.64
10:A:69:ILE:HG22	11:J:62:ALA:HB1	1.79	0.64
15:N:345:LYS:NZ	15:N:368:SER:OG	2.30	0.64
7:O:41:HIS:HB3	7:O:113:ILE:HD11	1.77	0.64
10:P:77:PHE:O	10:P:80:PRO:HD2	1.97	0.64
14:U:33:PHE:HA	14:U:79:ALA:HB1	1.79	0.64
9:W:59:VAL:HG11	9:W:63:PHE:CE2	2.32	0.64
1:B:165:THR:HG23	1:B:167:PHE:H	1.63	0.64
3:D:193:GLU:O	3:D:443:ARG:NH2	2.26	0.64
3:3:224:GLY:O	3:3:227:THR:HB	1.98	0.64
3:3:720:PRO:HG2	3:3:751:GLU:HG3	1.78	0.64
4:E:52:VAL:O	4:E:387:GLY:N	2.24	0.64
11:R:68:LEU:HD23	11:R:71:ILE:HD11	1.78	0.64
3:3:39:LEU:HB3	3:3:189:ARG:HE	1.63	0.64
14:M:43:HIS:NE2	14:M:45:GLY:O	2.31	0.64
4:4:248:VAL:HB	4:4:347:GLU:HB2	1.80	0.64
14:M:335:ARG:NH2	14:M:429:GLU:OE1	2.30	0.64
3:3:34:CYS:SG	3:3:35:SER:N	2.71	0.64
5:5:126:PHE:H	5:5:132:LEU:HD11	1.63	0.64
11:J:135:TRP:HZ3	15:N:105:LEU:HD22	1.62	0.64
13:L:17:LEU:HB2	13:L:106:ALA:HB2	1.79	0.64
5:F:10:ALA:HB1	5:F:15:TYR:HB2	1.80	0.64
15:V:187:ALA:O	15:V:216:LYS:NZ	2.31	0.64
4:4:230:ILE:HG21	5:5:47:ASN:HB3	1.80	0.64
3:D:149:LEU:HD11	4:E:110:PRO:HG3	1.79	0.64
4:E:281:ARG:HD3	4:E:284:ARG:HH12	1.63	0.64
1:1:400:CYS:SG	17:1:501:SF4:FE3	1.88	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:4:328:PHE:CE2	7:9:58:LEU:HD21	2.33	0.64
6:6:80:VAL:HG11	6:6:127:VAL:HG11	1.80	0.64
4:E:80:THR:O	4:E:84:ARG:NH1	2.29	0.64
12:S:88:ASP:OD2	13:T:587:ARG:NH1	2.31	0.64
14:U:85:GLY:O	14:U:89:ALA:HB2	1.97	0.64
6:G:17:GLU:HA	10:P:33:PRO:HG3	1.79	0.64
3:3:300:TRP:CD1	3:3:703:GLN:HA	2.33	0.63
4:4:31:GLY:HA3	10:A:45:GLU:OE2	1.98	0.63
13:L:574:LEU:HD22	15:N:246:LEU:HD13	1.80	0.63
7:O:40:ARG:NH1	7:O:41:HIS:O	2.31	0.63
3:3:567:TYR:HA	3:3:584:VAL:HG23	1.80	0.63
4:4:140:LEU:HD21	4:4:217:ARG:HH12	1.63	0.63
4:4:311:PRO:HD3	4:4:330:HIS:CE1	2.34	0.63
5:5:53:VAL:HG13	5:5:71:VAL:HB	1.79	0.63
3:3:592:PRO:HA	3:3:595:GLU:HG2	1.80	0.63
5:5:168:ALA:HA	5:5:171:ARG:HH11	1.62	0.63
10:A:27:VAL:HG12	16:H:67:ILE:HG21	1.79	0.63
10:P:56:ARG:HD3	11:R:74:LEU:HA	1.79	0.63
13:T:392:THR:HG22	13:T:399:GLY:O	1.98	0.63
4:4:144:THR:HG22	4:4:148:TYR:HE1	1.62	0.63
5:F:120:ASP:OD2	5:F:136:LEU:N	2.32	0.63
5:F:121:LEU:HA	5:F:145:PRO:HD2	1.80	0.63
6:G:18:GLY:HA2	6:G:28:VAL:HG11	1.80	0.63
13:T:234:THR:HG23	13:T:292:LYS:HE2	1.81	0.63
1:B:184:GLU:O	1:B:188:LEU:N	2.29	0.63
1:B:275:LEU:HA	1:B:279:TRP:HD1	1.63	0.63
2:C:66:PHE:O	3:D:205:ARG:NE	2.30	0.63
5:F:174:LEU:HB3	5:F:178:ASP:HB3	1.80	0.63
16:Q:120:LEU:HD22	16:Q:180:LEU:HD12	1.80	0.63
16:Q:332:LEU:HB2	16:Q:333:PRO:CD	2.27	0.63
2:2:110:GLU:OE2	8:7:114:ARG:NE	2.28	0.63
3:3:656:LEU:HD11	9:W:3:ARG:HD3	1.80	0.63
7:9:171:GLU:OE2	8:7:43:ARG:NH2	2.31	0.63
10:A:81:TYR:HE2	16:H:325:ALA:HB1	1.64	0.63
11:J:104:LEU:HA	15:N:174:LEU:HD21	1.80	0.63
4:E:201:ILE:HG21	4:E:284:ARG:HG3	1.81	0.63
4:4:285:GLU:O	4:4:289:ILE:HG12	1.99	0.63
14:M:306:GLU:OE2	14:M:386:LYS:NZ	2.25	0.63
15:N:98:LEU:HD23	15:N:218:ALA:HB1	1.81	0.63
5:F:35:LYS:NZ	5:F:103:THR:O	2.31	0.63
1:1:354:GLY:O	1:1:360:ARG:NH1	2.31	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:J:61:GLY:O	11:J:65:VAL:HG21	1.98	0.63
14:M:115:LEU:HD13	14:M:163:VAL:HG23	1.80	0.63
16:H:189:GLN:HG2	16:H:195:LEU:H	1.63	0.63
3:D:183:HIS:NE2	3:D:209:THR:O	2.31	0.63
3:3:605:PRO:HB2	3:3:609:GLU:HG3	1.79	0.62
8:7:40:PHE:HA	8:7:43:ARG:HG2	1.80	0.62
1:B:276:ILE:HA	1:B:280:ALA:HB3	1.81	0.62
1:1:196:ARG:NH2	3:3:204:GLU:O	2.30	0.62
15:V:14:THR:HA	15:V:86:LEU:HD21	1.81	0.62
15:V:317:ARG:NH1	15:V:384:ALA:O	2.31	0.62
6:6:58:ASN:ND2	6:6:145:GLU:OE2	2.33	0.62
13:L:151:TYR:HB3	13:L:231:ALA:HB1	1.80	0.62
16:H:332:LEU:HB2	16:H:333:PRO:CD	2.29	0.62
2:C:81:GLN:HB3	2:C:122:VAL:HG21	1.80	0.62
16:Q:43:GLN:O	16:Q:45:ARG:N	2.32	0.62
1:1:6:LEU:HD11	1:1:240:GLN:HE21	1.64	0.62
3:3:384:PRO:HG3	3:3:542:ARG:NH1	2.14	0.62
2:C:71:GLN:NE2	2:C:120:GLN:OE1	2.32	0.62
6:G:59:ASP:OD1	6:G:62:ARG:NH2	2.32	0.62
1:1:365:GLY:O	1:1:369:ASN:ND2	2.33	0.62
4:4:369:LYS:HG3	5:5:53:VAL:HG23	1.82	0.62
15:N:347:LEU:O	15:N:351:GLU:HG2	1.98	0.62
1:B:10:ASP:OD2	1:B:12:ARG:NE	2.26	0.62
15:V:108:LEU:HB2	15:V:147:PHE:HE2	1.62	0.62
16:Q:72:ILE:HG22	16:Q:237:SER:HB3	1.80	0.62
3:3:2:VAL:HG13	3:3:89:ASP:HA	1.81	0.62
7:9:164:PRO:HA	7:9:178:GLU:HB2	1.80	0.62
16:H:147:TYR:CD1	16:H:229:VAL:HG22	2.35	0.62
16:Q:29:ALA:O	16:Q:32:THR:OG1	2.13	0.62
16:H:60:LEU:O	16:H:64:ILE:HG13	2.00	0.62
16:H:205:VAL:HG21	16:H:317:ALA:HB2	1.80	0.62
1:B:201:LEU:HA	1:B:399:PHE:HZ	1.65	0.62
1:B:293:GLY:HA3	1:B:297:THR:HG21	1.80	0.62
14:U:70:LEU:O	14:U:73:LEU:HD23	1.99	0.62
1:1:195:LEU:HD23	2:2:24:ARG:HH12	1.64	0.62
3:D:243:ARG:HB3	3:D:275:LEU:HD22	1.81	0.62
3:D:737:GLU:HB2	3:D:776:LEU:HD11	1.81	0.62
3:3:716:LEU:HD21	3:3:758:LEU:HD23	1.80	0.62
4:4:261:THR:H	4:4:292:GLN:NE2	1.95	0.62
5:5:103:THR:HG22	5:5:126:PHE:HB3	1.81	0.62
16:H:267:TRP:CG	16:H:268:THR:N	2.65	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:T:291:ILE:HD12	13:T:336:SER:HB3	1.81	0.62
1:1:275:LEU:HA	1:1:279:TRP:HD1	1.63	0.61
1:1:359:CYS:HB2	1:1:403:ALA:HB2	1.80	0.61
14:M:333:TYR:O	14:M:337:GLY:N	2.32	0.61
1:B:243:THR:HG22	1:B:244:GLU:H	1.63	0.61
1:1:46:LYS:HE2	1:1:163:PHE:HB3	1.82	0.61
8:7:23:TYR:OH	8:7:123:ARG:NH1	2.22	0.61
13:T:278:ALA:HB1	13:T:409:VAL:HG11	1.82	0.61
15:V:95:MET:HG2	15:V:114:LEU:HD22	1.82	0.61
16:Q:292:TRP:O	16:Q:296:THR:OG1	2.07	0.61
16:Q:302:TYR:HA	16:Q:305:LEU:HB3	1.82	0.61
3:3:243:ARG:HB3	3:3:275:LEU:HD22	1.82	0.61
8:7:105:THR:HG23	8:7:110:LEU:HB2	1.82	0.61
13:L:490:GLU:O	13:L:494:ILE:HG12	2.00	0.61
4:E:123:LEU:HG	4:E:156:ILE:HG23	1.83	0.61
5:F:159:PHE:HB2	5:F:163:ARG:O	1.99	0.61
7:O:28:ASP:OD2	16:Q:50:ARG:NH1	2.33	0.61
16:Q:216:ARG:HB2	16:Q:294:ARG:HD2	1.82	0.61
3:3:364:LEU:HB2	3:3:650:VAL:HG21	1.82	0.61
14:M:54:PRO:HA	14:M:62:TYR:HD1	1.65	0.61
3:D:51:ARG:HB3	3:D:94:ASP:HB3	1.82	0.61
5:F:66:GLU:HB2	5:F:93:TYR:HB3	1.83	0.61
6:G:21:PHE:HD1	6:G:23:THR:H	1.47	0.61
14:U:109:LEU:HD21	14:U:236:VAL:HG21	1.82	0.61
16:Q:2:THR:HA	16:Q:5:TYR:HD2	1.65	0.61
13:T:490:GLU:O	13:T:494:ILE:HG12	2.01	0.61
16:Q:127:ALA:O	16:Q:131:LEU:HG	2.00	0.61
5:5:38:MET:HA	5:5:41:TYR:HD2	1.66	0.61
14:M:167:ARG:NH2	14:M:173:PRO:O	2.31	0.61
3:3:722:THR:HG21	3:3:756:GLY:H	1.65	0.61
15:N:128:GLN:NE2	15:N:305:ASP:OD1	2.34	0.61
1:B:254:ILE:HD11	1:B:330:LEU:HD11	1.82	0.61
15:V:59:SER:OG	15:V:100:SER:OG	2.13	0.61
12:K:88:ASP:OD2	13:L:587:ARG:NH1	2.33	0.61
14:M:354:LEU:HD13	14:M:425:LEU:HG	1.83	0.61
13:T:432:HIS:CE1	13:T:434:HIS:HB2	2.36	0.61
6:6:178:ARG:NH1	9:W:122:ASP:OD2	2.33	0.61
6:6:143:ARG:NE	6:6:145:GLU:OE1	2.33	0.61
11:J:50:PHE:HB2	11:J:124:PRO:HD3	1.83	0.61
13:L:325:HIS:NE2	13:L:329:LYS:HG3	2.15	0.61
1:B:6:LEU:HB2	1:B:241:MET:HA	1.82	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:F:171:ARG:NE	7:O:66:TYR:OH	2.34	0.61
14:U:24:LEU:HD22	14:U:27:LEU:HD21	1.83	0.61
15:V:217:ALA:HA	15:V:285:LEU:HD23	1.82	0.61
16:Q:39:LEU:O	16:Q:43:GLN:HG2	2.00	0.61
16:Q:86:PRO:HG3	16:Q:244:PHE:CE2	2.35	0.60
4:4:148:TYR:OH	16:H:42:PHE:O	2.17	0.60
9:W:59:VAL:HG11	9:W:63:PHE:HE2	1.66	0.60
1:B:101:PHE:CZ	1:B:253:GLN:HB2	2.35	0.60
1:B:288:GLN:HE21	1:B:331:ILE:HG22	1.66	0.60
3:3:9:ARG:NH1	3:3:26:ALA:O	2.33	0.60
6:6:117:MET:HE1	7:9:99:ILE:HG12	1.83	0.60
15:N:14:THR:HA	15:N:86:LEU:HD21	1.81	0.60
3:3:229:ILE:HD11	3:3:289:TRP:HZ3	1.65	0.60
3:3:352:GLU:OE2	3:3:661:GLN:NE2	2.35	0.60
4:4:218:ALA:HA	4:4:221:VAL:HG22	1.82	0.60
9:W:31:VAL:HG11	9:W:81:LEU:HD13	1.83	0.60
7:O:108:CYS:HA	17:O:202:SF4:S3	2.41	0.60
10:P:62:TYR:CD2	11:R:66:LEU:HD11	2.35	0.60
12:K:49:TYR:OH	15:N:156:GLY:O	2.13	0.60
10:P:65:ALA:O	10:P:69:ILE:HG23	2.01	0.60
10:P:70:LEU:HD13	11:R:150:THR:HG22	1.83	0.60
4:4:250:LYS:HE2	4:4:262:PHE:HB3	1.84	0.60
12:K:19:LEU:HD22	13:L:591:LEU:HD12	1.82	0.60
14:M:16:LEU:HD22	14:M:97:GLY:H	1.67	0.60
15:N:126:ARG:HD2	15:N:128:GLN:HG2	1.82	0.60
16:Q:222:PRO:HD2	16:Q:230:GLY:HA2	1.82	0.60
13:L:432:HIS:CE1	13:L:434:HIS:HB2	2.36	0.60
15:N:317:ARG:NH1	15:N:384:ALA:O	2.35	0.60
3:D:40:SER:O	3:D:189:ARG:NE	2.31	0.60
15:V:180:LEU:HD21	15:V:228:ALA:HB2	1.83	0.60
10:A:65:ALA:O	10:A:69:ILE:HG23	2.02	0.60
13:L:53:ALA:HB3	13:L:69:LEU:HB3	1.84	0.60
13:L:68:LEU:HD23	13:L:255:ARG:HH22	1.66	0.60
9:W:51:HIS:ND1	9:W:56:ASP:OD1	2.35	0.60
1:B:253:GLN:NE2	1:B:325:THR:O	2.35	0.60
14:U:201:PHE:HD2	14:U:245:ALA:HB2	1.66	0.60
15:N:279:GLN:HG3	15:N:423:LEU:HB2	1.83	0.59
6:G:90:PRO:O	6:G:93:ARG:HB3	2.02	0.59
3:3:223:SER:O	3:3:226:ILE:HG12	2.02	0.59
7:9:9:SER:O	7:9:12:ILE:HG13	2.01	0.59
10:A:65:ALA:HB3	11:J:66:LEU:HD13	1.84	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:19:VAL:HG22	3:D:91:MET:HE3	1.84	0.59
13:T:287:GLY:HA3	13:T:528:SER:HB2	1.83	0.59
4:4:216:GLU:OE2	16:H:304:GLN:NE2	2.35	0.59
13:L:287:GLY:HA3	13:L:528:SER:HB2	1.84	0.59
13:L:581:LEU:HD23	15:N:194:PHE:HE1	1.67	0.59
16:H:96:ALA:HB2	16:H:128:VAL:HG21	1.83	0.59
3:D:198:GLU:OE2	3:D:440:ARG:NH1	2.36	0.59
3:D:154:TYR:HB3	4:E:322:GLU:HB2	1.84	0.59
1:1:10:ASP:OD2	1:1:12:ARG:NE	2.29	0.59
3:D:592:PRO:HA	3:D:595:GLU:HG2	1.83	0.59
16:Q:202:ALA:HA	16:Q:205:VAL:HG22	1.84	0.59
1:1:390:LEU:HA	1:1:393:LEU:HD12	1.83	0.59
13:L:153:ASP:OD1	14:M:411:GLN:NE2	2.22	0.59
3:D:538:ALA:HB3	3:D:541:ALA:HB2	1.85	0.59
6:G:19:ILE:HG12	6:G:20:LEU:H	1.67	0.59
14:U:448:GLY:O	14:U:452:ARG:HG2	2.02	0.59
15:V:52:PRO:HB3	15:V:103:HIS:HB2	1.85	0.59
3:3:523:LEU:HD22	3:3:527:ARG:HH21	1.67	0.59
7:9:99:ILE:HG22	17:9:201:SF4:S3	2.42	0.59
1:1:243:THR:HG22	1:1:244:GLU:H	1.68	0.59
4:4:64:THR:OG1	6:6:83:ARG:HD2	2.03	0.59
5:5:55:LEU:HD23	5:5:57:TYR:OH	2.02	0.59
1:B:201:LEU:HG	1:B:203:PRO:HD2	1.85	0.59
3:D:614:LEU:HD11	3:D:624:LEU:HG	1.83	0.59
16:Q:290:PHE:O	16:Q:294:ARG:HG2	2.03	0.59
1:1:92:ASN:ND2	18:1:502:FMN:O3'	2.32	0.59
11:J:146:LEU:HD23	12:K:66:ALA:HB2	1.85	0.59
2:C:106:ILE:HG22	2:C:107:GLY:O	2.03	0.59
4:E:201:ILE:HA	4:E:204:TYR:HD2	1.68	0.59
5:F:151:PRO:HD3	9:X:112:LYS:HE2	1.83	0.59
3:3:369:LEU:HD12	3:3:369:LEU:O	2.03	0.58
16:H:302:TYR:HA	16:H:305:LEU:HB3	1.86	0.58
3:D:94:ASP:OD2	3:D:97:SER:OG	2.18	0.58
4:E:26:MET:N	4:E:47:LEU:O	2.36	0.58
4:E:185:GLU:OE2	7:O:165:TYR:OH	2.13	0.58
5:F:175:THR:HG22	5:F:178:ASP:HB2	1.83	0.58
3:3:81:ALA:O	3:3:85:THR:OG1	2.10	0.58
14:M:22:ARG:HG3	14:M:92:GLU:OE1	2.02	0.58
14:M:109:LEU:HD21	14:M:236:VAL:HG21	1.85	0.58
16:H:225:GLU:HB3	16:H:226:GLN:HG2	1.85	0.58
16:H:227:GLU:HG2	16:H:228:LEU:H	1.67	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:249:MET:HA	1:B:267:PRO:HA	1.85	0.58
4:E:148:TYR:OH	16:Q:42:PHE:O	2.13	0.58
16:Q:137:PHE:HA	16:Q:152:SER:HB2	1.83	0.58
1:1:312:SER:OG	1:1:315:HIS:ND1	2.22	0.58
4:4:87:TYR:CB	6:6:45:CYS:HB3	2.34	0.58
8:7:74:PRO:HG2	8:7:77:ALA:HB2	1.85	0.58
14:M:128:PRO:O	14:M:132:MET:HG2	2.03	0.58
16:H:274:VAL:HG12	16:H:278:TRP:CD1	2.37	0.58
3:D:690:GLY:HA2	3:D:770:ARG:HB3	1.84	0.58
13:T:255:ARG:HA	13:T:477:LEU:HD23	1.85	0.58
14:U:232:THR:HG21	14:U:322:THR:HB	1.86	0.58
15:V:132:ALA:HB1	15:V:199:VAL:HA	1.85	0.58
16:Q:227:GLU:HG2	16:Q:228:LEU:H	1.67	0.58
2:2:110:GLU:HA	8:7:121:ARG:HH12	1.68	0.58
13:L:278:ALA:HB1	13:L:409:VAL:HG11	1.83	0.58
5:F:28:VAL:HA	5:F:91:ARG:O	2.04	0.58
13:T:147:LYS:NZ	14:U:349:GLN:OE1	2.33	0.58
16:Q:168:LEU:HD23	16:Q:171:LEU:HD12	1.86	0.58
11:J:104:LEU:HD23	15:N:174:LEU:HD21	1.85	0.58
3:D:297:GLY:O	3:D:300:TRP:NE1	2.36	0.58
16:Q:71:ASP:OD1	16:Q:240:LYS:NZ	2.23	0.58
10:A:113:LYS:NZ	15:N:83:GLU:OE2	2.34	0.58
11:J:69:PHE:O	11:J:73:LEU:HG	2.04	0.58
11:J:152:VAL:HG13	15:N:120:ALA:HB2	1.85	0.58
13:L:104:PHE:CE2	13:L:108:PHE:CE2	2.91	0.58
16:H:190:LYS:HB2	16:H:268:THR:HG21	1.86	0.58
6:G:69:ARG:NH2	16:Q:223:GLU:OE2	2.32	0.58
6:G:163:TYR:HD1	7:O:152:ARG:HD2	1.69	0.58
10:P:13:TYR:CZ	16:Q:95:LEU:HA	2.38	0.58
10:P:63:VAL:HG11	10:P:115:VAL:HG21	1.84	0.58
16:Q:352:VAL:HG12	16:Q:353:LEU:HD12	1.85	0.58
13:L:355:LEU:HB3	13:L:359:LEU:HD12	1.85	0.58
1:1:118:MET:HG2	1:1:224:LEU:HD13	1.84	0.58
1:B:195:LEU:HD23	2:C:24:ARG:NH1	2.18	0.58
3:D:247:TRP:HE1	7:O:61:ALA:HB2	1.68	0.58
14:U:201:PHE:CD2	14:U:245:ALA:HB2	2.39	0.58
16:Q:159:LEU:O	16:Q:163:GLU:HB2	2.02	0.58
4:4:172:TYR:OH	4:4:180:GLU:O	2.13	0.58
9:W:102:LEU:O	9:W:110:LEU:HD13	2.04	0.58
10:A:62:TYR:CD2	11:J:66:LEU:HD11	2.39	0.58
16:H:150:LEU:HD22	16:H:228:LEU:HD12	1.85	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:268:ASP:OD2	3:D:278:ARG:NH1	2.30	0.58
3:D:415:GLU:HG2	3:D:418:ARG:HH21	1.69	0.58
4:4:77:GLN:O	4:4:80:THR:OG1	2.16	0.58
5:5:33:ARG:NH1	5:5:36:GLU:OE2	2.37	0.58
11:J:85:PRO:O	13:L:587:ARG:NH2	2.34	0.58
13:L:463:HIS:CE1	13:L:487:LEU:HD22	2.38	0.58
14:M:206:PRO:HG3	14:M:214:LEU:HD22	1.85	0.58
16:H:147:TYR:HD1	16:H:229:VAL:HG22	1.69	0.58
16:Q:265:GLY:O	16:Q:282:LYS:NZ	2.25	0.58
4:4:62:LEU:HD11	6:6:43:LEU:O	2.04	0.57
9:W:90:TYR:HB3	9:W:118:ALA:HB1	1.86	0.57
3:D:285:VAL:HG13	3:D:286:ASN:H	1.69	0.57
3:D:363:ALA:HB1	3:D:650:VAL:HG11	1.86	0.57
7:O:69:TYR:HE1	7:O:71:GLU:HG3	1.68	0.57
13:T:267:SER:HB3	13:T:311:GLY:O	2.04	0.57
13:T:380:SER:HB3	13:T:456:ALA:HB3	1.86	0.57
13:L:88:HIS:O	13:L:92:ILE:HG13	2.03	0.57
16:H:292:TRP:O	16:H:296:THR:OG1	2.08	0.57
10:P:2:ALA:HB3	16:Q:119:ASP:OD2	2.04	0.57
15:V:98:LEU:HD12	15:V:107:MET:HG2	1.87	0.57
3:3:274:LEU:H	3:3:302:ASP:HB3	1.69	0.57
4:4:30:VAL:HB	4:4:43:LEU:HB2	1.84	0.57
9:W:87:ARG:HH12	10:A:38:ARG:HH12	1.52	0.57
14:M:29:ALA:HB1	14:M:83:PHE:HA	1.87	0.57
14:M:264:ALA:HB1	14:M:294:GLY:O	2.04	0.57
4:E:272:VAL:HG13	4:E:399:SER:HB3	1.86	0.57
7:O:59:CYS:SG	7:O:91:TYR:OH	2.59	0.57
7:O:164:PRO:HA	7:O:178:GLU:HB2	1.86	0.57
8:I:13:TRP:CE3	8:I:72:VAL:HB	2.38	0.57
1:1:17:LEU:HD22	1:1:113:LEU:HD21	1.87	0.57
4:4:218:ALA:HB1	4:4:272:VAL:HB	1.87	0.57
8:7:105:THR:OG1	8:7:114:ARG:NH2	2.35	0.57
13:L:291:ILE:HD12	13:L:336:SER:HB3	1.87	0.57
3:D:152:PRO:HD3	4:E:305:PRO:HB2	1.86	0.57
3:D:656:LEU:HD11	9:X:3:ARG:HD3	1.86	0.57
13:T:433:HIS:ND1	13:T:433:HIS:O	2.38	0.57
16:Q:54:PHE:HB3	16:Q:56:LEU:HD23	1.86	0.57
4:4:336:HIS:HE1	5:5:174:LEU:HD12	1.68	0.57
7:9:71:GLU:HB2	7:9:90:VAL:HB	1.86	0.57
2:C:9:ASP:OD1	2:C:9:ASP:N	2.37	0.57
16:Q:150:LEU:HD21	16:Q:154:ARG:HH11	1.69	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
16:Q:226:GLN:HB2	16:Q:299:ARG:HH22	1.70	0.57
8:7:44:MET:HE2	8:7:46:ARG:HH22	1.69	0.57
10:A:83:VAL:HG23	10:A:84:SER:N	2.20	0.57
13:L:433:HIS:ND1	13:L:433:HIS:O	2.37	0.57
3:D:614:LEU:O	3:D:621:VAL:HA	2.04	0.57
16:Q:17:ALA:O	16:Q:21:VAL:HG23	2.05	0.57
3:3:664:LEU:O	3:3:669:VAL:HG12	2.03	0.57
4:4:140:LEU:HD21	4:4:217:ARG:NH1	2.19	0.57
6:6:102:PRO:HD3	10:A:33:PRO:HG2	1.87	0.57
6:6:155:GLN:O	6:6:159:ARG:HG3	2.04	0.57
3:D:131:GLN:HG2	4:E:325:ILE:HG23	1.85	0.57
3:D:678:PHE:CZ	3:D:680:LEU:HD13	2.39	0.57
4:E:224:ILE:HB	4:E:270:GLY:HA3	1.86	0.57
7:O:71:GLU:HB2	7:O:90:VAL:HB	1.85	0.57
15:V:63:THR:HG22	15:V:96:HIS:HA	1.87	0.57
16:Q:150:LEU:HD23	16:Q:154:ARG:HD2	1.87	0.57
1:1:72:THR:HG21	1:1:223:THR:HG21	1.85	0.57
7:9:108:CYS:SG	7:9:112:ALA:N	2.78	0.57
7:9:162:VAL:HA	7:9:176:PRO:HG2	1.87	0.57
14:M:232:THR:HA	14:M:235:LYS:HZ2	1.70	0.57
4:E:171:ASN:OD1	4:E:174:ARG:NH1	2.33	0.57
10:P:6:GLU:OE2	16:Q:2:THR:OG1	2.16	0.57
16:H:159:LEU:O	16:H:163:GLU:HB2	2.04	0.57
3:D:185:LYS:O	3:D:189:ARG:HB2	2.05	0.57
6:G:148:ILE:O	6:G:151:VAL:HG22	2.04	0.57
13:T:187:GLU:HA	13:T:190:GLU:HG2	1.85	0.57
11:J:19:VAL:O	12:K:21:ARG:NH2	2.33	0.57
16:Q:25:LEU:O	16:Q:28:PHE:CD1	2.58	0.57
14:M:402:SER:HA	14:M:405:TYR:CE2	2.40	0.56
16:H:39:LEU:O	16:H:43:GLN:HG2	2.04	0.56
11:R:72:MET:HE3	16:Q:149:LEU:HD21	1.85	0.56
14:U:91:VAL:HG23	14:U:92:GLU:H	1.69	0.56
16:Q:221:LEU:N	16:Q:222:PRO:HA	2.19	0.56
11:J:75:PHE:CZ	11:J:78:GLN:HG2	2.40	0.56
4:E:30:VAL:HB	4:E:43:LEU:HB2	1.86	0.56
9:X:34:ILE:HA	9:X:92:ALA:HB3	1.86	0.56
13:T:601:LEU:HD21	15:V:178:LEU:HD21	1.87	0.56
3:3:285:VAL:HG13	3:3:286:ASN:H	1.71	0.56
6:6:164:ASN:HD21	6:6:168:GLU:HB2	1.70	0.56
13:L:187:GLU:HA	13:L:190:GLU:HG2	1.87	0.56
14:M:17:LEU:HD21	14:M:98:LEU:HG	1.87	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:222:GLU:HG3	1:B:251:LEU:HD22	1.86	0.56
7:O:59:CYS:HB2	7:O:104:CYS:HB3	1.88	0.56
14:U:346:GLY:HA3	14:U:418:GLY:HA2	1.86	0.56
1:1:41:ALA:HB2	1:1:116:GLU:HG3	1.86	0.56
4:4:337:PRO:O	4:4:361:GLY:HA2	2.06	0.56
15:N:245:ASN:ND2	15:N:367:THR:HB	2.21	0.56
15:V:201:GLN:HA	15:V:255:LYS:HE3	1.88	0.56
3:3:269:THR:HG21	3:3:629:ILE:HG12	1.88	0.56
6:6:19:ILE:HG12	6:6:20:LEU:H	1.70	0.56
13:L:293:LYS:O	13:L:297:TYR:HD1	1.89	0.56
3:D:373:GLY:HA3	3:D:538:ALA:HB2	1.88	0.56
3:3:31:PRO:HG3	3:3:137:TYR:CD2	2.40	0.56
10:A:33:PRO:HD2	16:H:70:GLU:HB2	1.87	0.56
13:L:87:ILE:HD12	13:L:239:LEU:HD13	1.88	0.56
16:H:291:ILE:HA	16:H:294:ARG:HG3	1.87	0.56
3:D:370:ASP:OD2	3:D:558:TRP:HD1	1.89	0.56
4:E:174:ARG:N	4:E:177:GLY:O	2.34	0.56
4:E:336:HIS:HB2	5:F:189:ARG:HA	1.88	0.56
4:E:341:GLU:OE1	4:E:356:TYR:OH	2.24	0.56
13:T:60:LEU:HD21	14:U:375:PRO:HB3	1.87	0.56
13:T:240:ILE:HG22	13:T:241:HIS:HD2	1.71	0.56
1:1:6:LEU:HB2	1:1:241:MET:HA	1.88	0.56
4:4:341:GLU:HG2	4:4:358:VAL:HG22	1.88	0.56
16:H:8:ASP:OD2	16:H:112:GLN:HB2	2.06	0.56
3:D:19:VAL:HG11	3:D:50:VAL:HG21	1.88	0.56
14:U:122:PHE:O	14:U:234:TYR:OH	2.21	0.56
16:Q:205:VAL:HG21	16:Q:317:ALA:HB2	1.86	0.56
18:1:502:FMN:H1'1	19:1:503:NAI:H52N	1.88	0.56
4:4:314:ARG:NH2	8:7:44:MET:SD	2.78	0.56
2:C:146:THR:HG23	2:C:149:ARG:H	1.71	0.56
3:D:616:ASN:HD22	3:D:622:LEU:HD11	1.70	0.56
16:Q:219:PHE:HB3	16:Q:299:ARG:HG2	1.87	0.56
15:N:168:GLU:HG2	15:N:169:GLY:H	1.71	0.55
7:O:6:LEU:HD23	16:Q:297:TRP:CE2	2.41	0.55
14:U:194:PHE:HB2	14:U:249:ALA:HB3	1.87	0.55
3:3:558:TRP:HB2	3:3:570:PHE:CZ	2.40	0.55
1:B:293:GLY:O	1:B:327:GLY:N	2.39	0.55
3:D:43:GLY:HA2	20:D:804:FES:S1	2.46	0.55
10:P:57:PHE:HB3	10:P:58:PRO:HD2	1.88	0.55
13:T:115:MET:HG2	13:T:244:THR:HG22	1.88	0.55
2:2:85:THR:HG22	2:2:86:LEU:N	2.21	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:5:99:PRO:HB2	5:5:124:ILE:HA	1.87	0.55
11:J:64:VAL:HA	11:J:67:PHE:HB2	1.86	0.55
14:M:126:LEU:HD11	14:M:149:VAL:HG13	1.89	0.55
1:B:184:GLU:HB3	1:B:187:ALA:HB3	1.89	0.55
3:D:466:GLU:HB2	3:D:489:MET:HG3	1.87	0.55
4:E:201:ILE:HA	4:E:204:TYR:CD2	2.42	0.55
8:I:104:VAL:HG12	8:I:109:PRO:HA	1.88	0.55
14:U:54:PRO:HA	14:U:62:TYR:HD1	1.70	0.55
16:Q:16:LYS:HB3	16:Q:115:VAL:HG22	1.89	0.55
16:Q:35:GLU:OE2	16:Q:294:ARG:NE	2.32	0.55
16:Q:48:PRO:C	16:Q:50:ARG:H	2.10	0.55
7:9:149:GLU:O	7:9:153:THR:OG1	2.18	0.55
14:U:41:LEU:O	14:U:42:THR:HG22	2.05	0.55
2:2:9:ASP:OD1	2:2:9:ASP:N	2.36	0.55
3:3:343:LEU:HD12	3:3:361:ALA:HB2	1.89	0.55
3:3:459:MET:HG2	3:3:465:HIS:HB2	1.89	0.55
12:K:7:SER:O	12:K:37:ALA:HB1	2.07	0.55
16:H:133:VAL:HG11	16:H:160:ILE:HG13	1.88	0.55
3:D:248:GLU:HG2	5:F:170:PHE:CE1	2.42	0.55
2:2:87:SER:HB2	20:2:201:FES:S2	2.47	0.55
5:5:75:VAL:HG13	5:5:87:ARG:HB2	1.88	0.55
13:L:139:PHE:HA	13:L:155:ALA:HB1	1.89	0.55
4:E:53:LEU:O	4:E:386:LYS:HG3	2.07	0.55
13:T:213:ALA:HB2	13:T:252:LEU:HD23	1.88	0.55
13:T:325:HIS:CD2	13:T:329:LYS:HG3	2.41	0.55
1:1:160:LYS:O	1:1:168:SER:OG	2.10	0.55
1:1:373:LYS:HD3	1:1:383:ASP:OD2	2.07	0.55
3:3:131:GLN:HG2	4:4:325:ILE:HG23	1.87	0.55
3:3:297:GLY:O	3:3:703:GLN:NE2	2.38	0.55
3:3:305:ARG:NH2	3:3:605:PRO:HA	2.20	0.55
4:4:363:SER:HB2	5:5:174:LEU:H	1.72	0.55
5:5:164:TYR:HB3	9:W:37:TRP:HZ3	1.71	0.55
4:E:163:VAL:HG13	4:E:164:THR:HG23	1.88	0.55
15:V:79:SER:O	15:V:85:TYR:OH	2.14	0.55
3:3:391:LEU:HD12	3:3:422:PRO:HG3	1.88	0.55
6:6:117:MET:CE	7:9:99:ILE:HG12	2.37	0.55
8:7:63:LEU:HD22	8:7:128:PHE:HB2	1.88	0.55
8:7:104:VAL:HG12	8:7:109:PRO:HA	1.88	0.55
13:L:124:TYR:HH	13:L:256:SER:HG	1.52	0.55
3:D:34:CYS:HB2	3:D:44:ALA:HB3	1.89	0.55
3:D:293:ALA:HB2	3:D:698:MET:HG2	1.89	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:E:159:LEU:O	4:E:163:VAL:HG12	2.07	0.55
13:T:156:ARG:HG3	14:U:407:LEU:HB3	1.89	0.55
14:U:332:LEU:HA	14:U:335:ARG:HG2	1.89	0.55
1:1:8:GLY:HA2	1:1:270:THR:HG22	1.89	0.55
13:L:392:THR:HG22	13:L:399:GLY:HA3	1.89	0.55
13:L:490:GLU:HG3	13:L:491:TRP:N	2.21	0.55
1:B:18:TYR:N	1:B:265:GLU:OE1	2.33	0.55
1:B:26:SER:HA	1:B:31:TYR:CG	2.42	0.55
1:B:291:ILE:HG12	1:B:299:PRO:HB3	1.88	0.55
3:D:419:ASP:OD1	3:D:447:LYS:NZ	2.23	0.55
5:F:2:ARG:HG3	5:F:84:ASP:OD2	2.06	0.55
13:T:325:HIS:NE2	13:T:329:LYS:HG3	2.22	0.55
4:4:60:GLY:N	4:4:408:ASP:OD1	2.36	0.55
4:4:98:ALA:O	4:4:102:GLU:HG3	2.07	0.55
13:L:356:TRP:O	13:L:363:ARG:HD3	2.07	0.55
14:M:332:LEU:O	14:M:336:THR:OG1	2.11	0.55
4:E:87:TYR:CB	6:G:45:CYS:HB3	2.37	0.55
13:T:9:LEU:HB2	13:T:10:PRO:HD3	1.89	0.55
13:T:312:VAL:HA	13:T:397:PHE:HD2	1.72	0.55
16:Q:43:GLN:HE21	16:Q:45:ARG:NH2	2.05	0.55
3:3:166:LYS:NZ	3:3:179:GLU:OE1	2.36	0.54
4:4:88:LEU:HD21	6:6:48:ILE:HD13	1.88	0.54
13:L:223:MET:HE3	13:L:534:VAL:HG11	1.88	0.54
14:M:357:LEU:HD22	14:M:433:ALA:HB2	1.89	0.54
3:D:228:ASP:OD2	3:D:295:ARG:NH2	2.28	0.54
3:D:269:THR:HG22	3:D:274:LEU:HA	1.88	0.54
1:1:184:GLU:HG2	18:1:502:FMN:HM82	1.88	0.54
3:3:33:PHE:HB2	3:3:45:CYS:SG	2.46	0.54
6:6:145:GLU:HG2	7:9:31:VAL:HG21	1.89	0.54
10:A:7:TYR:HD2	11:J:44:VAL:HG11	1.72	0.54
11:R:50:PHE:O	11:R:54:ILE:HG12	2.07	0.54
11:R:64:VAL:HG13	16:Q:134:TYR:OH	2.07	0.54
16:Q:71:ASP:HB2	16:Q:238:SER:HB3	1.89	0.54
4:4:144:THR:HG22	4:4:148:TYR:CE1	2.42	0.54
4:4:341:GLU:OE1	4:4:356:TYR:OH	2.16	0.54
11:J:101:ALA:HB2	12:K:12:ALA:HB2	1.89	0.54
1:B:153:ARG:NH2	1:B:171:LEU:O	2.40	0.54
1:B:177:ALA:HA	2:C:32:ARG:NH2	2.22	0.54
4:E:140:LEU:HD11	4:E:217:ARG:HH12	1.72	0.54
4:E:200:ARG:NH1	4:E:203:GLU:OE1	2.40	0.54
4:E:224:ILE:HD11	4:E:275:ARG:CZ	2.37	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:I:23:TYR:OH	8:I:123:ARG:NH1	2.39	0.54
14:U:331:ARG:NH1	14:U:334:GLU:OE1	2.41	0.54
14:M:21:PRO:HD2	14:M:24:LEU:HG	1.90	0.54
4:E:64:THR:OG1	6:G:83:ARG:HD2	2.08	0.54
10:P:9:GLY:HA2	16:Q:13:VAL:HG11	1.88	0.54
15:V:62:PHE:CE2	15:V:285:LEU:HD22	2.42	0.54
4:4:205:GLU:OE1	4:4:284:ARG:NH2	2.37	0.54
6:6:162:ALA:HB1	7:9:124:TYR:CZ	2.43	0.54
7:9:10:LEU:HA	16:H:296:THR:HG21	1.89	0.54
3:D:8:ASP:OD1	3:D:9:ARG:HG3	2.06	0.54
3:D:413:LEU:O	3:D:417:VAL:HG23	2.07	0.54
4:E:144:THR:OG1	16:Q:295:ALA:O	2.24	0.54
8:I:13:TRP:CD2	8:I:72:VAL:HB	2.43	0.54
11:R:119:LEU:HD11	12:S:47:ARG:HA	1.88	0.54
15:V:62:PHE:HE2	15:V:285:LEU:HD22	1.72	0.54
15:V:204:PRO:O	15:V:208:VAL:HG23	2.07	0.54
9:W:6:MET:HG3	9:W:9:ALA:HB3	1.90	0.54
12:K:78:ILE:HG12	15:N:130:LEU:HD22	1.89	0.54
11:R:101:ALA:HB2	12:S:12:ALA:HB2	1.88	0.54
16:Q:122:ILE:HG13	16:Q:123:LEU:HD12	1.89	0.54
14:U:7:LEU:O	14:U:11:VAL:HG12	2.08	0.54
1:1:201:LEU:HG	1:1:203:PRO:HD2	1.89	0.54
4:4:162:TRP:CE2	7:9:34:LYS:HD2	2.43	0.54
13:L:129:ILE:HG12	14:M:369:PRO:HB2	1.90	0.54
13:L:240:ILE:HG22	13:L:241:HIS:HD2	1.72	0.54
14:M:304:THR:O	14:M:307:GLY:N	2.40	0.54
16:H:143:SER:HB2	16:H:235:GLU:HG3	1.89	0.54
3:D:18:SER:HB3	3:D:21:ASP:OD2	2.07	0.54
15:N:56:ASP:OD1	15:N:225:ARG:NH1	2.41	0.54
16:H:290:PHE:O	16:H:294:ARG:HG2	2.06	0.54
1:B:203:PRO:HB2	1:B:204:PRO:HD3	1.90	0.54
3:D:31:PRO:HG3	3:D:137:TYR:CD2	2.43	0.54
7:O:17:LEU:HD12	16:Q:42:PHE:CE1	2.43	0.54
3:3:713:ARG:HH21	3:3:746:ARG:HH21	1.56	0.54
3:D:459:MET:HG2	3:D:465:HIS:HB2	1.89	0.54
4:E:185:GLU:O	4:E:189:GLU:HG2	2.08	0.54
16:Q:267:TRP:CG	16:Q:268:THR:N	2.76	0.54
2:2:35:GLN:NE2	2:2:35:GLN:C	2.62	0.53
4:4:26:MET:N	4:4:47:LEU:O	2.41	0.53
4:4:28:LEU:HD12	10:A:51:ALA:HA	1.90	0.53
4:4:32:PRO:HB2	6:6:88:MET:HE1	1.90	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:4:278:VAL:O	4:4:282:GLU:HG3	2.08	0.53
5:5:80:TRP:HA	5:5:80:TRP:CE3	2.43	0.53
7:9:6:LEU:HB3	16:H:297:TRP:CZ2	2.42	0.53
5:F:31:ARG:NH2	5:F:98:ASP:OD2	2.41	0.53
5:F:53:VAL:HG13	5:F:71:VAL:HB	1.90	0.53
11:R:19:VAL:HG23	11:R:28:ALA:O	2.07	0.53
14:U:43:HIS:NE2	14:U:45:GLY:O	2.41	0.53
3:3:728:LEU:HB3	3:3:747:VAL:HG11	1.90	0.53
4:4:379:GLN:NE2	5:5:110:SER:O	2.35	0.53
10:A:83:VAL:HG23	10:A:84:SER:H	1.74	0.53
14:U:402:SER:HA	14:U:405:TYR:CE2	2.43	0.53
16:Q:52:GLY:HA3	16:Q:55:GLY:N	2.23	0.53
3:3:347:HIS:CD2	3:3:765:PRO:HG3	2.44	0.53
2:C:88:CYS:HA	2:C:131:ALA:HB1	1.90	0.53
3:D:126:GLY:O	4:E:329:LYS:NZ	2.41	0.53
1:1:250:LYS:NZ	1:1:325:THR:O	2.41	0.53
3:3:194:VAL:HG12	3:3:411:LEU:HD22	1.90	0.53
10:P:44:TYR:HB3	10:P:50:PRO:HB3	1.90	0.53
14:U:313:TYR:OH	14:U:443:MET:O	2.22	0.53
3:3:661:GLN:NE2	3:3:664:LEU:HD12	2.23	0.53
11:J:29:ALA:O	11:J:33:ILE:HG13	2.08	0.53
11:J:69:PHE:HZ	16:H:156:SER:HG	1.56	0.53
4:E:68:LYS:HG3	5:F:152:LEU:HD13	1.90	0.53
4:E:86:ASP:HB2	4:E:406:ASP:OD2	2.09	0.53
7:O:11:GLY:O	7:O:15:LYS:HG3	2.09	0.53
11:R:102:GLY:O	11:R:106:ALA:N	2.38	0.53
15:V:251:GLN:OE1	15:V:256:ARG:HD3	2.08	0.53
15:V:294:LEU:HG	15:V:402:VAL:HG13	1.89	0.53
1:1:75:LYS:NZ	1:1:218:ILE:O	2.32	0.53
2:2:107:GLY:H	2:2:110:GLU:HG3	1.73	0.53
3:3:85:THR:HG22	3:3:86:ALA:O	2.08	0.53
3:3:405:GLU:OE1	3:3:509:ALA:N	2.42	0.53
3:3:544:LEU:HD22	3:3:549:VAL:HG21	1.90	0.53
3:3:621:VAL:HG23	3:3:672:ALA:HA	1.91	0.53
4:4:68:LYS:HG3	5:5:152:LEU:HD13	1.91	0.53
10:A:57:PHE:HE2	16:H:149:LEU:HD13	1.74	0.53
16:H:127:ALA:O	16:H:131:LEU:HG	2.08	0.53
2:C:74:PRO:HD3	8:I:125:ALA:HB2	1.89	0.53
6:G:61:ALA:HB1	6:G:66:GLU:OE1	2.08	0.53
14:M:235:LYS:HD3	14:M:293:MET:HG3	1.90	0.53
1:B:160:LYS:O	1:B:168:SER:OG	2.18	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:I:22:GLU:HG2	8:I:116:PHE:HZ	1.72	0.53
13:T:539:ASN:HA	13:T:543:VAL:HB	1.89	0.53
14:U:56:LEU:HB2	14:U:61:VAL:HB	1.91	0.53
15:V:2:THR:HG23	15:V:36:ALA:HB1	1.90	0.53
15:V:345:LYS:NZ	15:V:368:SER:OG	2.42	0.53
3:3:42:ILE:O	3:3:42:ILE:CD1	2.48	0.53
3:3:42:ILE:HD13	3:3:44:ALA:HB2	1.91	0.53
6:6:138:PRO:HG2	7:9:121:MET:HG3	1.90	0.53
14:M:41:LEU:O	14:M:42:THR:HG22	2.08	0.53
16:H:186:VAL:HG11	16:H:267:TRP:CZ3	2.44	0.53
1:B:292:PRO:HG3	1:B:316:LEU:HD22	1.91	0.53
3:D:326:PHE:CZ	3:D:330:LYS:HE3	2.43	0.53
6:G:99:MET:HB3	6:G:103:LYS:HD3	1.90	0.53
12:S:19:LEU:HD22	13:T:591:LEU:HD12	1.90	0.53
14:U:346:GLY:O	14:U:349:GLN:HG2	2.07	0.53
3:3:463:ALA:O	3:3:465:HIS:ND1	2.31	0.53
11:J:75:PHE:HZ	11:J:78:GLN:HG2	1.74	0.53
3:D:123:ASP:OD2	3:D:241:ARG:HA	2.08	0.53
3:D:474:ARG:HB3	3:D:514:ASP:OD2	2.09	0.53
1:1:152:ALA:HB1	1:1:157:TYR:HB2	1.90	0.53
16:H:213:GLU:OE1	16:H:213:GLU:N	2.42	0.53
6:G:66:GLU:HG2	16:Q:36:ARG:HD3	1.90	0.53
14:U:215:PRO:HG2	14:U:216:PRO:HD3	1.91	0.53
14:U:264:ALA:HB1	14:U:294:GLY:O	2.08	0.53
15:V:228:ALA:HB1	15:V:233:LEU:CD1	2.39	0.53
16:Q:99:LEU:HD12	16:Q:116:ILE:HG13	1.90	0.53
1:1:203:PRO:HB2	1:1:204:PRO:HD3	1.90	0.52
3:3:127:ALA:HB3	3:3:246:ASN:HD22	1.74	0.52
3:3:317:LEU:HD21	3:3:595:GLU:HA	1.92	0.52
4:4:115:THR:HG21	4:4:297:LEU:HD13	1.91	0.52
7:9:94:ASN:HB3	7:9:97:ARG:HB2	1.91	0.52
14:M:215:PRO:HG2	14:M:216:PRO:HD3	1.90	0.52
3:D:247:TRP:HE1	7:O:61:ALA:CB	2.21	0.52
6:G:39:ALA:HB2	6:G:75:ALA:HB3	1.91	0.52
6:G:153:GLN:HG3	7:O:124:TYR:CZ	2.44	0.52
11:R:64:VAL:HA	11:R:67:PHE:HB2	1.90	0.52
15:V:83:GLU:O	15:V:87:LEU:HG	2.09	0.52
16:Q:147:TYR:HE1	16:Q:229:VAL:H	1.55	0.52
3:3:94:ASP:OD2	3:3:97:SER:OG	2.23	0.52
3:3:237:ASP:OD1	3:3:239:THR:HG22	2.10	0.52
4:4:341:GLU:CD	5:5:91:ARG:HH22	2.11	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:E:211:SER:HB2	4:E:215:TYR:N	2.24	0.52
16:Q:140:GLY:HA3	16:Q:152:SER:HB3	1.90	0.52
1:1:111:PRO:HB3	1:1:145:LEU:HD23	1.91	0.52
10:A:68:PHE:CD2	16:H:164:LEU:HB2	2.45	0.52
2:C:76:GLY:N	2:C:118:SER:OG	2.35	0.52
3:D:715:GLU:H	3:D:761:SER:HB2	1.75	0.52
6:G:153:GLN:HG3	7:O:124:TYR:OH	2.08	0.52
11:R:24:ASN:HB3	11:R:27:HIS:HB2	1.90	0.52
1:1:159:GLY:H	1:1:162:LEU:HD21	1.72	0.52
3:3:190:TYR:O	3:3:195:PRO:HD2	2.10	0.52
3:3:479:ALA:O	3:3:494:LYS:HD2	2.10	0.52
6:6:73:ARG:HD3	6:6:98:GLN:O	2.09	0.52
13:L:380:SER:CB	13:L:457:GLY:H	2.21	0.52
14:M:13:GLY:HA2	14:M:97:GLY:HA2	1.91	0.52
3:D:81:ALA:O	3:D:85:THR:OG1	2.23	0.52
5:F:155:THR:N	6:G:119:ASN:OD1	2.30	0.52
7:O:123:ASP:CG	7:O:148:ARG:HH22	2.13	0.52
8:I:86:LEU:HB3	8:I:126:LEU:HD11	1.91	0.52
3:3:32:LEU:HD11	3:3:35:SER:HB2	1.91	0.52
7:9:40:ARG:NH1	7:9:41:HIS:O	2.43	0.52
14:M:448:GLY:O	14:M:452:ARG:HG2	2.10	0.52
15:N:319:ASP:HB3	15:N:322:LEU:HB2	1.91	0.52
3:D:283:PRO:HG3	3:D:430:THR:OG1	2.10	0.52
4:E:240:ARG:NH1	4:E:282:GLU:OE2	2.43	0.52
6:G:160:GLY:O	6:G:169:ARG:NH1	2.43	0.52
10:P:29:ALA:O	10:P:34:LYS:NZ	2.42	0.52
18:1:502:FMN:H9	19:1:503:NAI:H52N	1.91	0.52
3:3:34:CYS:HB3	3:3:45:CYS:H	1.75	0.52
3:3:175:ILE:O	3:3:235:LEU:HA	2.10	0.52
3:3:503:PRO:HG3	3:3:528:LYS:HD3	1.91	0.52
4:4:47:LEU:HD13	4:4:51:GLU:O	2.10	0.52
4:4:143:LEU:H	4:4:143:LEU:HD23	1.74	0.52
15:N:317:ARG:NH1	15:N:383:PHE:O	2.31	0.52
1:B:238:PHE:CZ	1:B:248:GLY:HA3	2.45	0.52
2:C:85:THR:HG22	2:C:86:LEU:H	1.74	0.52
4:E:42:ARG:O	4:E:43:LEU:HD23	2.10	0.52
6:G:104:TRP:HE1	6:G:173:VAL:HA	1.74	0.52
13:T:88:HIS:O	13:T:92:ILE:HG13	2.09	0.52
14:U:134:TYR:HB2	14:U:145:LEU:HD13	1.92	0.52
4:4:202:ASP:OD1	4:4:284:ARG:NE	2.41	0.52
11:J:12:LEU:HD22	12:K:10:LEU:HD11	1.91	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
14:M:224:SER:HA	14:M:330:GLY:HA3	1.91	0.52
16:H:216:ARG:NH1	16:H:294:ARG:O	2.42	0.52
3:D:199:VAL:HG11	3:D:219:PRO:HD2	1.91	0.52
4:E:222:GLY:HA2	4:E:396:ILE:HD11	1.92	0.52
6:G:147:LEU:O	6:G:151:VAL:HG13	2.10	0.52
9:X:4:VAL:HG22	9:X:57:LEU:HD21	1.92	0.52
14:U:8:LEU:HD21	14:U:31:LEU:HB3	1.91	0.52
15:V:280:ALA:HB1	15:V:347:LEU:HB3	1.91	0.52
3:3:28:TYR:CE2	3:3:96:LEU:HD11	2.45	0.52
10:A:7:TYR:CD2	11:J:44:VAL:HG11	2.44	0.52
6:G:104:TRP:NE1	6:G:173:VAL:HA	2.25	0.52
6:G:114:SER:OG	7:O:96:LEU:O	2.28	0.52
7:O:13:THR:HG21	16:Q:296:THR:HG23	1.92	0.52
1:1:407:VAL:O	1:1:411:LYS:N	2.27	0.52
2:2:88:CYS:HA	2:2:131:ALA:HB1	1.91	0.52
4:4:234:LEU:O	4:4:239:LEU:HB2	2.10	0.52
4:4:338:PRO:HG3	5:5:193:ARG:HB2	1.91	0.52
5:5:67:ARG:HH22	5:5:149:ASP:CG	2.13	0.52
5:5:167:PRO:HB3	7:9:66:TYR:CD2	2.45	0.52
13:L:171:LEU:O	13:L:175:ILE:HG13	2.10	0.52
14:M:91:VAL:HG23	14:M:92:GLU:H	1.74	0.52
16:H:333:PRO:HG2	16:H:336:TYR:CD1	2.45	0.52
3:D:33:PHE:HB2	3:D:45:CYS:CB	2.40	0.52
3:D:565:TYR:HA	3:D:582:PHE:O	2.10	0.52
3:D:717:TRP:HB3	3:D:753:VAL:HG21	1.91	0.52
4:E:169:HIS:CE1	6:G:45:CYS:SG	3.03	0.52
5:F:71:VAL:HG11	5:F:89:PHE:HD2	1.75	0.52
5:F:120:ASP:OD1	5:F:134:LYS:HG3	2.10	0.52
6:G:21:PHE:O	6:G:25:GLU:HG2	2.10	0.52
13:T:463:HIS:CG	13:T:464:PRO:HD3	2.44	0.52
14:U:22:ARG:NH1	14:U:92:GLU:HB3	2.25	0.52
14:U:345:ARG:HG2	14:U:412:LYS:O	2.10	0.52
1:1:287:ILE:HG12	1:1:330:LEU:HB3	1.91	0.52
3:3:48:CYS:SG	3:3:82:SER:N	2.82	0.52
3:3:451:PHE:HD1	3:3:466:GLU:HB3	1.75	0.52
14:M:91:VAL:HB	14:M:95:PHE:HE1	1.73	0.52
15:N:44:TRP:CZ3	15:N:60:GLN:HB3	2.44	0.52
6:G:143:ARG:NE	6:G:145:GLU:OE1	2.43	0.52
10:P:66:MET:HG3	12:S:69:ALA:HB1	1.91	0.52
13:T:122:ASP:O	13:T:185:ILE:N	2.40	0.52
1:1:95:GLU:O	1:1:135:ARG:NH1	2.30	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:3:657:HIS:O	3:3:661:GLN:HG2	2.10	0.51
5:5:50:ALA:HB3	5:5:73:GLU:HB3	1.92	0.51
8:7:48:TYR:CZ	8:7:50:LEU:HB2	2.45	0.51
15:N:190:ALA:HB3	15:N:240:SER:HA	1.90	0.51
15:N:198:ASP:OD1	15:N:256:ARG:NH2	2.44	0.51
2:C:24:ARG:HE	2:C:55:THR:CB	2.22	0.51
3:D:270:ARG:HB3	3:D:275:LEU:HD11	1.90	0.51
8:I:37:PHE:CE1	8:I:74:PRO:HA	2.31	0.51
16:Q:260:PRO:HG3	16:Q:286:PHE:CD2	2.45	0.51
3:3:614:LEU:O	3:3:621:VAL:HA	2.10	0.51
6:6:163:TYR:CD1	7:9:152:ARG:HD2	2.45	0.51
1:B:50:PRO:HA	1:B:53:VAL:HG12	1.91	0.51
1:B:135:ARG:HE	1:B:137:GLU:HB2	1.75	0.51
4:E:363:SER:N	5:F:174:LEU:O	2.43	0.51
14:U:65:PHE:HA	14:U:111:ALA:O	2.09	0.51
15:V:53:TYR:HA	15:V:101:THR:HG22	1.92	0.51
1:1:106:ILE:HD11	1:1:251:LEU:HD21	1.92	0.51
3:3:127:ALA:HB3	3:3:246:ASN:ND2	2.24	0.51
3:3:416:PHE:HE2	3:3:448:MET:HB3	1.76	0.51
10:A:23:ALA:O	10:A:27:VAL:HG23	2.10	0.51
13:L:104:PHE:CE2	13:L:108:PHE:HE2	2.28	0.51
1:B:118:MET:HG2	1:B:224:LEU:HD13	1.92	0.51
13:T:348:ASP:OD1	13:T:349:VAL:N	2.42	0.51
13:L:66:SER:CB	13:L:122:ASP:HB3	2.39	0.51
13:L:321:HIS:HD2	13:L:388:ILE:HD12	1.75	0.51
4:E:222:GLY:HA3	4:E:275:ARG:NH2	2.26	0.51
6:6:84:LEU:HD12	6:6:124:VAL:HG21	1.91	0.51
12:K:79:PHE:CD2	12:K:85:THR:HA	2.46	0.51
15:N:53:TYR:HA	15:N:101:THR:HG22	1.92	0.51
16:H:65:LYS:O	16:H:69:LYS:HB2	2.11	0.51
1:B:201:LEU:HA	1:B:399:PHE:CZ	2.46	0.51
2:C:24:ARG:HA	2:C:53:VAL:CG2	2.40	0.51
4:E:81:TYR:CZ	6:G:117:MET:HG3	2.46	0.51
5:F:170:PHE:CE2	7:O:61:ALA:HA	2.45	0.51
6:G:97:GLU:HB3	10:P:39:ALA:HB3	1.91	0.51
8:I:43:ARG:HG3	8:I:43:ARG:O	2.11	0.51
1:1:65:ARG:HD2	1:1:222:GLU:OE2	2.10	0.51
4:4:190:LEU:CD1	4:4:194:LEU:HD11	2.41	0.51
10:A:93:PHE:CE2	16:H:326:LEU:HD13	2.46	0.51
12:K:59:MET:HB2	15:N:105:LEU:HD21	1.93	0.51
13:L:12:LEU:O	13:L:16:LEU:HG	2.11	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:L:214:VAL:HG13	13:L:219:GLN:HB2	1.93	0.51
13:L:454:VAL:HB	13:L:455:LEU:HD22	1.93	0.51
1:B:364:ALA:HB3	3:D:207:VAL:HG13	1.92	0.51
3:D:246:ASN:ND2	3:D:276:ARG:HH12	2.09	0.51
3:D:609:GLU:HA	3:D:627:ALA:H	1.76	0.51
3:D:620:ARG:HA	3:D:675:ARG:HA	1.91	0.51
13:T:26:GLU:HB3	13:T:27:PRO:HD3	1.91	0.51
13:T:340:ILE:O	13:T:345:GLY:N	2.28	0.51
14:U:157:LEU:HD12	15:V:369:ALA:HB2	1.92	0.51
15:V:61:VAL:O	15:V:64:LEU:HB3	2.11	0.51
3:3:385:ALA:HB2	3:3:531:LYS:HB2	1.92	0.51
3:3:465:HIS:O	3:3:489:MET:HG3	2.11	0.51
12:K:46:ALA:HB2	12:K:53:GLY:HA3	1.92	0.51
1:B:276:ILE:O	1:B:282:GLY:N	2.24	0.51
1:B:421:TYR:O	1:B:425:ALA:N	2.42	0.51
5:F:71:VAL:HA	5:F:90:VAL:O	2.08	0.51
16:Q:134:TYR:HA	16:Q:137:PHE:CE2	2.45	0.51
1:1:381:GLU:OE1	1:1:426:ARG:NH2	2.42	0.51
2:2:171:LYS:NZ	2:2:178:GLU:O	2.44	0.51
3:3:355:LEU:HB2	3:3:547:MET:SD	2.51	0.51
4:4:310:THR:HG22	4:4:311:PRO:O	2.11	0.51
5:5:34:PHE:CD1	5:5:92:VAL:HG11	2.46	0.51
8:7:89:ALA:O	8:7:90:HIS:ND1	2.44	0.51
11:J:2:SER:HA	11:J:5:GLU:HB3	1.93	0.51
14:M:95:PHE:HB3	14:M:136:TYR:CZ	2.45	0.51
3:D:173:PHE:O	3:D:238:LEU:N	2.43	0.51
6:G:152:MET:SD	7:O:27:PRO:HG3	2.50	0.51
14:U:281:PHE:CE1	14:U:341:ILE:HG22	2.46	0.51
16:Q:332:LEU:H	16:Q:332:LEU:HD12	1.75	0.51
1:1:165:THR:HG23	1:1:167:PHE:H	1.76	0.51
2:2:3:PHE:HB2	2:2:45:ARG:HH11	1.76	0.51
3:3:274:LEU:HD21	3:3:298:HIS:HB2	1.92	0.51
4:4:38:HIS:ND1	4:4:139:ASP:OD2	2.44	0.51
7:9:17:LEU:HD12	16:H:42:PHE:CE1	2.46	0.51
12:K:21:ARG:CZ	12:K:26:LEU:HD23	2.41	0.51
14:M:203:ILE:HG13	14:M:210:LEU:HB3	1.92	0.51
15:N:262:SER:OG	15:N:288:TYR:OH	2.27	0.51
16:H:136:ILE:HG23	16:H:232:TYR:CD2	2.45	0.51
1:B:190:ASN:OD1	1:B:200:ARG:NE	2.27	0.51
2:C:66:PHE:CE1	3:D:205:ARG:HD3	2.45	0.51
8:I:120:ASP:O	8:I:124:GLU:HG3	2.11	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
15:V:13:LEU:HD22	15:V:25:VAL:HG13	1.93	0.51
15:V:98:LEU:HD23	15:V:218:ALA:HB1	1.93	0.51
16:Q:205:VAL:HG12	16:Q:313:LEU:HD22	1.93	0.51
16:Q:291:ILE:HA	16:Q:294:ARG:CG	2.40	0.51
1:1:192:LEU:HD22	1:1:211:LEU:HD21	1.93	0.51
1:1:259:LYS:HA	1:1:284:LEU:HD21	1.93	0.51
4:4:190:LEU:HD12	4:4:194:LEU:CD1	2.41	0.51
5:5:33:ARG:O	5:5:37:GLU:HB2	2.11	0.51
16:H:114:TRP:NE1	16:H:117:ASN:HB2	2.26	0.51
16:H:201:PRO:O	16:H:204:LEU:HB2	2.10	0.51
2:C:97:TRP:CH2	2:C:119:VAL:HB	2.45	0.51
5:F:120:ASP:OD2	5:F:135:ILE:N	2.44	0.51
13:T:90:TYR:CG	13:T:334:LEU:HD13	2.46	0.51
15:V:29:THR:HG22	15:V:89:LEU:HD11	1.92	0.51
1:1:193:GLU:OE1	1:1:200:ARG:NH2	2.40	0.50
7:9:162:VAL:HG12	7:9:176:PRO:HB2	1.93	0.50
13:L:9:LEU:HB2	13:L:10:PRO:HD3	1.93	0.50
13:L:340:ILE:HB	13:L:345:GLY:HA2	1.92	0.50
6:G:36:LEU:O	6:G:38:PRO:HD3	2.10	0.50
14:U:208:PHE:N	14:U:267:SER:OG	2.44	0.50
15:V:101:THR:HG21	15:V:106:LEU:HD23	1.92	0.50
3:3:512:LEU:HD21	3:3:534:ALA:HB1	1.91	0.50
3:3:544:LEU:HB3	3:3:549:VAL:HB	1.92	0.50
5:5:98:ASP:OD1	5:5:100:ARG:HD3	2.11	0.50
15:N:283:PHE:O	15:N:287:THR:HG23	2.12	0.50
16:H:274:VAL:HG22	16:H:275:PRO:HD2	1.92	0.50
1:B:184:GLU:OE1	1:B:186:THR:OG1	2.21	0.50
3:D:249:MET:HB3	3:D:268:ASP:HB3	1.92	0.50
6:G:53:SER:O	6:G:60:LEU:N	2.36	0.50
7:O:44:THR:HA	7:O:138:VAL:HG13	1.92	0.50
13:T:359:LEU:HD21	13:T:437:GLU:HB3	1.93	0.50
15:V:16:LEU:O	15:V:20:LEU:N	2.44	0.50
16:Q:21:VAL:HG13	16:Q:94:LEU:HD22	1.92	0.50
1:1:121:ALA:O	1:1:125:ILE:HG12	2.11	0.50
1:1:220:ASN:N	18:1:502:FMN:O3P	2.30	0.50
3:3:445:THR:HB	3:3:463:ALA:HB2	1.92	0.50
4:4:169:HIS:NE2	6:6:45:CYS:SG	2.84	0.50
7:9:149:GLU:O	7:9:153:THR:CB	2.59	0.50
11:J:138:VAL:HG22	15:N:106:LEU:HB2	1.93	0.50
12:K:18:VAL:HG11	15:N:142:LEU:HD13	1.93	0.50
15:N:248:ALA:HA	15:N:251:GLN:HG2	1.92	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:173:GLY:HA3	2:C:176:VAL:O	2.12	0.50
3:D:351:LEU:HD12	3:D:540:ASN:HD21	1.76	0.50
13:T:463:HIS:CD2	13:T:464:PRO:HD3	2.46	0.50
13:T:490:GLU:HG3	13:T:491:TRP:N	2.26	0.50
16:Q:218:PRO:C	16:Q:220:ASP:H	2.13	0.50
1:1:260:ARG:HA	2:2:177:HIS:O	2.11	0.50
2:2:4:PHE:HB3	2:2:11:LEU:HD11	1.93	0.50
2:C:4:PHE:HB3	2:C:11:LEU:HD11	1.93	0.50
6:G:86:LYS:HG3	6:G:122:ALA:O	2.12	0.50
11:R:123:LEU:HD22	16:Q:120:LEU:HD11	1.93	0.50
4:4:73:ARG:NH2	6:6:117:MET:O	2.45	0.50
4:4:87:TYR:CG	6:6:45:CYS:HB3	2.46	0.50
10:A:86:GLY:HA2	16:H:329:ALA:HA	1.93	0.50
15:N:209:LEU:HB2	15:N:296:PHE:HB3	1.93	0.50
15:N:422:ALA:O	15:N:423:LEU:HD23	2.12	0.50
16:H:227:GLU:HG2	16:H:228:LEU:N	2.26	0.50
3:D:225:ASN:O	3:D:229:ILE:HG13	2.12	0.50
3:D:439:GLU:HG2	3:D:440:ARG:HG2	1.93	0.50
4:E:212:PRO:HG2	4:E:213:ILE:HD12	1.93	0.50
6:G:124:VAL:HG22	9:X:120:PRO:HD2	1.94	0.50
7:O:26:TYR:HE1	7:O:160:GLY:HA3	1.76	0.50
13:T:454:VAL:HB	13:T:455:LEU:HD22	1.94	0.50
13:T:586:LEU:HD13	15:V:138:LEU:HD12	1.93	0.50
3:3:165:ASP:HB2	8:7:66:PRO:HG2	1.93	0.50
3:3:245:ARG:NH1	7:9:56:CYS:O	2.45	0.50
3:3:694:LEU:HB3	3:3:762:ALA:HB2	1.93	0.50
5:5:38:MET:CE	5:5:104:VAL:HG11	2.39	0.50
13:L:435:PRO:HG2	13:L:436:HIS:CD2	2.46	0.50
14:M:281:PHE:CE1	14:M:341:ILE:HG22	2.47	0.50
16:H:159:LEU:HD11	16:H:221:LEU:HD21	1.92	0.50
4:E:222:GLY:O	4:E:271:ASP:HA	2.12	0.50
11:R:19:VAL:HG21	11:R:32:LEU:HB2	1.93	0.50
11:R:36:PHE:CE2	11:R:59:TYR:CD1	3.00	0.50
13:T:312:VAL:HA	13:T:397:PHE:CD2	2.47	0.50
1:1:20:HIS:CG	1:1:31:TYR:HE1	2.30	0.50
1:1:83:ASP:OD1	1:1:87:HIS:NE2	2.38	0.50
1:1:190:ASN:ND2	1:1:198:ASN:O	2.45	0.50
15:N:29:THR:HG21	15:N:85:TYR:HB3	1.94	0.50
16:H:120:LEU:HD22	16:H:180:LEU:HD12	1.92	0.50
3:D:247:TRP:CG	5:F:172:ALA:HB2	2.46	0.50
5:F:20:ASN:HD21	5:F:24:ASN:HB2	1.77	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
14:U:64:ALA:HB1	14:U:113:ARG:HB3	1.93	0.50
1:1:190:ASN:OD1	1:1:200:ARG:NE	2.38	0.50
3:3:229:ILE:HD11	3:3:289:TRP:CZ3	2.45	0.50
4:4:34:HIS:HA	4:4:36:SER:H	1.76	0.50
7:9:13:THR:HG21	16:H:296:THR:HG23	1.93	0.50
14:M:307:GLY:HA2	14:M:380:THR:HA	1.94	0.50
8:I:86:LEU:HB2	8:I:91:ILE:HB	1.93	0.50
14:U:305:PRO:HB3	14:U:459:GLU:HA	1.94	0.50
1:1:220:ASN:ND2	18:1:502:FMN:O2	2.45	0.50
4:4:213:ILE:HD11	7:9:6:LEU:HD21	1.92	0.50
11:J:19:VAL:HG11	12:K:33:LEU:HD13	1.94	0.50
14:M:46:GLY:HA2	14:M:68:ASP:HA	1.93	0.50
1:B:16:THR:HG23	1:B:233:ARG:HH21	1.77	0.50
1:B:91:CYS:HB3	1:B:132:ILE:HA	1.93	0.50
9:X:52:THR:OG1	9:X:55:LYS:O	2.23	0.50
12:S:79:PHE:CD2	12:S:85:THR:HA	2.47	0.50
1:1:179:ALA:HB3	1:1:182:CYS:SG	2.52	0.49
3:3:268:ASP:CG	3:3:278:ARG:HH11	2.13	0.49
3:3:444:ARG:HD3	3:3:447:LYS:HD2	1.94	0.49
4:4:93:HIS:ND1	4:4:355:TYR:OH	2.32	0.49
4:4:122:GLU:HB2	4:4:290:ILE:HD11	1.94	0.49
6:6:43:LEU:HD13	6:6:83:ARG:O	2.12	0.49
7:9:43:LEU:HA	7:9:112:ALA:O	2.11	0.49
16:H:2:THR:HA	16:H:5:TYR:HD2	1.77	0.49
1:B:437:TRP:HD1	2:C:95:GLU:OE1	1.94	0.49
3:D:133:ARG:NE	3:D:136:GLU:OE2	2.33	0.49
4:E:98:ALA:O	4:E:102:GLU:HG3	2.11	0.49
8:I:82:ILE:HG23	8:I:95:ALA:HB3	1.92	0.49
12:S:15:VAL:O	12:S:19:LEU:HG	2.11	0.49
15:V:168:GLU:HG2	15:V:169:GLY:H	1.77	0.49
15:V:279:GLN:NE2	15:V:420:LEU:O	2.43	0.49
4:4:201:ILE:HA	4:4:204:TYR:HD2	1.77	0.49
5:5:68:PHE:HB3	5:5:124:ILE:HD11	1.94	0.49
13:L:564:TYR:CG	14:M:151:PHE:HZ	2.30	0.49
15:N:194:PHE:O	15:N:197:PRO:HD2	2.11	0.49
1:B:341:MET:HB2	1:B:371:PHE:CE2	2.46	0.49
3:D:11:VAL:HG21	3:D:26:ALA:HB2	1.93	0.49
6:G:163:TYR:CD1	7:O:152:ARG:HD2	2.45	0.49
16:Q:102:PHE:CD1	16:Q:279:MET:HG2	2.47	0.49
3:3:133:ARG:HA	3:3:136:GLU:OE2	2.12	0.49
11:J:19:VAL:HG23	11:J:28:ALA:O	2.12	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:152:ALA:HB1	1:B:157:TYR:HB2	1.93	0.49
2:C:31:LEU:HD22	2:C:41:ILE:HD13	1.94	0.49
2:C:146:THR:HG22	2:C:149:ARG:HB2	1.93	0.49
2:C:161:LYS:HB3	2:C:166:ILE:HG12	1.93	0.49
3:D:414:SER:O	3:D:418:ARG:NE	2.44	0.49
4:E:285:GLU:O	4:E:289:ILE:HG12	2.11	0.49
5:F:18:GLU:HB2	5:F:26:TRP:HB2	1.94	0.49
8:I:29:VAL:HG21	8:I:67:PHE:CE2	2.47	0.49
10:P:90:LEU:HD12	16:Q:330:LEU:HD21	1.94	0.49
15:V:40:LEU:HD22	15:V:60:GLN:HG2	1.93	0.49
15:V:319:ASP:HB3	15:V:322:LEU:HB2	1.94	0.49
4:4:34:HIS:HA	4:4:36:SER:N	2.27	0.49
9:W:31:VAL:HG22	9:W:50:LEU:HD13	1.95	0.49
1:B:338:VAL:HG22	1:B:421:TYR:CE2	2.47	0.49
13:T:166:ASP:O	13:T:170:MET:HG3	2.12	0.49
13:T:217:SER:HB2	13:T:303:LEU:HD22	1.94	0.49
13:T:391:ALA:O	13:T:395:TYR:HB2	2.12	0.49
3:3:416:PHE:O	3:3:447:LYS:HD3	2.12	0.49
7:9:94:ASN:OD1	7:9:97:ARG:HG2	2.12	0.49
14:M:363:LEU:HD22	14:M:368:LEU:HD13	1.92	0.49
1:B:63:ARG:HB3	1:B:69:GLY:HA2	1.94	0.49
4:E:85:MET:HE1	4:E:370:VAL:HG21	1.94	0.49
7:O:35:PRO:O	7:O:117:TYR:OH	2.21	0.49
15:V:126:ARG:HD2	15:V:128:GLN:HG2	1.95	0.49
3:3:477:LEU:HA	3:3:480:LEU:HD12	1.94	0.49
4:4:118:VAL:HB	4:4:257:TYR:HE1	1.77	0.49
15:N:217:ALA:HA	15:N:285:LEU:HD23	1.95	0.49
16:H:221:LEU:N	16:H:222:PRO:HA	2.27	0.49
3:D:281:GLU:HB2	3:D:288:ILE:HG22	1.92	0.49
3:D:398:VAL:HG22	3:D:506:ILE:HD12	1.95	0.49
3:D:585:MET:SD	3:D:598:ALA:HB2	2.52	0.49
4:E:391:PRO:HG3	16:Q:227:GLU:OE2	2.13	0.49
6:G:163:TYR:H	7:O:152:ARG:NH1	2.10	0.49
13:T:196:LEU:HD23	13:T:202:LEU:HD23	1.94	0.49
15:V:62:PHE:CD2	15:V:221:ALA:HB2	2.47	0.49
4:4:114:GLU:O	4:4:118:VAL:HG13	2.12	0.49
5:5:103:THR:HG23	5:5:127:GLU:O	2.12	0.49
6:6:31:GLY:O	6:6:35:SER:HB3	2.12	0.49
15:N:247:ALA:O	15:N:251:GLN:NE2	2.34	0.49
3:D:716:LEU:HD21	3:D:758:LEU:HD23	1.94	0.49
4:E:114:GLU:O	4:E:118:VAL:HG13	2.12	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:F:47:ASN:O	5:F:108:TRP:NE1	2.43	0.49
11:R:75:PHE:CZ	11:R:78:GLN:HG2	2.48	0.49
15:V:315:LEU:O	15:V:319:ASP:N	2.37	0.49
1:1:402:LEU:O	1:1:405:ALA:HB3	2.13	0.49
3:3:451:PHE:CD1	3:3:466:GLU:HB3	2.47	0.49
4:4:254:TYR:CE2	4:4:346:THR:HA	2.47	0.49
13:L:44:GLY:HA3	13:L:77:LEU:HD21	1.94	0.49
4:E:173:ILE:O	4:E:174:ARG:NH1	2.46	0.49
12:S:31:ILE:O	12:S:35:LEU:HD13	2.13	0.49
15:V:14:THR:HG1	15:V:90:TYR:HH	1.58	0.49
16:Q:45:ARG:HG2	16:Q:46:MET:N	2.28	0.49
3:3:42:ILE:HG21	3:3:439:GLU:OE1	2.13	0.49
4:4:50:GLU:OE2	16:H:154:ARG:NH1	2.34	0.49
10:A:68:PHE:HD2	16:H:164:LEU:HB2	1.77	0.49
13:L:463:HIS:HE1	13:L:487:LEU:HD22	1.77	0.49
16:H:6:PRO:HG2	16:H:112:GLN:NE2	2.28	0.49
16:H:332:LEU:HD12	16:H:332:LEU:H	1.77	0.49
6:G:76:ASP:OD1	16:Q:65:LYS:NZ	2.38	0.49
11:R:75:PHE:CE2	11:R:78:GLN:HG2	2.48	0.49
13:T:461:LEU:HD13	13:T:465:LEU:HD13	1.95	0.49
10:A:67:LEU:HD21	10:A:110:GLU:OE2	2.13	0.49
1:B:106:ILE:HD11	1:B:251:LEU:HD21	1.93	0.49
4:E:50:GLU:OE2	16:Q:154:ARG:NH2	2.37	0.49
11:R:75:PHE:HZ	11:R:78:GLN:HE21	1.60	0.49
13:T:551:GLU:O	13:T:555:TYR:HD1	1.95	0.49
16:Q:51:VAL:O	16:Q:57:LEU:HB2	2.13	0.49
16:Q:302:TYR:O	16:Q:306:LEU:HG	2.12	0.49
1:1:264:TYR:CZ	1:1:279:TRP:HB3	2.48	0.48
1:1:387:LEU:HA	1:1:390:LEU:HD12	1.95	0.48
13:L:348:ASP:OD1	13:L:349:VAL:N	2.46	0.48
16:H:8:ASP:OD1	16:H:112:GLN:HG2	2.13	0.48
1:B:131:TYR:OH	2:C:17:LYS:O	2.16	0.48
3:D:42:ILE:HD12	3:D:42:ILE:O	2.12	0.48
3:D:271:SER:OG	7:O:69:TYR:OH	2.25	0.48
3:D:409:LEU:O	3:D:413:LEU:N	2.38	0.48
5:F:38:MET:HA	5:F:41:TYR:HB2	1.94	0.48
5:F:175:THR:H	5:F:178:ASP:HB2	1.77	0.48
6:G:130:VAL:HG13	9:X:120:PRO:O	2.14	0.48
10:P:7:TYR:CD1	16:Q:118:LEU:HD22	2.47	0.48
16:Q:232:TYR:HB2	16:Q:244:PHE:CE1	2.48	0.48
5:5:137:THR:HB	5:5:141:LEU:HD22	1.94	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
14:M:106:LEU:O	14:M:110:PHE:HD1	1.95	0.48
3:D:563:ALA:HB3	3:D:580:LYS:HE3	1.94	0.48
4:E:102:GLU:O	4:E:106:GLY:N	2.46	0.48
5:F:137:THR:HB	5:F:141:LEU:HD22	1.96	0.48
6:G:38:PRO:HG2	6:G:65:SER:HB3	1.95	0.48
13:T:163:ARG:NH2	14:U:366:VAL:O	2.45	0.48
14:U:127:ILE:HB	14:U:128:PRO:HD3	1.95	0.48
16:Q:81:LEU:HD13	16:Q:138:LEU:HD22	1.95	0.48
4:4:169:HIS:CE1	6:6:45:CYS:SG	3.06	0.48
13:L:90:TYR:O	13:L:94:TYR:HB2	2.13	0.48
13:L:255:ARG:HA	13:L:477:LEU:HD23	1.93	0.48
3:D:29:ASP:OD1	3:D:29:ASP:N	2.47	0.48
3:D:112:LEU:HD23	3:D:130:LEU:HD21	1.96	0.48
3:D:450:LEU:HD13	3:D:458:LEU:HB2	1.95	0.48
6:G:104:TRP:NE1	6:G:172:PRO:O	2.45	0.48
14:U:371:LEU:HD11	14:U:441:LEU:HD12	1.94	0.48
16:Q:35:GLU:OE1	16:Q:249:TYR:OH	2.14	0.48
6:6:76:ASP:O	6:6:104:TRP:N	2.31	0.48
6:6:94:ARG:HH11	10:A:46:SER:HB3	1.79	0.48
11:J:49:ARG:HD2	11:J:123:LEU:HD21	1.94	0.48
1:B:433:ARG:HH22	2:C:89:LYS:NZ	2.11	0.48
10:P:105:VAL:HG13	15:V:15:LEU:HD21	1.95	0.48
13:T:355:LEU:HB3	13:T:359:LEU:HD12	1.95	0.48
13:T:413:THR:HA	13:T:416:TYR:CE2	2.48	0.48
15:V:315:LEU:HD21	15:V:322:LEU:HB3	1.95	0.48
1:1:342:TRP:HZ3	1:1:346:ARG:HE	1.60	0.48
2:2:13:GLU:O	2:2:17:LYS:HG3	2.13	0.48
3:3:387:LEU:O	3:3:390:LEU:HB3	2.13	0.48
4:4:199:HIS:NE2	4:4:203:GLU:OE2	2.43	0.48
7:9:4:LYS:O	7:9:8:GLN:HG3	2.13	0.48
11:J:100:VAL:HA	13:L:598:LEU:HD21	1.95	0.48
13:L:159:PHE:CD2	14:M:407:LEU:HD11	2.45	0.48
1:B:374:ILE:HD13	1:B:421:TYR:HD2	1.79	0.48
4:E:275:ARG:O	4:E:279:ARG:HG3	2.13	0.48
7:O:149:GLU:HA	7:O:152:ARG:HG2	1.94	0.48
10:P:105:VAL:HG22	15:V:15:LEU:HD11	1.95	0.48
11:R:50:PHE:HB3	11:R:122:GLY:O	2.12	0.48
12:S:10:LEU:HD23	12:S:13:LEU:HD12	1.96	0.48
13:T:433:HIS:ND1	13:T:437:GLU:OE2	2.37	0.48
15:V:25:VAL:O	15:V:29:THR:HG23	2.13	0.48
15:V:99:ALA:O	15:V:225:ARG:NH1	2.46	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
16:Q:67:ILE:HG13	16:Q:68:PHE:CD1	2.49	0.48
16:Q:119:ASP:OD1	16:Q:120:LEU:HG	2.13	0.48
3:3:136:GLU:HG2	5:5:189:ARG:HG2	1.94	0.48
3:3:697:THR:OG1	3:3:762:ALA:O	2.23	0.48
15:N:313:ARG:HA	15:N:381:ALA:O	2.14	0.48
1:B:134:VAL:O	1:B:176:GLY:N	2.39	0.48
3:D:367:PRO:HB2	3:D:554:LYS:HB2	1.95	0.48
6:G:53:SER:HB3	6:G:144:PRO:HB3	1.96	0.48
7:O:56:CYS:N	17:O:202:SF4:S1	2.86	0.48
13:T:156:ARG:NH1	14:U:408:THR:OG1	2.46	0.48
1:1:358:PRO:HD3	3:3:107:MET:SD	2.54	0.48
3:3:117:LEU:H	4:4:321:MET:CE	2.26	0.48
3:3:136:GLU:HG2	5:5:186:GLY:O	2.14	0.48
5:5:104:VAL:HG12	5:5:107:LEU:HD22	1.95	0.48
6:6:138:PRO:HG3	7:9:129:LEU:HD22	1.95	0.48
13:L:327:PHE:CE1	13:L:452:GLY:HA3	2.48	0.48
13:L:356:TRP:CE3	13:L:363:ARG:HD2	2.48	0.48
14:M:221:ASN:ND2	14:M:228:ASP:OD1	2.47	0.48
14:M:241:PHE:HA	14:M:245:ALA:HB3	1.96	0.48
1:B:55:GLU:OE2	1:B:59:ARG:NH2	2.44	0.48
1:B:241:MET:O	1:B:248:GLY:N	2.46	0.48
3:D:154:TYR:CZ	4:E:312:PRO:HB3	2.48	0.48
4:E:385:CYS:HA	4:E:396:ILE:HD13	1.96	0.48
10:P:7:TYR:HD2	11:R:44:VAL:HG11	1.78	0.48
10:P:81:TYR:HB2	11:R:132:TYR:CZ	2.48	0.48
13:T:182:THR:HB	13:T:187:GLU:HG3	1.96	0.48
13:T:214:VAL:HG22	13:T:219:GLN:HB2	1.95	0.48
15:V:343:TRP:NE1	15:V:413:GLY:O	2.47	0.48
3:3:501:LYS:H	3:3:501:LYS:HD2	1.78	0.48
6:6:81:ALA:HA	6:6:108:MET:HB3	1.96	0.48
13:L:163:ARG:HD3	14:M:399:VAL:O	2.14	0.48
1:B:111:PRO:HB3	1:B:145:LEU:HD23	1.96	0.48
1:B:136:GLY:HA3	2:C:32:ARG:NH2	2.29	0.48
3:D:243:ARG:HH11	3:D:275:LEU:HD23	1.78	0.48
3:D:355:LEU:O	3:D:359:GLU:HG2	2.13	0.48
4:E:42:ARG:HB3	4:E:58:HIS:HB2	1.96	0.48
4:E:154:GLU:OE1	6:G:57:ARG:HD3	2.14	0.48
4:E:171:ASN:CG	4:E:174:ARG:HH22	2.17	0.48
6:G:99:MET:HB3	6:G:103:LYS:CD	2.44	0.48
13:T:241:HIS:HB3	13:T:299:THR:HG21	1.96	0.48
5:5:49:LEU:HD21	5:5:52:ILE:HD11	1.96	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:W:28:GLU:C	9:W:88:ARG:HH21	2.17	0.48
13:L:592:LEU:HB3	15:N:194:PHE:CZ	2.48	0.48
15:N:181:VAL:HA	15:N:192:PHE:CE2	2.49	0.48
15:N:207:VAL:O	15:N:211:MET:HG3	2.13	0.48
16:H:352:VAL:HG12	16:H:353:LEU:HD12	1.95	0.48
1:B:170:ASP:OD1	1:B:171:LEU:N	2.47	0.48
2:C:49:ILE:O	2:C:53:VAL:HG12	2.13	0.48
4:E:341:GLU:OE2	5:F:57:TYR:OH	2.31	0.48
10:P:10:THR:HA	16:Q:116:ILE:HD13	1.96	0.48
15:V:124:TRP:HZ3	15:V:305:ASP:HB2	1.78	0.48
4:4:306:ASN:HD21	5:5:192:TYR:HH	1.59	0.48
13:L:163:ARG:HE	14:M:399:VAL:HB	1.78	0.48
14:M:204:LYS:HE3	14:M:234:TYR:O	2.14	0.48
1:B:65:ARG:HH22	1:B:238:PHE:HZ	1.62	0.48
1:B:395:GLU:HB2	1:B:407:VAL:HG21	1.95	0.48
3:D:186:ARG:HD3	3:D:229:ILE:HG22	1.96	0.48
4:E:234:LEU:HD12	4:E:380:SER:HB2	1.95	0.48
4:E:304:ASP:O	4:E:310:THR:OG1	2.20	0.48
7:O:60:ALA:HB2	7:O:68:ILE:HG22	1.96	0.48
8:I:15:GLU:O	8:I:18:SER:HB3	2.14	0.48
13:T:30:GLY:HA3	13:T:92:ILE:HG12	1.95	0.48
13:T:219:GLN:NE2	13:T:277:THR:HG21	2.29	0.48
13:T:392:THR:HG22	13:T:399:GLY:HA3	1.96	0.48
14:U:70:LEU:HD13	14:U:312:LEU:HD13	1.96	0.48
14:U:338:THR:HG22	14:U:340:GLU:H	1.79	0.48
15:V:66:ALA:HB1	15:V:95:MET:HE3	1.94	0.48
1:1:176:GLY:O	2:2:32:ARG:NH2	2.44	0.47
3:3:505:LEU:HD21	3:3:521:ALA:HB1	1.96	0.47
6:6:61:ALA:O	16:H:48:PRO:HG3	2.13	0.47
10:A:57:PHE:CE2	16:H:149:LEU:HD13	2.49	0.47
13:L:4:LEU:HG	13:L:8:LEU:HG	1.96	0.47
13:L:17:LEU:HA	13:L:21:GLY:HA2	1.95	0.47
13:L:26:GLU:HB3	13:L:27:PRO:HD3	1.95	0.47
13:L:282:ALA:HA	13:L:416:TYR:HE2	1.79	0.47
15:N:25:VAL:HG11	15:N:82:PHE:HB2	1.96	0.47
15:N:269:MET:HB3	15:N:281:LEU:HD11	1.96	0.47
14:U:92:GLU:C	14:U:94:ARG:H	2.17	0.47
14:U:304:THR:HG21	14:U:386:LYS:HB2	1.95	0.47
15:V:63:THR:HG21	15:V:96:HIS:ND1	2.28	0.47
3:3:383:PRO:HG2	3:3:531:LYS:HA	1.96	0.47
4:4:105:LEU:HD21	4:4:335:PHE:CE1	2.50	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
14:M:36:ASN:OD1	14:M:79:ALA:HB2	2.14	0.47
14:M:126:LEU:HD11	14:M:149:VAL:HG22	1.96	0.47
14:M:359:LEU:O	14:M:363:LEU:HG	2.14	0.47
1:B:211:LEU:HB2	1:B:216:THR:HG21	1.96	0.47
3:D:463:ALA:O	3:D:465:HIS:ND1	2.47	0.47
4:E:341:GLU:HG2	4:E:358:VAL:HG22	1.96	0.47
13:T:293:LYS:O	13:T:297:TYR:HD1	1.97	0.47
15:V:108:LEU:HB2	15:V:147:PHE:CE2	2.48	0.47
1:1:343:ASN:O	1:1:346:ARG:HG2	2.14	0.47
3:3:115:HIS:CG	3:3:116:PRO:HD2	2.49	0.47
13:L:340:ILE:O	13:L:345:GLY:N	2.28	0.47
15:N:62:PHE:CD2	15:N:221:ALA:HB2	2.49	0.47
15:N:168:GLU:H	15:N:172:TYR:HB2	1.79	0.47
2:C:81:GLN:HB3	2:C:122:VAL:CG2	2.45	0.47
3:D:690:GLY:HA3	3:D:770:ARG:HH21	1.79	0.47
5:F:6:VAL:HG22	5:F:41:TYR:HE1	1.78	0.47
14:U:221:ASN:ND2	14:U:228:ASP:OD1	2.48	0.47
3:3:421:LYS:N	3:3:436:GLN:OE1	2.38	0.47
3:3:438:LYS:O	3:3:441:MET:HG3	2.14	0.47
3:3:670:PRO:HG3	3:3:675:ARG:O	2.14	0.47
6:6:28:VAL:O	6:6:32:ARG:HG3	2.14	0.47
9:W:41:ARG:NH1	9:W:91:GLU:OE1	2.47	0.47
11:J:20:VAL:HG11	12:K:13:LEU:O	2.15	0.47
13:L:582:GLN:HA	13:L:589:TYR:HE1	1.80	0.47
16:H:136:ILE:HG23	16:H:232:TYR:HD2	1.78	0.47
16:H:158:SER:HB2	16:H:305:LEU:HD21	1.95	0.47
4:E:236:GLY:O	4:E:238:SER:N	2.48	0.47
14:U:205:THR:HG23	14:U:238:VAL:HG23	1.96	0.47
16:Q:50:ARG:C	16:Q:52:GLY:H	2.15	0.47
16:Q:133:VAL:HG22	16:Q:159:LEU:HD23	1.96	0.47
4:4:371:ARG:HH22	4:4:376:VAL:HG21	1.76	0.47
13:L:463:HIS:CG	13:L:464:PRO:HD3	2.49	0.47
14:M:87:LEU:HD11	14:M:432:PHE:HB2	1.97	0.47
14:M:335:ARG:HG3	14:M:336:THR:HG23	1.96	0.47
16:H:194:TRP:CE2	16:H:265:GLY:HA3	2.50	0.47
3:D:7:ASN:ND2	3:D:94:ASP:OD1	2.45	0.47
3:D:694:LEU:HB3	3:D:762:ALA:CB	2.42	0.47
11:R:50:PHE:HB2	11:R:124:PRO:HD3	1.97	0.47
13:T:161:VAL:HG13	13:T:222:LEU:HD22	1.97	0.47
15:V:294:LEU:HD12	15:V:405:ALA:HB3	1.96	0.47
15:V:328:VAL:HG13	15:V:339:LEU:HD21	1.97	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:4:211:SER:HB2	4:4:215:TYR:N	2.29	0.47
13:L:90:TYR:OH	13:L:334:LEU:O	2.29	0.47
16:H:146:LYS:HA	16:H:149:LEU:HB2	1.97	0.47
3:D:297:GLY:HA3	3:D:703:GLN:NE2	2.29	0.47
3:D:621:VAL:O	3:D:622:LEU:HD23	2.14	0.47
4:E:44:MET:HB2	4:E:56:VAL:HB	1.96	0.47
7:O:43:LEU:CD1	7:O:133:LYS:HG3	2.44	0.47
13:T:88:HIS:NE2	13:T:108:PHE:HB3	2.28	0.47
13:T:176:LEU:HD11	13:T:209:LEU:HD11	1.96	0.47
14:U:318:SER:HA	14:U:321:TYR:CZ	2.50	0.47
1:1:201:LEU:O	1:1:204:PRO:HD2	2.15	0.47
3:3:123:ASP:OD2	3:3:241:ARG:HA	2.15	0.47
5:5:78:PRO:HA	5:5:83:GLY:HA3	1.96	0.47
7:9:105:GLU:OE2	7:9:167:ARG:NH2	2.47	0.47
13:L:358:HIS:HB3	13:L:433:HIS:CE1	2.49	0.47
14:M:194:PHE:HB2	14:M:249:ALA:HB3	1.97	0.47
15:N:17:GLY:HA3	15:N:82:PHE:CD2	2.49	0.47
16:H:224:ALA:HA	16:H:229:VAL:HA	1.97	0.47
3:D:301:ALA:O	3:D:305:ARG:HD2	2.14	0.47
3:D:615:VAL:HG22	3:D:621:VAL:HG12	1.97	0.47
4:E:84:ARG:O	6:G:83:ARG:NH2	2.47	0.47
4:E:248:VAL:HB	4:E:347:GLU:HB2	1.97	0.47
4:E:341:GLU:OE1	5:F:91:ARG:NH2	2.47	0.47
7:O:40:ARG:HH22	7:O:42:VAL:HG12	1.79	0.47
12:S:2:SER:HA	12:S:5:LEU:HD12	1.96	0.47
14:U:10:VAL:HG23	14:U:104:GLY:HA3	1.97	0.47
15:V:120:ALA:O	15:V:123:THR:OG1	2.27	0.47
15:V:415:LEU:HB3	15:V:418:LEU:HD13	1.96	0.47
1:1:386:ASN:O	1:1:390:LEU:HG	2.15	0.47
3:3:169:PRO:HA	3:3:175:ILE:HA	1.96	0.47
4:4:175:ILE:HG13	4:4:335:PHE:HZ	1.80	0.47
5:5:145:PRO:HA	5:5:150:TYR:CD1	2.50	0.47
13:L:394:THR:HB	13:L:484:HIS:O	2.15	0.47
14:M:331:ARG:HA	14:M:331:ARG:HD2	1.79	0.47
15:N:277:ASN:C	15:N:279:GLN:H	2.19	0.47
16:H:219:PHE:HD2	16:H:299:ARG:HE	1.60	0.47
1:B:211:LEU:HG	1:B:212:TRP:CE3	2.50	0.47
3:D:621:VAL:HG21	3:D:670:PRO:O	2.15	0.47
9:X:102:LEU:HG	9:X:110:LEU:HD13	1.97	0.47
10:P:56:ARG:HH11	11:R:75:PHE:H	1.62	0.47
11:R:2:SER:HA	11:R:5:GLU:HB3	1.96	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:1:372:ALA:O	1:1:376:THR:OG1	2.21	0.47
13:L:217:SER:HA	13:L:246:VAL:HG12	1.97	0.47
15:N:190:ALA:HA	15:N:192:PHE:H	1.80	0.47
15:V:41:LEU:O	15:V:44:TRP:HB2	2.15	0.47
16:Q:2:THR:HA	16:Q:5:TYR:CD2	2.47	0.47
3:3:476:ILE:O	3:3:480:LEU:HG	2.15	0.47
4:4:86:ASP:HB3	4:4:93:HIS:CD2	2.50	0.47
5:5:1:MET:HB3	5:5:5:ARG:NH2	2.30	0.47
11:J:19:VAL:HG21	11:J:32:LEU:HB2	1.95	0.47
13:L:439:PRO:HG2	13:L:442:MET:HE3	1.96	0.47
16:H:304:GLN:HE22	16:H:307:ARG:HD2	1.79	0.47
1:B:162:LEU:O	1:B:165:THR:HG22	2.15	0.47
1:B:341:MET:HE1	1:B:409:PRO:HB2	1.96	0.47
5:F:35:LYS:NZ	5:F:104:VAL:HA	2.30	0.47
6:G:25:GLU:HA	6:G:28:VAL:HG12	1.97	0.47
7:O:59:CYS:HB2	7:O:104:CYS:CB	2.44	0.47
13:T:572:ARG:NH2	15:V:373:TYR:OH	2.41	0.47
15:V:272:ALA:HB3	15:V:281:LEU:HD13	1.97	0.47
15:V:312:LEU:HD13	15:V:326:PHE:CZ	2.50	0.47
3:3:125:GLY:HA3	3:3:245:ARG:HH21	1.78	0.46
14:M:151:PHE:CD2	14:M:213:TRP:HB3	2.49	0.46
15:N:116:LEU:HD23	15:N:119:TYR:CE2	2.50	0.46
15:N:290:LEU:HD11	15:N:408:LEU:HD23	1.97	0.46
16:H:52:GLY:HA3	16:H:55:GLY:N	2.28	0.46
3:D:360:LEU:O	3:D:364:LEU:N	2.39	0.46
4:E:391:PRO:HB2	16:Q:301:ARG:HB2	1.97	0.46
5:F:34:PHE:CD2	5:F:102:PRO:HG2	2.51	0.46
13:T:132:GLU:OE2	13:T:163:ARG:NH1	2.47	0.46
14:U:75:PHE:CZ	14:U:111:ALA:HB2	2.50	0.46
15:V:283:PHE:O	15:V:287:THR:HG23	2.14	0.46
1:1:239:ALA:HA	1:1:247:LYS:HB3	1.96	0.46
3:3:230:CYS:SG	3:3:234:ALA:HB3	2.55	0.46
3:3:404:GLU:OE1	3:3:698:MET:N	2.27	0.46
4:4:173:ILE:O	4:4:174:ARG:NH1	2.48	0.46
7:9:158:LYS:HG3	7:9:158:LYS:O	2.15	0.46
11:J:105:ALA:O	11:J:109:TRP:HB2	2.15	0.46
13:L:63:ILE:HG21	13:L:125:PRO:HG2	1.98	0.46
14:M:331:ARG:HA	14:M:331:ARG:HH11	1.79	0.46
15:N:241:VAL:O	15:N:245:ASN:ND2	2.48	0.46
16:H:289:PHE:O	16:H:293:ILE:HG12	2.16	0.46
1:B:114:LEU:HD13	1:B:221:VAL:HG13	1.96	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:688:ARG:HD3	3:D:688:ARG:HA	1.56	0.46
4:E:143:LEU:HD23	4:E:143:LEU:H	1.80	0.46
4:E:205:GLU:OE1	4:E:284:ARG:NH2	2.49	0.46
6:G:163:TYR:O	7:O:152:ARG:NH1	2.49	0.46
11:R:65:VAL:HG23	16:Q:134:TYR:CZ	2.50	0.46
14:U:95:PHE:HB3	14:U:136:TYR:CZ	2.50	0.46
1:1:26:SER:HA	1:1:31:TYR:CG	2.50	0.46
1:1:257:PRO:HD2	1:1:330:LEU:HB2	1.97	0.46
2:2:112:THR:HG23	2:2:115:GLY:H	1.79	0.46
4:4:32:PRO:HG2	6:6:91:VAL:HG11	1.96	0.46
6:6:32:ARG:HD2	6:6:104:TRP:HH2	1.81	0.46
10:A:81:TYR:CE2	16:H:325:ALA:HB1	2.46	0.46
14:M:186:GLN:HG2	14:M:187:GLU:H	1.81	0.46
14:M:332:LEU:HA	14:M:335:ARG:HG2	1.97	0.46
15:N:299:LEU:HD22	15:N:307:VAL:HG11	1.98	0.46
1:B:122:GLY:HA2	1:B:127:ALA:HB3	1.98	0.46
1:B:302:PHE:CZ	1:B:307:LEU:HD21	2.50	0.46
3:D:611:ARG:NH2	9:X:101:ALA:HB1	2.24	0.46
10:P:68:PHE:CD2	16:Q:164:LEU:HB2	2.51	0.46
3:3:506:ILE:HG12	3:3:533:LEU:HB2	1.98	0.46
4:4:28:LEU:HD11	16:H:147:TYR:CD2	2.51	0.46
4:4:147:PHE:HE2	16:H:45:ARG:HD3	1.81	0.46
4:4:162:TRP:NE1	7:9:34:LYS:HD2	2.30	0.46
5:5:164:TYR:HB3	9:W:37:TRP:CZ3	2.51	0.46
13:L:458:TYR:HD1	13:L:461:LEU:HD21	1.80	0.46
13:L:461:LEU:N	13:L:467:ASN:OD1	2.48	0.46
14:M:260:LEU:HB3	14:M:301:PHE:CD2	2.50	0.46
3:D:203:ILE:HG21	8:I:88:ARG:HG2	1.96	0.46
4:E:50:GLU:O	4:E:390:VAL:HG23	2.15	0.46
7:O:10:LEU:HD12	16:Q:296:THR:HG21	1.97	0.46
10:P:67:LEU:HD23	16:Q:310:TRP:CZ2	2.51	0.46
15:V:176:LEU:HD23	15:V:176:LEU:HA	1.80	0.46
16:Q:25:LEU:O	16:Q:28:PHE:HD1	1.96	0.46
1:1:291:ILE:O	1:1:328:VAL:HA	2.16	0.46
18:1:502:FMN:O4'	18:1:502:FMN:O2'	2.33	0.46
2:2:146:THR:HG23	2:2:149:ARG:H	1.81	0.46
3:3:201:ASP:OD1	3:3:202:PHE:N	2.43	0.46
4:4:55:VAL:O	4:4:382:PRO:HG3	2.16	0.46
7:9:133:LYS:HG2	7:9:137:LEU:HD11	1.97	0.46
11:J:83:PHE:HB3	11:J:85:PRO:HG3	1.97	0.46
14:M:99:ALA:HB2	14:M:226:LEU:HD21	1.98	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:5:ILE:H	1:B:12:ARG:HH22	1.62	0.46
5:F:2:ARG:NH1	5:F:45:GLY:O	2.48	0.46
11:R:154:VAL:O	11:R:158:GLU:HB2	2.15	0.46
2:2:108:PRO:HA	2:2:119:VAL:HG23	1.98	0.46
4:4:193:LEU:HA	4:4:196:VAL:HG12	1.97	0.46
5:5:38:MET:HA	5:5:41:TYR:CD2	2.49	0.46
6:6:101:ASP:OD2	10:A:35:LYS:HB2	2.15	0.46
10:A:93:PHE:O	10:A:96:VAL:HG12	2.16	0.46
13:L:13:GLY:O	13:L:17:LEU:HG	2.15	0.46
13:L:325:HIS:HA	13:L:328:PHE:CE2	2.50	0.46
15:N:265:HIS:NE2	15:N:375:TYR:OH	2.48	0.46
1:B:250:LYS:HB3	1:B:252:TYR:CE1	2.50	0.46
1:B:291:ILE:O	1:B:328:VAL:HA	2.15	0.46
2:C:24:ARG:HE	2:C:55:THR:HB	1.80	0.46
4:E:409:ARG:NH2	5:F:117:GLU:OE2	2.49	0.46
6:G:28:VAL:O	6:G:32:ARG:HG3	2.16	0.46
8:I:58:SER:HB3	8:I:69:LEU:HD23	1.97	0.46
13:T:153:ASP:OD1	14:U:411:GLN:NE2	2.37	0.46
3:3:154:TYR:CZ	4:4:312:PRO:HB3	2.50	0.46
9:W:35:THR:OG1	9:W:36:ASP:N	2.49	0.46
14:M:338:THR:HG22	14:M:340:GLU:H	1.79	0.46
16:H:70:GLU:HG3	16:H:70:GLU:O	2.16	0.46
2:C:112:THR:HG22	2:C:117:PHE:H	1.80	0.46
3:D:223:SER:O	3:D:226:ILE:HG12	2.16	0.46
3:D:341:VAL:HB	3:D:364:LEU:HD21	1.97	0.46
4:E:140:LEU:HD13	4:E:217:ARG:HH22	1.80	0.46
4:E:350:ARG:O	4:E:373:PRO:HB2	2.16	0.46
6:G:115:GLY:HA3	6:G:125:GLN:CD	2.36	0.46
9:X:35:THR:N	9:X:92:ALA:O	2.34	0.46
16:Q:150:LEU:O	16:Q:154:ARG:HG3	2.15	0.46
1:1:189:MET:O	1:1:193:GLU:HB2	2.16	0.46
3:3:268:ASP:CG	3:3:278:ARG:NH1	2.68	0.46
3:3:269:THR:OG1	3:3:628:PRO:HD2	2.16	0.46
4:4:245:ASN:O	5:5:79:GLY:HA3	2.16	0.46
13:L:26:GLU:O	13:L:29:PRO:HD2	2.16	0.46
13:L:317:VAL:HG12	13:L:388:ILE:HG12	1.97	0.46
2:C:85:THR:HB	20:C:201:FES:S2	2.56	0.46
3:D:165:ASP:HB3	3:D:178:ARG:HD2	1.98	0.46
3:D:225:ASN:ND2	3:D:289:TRP:HB3	2.31	0.46
3:D:237:ASP:OD1	3:D:239:THR:HG22	2.15	0.46
4:E:85:MET:HE2	4:E:370:VAL:HG11	1.98	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:O:4:LYS:HE2	16:Q:352:VAL:O	2.15	0.46
3:3:300:TRP:NE1	3:3:703:GLN:HG2	2.31	0.46
3:3:397:LEU:HD21	3:3:480:LEU:CD1	2.34	0.46
4:4:105:LEU:HD13	4:4:309:ILE:HD13	1.96	0.46
4:4:144:THR:HA	16:H:43:GLN:OE1	2.16	0.46
7:9:30:PRO:HB2	7:9:162:VAL:HG22	1.96	0.46
15:N:313:ARG:HB2	15:N:384:ALA:HB3	1.97	0.46
18:B:502:FMN:H9	19:B:503:NAI:H52N	1.96	0.46
2:C:61:MET:O	2:C:65:SER:OG	2.29	0.46
11:R:29:ALA:O	11:R:33:ILE:HG13	2.16	0.46
13:T:41:PHE:HB2	13:T:81:THR:HB	1.98	0.46
13:T:246:VAL:HB	13:T:303:LEU:HD21	1.98	0.46
15:V:198:ASP:OD1	15:V:256:ARG:NH2	2.47	0.46
16:Q:43:GLN:HE21	16:Q:45:ARG:CZ	2.28	0.46
9:W:24:LEU:HD21	9:W:52:THR:HG21	1.96	0.46
16:H:138:LEU:HD23	16:H:138:LEU:HA	1.77	0.46
1:B:352:SER:OG	1:B:359:CYS:SG	2.61	0.46
3:D:190:TYR:O	3:D:195:PRO:HD2	2.16	0.46
3:D:654:PHE:CE2	3:D:660:ALA:HA	2.51	0.46
4:E:59:ILE:O	6:G:87:LYS:NZ	2.46	0.46
4:E:144:THR:HG22	4:E:148:TYR:CE1	2.41	0.46
4:E:379:GLN:HG2	5:F:113:PHE:CD2	2.51	0.46
4:E:390:VAL:HB	4:E:391:PRO:HD3	1.98	0.46
5:F:82:ASP:OD1	5:F:82:ASP:N	2.49	0.46
6:G:82:GLY:HA2	17:G:201:SF4:S4	2.56	0.46
14:U:411:GLN:NE2	14:U:416:GLU:OE2	2.26	0.46
15:V:257:LEU:HD11	15:V:374:TYR:HB2	1.98	0.46
3:3:719:HIS:ND1	3:3:753:VAL:O	2.41	0.45
4:4:62:LEU:HD23	4:4:62:LEU:HA	1.72	0.45
14:M:119:TYR:OH	14:M:160:LEU:HB2	2.16	0.45
16:H:17:ALA:O	16:H:21:VAL:HG23	2.16	0.45
16:H:293:ILE:HG23	16:H:297:TRP:CE3	2.51	0.45
1:B:159:GLY:H	1:B:162:LEU:HD21	1.81	0.45
1:B:356:CYS:N	17:B:501:SF4:S3	2.78	0.45
2:C:50:ALA:HA	2:C:53:VAL:HG12	1.98	0.45
3:D:38:HIS:NE2	3:D:430:THR:HG21	2.31	0.45
3:D:642:ALA:O	3:D:652:PRO:HG3	2.17	0.45
5:F:80:TRP:CE3	5:F:80:TRP:HA	2.51	0.45
14:U:75:PHE:HZ	14:U:111:ALA:HB2	1.81	0.45
14:U:119:TYR:HE1	15:V:342:PHE:CE1	2.35	0.45
15:V:25:VAL:HG11	15:V:82:PHE:HB2	1.96	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
16:Q:20:VAL:O	16:Q:24:LEU:HD13	2.16	0.45
3:3:290:ILE:HB	3:3:295:ARG:NH2	2.30	0.45
4:4:48:SER:H	4:4:53:LEU:HD23	1.80	0.45
4:4:356:TYR:HE1	5:5:26:TRP:HZ2	1.64	0.45
7:9:112:ALA:HB3	17:9:202:SF4:S4	2.57	0.45
11:J:92:LEU:O	11:J:95:LEU:HB3	2.16	0.45
11:J:119:LEU:HD11	12:K:47:ARG:HA	1.97	0.45
15:N:303:SER:HB3	15:N:307:VAL:HG22	1.97	0.45
1:B:303:THR:H	1:B:306:VAL:HB	1.80	0.45
2:C:106:ILE:CD1	2:C:112:THR:CA	2.91	0.45
3:D:40:SER:HB3	3:D:437:ILE:HG22	1.99	0.45
3:D:124:LYS:HG2	3:D:236:LEU:HD21	1.98	0.45
3:D:651:ARG:NH1	3:D:652:PRO:O	2.50	0.45
4:E:236:GLY:C	4:E:238:SER:H	2.20	0.45
5:F:123:GLY:HA2	5:F:144:HIS:CE1	2.52	0.45
6:G:36:LEU:HD11	6:G:155:GLN:HG3	1.99	0.45
7:O:163:VAL:O	7:O:177:THR:HA	2.17	0.45
8:I:27:LYS:HA	8:I:27:LYS:HD3	1.82	0.45
11:R:105:ALA:O	11:R:109:TRP:HB2	2.16	0.45
13:T:340:ILE:HB	13:T:345:GLY:HA2	1.98	0.45
14:U:22:ARG:NH1	14:U:92:GLU:HG3	2.31	0.45
14:U:54:PRO:HA	14:U:62:TYR:CD1	2.51	0.45
15:V:38:ALA:HA	15:V:41:LEU:HD12	1.98	0.45
15:V:207:VAL:O	15:V:211:MET:HG3	2.15	0.45
3:3:76:GLN:HG3	3:3:77:PRO:HD2	1.98	0.45
3:3:132:ASP:O	3:3:136:GLU:HG3	2.17	0.45
3:3:734:VAL:HG13	3:3:775:VAL:HG13	1.99	0.45
4:4:163:VAL:HG13	4:4:164:THR:HG23	1.98	0.45
4:4:214:PHE:CE2	4:4:273:PHE:HD2	2.34	0.45
6:6:59:ASP:OD1	6:6:62:ARG:NH2	2.49	0.45
7:9:63:CYS:HA	17:9:201:SF4:S2	2.56	0.45
11:J:103:ILE:HG13	15:N:174:LEU:HD13	1.98	0.45
12:K:7:SER:HB2	12:K:37:ALA:O	2.17	0.45
13:L:111:PHE:CZ	13:L:134:VAL:HG13	2.51	0.45
16:H:300:LEU:O	16:H:301:ARG:HG2	2.17	0.45
2:C:6:ASP:HB3	2:C:7:LYS:HE3	1.99	0.45
3:D:120:PRO:O	3:D:245:ARG:NH1	2.49	0.45
3:D:329:LEU:HD12	3:D:584:VAL:HG11	1.98	0.45
3:D:657:HIS:O	3:D:661:GLN:HG2	2.16	0.45
13:T:291:ILE:O	13:T:295:VAL:HG23	2.16	0.45
13:T:380:SER:HB3	13:T:457:GLY:H	1.81	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
15:V:62:PHE:CG	15:V:221:ALA:HB2	2.51	0.45
16:Q:76:GLN:O	16:Q:144:GLY:HA3	2.15	0.45
16:Q:136:ILE:HG23	16:Q:232:TYR:HD2	1.81	0.45
7:9:42:VAL:HA	7:9:136:MET:O	2.16	0.45
10:A:38:ARG:O	10:A:42:MET:HG3	2.16	0.45
11:J:64:VAL:HG13	16:H:134:TYR:OH	2.16	0.45
13:L:356:TRP:CD2	13:L:363:ARG:HD2	2.51	0.45
13:L:385:LYS:NZ	13:L:413:THR:OG1	2.50	0.45
16:H:215:ALA:O	16:H:294:ARG:NH1	2.39	0.45
16:H:293:ILE:HD12	16:H:297:TRP:CZ3	2.51	0.45
1:B:32:TYR:OH	1:B:116:GLU:OE1	2.21	0.45
1:B:193:GLU:OE1	1:B:200:ARG:NH2	2.47	0.45
4:E:40:VAL:HG21	6:G:88:MET:HE1	1.98	0.45
4:E:193:LEU:HA	4:E:196:VAL:HG12	1.98	0.45
9:X:125:ILE:HD11	9:X:126:TYR:CZ	2.51	0.45
10:P:23:ALA:O	10:P:27:VAL:HG23	2.17	0.45
10:P:66:MET:O	10:P:69:ILE:HG12	2.15	0.45
11:R:16:GLY:O	11:R:19:VAL:HG12	2.15	0.45
13:T:373:LEU:HD21	13:T:416:TYR:HE1	1.81	0.45
14:U:238:VAL:O	14:U:241:PHE:HB2	2.17	0.45
3:3:180:ARG:O	3:3:232:VAL:HG21	2.17	0.45
3:3:715:GLU:O	3:3:760:LEU:HD12	2.16	0.45
4:4:197:LEU:N	4:4:198:PRO:HD2	2.31	0.45
4:4:385:CYS:HB3	4:4:396:ILE:HG21	1.97	0.45
5:5:82:ASP:OD1	5:5:82:ASP:N	2.48	0.45
13:L:33:ALA:O	13:L:37:VAL:HG23	2.17	0.45
13:L:79:ILE:HD11	13:L:323:PHE:HD1	1.82	0.45
13:L:147:LYS:NZ	14:M:349:GLN:OE1	2.47	0.45
16:H:147:TYR:CE1	16:H:228:LEU:HD13	2.51	0.45
1:B:121:ALA:O	1:B:125:ILE:HG12	2.17	0.45
3:D:304:ASN:O	3:D:589:HIS:NE2	2.50	0.45
3:D:472:GLU:O	3:D:476:ILE:HD12	2.16	0.45
4:E:147:PHE:HE2	16:Q:45:ARG:HD3	1.81	0.45
4:E:283:MET:O	4:E:287:VAL:HG23	2.16	0.45
7:O:4:LYS:O	7:O:8:GLN:HG3	2.16	0.45
8:I:68:LEU:HD11	8:I:115:PHE:CE1	2.52	0.45
13:T:379:LEU:HD22	13:T:454:VAL:HA	1.99	0.45
14:U:332:LEU:O	14:U:336:THR:OG1	2.20	0.45
15:V:272:ALA:O	15:V:276:GLY:N	2.45	0.45
3:3:406:ALA:O	3:3:409:LEU:HB2	2.16	0.45
6:6:37:TRP:NE1	6:6:67:VAL:HB	2.32	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:A:7:TYR:N	10:A:7:TYR:CD1	2.84	0.45
10:A:7:TYR:N	10:A:7:TYR:HD1	2.15	0.45
13:L:391:ALA:HA	13:L:394:THR:OG1	2.17	0.45
15:N:40:LEU:HD12	15:N:67:LEU:HD12	1.99	0.45
15:N:126:ARG:O	15:N:129:GLY:N	2.48	0.45
1:B:67:GLY:HA3	19:B:503:NAI:H1D	1.99	0.45
3:D:563:ALA:O	3:D:580:LYS:HG2	2.17	0.45
4:E:250:LYS:HE2	4:E:262:PHE:HB3	1.97	0.45
4:E:369:LYS:HG3	5:F:53:VAL:HG23	1.98	0.45
5:F:145:PRO:O	5:F:150:TYR:HB3	2.17	0.45
10:P:34:LYS:N	16:Q:70:GLU:OE1	2.47	0.45
14:U:16:LEU:HD22	14:U:97:GLY:H	1.82	0.45
14:U:159:MET:HG3	14:U:197:PHE:CE1	2.52	0.45
14:U:201:PHE:CZ	14:U:240:ALA:HB1	2.51	0.45
14:U:204:LYS:HE3	14:U:234:TYR:O	2.17	0.45
16:Q:15:LEU:O	16:Q:19:LEU:HG	2.17	0.45
16:Q:138:LEU:HD23	16:Q:138:LEU:HA	1.84	0.45
16:Q:216:ARG:HD2	16:Q:294:ARG:HD2	1.98	0.45
16:Q:274:VAL:CG2	16:Q:275:PRO:HD2	2.47	0.45
8:7:82:ILE:HG23	8:7:95:ALA:HB3	1.97	0.45
13:L:34:SER:OG	13:L:88:HIS:HB3	2.16	0.45
13:L:413:THR:HG22	13:L:416:TYR:OH	2.16	0.45
15:N:234:ALA:HB1	15:N:360:VAL:HG21	1.99	0.45
1:B:275:LEU:O	1:B:279:TRP:HB2	2.16	0.45
1:B:297:THR:HG22	1:B:322:MET:HG3	1.99	0.45
4:E:314:ARG:NH1	7:O:106:GLU:O	2.49	0.45
9:X:36:ASP:OD1	9:X:36:ASP:N	2.48	0.45
14:U:310:GLY:HA2	14:U:376:GLY:HA2	1.97	0.45
2:2:154:LEU:HD23	2:2:154:LEU:HA	1.87	0.45
11:J:104:LEU:HD21	15:N:178:LEU:HD11	1.99	0.45
13:L:379:LEU:HD23	13:L:379:LEU:HA	1.84	0.45
13:L:426:LEU:HB3	13:L:513:GLN:HE22	1.82	0.45
16:H:190:LYS:HB2	16:H:268:THR:CG2	2.46	0.45
2:C:135:GLN:HB2	2:C:141:TYR:HD1	1.81	0.45
3:D:119:CYS:N	17:D:801:SF4:S1	2.90	0.45
3:D:224:GLY:HA3	3:D:295:ARG:HD2	1.98	0.45
4:E:48:SER:H	4:E:53:LEU:HD23	1.82	0.45
6:G:178:ARG:NE	9:X:125:ILE:HG22	2.31	0.45
7:O:52:LYS:NZ	7:O:171:GLU:OE2	2.34	0.45
5:5:35:LYS:HD3	5:5:102:PRO:HB2	1.99	0.45
14:M:313:TYR:OH	14:M:443:MET:O	2.23	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
16:H:67:ILE:HG13	16:H:68:PHE:CD1	2.52	0.45
1:B:223:THR:O	1:B:227:VAL:HG23	2.17	0.45
3:D:474:ARG:O	3:D:520:ARG:NH1	2.48	0.45
3:D:513:GLN:HG2	3:D:769:LEU:HD23	1.98	0.45
3:D:654:PHE:CD2	3:D:660:ALA:HA	2.51	0.45
3:D:664:LEU:O	3:D:669:VAL:HG12	2.16	0.45
6:G:108:MET:HA	6:G:137:VAL:HG13	1.99	0.45
16:Q:122:ILE:HA	16:Q:125:LEU:HD12	1.98	0.45
16:Q:147:TYR:CD1	16:Q:229:VAL:HG22	2.52	0.45
1:1:338:VAL:O	1:1:342:TRP:HB2	2.17	0.45
3:3:568:TYR:CD1	3:3:572:PRO:HG3	2.52	0.45
4:4:73:ARG:CZ	4:4:81:TYR:OH	2.65	0.45
7:9:59:CYS:HB3	7:9:113:ILE:HG21	1.99	0.45
7:9:149:GLU:HA	7:9:152:ARG:HG2	1.98	0.45
9:W:41:ARG:HH12	9:W:91:GLU:CD	2.20	0.45
9:W:74:LEU:HD21	9:W:126:TYR:HD1	1.81	0.45
10:A:28:GLY:HA3	16:H:239:ILE:HG21	1.99	0.45
13:L:166:ASP:O	13:L:170:MET:HG3	2.17	0.45
1:B:270:THR:O	1:B:311:MET:HG3	2.17	0.45
5:F:74:LEU:HD12	5:F:88:PHE:CZ	2.52	0.45
6:G:56:ALA:HA	16:Q:45:ARG:HB2	1.97	0.45
9:X:35:THR:OG1	9:X:36:ASP:N	2.49	0.45
10:P:80:PRO:HA	11:R:124:PRO:HB2	1.98	0.45
11:R:152:VAL:HG22	15:V:87:LEU:HD22	1.99	0.45
13:T:90:TYR:OH	13:T:334:LEU:O	2.14	0.45
14:U:354:LEU:HD12	14:U:354:LEU:HA	1.77	0.45
16:Q:40:ALA:HA	16:Q:45:ARG:HH21	1.82	0.45
16:Q:177:VAL:HG11	16:Q:185:ILE:HA	1.99	0.45
3:3:616:ASN:HB2	3:3:620:ARG:O	2.17	0.44
6:6:21:PHE:HD1	6:6:23:THR:H	1.65	0.44
6:6:105:VAL:N	6:6:134:ASP:OD2	2.36	0.44
14:M:70:LEU:HD13	14:M:312:LEU:HD13	1.99	0.44
2:C:130:THR:HB	2:C:143:GLU:HB3	1.99	0.44
3:D:453:PRO:HA	3:D:468:HIS:O	2.17	0.44
4:E:62:LEU:HD11	6:G:43:LEU:O	2.17	0.44
5:F:55:LEU:HD23	5:F:57:TYR:OH	2.17	0.44
11:R:48:ALA:HB1	11:R:51:LEU:HB3	1.98	0.44
11:R:92:LEU:O	11:R:95:LEU:HB3	2.17	0.44
16:Q:225:GLU:HB3	16:Q:226:GLN:HG2	1.99	0.44
16:Q:314:PHE:HB2	16:Q:315:PRO:HD3	1.98	0.44
1:1:288:GLN:NE2	1:1:332:PRO:O	2.50	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:1:337:MET:O	1:1:341:MET:HG2	2.17	0.44
1:1:370:LEU:HD13	1:1:383:ASP:HB3	1.99	0.44
3:3:76:GLN:CG	3:3:77:PRO:HD2	2.47	0.44
3:3:119:CYS:HB2	4:4:324:VAL:HG12	1.99	0.44
3:3:408:ILE:HG23	17:3:803:SF4:S1	2.57	0.44
3:3:464:ILE:HA	3:3:489:MET:SD	2.57	0.44
4:4:81:TYR:CZ	6:6:117:MET:HG3	2.52	0.44
4:4:374:SER:O	4:4:407:VAL:HG22	2.17	0.44
7:9:83:ALA:HB3	8:7:41:ILE:HG12	1.99	0.44
16:H:224:ALA:HA	16:H:230:GLY:H	1.82	0.44
16:H:260:PRO:HG3	16:H:286:PHE:CD2	2.52	0.44
1:B:225:ALA:O	1:B:229:PRO:HD2	2.16	0.44
3:D:225:ASN:HD21	3:D:289:TRP:HB3	1.83	0.44
3:D:689:LYS:H	3:D:689:LYS:HG2	1.52	0.44
7:O:45:ARG:NH2	7:O:139:ASP:OD2	2.48	0.44
7:O:149:GLU:O	7:O:153:THR:OG1	2.23	0.44
8:I:96:HIS:O	8:I:103:LEU:HD12	2.17	0.44
15:V:7:ALA:O	15:V:11:VAL:HG23	2.17	0.44
3:3:307:LYS:HE3	3:3:632:GLY:HA2	1.99	0.44
3:3:343:LEU:HB2	3:3:369:LEU:HB3	1.99	0.44
8:7:105:THR:N	8:7:108:ILE:O	2.49	0.44
9:W:98:GLU:O	9:W:102:LEU:HB2	2.17	0.44
11:J:90:ARG:HG2	12:K:20:THR:HG23	1.99	0.44
13:L:361:GLN:O	13:L:365:HIS:ND1	2.49	0.44
14:M:90:ARG:HD2	14:M:90:ARG:HA	1.80	0.44
14:M:452:ARG:HD3	14:M:452:ARG:HA	1.74	0.44
16:H:50:ARG:C	16:H:52:GLY:H	2.11	0.44
16:H:274:VAL:HG12	16:H:278:TRP:HD1	1.79	0.44
1:B:179:ALA:HB3	1:B:182:CYS:SG	2.57	0.44
1:B:427:GLU:OE1	1:B:429:ARG:NH1	2.50	0.44
3:D:383:PRO:HD3	3:D:679:ARG:HH21	1.81	0.44
3:D:497:TRP:O	3:D:528:LYS:HE3	2.17	0.44
3:D:568:TYR:CD1	3:D:572:PRO:HG3	2.53	0.44
4:E:230:ILE:HG21	5:F:47:ASN:HB3	1.98	0.44
5:F:31:ARG:NH2	5:F:98:ASP:O	2.50	0.44
5:F:34:PHE:HD2	5:F:102:PRO:HG2	1.83	0.44
10:P:71:PHE:O	10:P:75:VAL:HG23	2.16	0.44
4:4:367:ARG:HH21	5:5:146:LEU:CD1	2.30	0.44
13:L:20:PHE:O	13:L:22:LYS:N	2.48	0.44
14:M:12:PHE:HB3	14:M:100:LEU:HD13	1.99	0.44
14:M:318:SER:HA	14:M:321:TYR:CZ	2.53	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
16:H:204:LEU:HD23	16:H:204:LEU:HA	1.85	0.44
1:B:197:ALA:HB3	2:C:66:PHE:CE2	2.53	0.44
1:B:201:LEU:O	1:B:204:PRO:HD2	2.18	0.44
1:B:250:LYS:NZ	1:B:251:LEU:O	2.50	0.44
4:E:115:THR:HG21	4:E:297:LEU:HD13	1.99	0.44
11:R:155:ALA:HB2	15:V:83:GLU:HG2	2.00	0.44
3:3:270:ARG:HB3	3:3:275:LEU:HD11	1.99	0.44
3:3:344:TYR:HA	3:3:370:ASP:O	2.18	0.44
3:3:635:GLU:OE2	9:W:7:ARG:HD2	2.17	0.44
4:4:136:GLY:HA2	4:4:398:ALA:HB1	1.99	0.44
4:4:246:TYR:CD1	5:5:78:PRO:HD2	2.52	0.44
5:5:68:PHE:HE1	5:5:96:GLU:HA	1.82	0.44
5:5:105:THR:HA	5:5:108:TRP:O	2.18	0.44
6:6:34:ASN:O	6:6:64:GLY:HA3	2.18	0.44
6:6:84:LEU:HD11	6:6:89:ALA:HA	2.00	0.44
6:6:96:TRP:HZ2	6:6:175:ALA:HB1	1.83	0.44
10:A:66:MET:O	10:A:69:ILE:HG12	2.17	0.44
13:L:183:LEU:HD23	13:L:183:LEU:HA	1.78	0.44
13:L:325:HIS:CD2	13:L:329:LYS:HG3	2.53	0.44
16:H:6:PRO:HG2	16:H:112:GLN:HE21	1.83	0.44
16:H:72:ILE:HG22	16:H:237:SER:HB3	2.00	0.44
3:D:224:GLY:O	3:D:227:THR:HB	2.18	0.44
4:E:261:THR:H	4:E:292:GLN:NE2	2.06	0.44
5:F:16:PRO:HD2	5:F:28:VAL:HG13	2.00	0.44
5:F:149:ASP:O	9:X:112:LYS:NZ	2.30	0.44
6:G:16:ARG:O	6:G:19:ILE:HG22	2.18	0.44
13:T:158:ALA:HA	13:T:225:TRP:HB2	1.99	0.44
15:V:86:LEU:O	15:V:89:LEU:HB2	2.17	0.44
1:1:382:LYS:O	1:1:386:ASN:ND2	2.51	0.44
2:2:146:THR:HG22	2:2:149:ARG:HB2	1.99	0.44
3:3:143:TYR:OH	5:5:195:LEU:O	2.20	0.44
3:3:285:VAL:HG21	3:3:616:ASN:HD21	1.83	0.44
4:4:61:TYR:O	6:6:85:SER:HB3	2.17	0.44
5:5:131:ASP:HB2	5:5:133:ARG:HE	1.82	0.44
10:A:57:PHE:HB3	10:A:58:PRO:HD2	2.00	0.44
1:B:310:PRO:O	1:B:315:HIS:HB2	2.18	0.44
3:D:583:VAL:HG21	3:D:597:TYR:O	2.18	0.44
3:D:694:LEU:CB	3:D:762:ALA:HB2	2.45	0.44
3:D:734:VAL:HG13	3:D:775:VAL:HG13	1.99	0.44
4:E:186:PHE:CZ	4:E:190:LEU:HD22	2.52	0.44
9:X:46:TYR:N	9:X:63:PHE:O	2.48	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
14:U:279:LYS:HD3	14:U:279:LYS:HA	1.80	0.44
16:Q:35:GLU:CD	16:Q:294:ARG:HH21	2.20	0.44
16:Q:293:ILE:HD12	16:Q:297:TRP:CZ3	2.53	0.44
4:4:30:VAL:HG13	4:4:35:PRO:HD2	2.00	0.44
4:4:193:LEU:HD23	4:4:194:LEU:HD12	1.99	0.44
4:4:336:HIS:CE1	5:5:174:LEU:HD12	2.50	0.44
5:5:163:ARG:O	9:W:37:TRP:HH2	2.01	0.44
6:6:21:PHE:O	6:6:25:GLU:HG2	2.18	0.44
6:6:163:TYR:H	7:9:152:ARG:NH1	2.15	0.44
11:J:63:ILE:HG23	12:K:68:VAL:HG11	1.99	0.44
11:J:72:MET:HE3	16:H:149:LEU:HD21	1.99	0.44
13:L:115:MET:HG2	13:L:244:THR:HG22	2.00	0.44
13:L:553:LEU:O	14:M:270:TYR:OH	2.15	0.44
1:B:201:LEU:HD12	1:B:399:PHE:CZ	2.52	0.44
3:D:409:LEU:HA	3:D:409:LEU:HD23	1.61	0.44
4:E:341:GLU:HG2	4:E:358:VAL:HG13	1.99	0.44
4:E:350:ARG:HG2	4:E:401:ASP:O	2.18	0.44
6:G:26:LYS:HA	6:G:26:LYS:HD3	1.82	0.44
6:G:58:ASN:ND2	6:G:145:GLU:OE2	2.51	0.44
6:G:155:GLN:O	6:G:159:ARG:HG3	2.18	0.44
12:S:28:PHE:CZ	15:V:137:PHE:HZ	2.36	0.44
14:U:143:ARG:HD3	14:U:143:ARG:HA	1.67	0.44
14:U:169:LEU:HD21	15:V:358:TRP:HZ2	1.82	0.44
15:V:10:SER:HB3	15:V:90:TYR:HE1	1.82	0.44
15:V:190:ALA:HA	15:V:192:PHE:H	1.81	0.44
16:Q:224:ALA:HA	16:Q:230:GLY:H	1.83	0.44
2:2:161:LYS:NZ	2:2:166:ILE:HA	2.32	0.44
3:3:405:GLU:HG2	3:3:696:PRO:HB2	2.00	0.44
4:4:205:GLU:OE2	4:4:281:ARG:NE	2.50	0.44
4:4:239:LEU:HG	4:4:244:VAL:HB	2.00	0.44
4:4:333:GLU:O	4:4:363:SER:OG	2.19	0.44
4:4:369:LYS:HE2	5:5:53:VAL:HA	2.00	0.44
5:5:49:LEU:HD12	5:5:73:GLU:O	2.18	0.44
8:7:27:LYS:HA	8:7:27:LYS:HD3	1.90	0.44
12:K:87:VAL:HG23	15:N:134:LEU:HD21	2.00	0.44
13:L:10:PRO:HB2	13:L:109:ASN:O	2.17	0.44
16:H:292:TRP:HD1	16:H:296:THR:OG1	2.01	0.44
1:B:98:PRO:HB2	1:B:295:SER:HB2	1.99	0.44
1:B:245:GLN:HB2	1:B:314:GLU:CD	2.38	0.44
2:C:83:CYS:HA	2:C:122:VAL:O	2.17	0.44
3:D:352:GLU:OE2	3:D:612:GLY:HA2	2.16	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:E:64:THR:HG23	6:G:123:ILE:HG13	2.00	0.44
4:E:87:TYR:HB3	4:E:169:HIS:HE1	1.82	0.44
4:E:176:GLY:HA3	4:E:303:ARG:HB2	1.98	0.44
14:U:87:LEU:HD11	14:U:432:PHE:HB2	2.00	0.44
15:V:95:MET:HB3	15:V:218:ALA:HB2	1.99	0.44
15:V:188:ALA:HB3	15:V:216:LYS:HZ1	1.82	0.44
1:1:48:LYS:O	1:1:123:TYR:OH	2.17	0.44
1:1:296:SER:OG	1:1:348:TYR:OH	2.25	0.44
2:2:26:ALA:O	2:2:30:LEU:HG	2.18	0.44
3:3:453:PRO:HA	3:3:468:HIS:O	2.17	0.44
3:3:586:HIS:NE2	3:3:640:VAL:HG21	2.33	0.44
3:3:615:VAL:HG22	3:3:621:VAL:HG12	2.00	0.44
7:9:14:LEU:HB2	16:H:292:TRP:CZ2	2.52	0.44
14:M:314:LEU:HB2	14:M:376:GLY:HA3	2.00	0.44
15:N:196:THR:HG22	15:N:259:ALA:HB1	2.00	0.44
16:H:35:GLU:OE1	16:H:249:TYR:OH	2.28	0.44
16:H:122:ILE:HA	16:H:125:LEU:HD12	2.00	0.44
1:B:186:THR:O	1:B:200:ARG:HG3	2.17	0.44
1:B:438:ARG:OXT	2:C:146:THR:OG1	2.35	0.44
3:D:382:PHE:HB3	3:D:532:VAL:HB	1.99	0.44
4:E:87:TYR:HD1	6:G:48:ILE:HD12	1.83	0.44
4:E:369:LYS:HD3	4:E:370:VAL:N	2.32	0.44
14:U:344:TYR:O	14:U:347:LEU:HD23	2.18	0.44
16:Q:327:VAL:O	16:Q:331:ASP:N	2.51	0.44
1:1:185:GLU:HB2	1:1:218:ILE:HD13	1.99	0.43
4:4:50:GLU:C	4:4:389:GLN:HE21	2.19	0.43
13:L:104:PHE:HE2	13:L:108:PHE:HE2	1.66	0.43
13:L:287:GLY:HA2	13:L:525:GLU:CG	2.48	0.43
13:L:380:SER:HA	13:L:457:GLY:HA2	2.00	0.43
16:H:203:PHE:HB2	16:H:263:PHE:CD2	2.52	0.43
1:B:18:TYR:OH	1:B:102:LYS:O	2.27	0.43
1:B:310:PRO:HG2	1:B:315:HIS:CD2	2.52	0.43
4:E:100:ALA:HB2	4:E:344:VAL:HG22	1.99	0.43
4:E:171:ASN:ND2	4:E:174:ARG:HH22	2.15	0.43
5:F:74:LEU:HD22	5:F:108:TRP:CH2	2.52	0.43
6:G:41:PHE:CE2	6:G:43:LEU:HD21	2.52	0.43
14:U:350:SER:OG	14:U:421:GLY:HA2	2.18	0.43
15:V:93:LEU:O	15:V:96:HIS:HB3	2.18	0.43
16:Q:28:PHE:O	16:Q:32:THR:HG23	2.17	0.43
16:Q:216:ARG:NH1	16:Q:294:ARG:HB3	2.33	0.43
3:3:185:LYS:O	3:3:189:ARG:HB2	2.17	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:3:281:GLU:HB2	3:3:288:ILE:HG22	2.01	0.43
9:W:1:MET:HG3	9:W:56:ASP:HB2	1.99	0.43
14:M:242:PHE:CE2	14:M:461:PHE:HD2	2.36	0.43
14:M:346:GLY:HA3	14:M:419:GLY:H	1.82	0.43
15:N:299:LEU:HD23	15:N:299:LEU:HA	1.83	0.43
3:D:526:GLU:HG2	3:D:679:ARG:HH22	1.83	0.43
6:G:64:GLY:HA2	16:Q:58:GLN:NE2	2.33	0.43
7:O:6:LEU:O	7:O:10:LEU:HD13	2.18	0.43
8:I:97:TYR:CE1	8:I:102:GLY:HA2	2.53	0.43
13:T:12:LEU:O	13:T:16:LEU:HG	2.18	0.43
14:U:24:LEU:O	14:U:27:LEU:HG	2.17	0.43
3:3:279:ALA:HB2	3:3:295:ARG:HH22	1.83	0.43
3:3:695:ARG:O	3:3:762:ALA:HB3	2.18	0.43
4:4:329:LYS:HA	4:4:329:LYS:HD2	1.80	0.43
5:5:68:PHE:CE1	5:5:96:GLU:HA	2.53	0.43
6:6:25:GLU:HA	6:6:28:VAL:HG12	1.99	0.43
13:L:538:TYR:O	13:L:542:ILE:HB	2.19	0.43
15:N:206:PRO:O	15:N:209:LEU:HB3	2.18	0.43
16:H:45:ARG:HG2	16:H:46:MET:N	2.33	0.43
1:B:157:TYR:O	1:B:158:LEU:HD23	2.18	0.43
3:D:200:LEU:HD12	3:D:213:THR:HB	2.00	0.43
3:D:356:LEU:HD22	3:D:638:LEU:HD12	2.01	0.43
7:O:52:LYS:HB2	7:O:112:ALA:HB2	1.99	0.43
13:T:255:ARG:HA	13:T:255:ARG:HD2	1.83	0.43
14:U:61:VAL:HG22	14:U:175:PHE:CD2	2.54	0.43
14:U:91:VAL:HB	14:U:95:PHE:CE1	2.53	0.43
16:Q:204:LEU:HD23	16:Q:204:LEU:HA	1.89	0.43
3:3:33:PHE:HZ	3:3:130:LEU:HA	1.82	0.43
3:3:123:ASP:HB2	3:3:236:LEU:HD13	2.00	0.43
4:4:288:LYS:HA	4:4:288:LYS:HD3	1.74	0.43
7:9:163:VAL:O	7:9:177:THR:HA	2.18	0.43
14:M:69:GLY:HA3	14:M:453:GLY:HA3	2.00	0.43
3:D:9:ARG:NH1	3:D:26:ALA:O	2.51	0.43
4:E:31:GLY:HA3	10:P:45:GLU:OE2	2.18	0.43
13:T:7:ILE:O	13:T:10:PRO:HD2	2.19	0.43
13:T:477:LEU:HA	13:T:477:LEU:HD12	1.86	0.43
15:V:124:TRP:CZ3	15:V:305:ASP:HB2	2.53	0.43
16:Q:90:VAL:HG21	16:Q:243:LEU:HB3	2.00	0.43
5:5:38:MET:HA	5:5:41:TYR:HB2	2.00	0.43
11:J:53:PHE:HE2	16:H:120:LEU:O	2.01	0.43
14:M:274:VAL:O	14:M:277:ALA:N	2.51	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
14:M:279:LYS:HD3	14:M:279:LYS:HA	1.77	0.43
16:H:255:ALA:O	16:H:259:ILE:HG13	2.18	0.43
16:H:287:LEU:O	16:H:291:ILE:HG13	2.19	0.43
1:B:298:PRO:HG3	1:B:408:TRP:HB3	2.00	0.43
1:B:374:ILE:HD13	1:B:421:TYR:CD2	2.54	0.43
3:D:13:VAL:HG21	3:D:17:THR:HG21	2.01	0.43
3:D:326:PHE:CD2	3:D:643:LEU:HD11	2.54	0.43
10:P:88:LEU:HD23	11:R:132:TYR:HB2	2.00	0.43
13:T:210:PHE:CD1	13:T:270:ILE:HG12	2.52	0.43
13:T:409:VAL:HA	13:T:412:LEU:HD12	2.00	0.43
15:V:98:LEU:HD12	15:V:107:MET:CG	2.47	0.43
16:Q:300:LEU:HD23	16:Q:305:LEU:HA	2.00	0.43
2:2:98:ASP:HB3	8:7:107:LYS:HZ2	1.84	0.43
4:4:115:THR:O	4:4:118:VAL:HG22	2.19	0.43
4:4:165:GLY:HA3	7:9:36:ARG:O	2.18	0.43
4:4:207:LEU:HD21	7:9:12:ILE:HD11	2.00	0.43
9:W:102:LEU:HG	9:W:110:LEU:HD13	2.00	0.43
10:A:110:GLU:HG3	10:A:111:TRP:N	2.31	0.43
13:L:477:LEU:HD12	13:L:477:LEU:HA	1.85	0.43
14:M:131:LEU:O	14:M:135:LEU:HD23	2.18	0.43
15:N:26:LYS:HD3	15:N:85:TYR:OH	2.19	0.43
16:H:43:GLN:HG2	16:H:43:GLN:H	1.71	0.43
1:B:275:LEU:HA	1:B:279:TRP:CD1	2.48	0.43
1:B:364:ALA:HB1	3:D:207:VAL:HG22	2.00	0.43
4:E:39:GLY:O	4:E:404:MET:HG3	2.18	0.43
10:P:44:TYR:O	10:P:50:PRO:HG3	2.18	0.43
13:T:94:TYR:CE1	13:T:341:HIS:HB2	2.37	0.43
13:T:287:GLY:HA2	13:T:525:GLU:HG3	2.00	0.43
14:U:347:LEU:HB2	14:U:414:PHE:HA	2.00	0.43
1:1:223:THR:O	1:1:227:VAL:HG23	2.19	0.43
1:1:288:GLN:HE21	1:1:331:ILE:HG22	1.84	0.43
1:1:293:GLY:O	1:1:327:GLY:N	2.52	0.43
3:3:358:SER:HB2	3:3:548:GLY:O	2.19	0.43
5:5:116:ARG:HB3	5:5:135:ILE:HG13	2.01	0.43
6:6:19:ILE:HG12	6:6:20:LEU:N	2.34	0.43
7:9:9:SER:OG	16:H:296:THR:HG22	2.18	0.43
7:9:94:ASN:OD1	7:9:97:ARG:N	2.52	0.43
7:9:133:LYS:O	7:9:137:LEU:CD1	2.47	0.43
8:7:43:ARG:HA	8:7:46:ARG:HH21	1.84	0.43
13:L:433:HIS:O	13:L:433:HIS:CG	2.71	0.43
16:H:2:THR:HG23	16:H:5:TYR:HB2	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
16:H:20:VAL:O	16:H:24:LEU:HD13	2.19	0.43
1:B:272:PHE:CZ	1:B:311:MET:HG2	2.54	0.43
6:G:43:LEU:HB2	6:G:82:GLY:HA3	2.00	0.43
6:G:154:LEU:O	6:G:158:VAL:HG13	2.18	0.43
7:O:42:VAL:HG22	7:O:114:VAL:O	2.19	0.43
14:U:22:ARG:HH11	14:U:92:GLU:HG3	1.83	0.43
16:Q:181:ASN:O	16:Q:185:ILE:HG13	2.18	0.43
4:4:26:MET:HG2	10:A:54:VAL:HB	2.00	0.43
4:4:366:TYR:CZ	5:5:148:LYS:HE3	2.54	0.43
13:L:427:GLY:O	13:L:428:GLU:HG2	2.18	0.43
1:B:246:SER:OG	1:B:312:SER:HB2	2.19	0.43
1:B:433:ARG:NH1	2:C:89:LYS:HE2	2.26	0.43
4:E:62:LEU:HA	4:E:62:LEU:HD23	1.78	0.43
4:E:381:LEU:HB3	4:E:382:PRO:HD3	2.01	0.43
6:G:99:MET:HG2	6:G:100:PRO:HD2	2.00	0.43
14:U:27:LEU:O	14:U:31:LEU:HD13	2.19	0.43
14:U:206:PRO:HD2	14:U:293:MET:HG3	2.01	0.43
16:Q:147:TYR:CE1	16:Q:228:LEU:HD13	2.54	0.43
16:Q:212:ALA:HA	16:Q:218:PRO:HG3	2.00	0.43
16:Q:289:PHE:O	16:Q:293:ILE:HG12	2.19	0.43
1:1:18:TYR:CZ	1:1:263:VAL:HG11	2.53	0.43
3:3:266:THR:HG21	3:3:278:ARG:HH12	1.83	0.43
3:3:347:HIS:HB2	3:3:538:ALA:CB	2.49	0.43
3:3:583:VAL:HG23	3:3:598:ALA:HA	2.01	0.43
6:6:140:CYS:SG	7:9:99:ILE:HG13	2.59	0.43
6:6:164:ASN:ND2	6:6:168:GLU:HB2	2.33	0.43
11:J:36:PHE:CE2	11:J:59:TYR:HB3	2.54	0.43
15:N:87:LEU:HB3	15:N:117:PRO:HB2	2.01	0.43
3:D:5:LYS:O	3:D:93:VAL:N	2.48	0.43
3:D:149:LEU:HD12	4:E:108:VAL:HG23	2.01	0.43
5:F:144:HIS:HB2	5:F:147:ARG:HD3	2.00	0.43
7:O:93:ILE:HD12	7:O:136:MET:SD	2.59	0.43
13:T:214:VAL:HG12	13:T:222:LEU:HB2	2.01	0.43
14:U:88:VAL:HG22	14:U:331:ARG:HE	1.84	0.43
14:U:148:PHE:O	14:U:152:THR:HG23	2.19	0.43
15:V:181:VAL:HA	15:V:192:PHE:CE2	2.54	0.43
16:Q:150:LEU:HD21	16:Q:154:ARG:NH1	2.33	0.43
1:1:50:PRO:HA	1:1:53:VAL:HG12	2.01	0.43
1:1:171:LEU:HD23	1:1:171:LEU:HA	1.79	0.43
3:3:34:CYS:HB2	3:3:44:ALA:HB3	2.01	0.43
3:3:398:VAL:HG22	3:3:506:ILE:HD12	2.01	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:4:73:ARG:NH2	7:9:64:PRO:O	2.52	0.43
6:6:106:ILE:HD11	6:6:154:LEU:HD22	2.00	0.43
13:L:30:GLY:HA3	13:L:92:ILE:HG12	2.01	0.43
14:M:75:PHE:CZ	14:M:111:ALA:HB2	2.54	0.43
14:M:217:PHE:CE2	14:M:231:GLY:HA3	2.54	0.43
3:D:5:LYS:HA	3:D:9:ARG:O	2.19	0.43
3:D:526:GLU:OE2	3:D:679:ARG:NH1	2.51	0.43
3:D:585:MET:HB3	3:D:587:LEU:CD1	2.49	0.43
5:F:78:PRO:HA	5:F:83:GLY:HA3	2.00	0.43
16:Q:96:ALA:HB2	16:Q:128:VAL:HG21	2.01	0.43
16:Q:141:TRP:CE3	16:Q:149:LEU:HD11	2.54	0.43
16:Q:236:TYR:HB2	16:Q:241:TRP:HB2	2.01	0.43
2:2:162:ARG:NH2	2:2:165:GLU:OE1	2.51	0.42
3:3:356:LEU:CD1	3:3:653:PRO:HD2	2.49	0.42
4:4:130:LEU:HD22	4:4:149:ALA:HB1	2.01	0.42
4:4:382:PRO:O	4:4:386:LYS:HB2	2.19	0.42
13:L:202:LEU:HD12	13:L:202:LEU:HA	1.82	0.42
13:L:285:ALA:O	13:L:294:ILE:HG13	2.18	0.42
13:L:549:LEU:O	13:L:553:LEU:HG	2.19	0.42
14:M:114:ASP:HB3	14:M:176:LEU:HD23	1.99	0.42
14:M:138:GLY:HA3	14:M:220:GLU:HB3	2.00	0.42
15:N:260:TYR:HA	15:N:263:ILE:HD12	2.01	0.42
16:H:208:ILE:HG21	16:H:308:PHE:CE1	2.54	0.42
2:C:106:ILE:HG22	2:C:107:GLY:N	2.34	0.42
3:D:310:LEU:HD23	3:D:319:GLU:HA	1.99	0.42
3:D:648:LEU:HD23	3:D:648:LEU:HA	1.83	0.42
4:E:138:LEU:HD13	4:E:143:LEU:HA	2.01	0.42
4:E:247:ASP:OD1	4:E:249:ARG:HG3	2.19	0.42
4:E:306:ASN:HD21	5:F:192:TYR:HH	1.61	0.42
8:I:71:ASP:OD2	8:I:81:ARG:NH2	2.46	0.42
8:I:105:THR:N	8:I:108:ILE:O	2.45	0.42
13:T:561:LEU:HG	13:T:565:PHE:CE2	2.54	0.42
14:U:157:LEU:HD23	14:U:157:LEU:HA	1.87	0.42
16:Q:39:LEU:CD2	16:Q:295:ALA:HB2	2.48	0.42
1:1:404:ASP:OD1	1:1:404:ASP:N	2.50	0.42
18:1:502:FMN:C9	19:1:503:NAI:H52N	2.49	0.42
3:3:50:VAL:HG12	3:3:95:THR:HG22	2.01	0.42
3:3:368:HIS:HB2	3:3:556:ALA:O	2.19	0.42
3:3:585:MET:HB3	3:3:587:LEU:HD13	2.00	0.42
4:4:86:ASP:HB3	4:4:93:HIS:HD2	1.85	0.42
4:4:350:ARG:O	4:4:373:PRO:HB2	2.18	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:5:41:TYR:HD1	5:5:46:PHE:HE2	1.67	0.42
9:W:72:GLU:O	9:W:76:GLU:HG3	2.19	0.42
9:W:102:LEU:HG	9:W:110:LEU:CD1	2.49	0.42
13:L:162:ASN:ND2	13:L:166:ASP:OD2	2.51	0.42
14:M:371:LEU:HD13	14:M:371:LEU:HA	1.87	0.42
1:B:104:ARG:O	1:B:108:GLU:HG3	2.19	0.42
4:E:72:HIS:ND1	5:F:152:LEU:HD22	2.34	0.42
4:E:240:ARG:HG3	4:E:278:VAL:HG11	2.00	0.42
5:F:176:GLY:O	5:F:185:LYS:NZ	2.43	0.42
6:G:115:GLY:HA3	6:G:125:GLN:OE1	2.18	0.42
13:T:321:HIS:HD2	13:T:388:ILE:HD12	1.84	0.42
13:T:419:ARG:HB2	13:T:512:PHE:CE2	2.53	0.42
1:1:241:MET:SD	1:1:249:MET:HB3	2.59	0.42
3:3:688:ARG:HD3	3:3:688:ARG:HA	1.65	0.42
4:4:115:THR:O	4:4:119:ILE:HG13	2.19	0.42
4:4:131:VAL:HG23	4:4:153:ARG:HD2	2.01	0.42
4:4:304:ASP:O	4:4:310:THR:OG1	2.11	0.42
13:L:33:ALA:HB2	13:L:109:ASN:HD21	1.84	0.42
13:L:39:ALA:O	13:L:43:LEU:HG	2.19	0.42
2:C:66:PHE:CZ	3:D:205:ARG:HD3	2.54	0.42
3:D:188:VAL:HG11	3:D:201:ASP:HA	2.02	0.42
4:E:310:THR:HG22	4:E:311:PRO:O	2.18	0.42
5:F:41:TYR:HA	5:F:44:MET:HE3	2.01	0.42
6:G:19:ILE:HG12	6:G:20:LEU:N	2.33	0.42
6:G:56:ALA:O	7:O:22:VAL:HG12	2.19	0.42
8:I:23:TYR:OH	8:I:120:ASP:HA	2.18	0.42
14:U:131:LEU:O	14:U:135:LEU:HD23	2.19	0.42
15:V:3:LEU:HD13	15:V:96:HIS:CD2	2.54	0.42
15:V:114:LEU:C	15:V:114:LEU:HD12	2.39	0.42
1:1:253:GLN:HG2	1:1:327:GLY:HA2	2.01	0.42
1:1:291:ILE:HD11	1:1:331:ILE:HD11	2.01	0.42
3:3:46:ARG:HH22	3:3:81:ALA:HB2	1.84	0.42
3:3:722:THR:HG21	3:3:756:GLY:N	2.34	0.42
4:4:261:THR:N	4:4:292:GLN:HE22	2.03	0.42
6:6:83:ARG:HB2	6:6:123:ILE:HD12	2.01	0.42
6:6:143:ARG:HG3	6:6:144:PRO:HD2	2.00	0.42
10:A:97:LEU:O	10:A:101:LEU:HG	2.19	0.42
11:J:146:LEU:O	11:J:150:THR:HG23	2.19	0.42
12:K:15:VAL:O	12:K:19:LEU:HG	2.19	0.42
13:L:239:LEU:HD12	13:L:239:LEU:HA	1.86	0.42
13:L:348:ASP:OD1	13:L:350:ARG:HG2	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:L:380:SER:CB	13:L:456:ALA:HB3	2.49	0.42
13:L:459:LEU:HD23	13:L:459:LEU:HA	1.90	0.42
15:N:97:LEU:HD23	15:N:97:LEU:HA	1.94	0.42
1:B:145:LEU:HD23	1:B:145:LEU:HA	1.89	0.42
1:B:189:MET:HE1	1:B:210:GLY:HA2	2.02	0.42
2:C:132:PRO:HG2	2:C:145:VAL:HB	2.00	0.42
3:D:256:CYS:O	3:D:262:GLY:HA2	2.19	0.42
3:D:341:VAL:HA	3:D:565:TYR:O	2.19	0.42
3:D:513:GLN:NE2	3:D:769:LEU:HD21	2.35	0.42
6:G:62:ARG:HB3	16:Q:50:ARG:HB2	2.00	0.42
11:R:72:MET:HG2	16:Q:141:TRP:CE3	2.54	0.42
12:S:78:ILE:CD1	15:V:134:LEU:HB2	2.48	0.42
14:U:318:SER:HA	14:U:321:TYR:CE1	2.54	0.42
16:Q:185:ILE:HG22	16:Q:189:GLN:OE1	2.19	0.42
16:Q:267:TRP:CD1	16:Q:275:PRO:HA	2.53	0.42
3:3:46:ARG:NH2	3:3:81:ALA:HB2	2.34	0.42
3:3:271:SER:HG	7:9:69:TYR:HH	1.55	0.42
4:4:127:ALA:O	4:4:153:ARG:NH1	2.52	0.42
6:6:43:LEU:HD11	6:6:84:LEU:HD23	2.01	0.42
14:M:33:PHE:HA	14:M:79:ALA:HB1	2.00	0.42
15:N:61:VAL:O	15:N:65:LEU:HG	2.20	0.42
1:B:292:PRO:HA	1:B:328:VAL:HG13	2.01	0.42
3:D:385:ALA:O	3:D:533:LEU:HD21	2.19	0.42
3:D:445:THR:HB	3:D:463:ALA:HB2	2.02	0.42
4:E:29:ASN:HD22	10:P:49:ASP:HB3	1.84	0.42
6:G:151:VAL:O	6:G:155:GLN:HB2	2.19	0.42
10:P:41:LEU:HD23	16:Q:72:ILE:HD11	2.02	0.42
14:U:13:GLY:HA2	14:U:97:GLY:HA2	2.01	0.42
14:U:55:LEU:HD11	15:V:416:PRO:HD2	2.00	0.42
14:U:304:THR:O	14:U:306:GLU:N	2.52	0.42
14:U:436:SER:O	14:U:440:LEU:HD13	2.19	0.42
15:V:77:VAL:HG12	15:V:85:TYR:HE1	1.83	0.42
1:1:245:GLN:HB2	1:1:314:GLU:CD	2.40	0.42
2:2:15:PHE:HE1	2:2:53:VAL:HG23	1.84	0.42
2:2:110:GLU:OE1	8:7:114:ARG:HG3	2.20	0.42
3:3:470:PRO:HD3	3:3:759:TYR:OH	2.19	0.42
9:W:113:ARG:O	9:W:117:ILE:HG12	2.20	0.42
13:L:128:PHE:CZ	13:L:166:ASP:HB3	2.55	0.42
15:N:332:SER:O	15:N:341:GLY:HA3	2.20	0.42
16:H:99:LEU:HD12	16:H:116:ILE:HG13	2.02	0.42
16:H:131:LEU:HA	16:H:134:TYR:HB2	2.02	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
16:H:218:PRO:C	16:H:220:ASP:H	2.22	0.42
1:B:90:ILE:HB	1:B:218:ILE:HG12	2.01	0.42
2:C:162:ARG:NH2	2:C:165:GLU:OE2	2.53	0.42
3:D:572:PRO:HD2	3:D:577:LEU:HD21	2.01	0.42
3:D:697:THR:OG1	3:D:763:LEU:HA	2.19	0.42
10:P:61:PHE:HE1	16:Q:302:TYR:OH	2.03	0.42
11:R:40:ALA:O	11:R:44:VAL:HG23	2.20	0.42
11:R:146:LEU:O	11:R:150:THR:HG23	2.20	0.42
13:T:287:GLY:HA2	13:T:525:GLU:CG	2.50	0.42
13:T:365:HIS:HD2	13:T:450:ALA:HB2	1.85	0.42
14:U:452:ARG:HA	14:U:452:ARG:HD3	1.83	0.42
15:V:368:SER:O	15:V:371:SER:OG	2.25	0.42
1:1:211:LEU:HD12	1:1:211:LEU:HA	1.75	0.42
3:3:574:GLU:HG3	3:3:593:LEU:HD11	2.00	0.42
3:3:672:ALA:O	3:3:673:MET:HB2	2.19	0.42
4:4:236:GLY:O	4:4:238:SER:N	2.51	0.42
11:J:53:PHE:O	11:J:57:ILE:HG13	2.19	0.42
13:L:90:TYR:CG	13:L:334:LEU:HD13	2.54	0.42
13:L:214:VAL:HG22	13:L:219:GLN:HB2	2.01	0.42
13:L:582:GLN:CD	15:N:194:PHE:HA	2.40	0.42
14:M:329:ALA:O	14:M:332:LEU:HG	2.19	0.42
15:N:204:PRO:O	15:N:208:VAL:HG23	2.20	0.42
15:N:290:LEU:HD13	15:N:408:LEU:HB3	2.02	0.42
1:B:193:GLU:OE1	1:B:211:LEU:HD12	2.20	0.42
1:B:334:ARG:HG2	1:B:434:PRO:HG3	2.02	0.42
1:B:381:GLU:O	1:B:385:GLU:HG3	2.20	0.42
3:D:381:LEU:HD12	3:D:522:ARG:HD3	2.02	0.42
4:E:46:THR:O	4:E:53:LEU:HB2	2.19	0.42
4:E:73:ARG:NH2	6:G:117:MET:O	2.52	0.42
6:G:30:TRP:O	6:G:34:ASN:ND2	2.48	0.42
13:T:290:ASP:OD1	13:T:291:ILE:N	2.53	0.42
1:1:3:GLY:HA2	1:1:4:PRO:HD3	1.87	0.42
3:3:248:GLU:HG2	5:5:170:PHE:CE1	2.54	0.42
6:6:163:TYR:OH	6:6:169:ARG:NH2	2.53	0.42
10:A:71:PHE:O	10:A:74:GLU:HB3	2.20	0.42
11:J:102:GLY:O	11:J:106:ALA:N	2.50	0.42
11:J:104:LEU:O	11:J:108:LEU:HD12	2.20	0.42
11:J:135:TRP:CZ3	15:N:105:LEU:HD22	2.49	0.42
13:L:7:ILE:O	13:L:10:PRO:HD2	2.20	0.42
14:M:203:ILE:HA	14:M:210:LEU:HB3	2.01	0.42
14:M:244:PHE:O	14:M:248:LEU:HB2	2.20	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
15:N:190:ALA:HA	15:N:192:PHE:N	2.35	0.42
16:H:48:PRO:C	16:H:50:ARG:H	2.23	0.42
16:H:82:PHE:HA	16:H:236:TYR:OH	2.20	0.42
16:H:108:PHE:O	16:H:108:PHE:CG	2.73	0.42
1:B:176:GLY:O	2:C:32:ARG:NH2	2.51	0.42
2:C:4:PHE:HB2	2:C:48:GLU:OE2	2.20	0.42
3:D:507:LEU:HD22	3:D:511:VAL:HG11	2.01	0.42
3:D:716:LEU:HD21	3:D:758:LEU:HB3	2.00	0.42
4:E:60:GLY:N	4:E:408:ASP:OD1	2.48	0.42
9:X:51:HIS:HA	9:X:56:ASP:OD1	2.20	0.42
11:R:144:PHE:CE1	15:V:93:LEU:HD22	2.55	0.42
12:S:46:ALA:HB2	12:S:53:GLY:HA3	2.01	0.42
13:T:27:PRO:O	13:T:31:VAL:HG23	2.19	0.42
13:T:291:ILE:O	13:T:294:ILE:HG22	2.19	0.42
14:U:37:LEU:O	14:U:41:LEU:HG	2.20	0.42
3:3:585:MET:SD	3:3:594:ALA:HB2	2.60	0.42
4:4:202:ASP:HA	4:4:284:ARG:HH21	1.84	0.42
4:4:236:GLY:C	4:4:238:SER:H	2.23	0.42
10:A:18:LEU:O	10:A:22:VAL:HG23	2.19	0.42
13:L:290:ASP:OD1	13:L:291:ILE:N	2.53	0.42
13:L:554:PHE:CZ	14:M:283:THR:HG21	2.54	0.42
13:L:574:LEU:HD22	15:N:246:LEU:CD1	2.49	0.42
14:M:30:GLY:O	14:M:34:LEU:HG	2.20	0.42
14:M:327:LEU:O	14:M:331:ARG:HG2	2.20	0.42
14:M:348:ALA:HB2	14:M:414:PHE:HB3	2.02	0.42
15:N:217:ALA:HA	15:N:285:LEU:CD2	2.49	0.42
15:N:259:ALA:O	15:N:263:ILE:HG13	2.20	0.42
3:D:459:MET:HG2	3:D:465:HIS:CB	2.49	0.42
3:D:470:PRO:HD3	3:D:759:TYR:OH	2.20	0.42
4:E:101:VAL:O	4:E:105:LEU:HG	2.20	0.42
4:E:239:LEU:HG	4:E:244:VAL:HB	2.01	0.42
6:G:109:GLY:HA2	6:G:142:PRO:HD3	2.01	0.42
6:G:135:VAL:HG21	6:G:154:LEU:HB2	2.02	0.42
7:O:33:LEU:HB2	7:O:163:VAL:HG12	2.00	0.42
14:U:186:GLN:HG2	14:U:187:GLU:H	1.85	0.42
15:V:73:THR:HG21	15:V:210:PHE:HB2	2.02	0.42
16:Q:147:TYR:CE1	16:Q:229:VAL:HG22	2.54	0.42
16:Q:237:SER:OG	16:Q:238:SER:N	2.52	0.42
16:Q:293:ILE:HG23	16:Q:297:TRP:CE3	2.55	0.42
16:Q:343:LEU:O	16:Q:347:VAL:HG23	2.20	0.42
1:1:343:ASN:HA	1:1:346:ARG:HG2	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:3:268:ASP:OD1	3:3:278:ARG:NH1	2.53	0.42
8:7:20:MET:HG2	8:7:115:PHE:CZ	2.55	0.42
13:L:435:PRO:HG2	13:L:436:HIS:HD2	1.84	0.42
15:N:190:ALA:N	15:N:240:SER:OG	2.53	0.42
16:H:189:GLN:O	16:H:193:GLY:HA2	2.20	0.42
16:H:310:TRP:HA	16:H:314:PHE:CD2	2.55	0.42
1:B:75:LYS:NZ	1:B:218:ILE:O	2.48	0.42
13:T:159:PHE:HD2	14:U:407:LEU:HD11	1.85	0.42
13:T:313:GLY:HA2	13:T:315:TYR:CZ	2.54	0.42
1:1:339:ASP:OD1	1:1:433:ARG:NH2	2.53	0.41
3:3:384:PRO:O	3:3:531:LYS:HD3	2.19	0.41
3:3:409:LEU:HD23	3:3:409:LEU:HA	1.63	0.41
4:4:50:GLU:O	4:4:390:VAL:HG23	2.20	0.41
4:4:59:ILE:HB	4:4:408:ASP:OD1	2.20	0.41
4:4:167:ARG:HD3	6:6:143:ARG:NH1	2.28	0.41
4:4:172:TYR:CE2	4:4:178:VAL:HB	2.55	0.41
4:4:176:GLY:HA3	4:4:304:ASP:H	1.83	0.41
8:7:120:ASP:O	8:7:124:GLU:HG3	2.20	0.41
9:W:38:GLN:HG3	9:W:93:VAL:HG21	2.02	0.41
13:L:433:HIS:ND1	13:L:437:GLU:OE2	2.44	0.41
14:M:131:LEU:HD23	14:M:131:LEU:HA	1.85	0.41
14:M:371:LEU:HD11	14:M:441:LEU:HD12	2.02	0.41
15:N:3:LEU:HD13	15:N:96:HIS:HD2	1.84	0.41
15:N:63:THR:HG22	15:N:96:HIS:HA	2.02	0.41
1:B:404:ASP:HA	1:B:407:VAL:HG22	2.02	0.41
3:D:248:GLU:OE2	7:O:57:SER:OG	2.36	0.41
4:E:84:ARG:CZ	4:E:169:HIS:HB3	2.50	0.41
7:O:43:LEU:HD12	7:O:133:LYS:HG3	2.01	0.41
14:U:163:VAL:HG22	14:U:175:PHE:CE1	2.55	0.41
14:U:292:HIS:NE2	14:U:365:MET:HG3	2.35	0.41
14:U:426:ALA:HB3	14:U:429:GLU:HG3	2.02	0.41
15:V:196:THR:HB	15:V:197:PRO:HD3	2.01	0.41
3:3:29:ASP:OD1	3:3:29:ASP:N	2.54	0.41
3:3:387:LEU:HA	3:3:387:LEU:HD23	1.74	0.41
3:3:460:LYS:HA	3:3:460:LYS:HD3	1.94	0.41
3:3:504:VAL:HG12	3:3:506:ILE:HG13	2.02	0.41
3:3:533:LEU:HA	3:3:533:LEU:HD23	1.75	0.41
3:3:689:LYS:H	3:3:689:LYS:HG2	1.34	0.41
4:4:314:ARG:NH1	7:9:106:GLU:O	2.53	0.41
8:7:23:TYR:OH	8:7:123:ARG:HD3	2.20	0.41
11:J:16:GLY:O	11:J:19:VAL:HG12	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
14:M:8:LEU:HB3	14:M:9:PRO:HD3	2.02	0.41
14:M:17:LEU:HD11	14:M:98:LEU:HD23	2.01	0.41
14:M:321:TYR:CE1	14:M:365:MET:HA	2.55	0.41
14:M:346:GLY:HA3	14:M:418:GLY:HA2	2.02	0.41
15:N:101:THR:HG21	15:N:106:LEU:HD23	2.01	0.41
3:D:149:LEU:HG	4:E:305:PRO:HD2	2.01	0.41
3:D:561:PRO:HB3	3:D:575:GLU:O	2.20	0.41
4:E:59:ILE:HB	4:E:408:ASP:OD1	2.19	0.41
4:E:88:LEU:HD21	6:G:48:ILE:HD13	2.02	0.41
5:F:31:ARG:HH22	5:F:98:ASP:CG	2.23	0.41
10:P:7:TYR:N	10:P:7:TYR:HD1	2.18	0.41
11:R:100:VAL:O	11:R:104:LEU:HG	2.20	0.41
13:T:437:GLU:O	13:T:439:PRO:HD3	2.19	0.41
13:T:469:LEU:HA	13:T:469:LEU:HD12	1.82	0.41
14:U:426:ALA:N	14:U:429:GLU:OE1	2.39	0.41
16:Q:48:PRO:C	16:Q:50:ARG:N	2.73	0.41
16:Q:269:MET:HG3	16:Q:270:PRO:HD2	2.01	0.41
1:1:207:ALA:O	1:1:215:PRO:HB3	2.21	0.41
3:3:327:LEU:HD23	3:3:327:LEU:HA	1.83	0.41
3:3:715:GLU:H	3:3:761:SER:HB2	1.85	0.41
6:6:57:ARG:O	7:9:24:VAL:HG22	2.20	0.41
8:7:63:LEU:HD11	8:7:129:ALA:HB3	2.00	0.41
13:L:128:PHE:CE1	13:L:166:ASP:HB3	2.55	0.41
13:L:352:MET:SD	13:L:424:VAL:HG13	2.60	0.41
13:L:372:ALA:O	13:L:381:GLY:HA3	2.21	0.41
14:M:306:GLU:H	14:M:306:GLU:HG3	1.63	0.41
15:N:73:THR:O	15:N:77:VAL:HG23	2.20	0.41
16:H:153:LEU:HD23	16:H:153:LEU:HA	1.75	0.41
16:H:187:ASN:O	16:H:190:LYS:HB3	2.19	0.41
1:B:4:PRO:HA	1:B:12:ARG:NH1	2.29	0.41
1:B:298:PRO:HD2	1:B:321:SER:HA	2.02	0.41
2:C:79:HIS:N	2:C:137:ASN:OD1	2.52	0.41
3:D:175:ILE:HG22	3:D:236:LEU:HB2	2.02	0.41
3:D:347:HIS:HB2	3:D:538:ALA:HB1	2.02	0.41
4:E:272:VAL:N	4:E:275:ARG:HH21	2.18	0.41
5:F:116:ARG:CZ	5:F:135:ILE:HD11	2.49	0.41
6:G:36:LEU:CD1	6:G:155:GLN:HG3	2.50	0.41
8:I:8:GLU:HG2	8:I:97:TYR:CZ	2.55	0.41
9:X:113:ARG:O	9:X:117:ILE:HG12	2.20	0.41
10:P:10:THR:OG1	16:Q:118:LEU:HD21	2.21	0.41
12:S:7:SER:CB	12:S:40:LEU:HD23	2.47	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
15:V:136:TYR:HB2	15:V:199:VAL:HG21	2.02	0.41
16:Q:134:TYR:HA	16:Q:137:PHE:HE2	1.84	0.41
16:Q:224:ALA:HA	16:Q:229:VAL:HA	2.02	0.41
2:2:45:ARG:O	2:2:49:ILE:HG13	2.20	0.41
3:3:118:ASP:O	3:3:122:CYS:N	2.53	0.41
4:4:74:THR:HG22	4:4:75:TYR:N	2.35	0.41
7:9:34:LYS:HB3	7:9:35:PRO:HD2	2.02	0.41
12:K:23:THR:HG22	12:K:85:THR:OG1	2.21	0.41
13:L:450:ALA:O	13:L:454:VAL:HG23	2.21	0.41
1:B:97:GLU:HB2	19:B:503:NAI:H42N	2.02	0.41
2:C:129:HIS:CD2	2:C:130:THR:HG23	2.55	0.41
8:I:105:THR:HG1	8:I:108:ILE:HB	1.86	0.41
13:T:327:PHE:CE1	13:T:452:GLY:HA3	2.55	0.41
13:T:564:TYR:CZ	14:U:151:PHE:HZ	2.38	0.41
14:U:289:GLY:O	14:U:293:MET:HG2	2.19	0.41
15:V:302:ILE:HG12	15:V:391:PHE:HD1	1.84	0.41
1:1:29:LEU:HD23	1:1:155:ARG:HD2	2.02	0.41
3:3:127:ALA:HB2	5:5:181:LEU:HB3	2.03	0.41
3:3:242:PHE:HE2	7:9:85:GLU:O	2.04	0.41
3:3:661:GLN:HE22	3:3:664:LEU:HD12	1.85	0.41
4:4:154:GLU:OE1	6:6:57:ARG:HD3	2.21	0.41
4:4:374:SER:HB2	4:4:406:ASP:HB3	2.02	0.41
6:6:115:GLY:HA3	6:6:125:GLN:OE1	2.21	0.41
6:6:143:ARG:O	6:6:146:ALA:N	2.54	0.41
12:K:71:GLY:HA3	15:N:137:PHE:CZ	2.55	0.41
13:L:419:ARG:HB2	13:L:512:PHE:CE2	2.56	0.41
13:L:553:LEU:HB3	14:M:270:TYR:CE2	2.55	0.41
14:M:70:LEU:O	14:M:73:LEU:HD23	2.20	0.41
16:H:134:TYR:HA	16:H:137:PHE:CE2	2.55	0.41
1:B:343:ASN:OD1	2:C:86:LEU:N	2.54	0.41
2:C:154:LEU:HD23	2:C:154:LEU:HA	1.86	0.41
3:D:8:ASP:OD2	3:D:28:TYR:OH	2.39	0.41
4:E:125:ARG:HD2	4:E:286:SER:OG	2.21	0.41
5:F:6:VAL:HG22	5:F:41:TYR:CE1	2.56	0.41
13:T:356:TRP:O	13:T:363:ARG:HD3	2.20	0.41
15:V:140:GLY:HA2	15:V:185:PHE:CZ	2.56	0.41
15:V:334:LEU:HD13	15:V:375:TYR:HD2	1.85	0.41
16:Q:267:TRP:O	16:Q:269:MET:N	2.53	0.41
1:1:261:PRO:HD2	2:2:177:HIS:O	2.20	0.41
3:3:678:PHE:CZ	3:3:680:LEU:HD13	2.56	0.41
6:6:41:PHE:HE2	6:6:88:MET:HE2	1.85	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:7:74:PRO:HG2	8:7:77:ALA:CB	2.51	0.41
11:J:46:LEU:HD23	11:J:46:LEU:HA	1.81	0.41
13:L:267:SER:HB3	13:L:311:GLY:O	2.21	0.41
13:L:469:LEU:HA	13:L:469:LEU:HD12	1.79	0.41
13:L:517:PHE:O	13:L:522:LEU:HG	2.20	0.41
15:N:58:VAL:O	15:N:62:PHE:HD1	2.03	0.41
16:H:70:GLU:O	16:H:237:SER:OG	2.31	0.41
16:H:333:PRO:HG2	16:H:336:TYR:CG	2.55	0.41
1:B:261:PRO:HD2	2:C:177:HIS:O	2.21	0.41
3:D:140:TYR:CE2	3:D:142:LYS:HA	2.56	0.41
6:G:44:ALA:O	6:G:47:ALA:N	2.41	0.41
11:R:103:ILE:O	11:R:107:GLY:N	2.45	0.41
13:T:13:GLY:HA3	13:T:36:LEU:HD13	2.02	0.41
13:T:335:ALA:O	13:T:339:VAL:HG23	2.20	0.41
13:T:414:ALA:HB1	13:T:505:LEU:HD23	2.02	0.41
14:U:177:LEU:HD11	14:U:248:LEU:HD11	2.03	0.41
15:V:73:THR:O	15:V:77:VAL:HG23	2.20	0.41
15:V:74:VAL:HG23	15:V:88:VAL:HG11	2.02	0.41
1:1:51:ASP:OD1	1:1:81:LYS:HD3	2.20	0.41
2:2:77:LYS:H	2:2:116:LEU:HA	1.86	0.41
3:3:423:PRO:HB2	3:3:431:PRO:HG3	2.03	0.41
4:4:271:ASP:OD1	4:4:274:ASP:HB2	2.20	0.41
14:M:215:PRO:CG	14:M:216:PRO:HD3	2.50	0.41
14:M:221:ASN:HB3	14:M:227:ALA:HB3	2.03	0.41
14:M:344:TYR:O	14:M:347:LEU:HD23	2.20	0.41
15:N:62:PHE:CE2	15:N:285:LEU:HD22	2.56	0.41
16:H:202:ALA:O	16:H:205:VAL:HG22	2.21	0.41
1:B:183:GLY:HA3	18:B:502:FMN:O4	2.21	0.41
13:T:119:VAL:HA	13:T:251:TYR:CZ	2.55	0.41
14:U:102:MET:HB3	14:U:230:LEU:HD23	2.03	0.41
14:U:187:GLU:HG2	14:U:188:GLU:HG3	2.02	0.41
16:Q:8:ASP:OD2	16:Q:112:GLN:HB2	2.21	0.41
1:1:41:ALA:N	1:1:116:GLU:OE2	2.48	0.41
3:3:360:LEU:HD11	3:3:645:ALA:HB2	2.03	0.41
4:4:212:PRO:HG2	4:4:213:ILE:HD12	2.02	0.41
5:5:2:ARG:HG3	5:5:84:ASP:OD2	2.21	0.41
5:5:80:TRP:HA	5:5:80:TRP:HE3	1.85	0.41
13:L:321:HIS:HA	13:L:384:SER:HB2	2.02	0.41
13:L:391:ALA:O	13:L:395:TYR:HB2	2.19	0.41
13:L:598:LEU:HD23	13:L:598:LEU:HA	1.84	0.41
15:N:41:LEU:O	15:N:44:TRP:HB2	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:3:GLY:HA2	1:B:4:PRO:HD3	1.89	0.41
1:B:193:GLU:CD	1:B:200:ARG:HH22	2.24	0.41
3:D:533:LEU:HA	3:D:533:LEU:HD23	1.77	0.41
4:E:177:GLY:HA3	4:E:302:VAL:O	2.20	0.41
7:O:22:VAL:HB	16:Q:44:VAL:CG1	2.51	0.41
11:R:72:MET:CE	16:Q:153:LEU:HD21	2.51	0.41
13:T:154:SER:HB2	13:T:228:ASP:HB3	2.03	0.41
13:T:168:GLY:HA3	13:T:211:LEU:HD22	2.02	0.41
13:T:538:TYR:O	13:T:542:ILE:HB	2.20	0.41
14:U:164:LEU:HD21	15:V:346:TYR:HE1	1.85	0.41
16:Q:85:ALA:CB	16:Q:139:SER:HB2	2.50	0.41
16:Q:268:THR:HA	16:Q:273:GLU:OE1	2.21	0.41
1:1:63:ARG:HD3	1:1:313:TYR:CD2	2.56	0.41
1:1:354:GLY:HA2	1:1:360:ARG:HB2	2.02	0.41
2:2:89:LYS:HE3	2:2:94:GLU:HG2	2.02	0.41
2:2:147:ARG:HE	2:2:147:ARG:HB2	1.58	0.41
3:3:655:ARG:HH22	3:3:659:GLU:HG3	1.85	0.41
3:3:664:LEU:HB3	3:3:669:VAL:HG11	2.03	0.41
3:3:688:ARG:CZ	3:3:769:LEU:HD22	2.51	0.41
5:5:35:LYS:HA	5:5:35:LYS:HD2	1.88	0.41
6:6:18:GLY:HA3	6:6:32:ARG:HH21	1.85	0.41
6:6:163:TYR:H	7:9:152:ARG:HH12	1.67	0.41
10:A:56:ARG:HB3	11:J:73:LEU:O	2.21	0.41
13:L:49:LEU:HD23	13:L:49:LEU:HA	1.96	0.41
13:L:68:LEU:HD23	13:L:255:ARG:NH2	2.33	0.41
14:M:85:GLY:O	14:M:89:ALA:HB2	2.20	0.41
15:N:73:THR:HG21	15:N:210:PHE:HB2	2.03	0.41
16:H:119:ASP:OD1	16:H:120:LEU:HG	2.20	0.41
1:B:66:GLY:O	19:B:503:NAI:H2N	2.21	0.41
1:B:145:LEU:O	1:B:149:ILE:HG13	2.20	0.41
1:B:404:ASP:N	1:B:404:ASP:OD1	2.54	0.41
3:D:49:LEU:HD23	3:D:81:ALA:HA	2.02	0.41
3:D:201:ASP:OD1	3:D:202:PHE:N	2.49	0.41
3:D:567:TYR:HA	3:D:584:VAL:O	2.21	0.41
4:E:87:TYR:HB3	6:G:45:CYS:HB3	2.01	0.41
4:E:132:PHE:HE1	4:E:398:ALA:O	2.03	0.41
4:E:154:GLU:OE1	6:G:57:ARG:NH1	2.54	0.41
4:E:288:LYS:HD3	4:E:288:LYS:HA	1.69	0.41
6:G:132:PRO:HG3	6:G:178:ARG:CZ	2.51	0.41
7:O:98:CYS:SG	7:O:100:PHE:CD1	3.14	0.41
9:X:49:LEU:HD13	9:X:58:LEU:HD13	2.03	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:R:5:GLU:O	11:R:9:LEU:HG	2.21	0.41
11:R:115:PHE:CD1	12:S:48:ALA:HB2	2.56	0.41
13:T:29:PRO:HB2	13:T:101:TYR:HD2	1.85	0.41
13:T:41:PHE:HD1	13:T:81:THR:OG1	2.04	0.41
13:T:324:THR:HG22	13:T:380:SER:HB2	2.03	0.41
13:T:450:ALA:O	13:T:454:VAL:HG23	2.21	0.41
13:T:541:LEU:C	13:T:545:PRO:HG2	2.41	0.41
14:U:99:ALA:HB2	14:U:226:LEU:HD21	2.03	0.41
14:U:331:ARG:HD2	14:U:331:ARG:HA	1.82	0.41
14:U:371:LEU:HD12	14:U:440:LEU:HB3	2.03	0.41
15:V:3:LEU:HD13	15:V:96:HIS:HD2	1.85	0.41
15:V:23:GLN:O	15:V:27:ARG:HG3	2.21	0.41
15:V:98:LEU:HD22	15:V:114:LEU:HD21	2.01	0.41
15:V:299:LEU:HD22	15:V:307:VAL:HG11	2.03	0.41
16:Q:274:VAL:CG1	16:Q:278:TRP:CD1	2.91	0.41
1:1:272:PHE:CE1	1:1:309:THR:HB	2.56	0.41
3:3:8:ASP:OD1	3:3:9:ARG:HG3	2.21	0.41
3:3:34:CYS:O	3:3:189:ARG:NH2	2.52	0.41
3:3:728:LEU:O	3:3:749:HIS:NE2	2.37	0.41
4:4:35:PRO:HB3	16:H:229:VAL:HG12	2.02	0.41
4:4:133:LEU:O	4:4:137:LEU:HD13	2.21	0.41
6:6:44:ALA:O	6:6:47:ALA:N	2.40	0.41
8:7:60:SER:HA	8:7:66:PRO:HA	2.02	0.41
11:J:61:GLY:O	11:J:65:VAL:CG2	2.66	0.41
13:L:291:ILE:HG13	13:L:292:LYS:N	2.36	0.41
13:L:360:PRO:HA	13:L:363:ARG:NH1	2.35	0.41
13:L:386:ASP:OD2	13:L:494:ILE:HA	2.21	0.41
14:M:5:ALA:HB1	14:M:36:ASN:HD21	1.85	0.41
14:M:214:LEU:HD11	14:M:235:LYS:HZ1	1.86	0.41
15:N:76:LEU:HD12	15:N:206:PRO:HB3	2.03	0.41
16:H:171:LEU:HB3	16:H:321:PHE:CD1	2.56	0.41
1:B:98:PRO:HA	2:C:124:CYS:SG	2.61	0.41
1:B:207:ALA:O	1:B:215:PRO:HB3	2.21	0.41
2:C:61:MET:CE	3:D:214:MET:HG3	2.51	0.41
3:D:176:LEU:HD13	3:D:235:LEU:CD2	2.51	0.41
3:D:384:PRO:O	3:D:531:LYS:HD3	2.21	0.41
3:D:403:THR:H	3:D:458:LEU:HD11	1.86	0.41
10:P:28:GLY:HA3	16:Q:239:ILE:HB	2.02	0.41
10:P:56:ARG:NH1	11:R:75:PHE:H	2.19	0.41
10:P:71:PHE:CZ	10:P:107:PHE:HB2	2.56	0.41
10:P:107:PHE:HE1	16:Q:310:TRP:CD1	2.39	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:R:72:MET:HE2	16:Q:153:LEU:HD21	2.03	0.41
13:T:111:PHE:CZ	13:T:134:VAL:HG13	2.56	0.41
4:4:42:ARG:O	4:4:43:LEU:HD23	2.21	0.40
10:A:100:THR:HG21	16:H:322:LEU:HD11	2.02	0.40
11:J:83:PHE:O	12:K:22:ARG:HD3	2.21	0.40
13:L:90:TYR:CD1	13:L:334:LEU:HD22	2.56	0.40
13:L:463:HIS:CD2	13:L:464:PRO:HD3	2.56	0.40
14:M:54:PRO:HA	14:M:62:TYR:CD1	2.51	0.40
14:M:148:PHE:O	14:M:152:THR:HG23	2.20	0.40
14:M:304:THR:O	14:M:306:GLU:N	2.54	0.40
16:H:74:VAL:HG23	16:H:82:PHE:CZ	2.56	0.40
1:B:65:ARG:NH2	1:B:238:PHE:HZ	2.19	0.40
3:D:170:LEU:HD11	3:D:176:LEU:HD22	2.03	0.40
3:D:368:HIS:CB	3:D:556:ALA:HB3	2.52	0.40
3:D:717:TRP:CE3	3:D:750:ARG:HD3	2.57	0.40
13:T:160:ILE:O	13:T:164:ILE:HG13	2.20	0.40
13:T:202:LEU:HD12	13:T:202:LEU:HA	1.87	0.40
13:T:427:GLY:O	13:T:428:GLU:HG2	2.20	0.40
14:U:29:ALA:HB1	14:U:83:PHE:HA	2.02	0.40
14:U:225:GLY:HA2	14:U:228:ASP:OD2	2.20	0.40
14:U:306:GLU:H	14:U:306:GLU:HG3	1.68	0.40
1:1:180:TYR:HB3	1:1:351:GLU:HB3	2.03	0.40
1:1:356:CYS:N	17:1:501:SF4:S3	2.86	0.40
2:2:79:HIS:ND1	2:2:118:SER:HB2	2.36	0.40
4:4:120:LEU:HD22	4:4:160:PHE:HE1	1.85	0.40
5:5:116:ARG:NH2	5:5:135:ILE:HG12	2.36	0.40
6:6:36:LEU:O	6:6:38:PRO:HD3	2.21	0.40
6:6:94:ARG:HD2	10:A:46:SER:CA	2.45	0.40
10:A:49:ASP:OD1	10:A:52:GLY:HA3	2.21	0.40
10:A:67:LEU:HD23	16:H:310:TRP:CZ2	2.56	0.40
14:M:56:LEU:HB3	14:M:59:ALA:HB3	2.03	0.40
14:M:224:SER:O	14:M:330:GLY:HA3	2.21	0.40
15:N:311:ALA:HA	15:N:389:THR:OG1	2.21	0.40
16:H:83:VAL:HA	16:H:240:LYS:HD3	2.03	0.40
16:H:196:PHE:O	16:H:200:PHE:N	2.55	0.40
1:B:116:GLU:O	1:B:120:LEU:HG	2.21	0.40
3:D:695:ARG:HH11	3:D:695:ARG:HD3	1.72	0.40
4:E:84:ARG:HA	4:E:169:HIS:CE1	2.57	0.40
4:E:106:GLY:O	5:F:194:SER:HB3	2.21	0.40
5:F:56:ASP:HB2	5:F:122:PHE:HE2	1.86	0.40
6:G:178:ARG:CZ	9:X:125:ILE:HG22	2.51	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:O:40:ARG:NH2	7:O:42:VAL:HG12	2.36	0.40
8:I:88:ARG:HH21	8:I:126:LEU:HB3	1.86	0.40
13:T:128:PHE:CZ	13:T:166:ASP:HB3	2.56	0.40
13:T:142:ILE:HD13	13:T:229:ALA:HA	2.02	0.40
13:T:404:VAL:O	13:T:408:LEU:HG	2.21	0.40
14:U:5:ALA:HB1	14:U:36:ASN:ND2	2.37	0.40
14:U:64:ALA:CB	14:U:113:ARG:HB3	2.51	0.40
3:3:233:GLY:O	3:3:236:LEU:HG	2.22	0.40
3:3:327:LEU:HD23	3:3:330:LYS:HD2	2.03	0.40
4:4:162:TRP:CD1	7:9:34:LYS:HD2	2.56	0.40
6:6:37:TRP:HB2	6:6:76:ASP:OD1	2.22	0.40
6:6:69:ARG:HD3	6:6:74:GLN:OE1	2.20	0.40
7:9:55:GLY:O	7:9:86:ARG:NE	2.46	0.40
10:A:6:GLU:OE2	16:H:2:THR:OG1	2.31	0.40
11:J:36:PHE:CD2	11:J:59:TYR:HB3	2.57	0.40
11:J:48:ALA:HA	11:J:122:GLY:HA3	2.03	0.40
12:K:13:LEU:HD23	12:K:13:LEU:HA	1.77	0.40
14:M:92:GLU:C	14:M:94:ARG:H	2.24	0.40
16:H:222:PRO:HD2	16:H:230:GLY:HA2	2.04	0.40
16:H:260:PRO:HG3	16:H:286:PHE:CE2	2.55	0.40
1:B:192:LEU:HD22	1:B:211:LEU:HD21	2.04	0.40
2:C:7:LYS:HE2	2:C:7:LYS:HB3	1.96	0.40
3:D:33:PHE:CE2	3:D:47:MET:HE3	2.57	0.40
3:D:250:GLU:HG3	5:F:169:GLU:OE1	2.22	0.40
4:E:367:ARG:HH12	5:F:53:VAL:HG23	1.87	0.40
5:F:147:ARG:H	5:F:147:ARG:HG2	1.68	0.40
7:O:67:ALA:O	7:O:93:ILE:HA	2.22	0.40
8:I:21:ARG:O	8:I:24:ALA:HB3	2.21	0.40
10:P:7:TYR:CD1	10:P:7:TYR:N	2.88	0.40
13:T:234:THR:N	13:T:235:PRO:HD2	2.37	0.40
13:T:239:LEU:HD12	13:T:239:LEU:HA	1.87	0.40
15:V:200:TYR:CE2	15:V:212:ALA:HB2	2.56	0.40
16:Q:50:ARG:HD3	16:Q:50:ARG:HA	1.93	0.40
1:1:122:GLY:HA3	1:1:169:PHE:HE1	1.86	0.40
1:1:270:THR:O	1:1:311:MET:HG3	2.21	0.40
2:2:143:GLU:O	2:2:149:ARG:NH1	2.55	0.40
3:3:170:LEU:HG	3:3:176:LEU:HB2	2.03	0.40
6:6:93:ARG:HD3	6:6:130:VAL:O	2.21	0.40
9:W:10:PRO:HG3	9:W:62:ALA:O	2.21	0.40
12:K:23:THR:OG1	12:K:26:LEU:HD13	2.21	0.40
13:L:184:SER:HB3	13:L:187:GLU:HG2	2.04	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:L:582:GLN:HA	13:L:589:TYR:CE1	2.57	0.40
1:B:413:SER:O	1:B:417:PHE:HB2	2.21	0.40
2:C:79:HIS:H	2:C:137:ASN:HD21	1.69	0.40
3:D:24:PHE:CE2	3:D:30:VAL:HG12	2.56	0.40
3:D:192:GLU:HG3	3:D:440:ARG:HH11	1.87	0.40
4:E:73:ARG:NH1	5:F:171:ARG:HH21	2.19	0.40
4:E:75:TYR:CZ	4:E:337:PRO:HG2	2.56	0.40
4:E:218:ALA:HA	4:E:221:VAL:HG22	2.03	0.40
5:F:122:PHE:O	5:F:144:HIS:ND1	2.55	0.40
6:G:46:CYS:SG	6:G:109:GLY:HA3	2.61	0.40
8:I:101:LYS:H	8:I:101:LYS:HG2	1.66	0.40
10:P:57:PHE:HE2	16:Q:149:LEU:HD13	1.85	0.40
11:R:104:LEU:O	11:R:108:LEU:HD12	2.21	0.40
13:T:291:ILE:HG13	13:T:292:LYS:N	2.36	0.40
14:U:281:PHE:CE2	14:U:332:LEU:HD21	2.56	0.40
16:Q:257:ALA:O	16:Q:260:PRO:HD2	2.20	0.40
1:1:170:ASP:OD1	1:1:171:LEU:N	2.55	0.40
3:3:42:ILE:HD12	3:3:42:ILE:C	2.37	0.40
3:3:473:GLU:O	3:3:476:ILE:N	2.55	0.40
4:4:317:LEU:HD12	4:4:317:LEU:HA	1.86	0.40
5:5:3:LEU:HB2	5:5:86:SER:HB2	2.02	0.40
7:9:68:ILE:HD11	17:9:201:SF4:S1	2.61	0.40
9:W:43:GLN:O	9:W:66:ALA:HB2	2.22	0.40
10:A:1:MET:HG3	11:J:123:LEU:HD11	2.03	0.40
11:J:131:LEU:HA	11:J:135:TRP:HB2	2.04	0.40
13:L:320:PHE:CE2	13:L:460:ALA:HB3	2.56	0.40
14:M:206:PRO:HD2	14:M:293:MET:HG3	2.04	0.40
14:M:232:THR:HA	14:M:235:LYS:NZ	2.34	0.40
16:H:275:PRO:HB2	16:H:276:TYR:HD1	1.87	0.40
16:H:314:PHE:HB2	16:H:315:PRO:HD3	2.02	0.40
2:C:125:LEU:HB3	2:C:141:TYR:CZ	2.55	0.40
3:D:7:ASN:ND2	3:D:94:ASP:HA	2.36	0.40
3:D:120:PRO:HA	4:E:328:PHE:HE2	1.86	0.40
4:E:102:GLU:HG2	4:E:175:ILE:O	2.21	0.40
5:F:77:LEU:HA	5:F:78:PRO:HD3	1.98	0.40
11:R:75:PHE:O	11:R:77:ALA:N	2.54	0.40
13:T:70:ASP:H	13:T:73:SER:HB2	1.85	0.40
13:T:386:ASP:OD2	13:T:494:ILE:HG23	2.22	0.40
14:U:215:PRO:CG	14:U:216:PRO:HD3	2.52	0.40
15:V:279:GLN:HG3	15:V:423:LEU:HB2	2.04	0.40
16:Q:340:LEU:HA	16:Q:340:LEU:HD23	1.83	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%)	404 (93%)	31 (7%)	0	100	100
2	2	176/181 (97%)	168 (96%)	8 (4%)	0	100	100
2	C	176/181 (97%)	168 (96%)	8 (4%)	0	100	100
3	3	750/783 (96%)	696 (93%)	54 (7%)	0	100	100
3	D	750/783 (96%)	703 (94%)	47 (6%)	0	100	100
4	4	382/409 (93%)	359 (94%)	23 (6%)	0	100	100
4	E	382/409 (93%)	360 (94%)	22 (6%)	0	100	100
5	5	194/207 (94%)	185 (95%)	9 (5%)	0	100	100
5	F	194/207 (94%)	187 (96%)	7 (4%)	0	100	100
6	6	164/181 (91%)	147 (90%)	16 (10%)	1 (1%)	25	64
6	G	164/181 (91%)	145 (88%)	19 (12%)	0	100	100
7	9	178/182 (98%)	172 (97%)	6 (3%)	0	100	100
7	O	178/182 (98%)	171 (96%)	7 (4%)	0	100	100
8	7	125/129 (97%)	116 (93%)	9 (7%)	0	100	100
8	I	125/129 (97%)	115 (92%)	10 (8%)	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%)	106 (92%)	9 (8%)	0	100	100
10	P	115/119 (97%)	106 (92%)	9 (8%)	0	100	100
11	J	158/176 (90%)	147 (93%)	11 (7%)	0	100	100
11	R	158/176 (90%)	146 (92%)	12 (8%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
12	K	93/95 (98%)	89 (96%)	4 (4%)	0	100	100
12	S	93/95 (98%)	89 (96%)	4 (4%)	0	100	100
13	L	603/606 (100%)	569 (94%)	33 (6%)	1 (0%)	47	79
13	T	603/606 (100%)	569 (94%)	33 (6%)	1 (0%)	47	79
14	M	465/469 (99%)	437 (94%)	28 (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%)	404 (95%)	21 (5%)	0	100	100
16	H	351/365 (96%)	303 (86%)	42 (12%)	6 (2%)	9	42
16	Q	351/365 (96%)	302 (86%)	42 (12%)	7 (2%)	7	38
All	All	9478/9796 (97%)	8845 (93%)	617 (6%)	16 (0%)	47	79

All (16) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
16	H	51	VAL
16	Q	51	VAL
16	H	50	ARG
16	H	218	PRO
16	H	44	VAL
13	T	435	PRO
16	Q	50	ARG
16	Q	268	THR
13	L	435	PRO
6	6	45	CYS
16	H	195	LEU
16	Q	218	PRO
16	Q	44	VAL
16	Q	332	LEU
16	Q	333	PRO
16	H	53	PRO

5.3.2 Protein sidechains (i)

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the sidechain conformation was

analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	1	355/356 (100%)	344 (97%)	11 (3%)	40	72
1	B	355/356 (100%)	344 (97%)	11 (3%)	40	72
2	2	150/152 (99%)	144 (96%)	6 (4%)	31	66
2	C	150/152 (99%)	144 (96%)	6 (4%)	31	66
3	3	609/628 (97%)	597 (98%)	12 (2%)	55	80
3	D	609/628 (97%)	599 (98%)	10 (2%)	62	84
4	4	332/355 (94%)	325 (98%)	7 (2%)	53	79
4	E	332/355 (94%)	325 (98%)	7 (2%)	53	79
5	5	167/175 (95%)	166 (99%)	1 (1%)	86	94
5	F	167/175 (95%)	164 (98%)	3 (2%)	59	82
6	6	135/149 (91%)	125 (93%)	10 (7%)	13	46
6	G	135/149 (91%)	125 (93%)	10 (7%)	13	46
7	9	148/150 (99%)	145 (98%)	3 (2%)	55	80
7	O	148/150 (99%)	146 (99%)	2 (1%)	67	86
8	7	104/106 (98%)	103 (99%)	1 (1%)	76	90
8	I	104/106 (98%)	102 (98%)	2 (2%)	57	81
9	W	99/101 (98%)	98 (99%)	1 (1%)	76	90
9	X	99/101 (98%)	97 (98%)	2 (2%)	55	80
10	A	90/92 (98%)	86 (96%)	4 (4%)	28	64
10	P	90/92 (98%)	89 (99%)	1 (1%)	73	88
11	J	118/130 (91%)	114 (97%)	4 (3%)	37	70
11	R	118/130 (91%)	115 (98%)	3 (2%)	47	77
12	K	71/71 (100%)	69 (97%)	2 (3%)	43	74
12	S	71/71 (100%)	70 (99%)	1 (1%)	67	86
13	L	453/454 (100%)	446 (98%)	7 (2%)	65	85
13	T	453/454 (100%)	446 (98%)	7 (2%)	65	85
14	M	332/332 (100%)	326 (98%)	6 (2%)	59	82
14	U	332/332 (100%)	323 (97%)	9 (3%)	44	75
15	N	302/302 (100%)	298 (99%)	4 (1%)	69	87
15	V	302/302 (100%)	297 (98%)	5 (2%)	60	83
16	H	293/300 (98%)	286 (98%)	7 (2%)	49	77

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
16	Q	293/300 (98%)	288 (98%)	5 (2%)	60	83
All	All	7516/7706 (98%)	7346 (98%)	170 (2%)	50	78

All (170) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	1	18	TYR
1	1	81	LYS
1	1	249	MET
1	1	342	TRP
1	1	353	CYS
1	1	355	LYS
1	1	359	CYS
1	1	366	PHE
1	1	397	ARG
1	1	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	123	ASP
3	3	132	ASP
3	3	184	CYS
3	3	259	CYS
3	3	260	PRO
3	3	337	ARG
3	3	369	LEU
3	3	651	ARG
3	3	655	ARG
3	3	761	SER
3	3	774	ARG
4	4	87	TYR
4	4	132	PHE
4	4	143	LEU
4	4	151	ARG
4	4	208	PHE
4	4	262	PHE
4	4	363	SER

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Mol	Chain	Res	Type
5	5	147	ARG
6	6	37	TRP
6	6	49	GLU
6	6	55	ASP
6	6	68	PHE
6	6	88	MET
6	6	98	GLN
6	6	101	ASP
6	6	120	ASN
6	6	153	GLN
6	6	156	LYS
7	9	4	LYS
7	9	38	HIS
7	9	118	ASP
8	7	43	ARG
9	W	37	TRP
10	A	13	TYR
10	A	49	ASP
10	A	79	TRP
10	A	110	GLU
11	J	32	LEU
11	J	59	TYR
11	J	118	ASP
11	J	119	LEU
12	K	28	PHE
12	K	82	ARG
13	L	56	GLN
13	L	59	TRP
13	L	169	PHE
13	L	275	LEU
13	L	506	TRP
13	L	511	PHE
13	L	554	PHE
14	M	22	ARG
14	M	135	LEU
14	M	148	PHE
14	M	241	PHE
14	M	255	GLN
14	M	455	HIS
15	N	50	PHE
15	N	125	ARG
15	N	126	ARG

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Mol	Chain	Res	Type
15	N	284	TYR
16	H	119	ASP
16	H	134	TYR
16	H	147	TYR
16	H	196	PHE
16	H	233	HIS
16	H	307	ARG
16	H	354	TYR
1	B	81	LYS
1	B	249	MET
1	B	337	MET
1	B	342	TRP
1	B	353	CYS
1	B	355	LYS
1	B	359	CYS
1	B	366	PHE
1	B	397	ARG
1	B	400	CYS
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	83	CYS
3	D	184	CYS
3	D	259	CYS
3	D	337	ARG
3	D	369	LEU
3	D	617	LEU
3	D	655	ARG
3	D	761	SER
3	D	774	ARG
4	E	87	TYR
4	E	129	HIS
4	E	143	LEU
4	E	151	ARG
4	E	152	GLU
4	E	208	PHE
4	E	262	PHE

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Mol	Chain	Res	Type
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	101	ASP
6	G	120	ASN
6	G	156	LYS
6	G	176	TRP
6	G	177	LYS
7	O	38	HIS
7	O	104	CYS
8	I	43	ARG
8	I	120	ASP
9	X	37	TRP
9	X	43	GLN
10	P	13	TYR
11	R	59	TYR
11	R	118	ASP
11	R	119	LEU
12	S	28	PHE
13	T	10	PRO
13	T	59	TRP
13	T	151	TYR
13	T	169	PHE
13	T	506	TRP
13	T	511	PHE
13	T	554	PHE
14	U	22	ARG
14	U	115	LEU
14	U	135	LEU
14	U	148	PHE
14	U	215	PRO
14	U	234	TYR
14	U	241	PHE
14	U	255	GLN
14	U	455	HIS
15	V	50	PHE
15	V	125	ARG

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Mol	Chain	Res	Type
15	V	126	ARG
15	V	284	TYR
15	V	313	ARG
16	Q	54	PHE
16	Q	134	TYR
16	Q	196	PHE
16	Q	307	ARG
16	Q	354	TYR

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

Mol	Chain	Res	Type
1	1	92	ASN
1	1	220	ASN
1	1	240	GLN
1	1	288	GLN
2	2	35	GLN
2	2	71	GLN
2	2	120	GLN
3	3	104	GLN
3	3	616	ASN
3	3	709	GLN
4	4	292	GLN
4	4	330	HIS
5	5	112	ASN
5	5	129	HIS
6	6	120	ASN
6	6	125	GLN
6	6	153	GLN
9	W	43	GLN
10	A	60	HIS
12	K	81	HIS
13	L	241	HIS
13	L	302	GLN
13	L	432	HIS
13	L	447	HIS
13	L	513	GLN
14	M	221	ASN
15	N	128	GLN
15	N	245	ASN
16	H	112	GLN
16	H	117	ASN

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Mol	Chain	Res	Type
16	H	304	GLN
1	B	240	GLN
1	B	288	GLN
3	D	104	GLN
3	D	246	ASN
3	D	436	GLN
3	D	709	GLN
4	E	29	ASN
4	E	292	GLN
4	E	308	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	241	HIS
13	T	288	GLN
13	T	325	HIS
13	T	432	HIS
13	T	447	HIS
14	U	36	ASN
14	U	218	HIS
14	U	221	ASN
14	U	255	GLN
15	V	277	ASN
16	Q	43	GLN

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

22 ligands are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
17	SF4	O	202	7	0,12,12	-	-	-		
20	FES	C	201	2	0,4,4	-	-	-		
17	SF4	6	201	6	0,12,12	-	-	-		
17	SF4	3	803	3	0,12,12	-	-	-		
17	SF4	D	801	3	0,12,12	-	-	-		
19	NAI	1	503	-	42,48,48	0.53	0	47,73,73	0.66	1 (2%)
17	SF4	9	202	7	0,12,12	-	-	-		
20	FES	2	201	2	0,4,4	-	-	-		
17	SF4	G	201	6	0,12,12	-	-	-		
18	FMN	B	502	-	33,33,33	1.12	2 (6%)	48,50,50	1.27	9 (18%)
17	SF4	1	501	1	0,12,12	-	-	-		
17	SF4	O	201	7	0,12,12	-	-	-		
17	SF4	3	801	3	0,12,12	-	-	-		
19	NAI	B	503	-	42,48,48	0.57	0	47,73,73	0.66	1 (2%)
17	SF4	D	802	3	0,12,12	-	-	-		
20	FES	3	804	3	0,4,4	-	-	-		
18	FMN	1	502	-	33,33,33	1.11	2 (6%)	48,50,50	1.31	9 (18%)
17	SF4	9	201	7	0,12,12	-	-	-		
17	SF4	B	501	1	0,12,12	-	-	-		
17	SF4	D	803	3	0,12,12	-	-	-		
20	FES	D	804	3	0,4,4	-	-	-		
17	SF4	3	802	3	0,12,12	-	-	-		

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
17	SF4	O	202	7	-	-	0/6/5/5
20	FES	C	201	2	-	-	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
17	SF4	6	201	6	-	-	0/6/5/5
17	SF4	3	803	3	-	-	0/6/5/5
17	SF4	D	801	3	-	-	0/6/5/5
19	NAI	1	503	-	-	11/25/72/72	0/5/5/5
17	SF4	9	202	7	-	-	0/6/5/5
20	FES	2	201	2	-	-	0/1/1/1
18	FMN	B	502	-	-	8/18/18/18	0/3/3/3
17	SF4	G	201	6	-	-	0/6/5/5
17	SF4	1	501	1	-	-	0/6/5/5
19	NAI	B	503	-	-	9/25/72/72	0/5/5/5
17	SF4	3	801	3	-	-	0/6/5/5
17	SF4	O	201	7	-	-	0/6/5/5
17	SF4	D	802	3	-	-	0/6/5/5
20	FES	3	804	3	-	-	0/1/1/1
18	FMN	1	502	-	-	8/18/18/18	0/3/3/3
17	SF4	9	201	7	-	-	0/6/5/5
17	SF4	B	501	1	-	-	0/6/5/5
17	SF4	D	803	3	-	-	0/6/5/5
20	FES	D	804	3	-	-	0/1/1/1
17	SF4	3	802	3	-	-	0/6/5/5

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
18	B	502	FMN	C4A-N5	3.84	1.38	1.30
18	1	502	FMN	C4A-N5	3.69	1.37	1.30
18	B	502	FMN	C10-N1	2.69	1.38	1.33
18	1	502	FMN	C10-N1	2.30	1.37	1.33

All (20) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
18	B	502	FMN	C4-N3-C2	-3.04	120.02	125.64
18	B	502	FMN	O4-C4-C4A	-2.90	118.92	126.60
18	1	502	FMN	C4-N3-C2	-2.88	120.32	125.64
18	B	502	FMN	C4A-C4-N3	2.79	120.27	113.19
18	1	502	FMN	O4-C4-C4A	-2.59	119.73	126.60
18	1	502	FMN	C4A-C10-N10	2.49	120.12	116.48
18	B	502	FMN	C4A-C10-N1	-2.47	118.99	124.73
18	1	502	FMN	C4A-C10-N1	-2.37	119.24	124.73
18	1	502	FMN	C4A-C4-N3	2.36	119.19	113.19

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
18	1	502	FMN	P-O5'-C5'	2.34	124.75	118.30
18	B	502	FMN	C9A-C5A-N5	-2.34	119.89	122.43
19	1	503	NAI	C5A-C6A-N6A	2.30	123.85	120.35
18	1	502	FMN	C5A-C9A-N10	2.30	120.33	117.95
19	B	503	NAI	C5A-C6A-N6A	2.29	123.84	120.35
18	1	502	FMN	C4-C4A-C10	2.24	120.56	116.79
18	1	502	FMN	C10-C4A-N5	-2.20	120.19	124.86
18	B	502	FMN	C5A-C9A-N10	2.12	120.14	117.95
18	B	502	FMN	C4A-C10-N10	2.09	119.53	116.48
18	B	502	FMN	C10-N1-C2	2.07	121.04	116.90
18	B	502	FMN	C10-C4A-N5	-2.07	120.46	124.86

There are no chirality outliers.

All (36) 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'
19	1	503	NAI	C5D-O5D-PN-O3
19	1	503	NAI	C5D-O5D-PN-O2N
19	1	503	NAI	C3D-C4D-C5D-O5D
19	B	503	NAI	C5D-O5D-PN-O2N
19	B	503	NAI	C3D-C4D-C5D-O5D
19	1	503	NAI	O4D-C4D-C5D-O5D
19	B	503	NAI	O4D-C4D-C5D-O5D
19	1	503	NAI	C2D-C1D-N1N-C2N
19	B	503	NAI	C2D-C1D-N1N-C2N
19	B	503	NAI	C2D-C1D-N1N-C6N
19	1	503	NAI	C2D-C1D-N1N-C6N
19	B	503	NAI	O4D-C1D-N1N-C2N

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Mol	Chain	Res	Type	Atoms
19	B	503	NAI	O4D-C1D-N1N-C6N
19	B	503	NAI	C5D-O5D-PN-O3
19	1	503	NAI	O4D-C1D-N1N-C2N
19	1	503	NAI	O4D-C1D-N1N-C6N
19	1	503	NAI	PA-O3-PN-O1N
19	1	503	NAI	PA-O3-PN-O2N
19	B	503	NAI	PA-O3-PN-O1N
18	1	502	FMN	C3'-C4'-C5'-O5'
18	B	502	FMN	C3'-C4'-C5'-O5'
19	1	503	NAI	C5B-O5B-PA-O1A

There are no ring outliers.

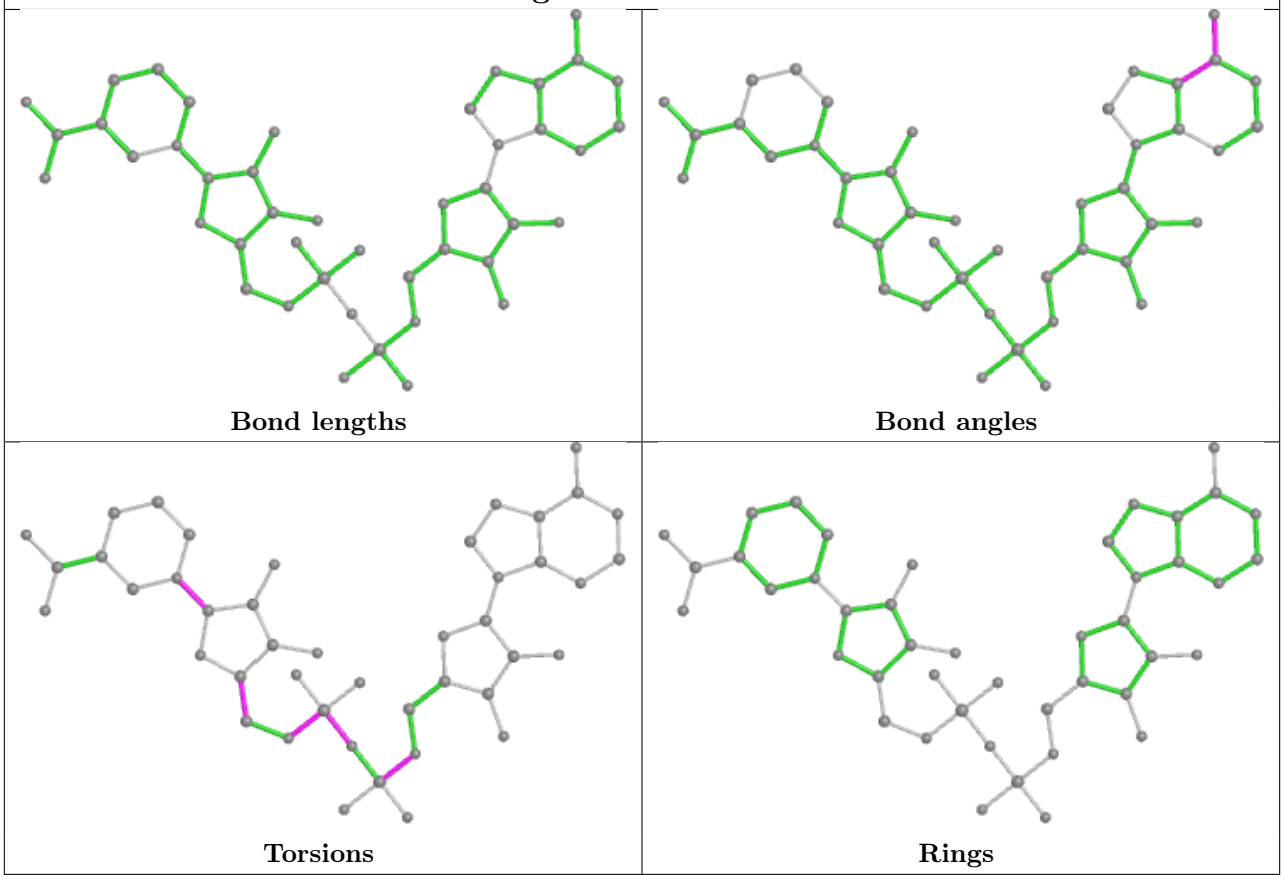
16 monomers are involved in 36 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
17	O	202	SF4	2	0
20	C	201	FES	2	0
17	3	803	SF4	2	0
17	D	801	SF4	1	0
19	1	503	NAI	3	0
17	9	202	SF4	2	0
20	2	201	FES	1	0
17	G	201	SF4	2	0
18	B	502	FMN	2	0
17	1	501	SF4	3	0
17	O	201	SF4	1	0
19	B	503	NAI	4	0
18	1	502	FMN	8	0
17	9	201	SF4	4	0
17	B	501	SF4	1	0
20	D	804	FES	2	0

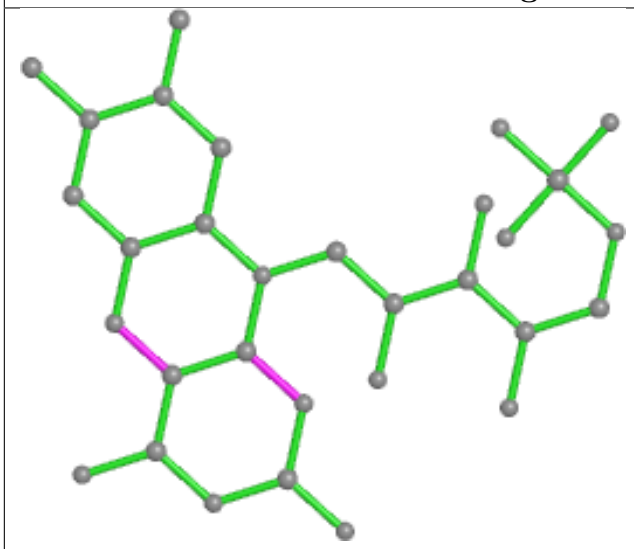
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

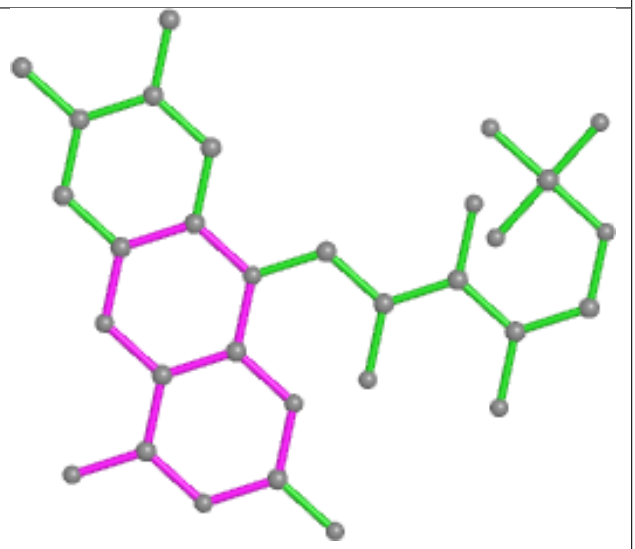
Ligand NAI 1 503



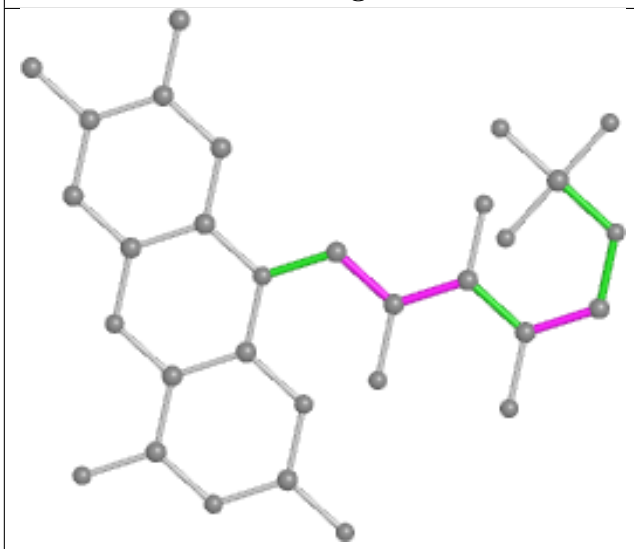
Ligand FMN B 502



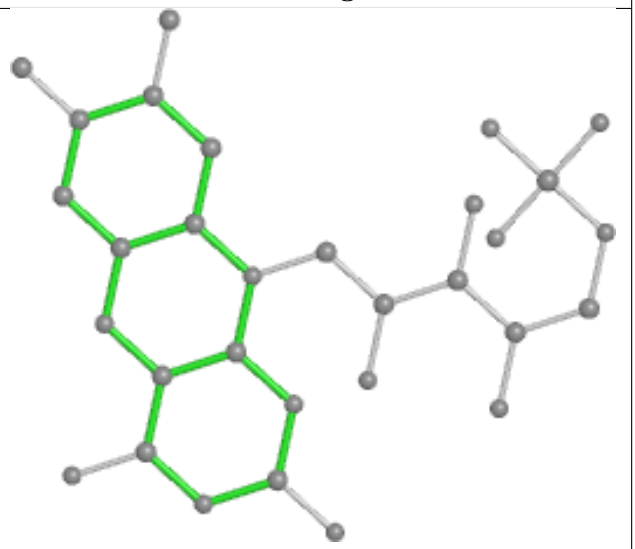
Bond lengths



Bond angles

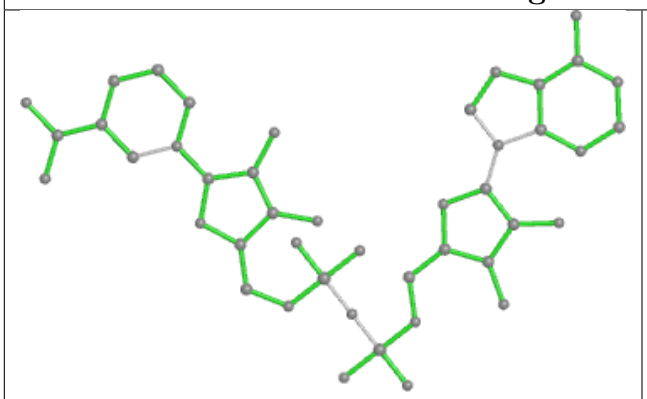


Torsions



Rings

Ligand NAI B 503



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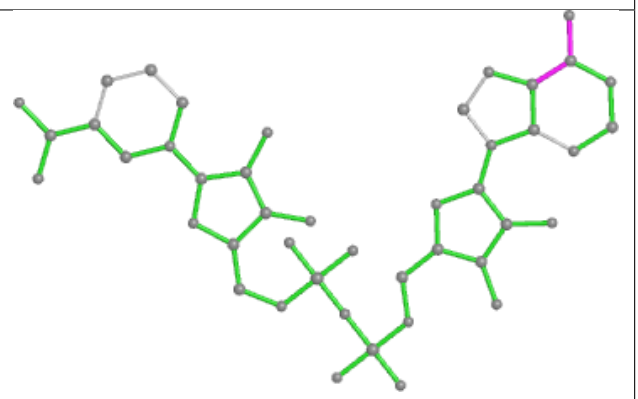

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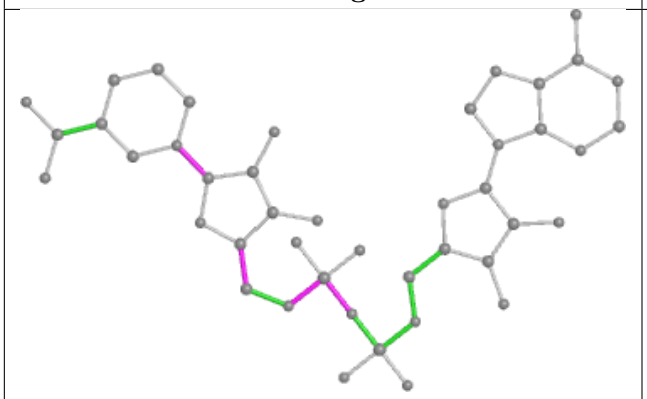
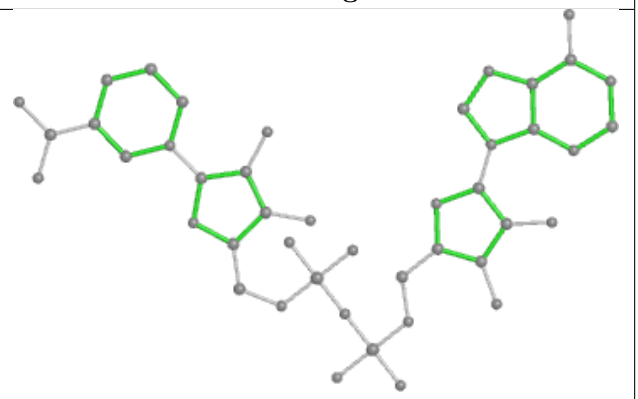
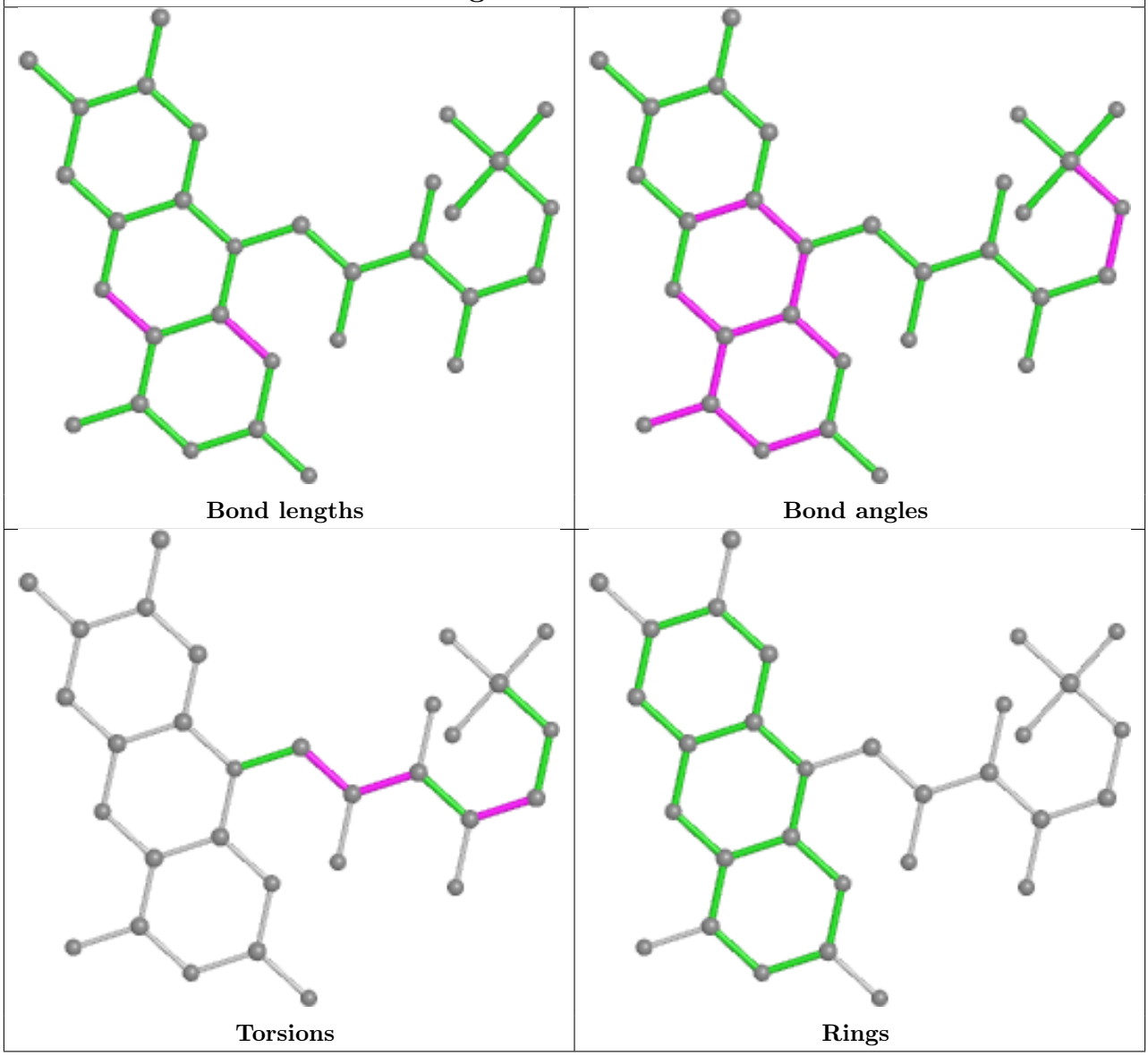


Torsions



Rings

Ligand FMN 1 502



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.