Full wwPDB X-ray Structure Validation Report ⓘ

Aug 31, 2020 – 07:34 AM BST

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

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

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

The following versions of software and data (see references ①) were used in the production of this report:

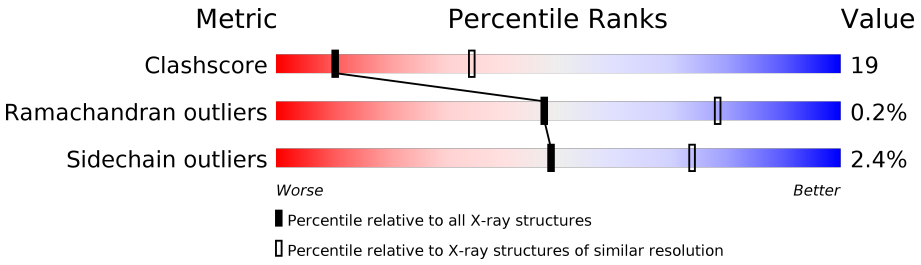
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	FAILED
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.13

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 3.40 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
Clashscore	141614	1055 (3.48-3.32)
Ramachandran outliers	138981	1038 (3.48-3.32)
Sidechain outliers	138945	1038 (3.48-3.32)

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

Note EDS failed to run properly.

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

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

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

ria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
17	SF4	1	501	-	-	X	-
17	SF4	B	501	-	-	X	-
19	FES	3	804	-	-	X	-
19	FES	C	201	-	-	X	-
19	FES	D	804	-	-	X	-

2 Entry composition

There are 20 unique types of molecules in this entry. The entry contains 74144 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

- Molecule 9 is a protein called Uncharacterized protein.

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

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

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

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

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

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

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

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

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

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

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

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

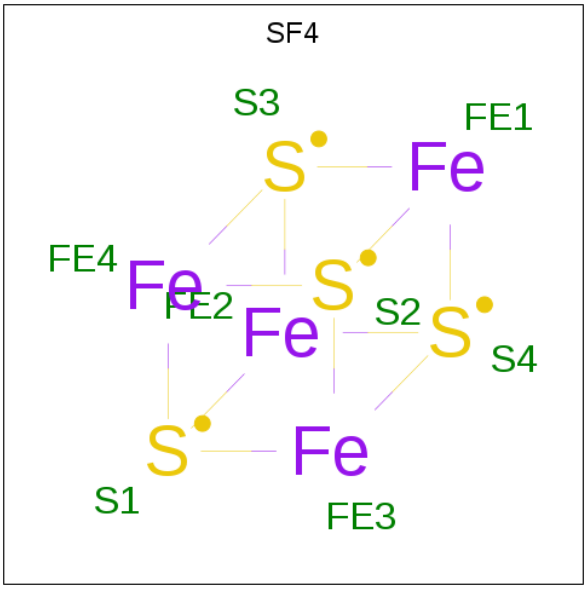
- Molecule 15 is a protein called NADH-quinone oxidoreductase subunit 14.

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

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

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

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



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

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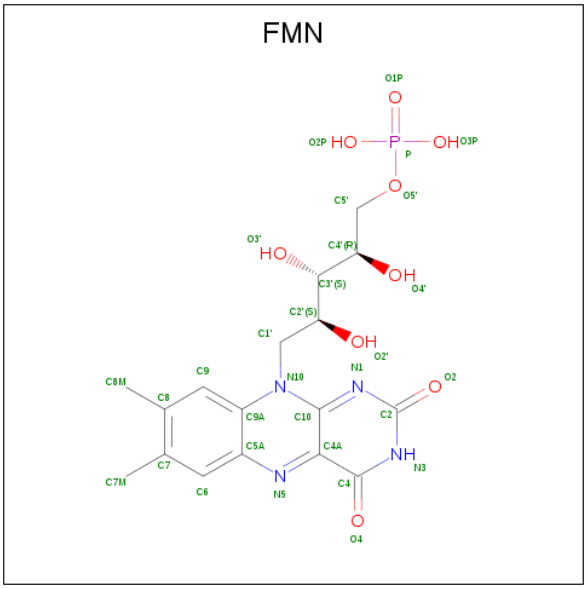
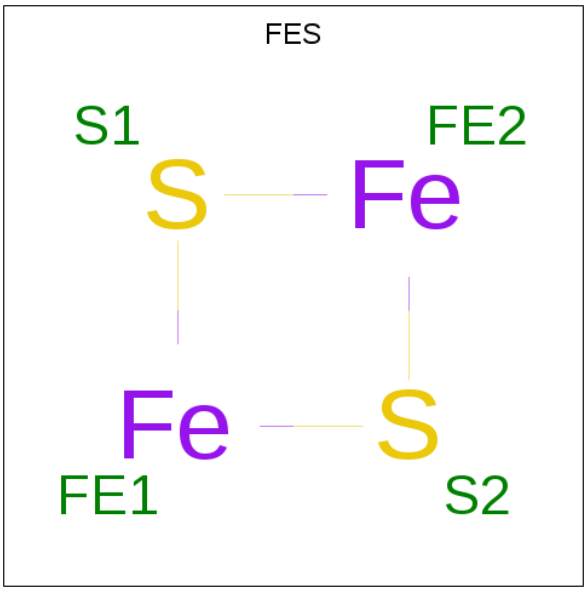
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
17	D	1	Total Fe S 8 4 4	0	0
17	D	1	Total Fe S 8 4 4	0	0
17	G	1	Total Fe S 8 4 4	0	0
17	O	1	Total Fe S 8 4 4	0	0
17	O	1	Total Fe S 8 4 4	0	0

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



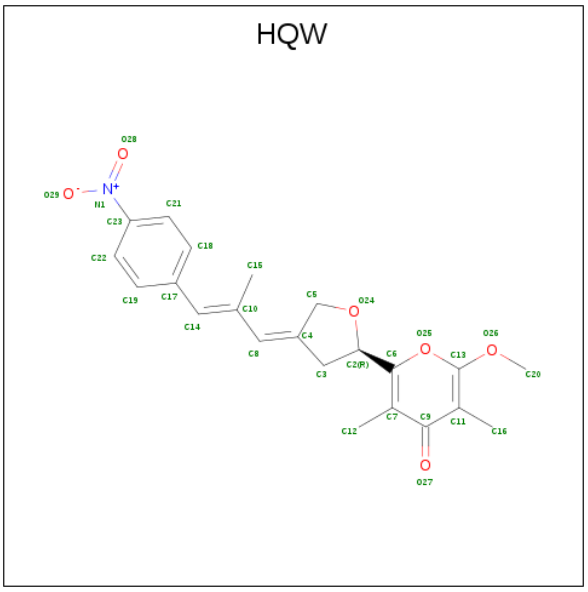
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
18	1	1	Total C N O P 31 17 4 9 1	0	0
18	B	1	Total C N O P 31 17 4 9 1	0	0

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



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

- Molecule 20 is Aureothin (three-letter code: HQW) (formula: $C_{22}H_{23}NO_6$) (labeled as "Ligand of Interest" by author).



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

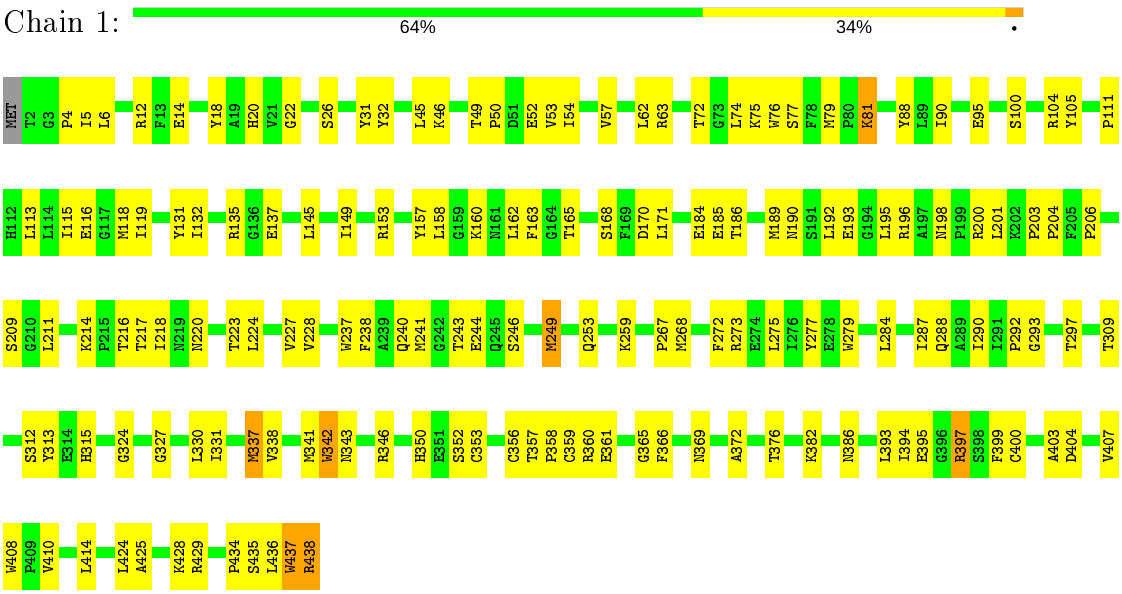
3 Residue-property plots (i)

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

Note EDS failed to run properly.

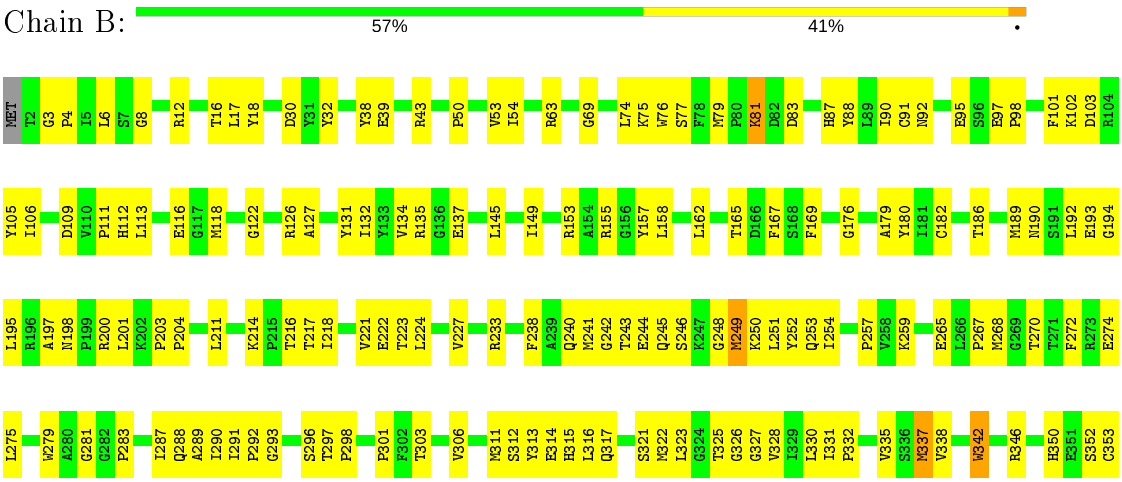
- Molecule 1: NADH-quinone oxidoreductase subunit 1

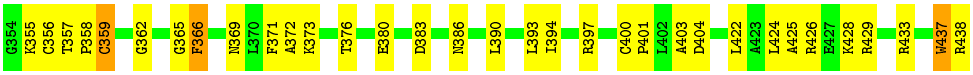
Chain 1:



- Molecule 1: NADH-quinone oxidoreductase subunit 1

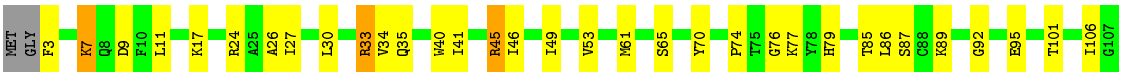
Chain B:

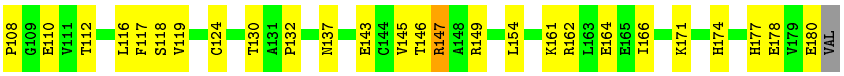




• Molecule 2: NADH-quinone oxidoreductase subunit 2

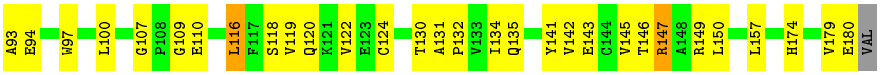
Chain 2:





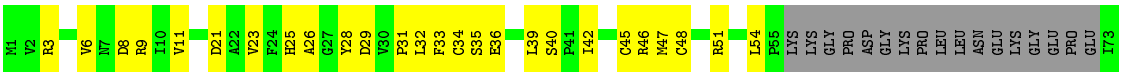
• Molecule 2: NADH-quinone oxidoreductase subunit 2

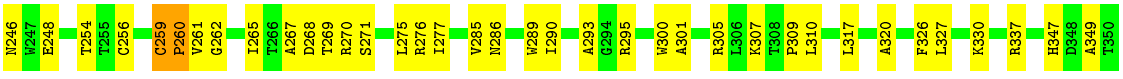
Chain C:

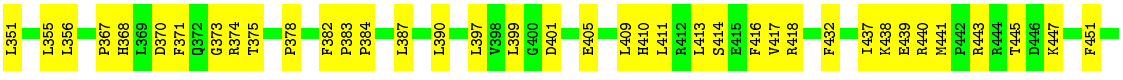


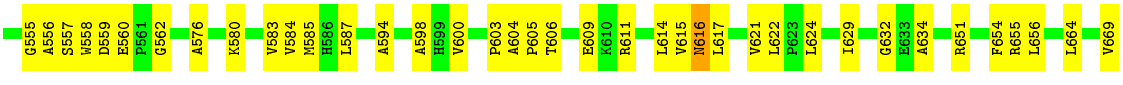
• Molecule 3: NADH-quinone oxidoreductase subunit 3

Chain 3:



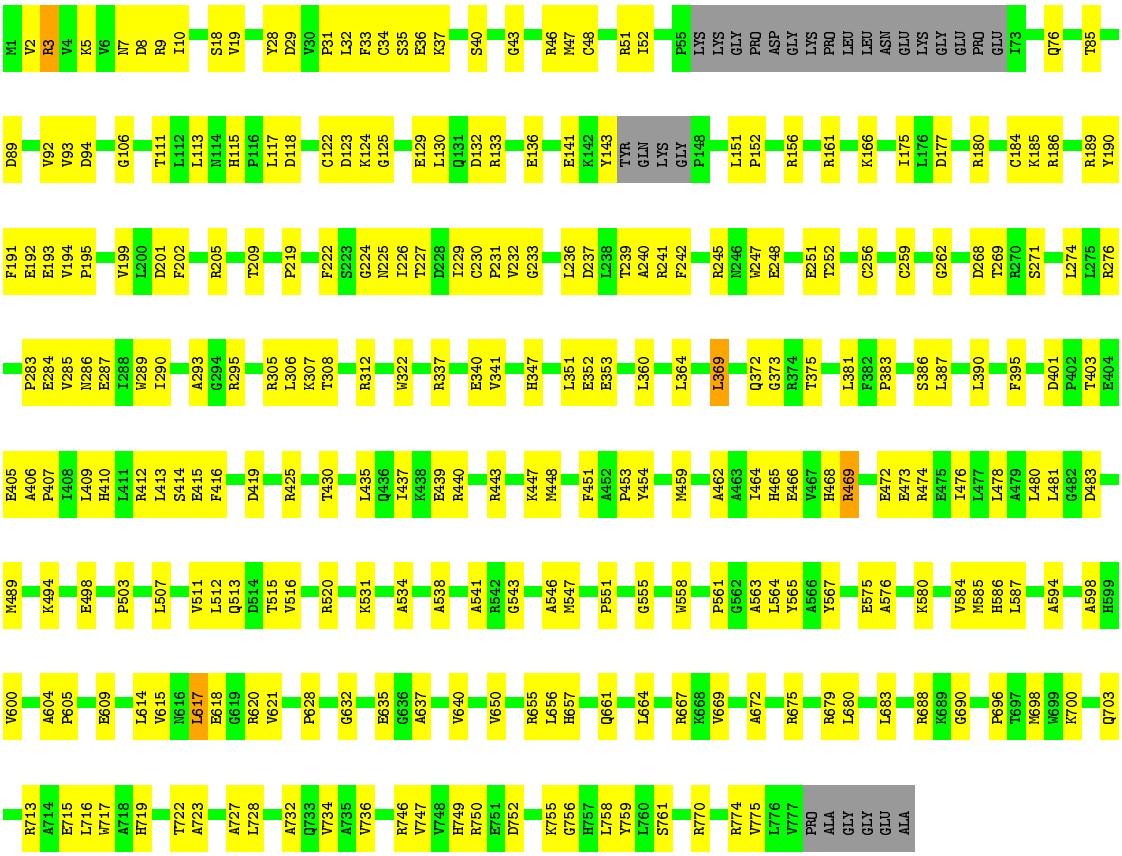






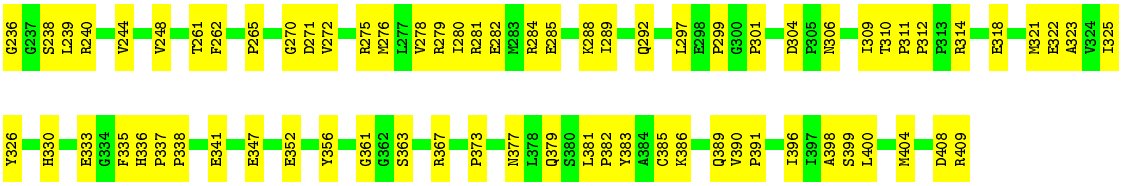
• Molecule 3: NADH-quinone oxidoreductase subunit 3

Chain D:



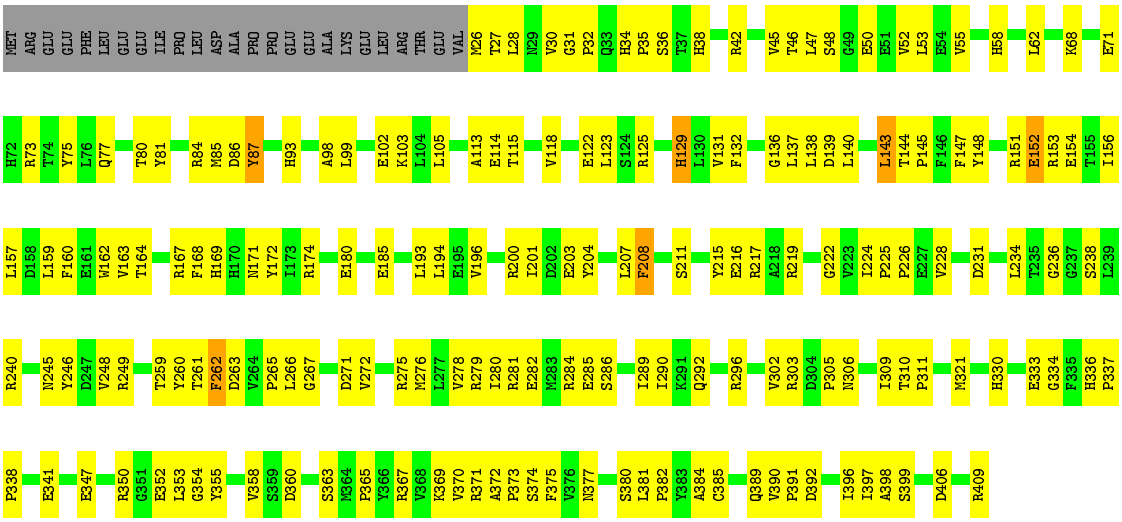
• Molecule 4: NADH-quinone oxidoreductase subunit 4

Chain 4:



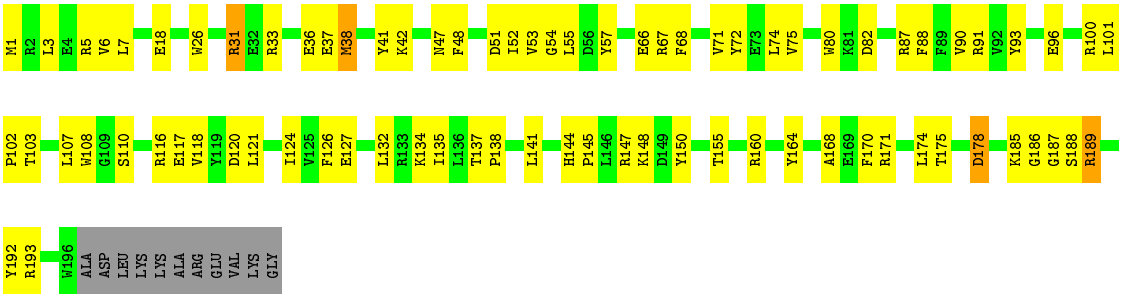
• Molecule 4: NADH-quinone oxidoreductase subunit 4

Chain E:



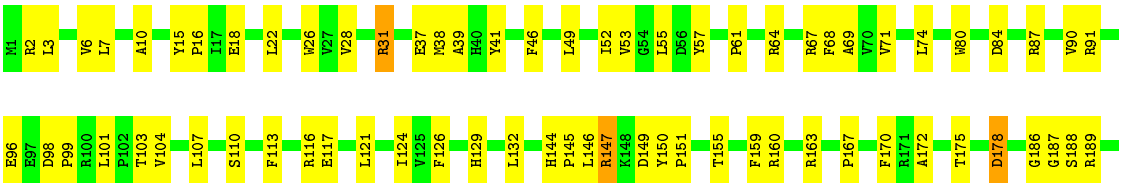
• Molecule 5: NADH-quinone oxidoreductase subunit 5

Chain 5:



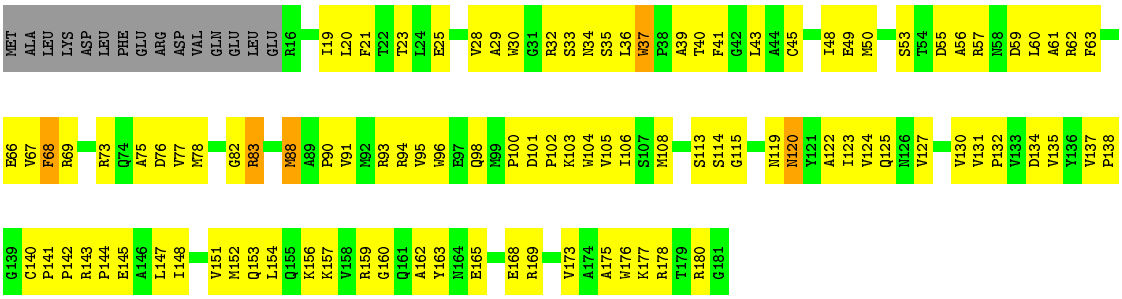
• Molecule 5: NADH-quinone oxidoreductase subunit 5

Chain F:



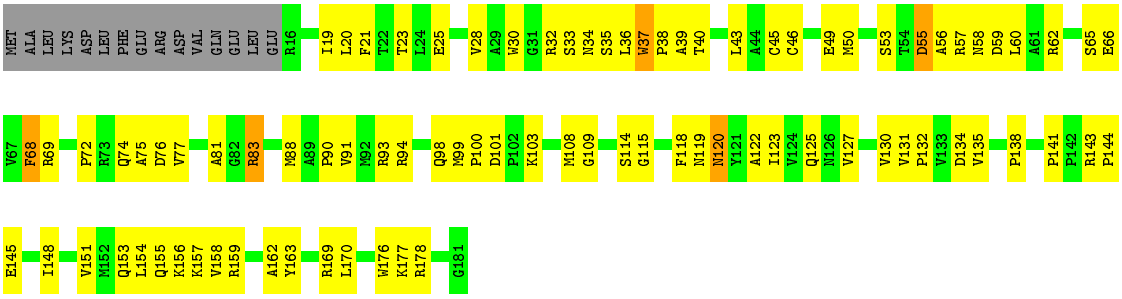
• Molecule 6: NADH-quinone oxidoreductase subunit 6

Chain 6:



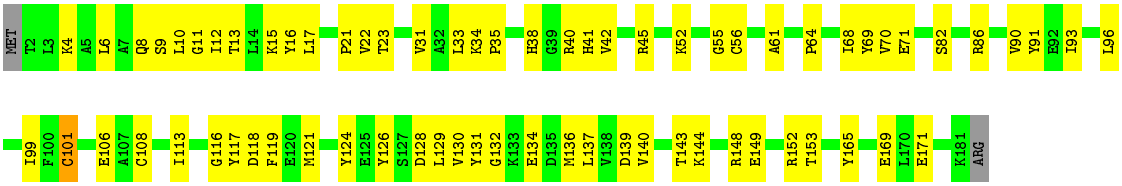
• Molecule 6: NADH-quinone oxidoreductase subunit 6

Chain G:



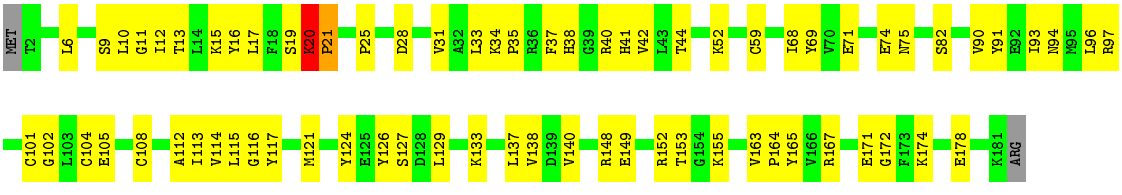
• Molecule 7: NADH-quinone oxidoreductase subunit 9

Chain 9:



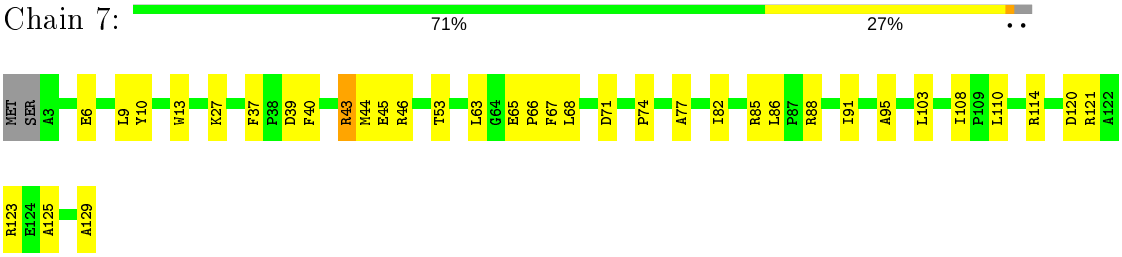
• Molecule 7: NADH-quinone oxidoreductase subunit 9

Chain O:



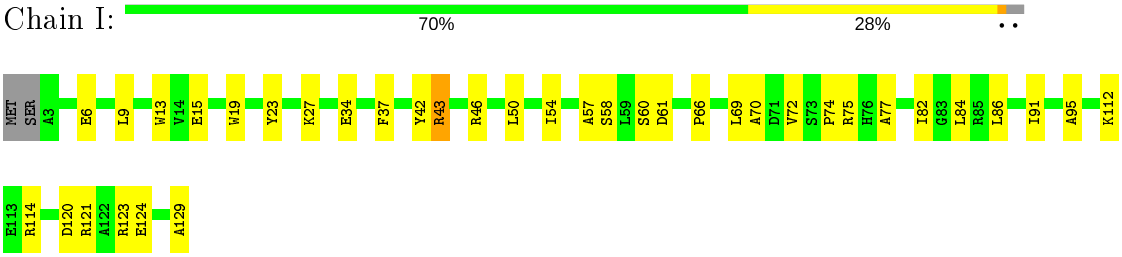
• Molecule 8: NADH-quinone oxidoreductase subunit 15

Chain 7:



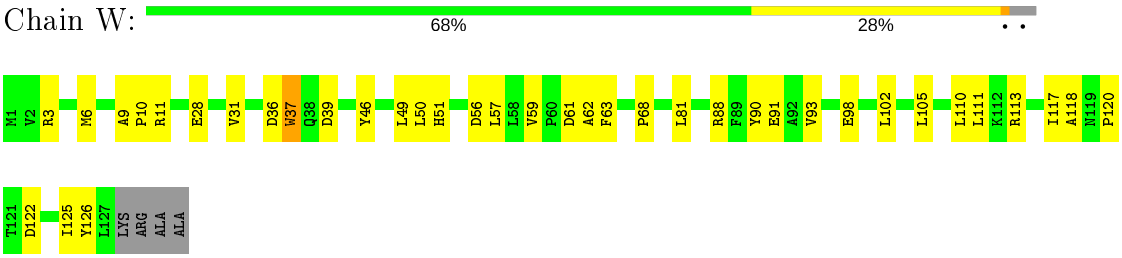
• Molecule 8: NADH-quinone oxidoreductase subunit 15

Chain I:



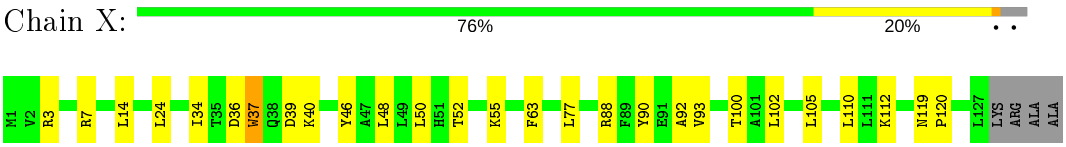
• Molecule 9: Uncharacterized protein

Chain W:



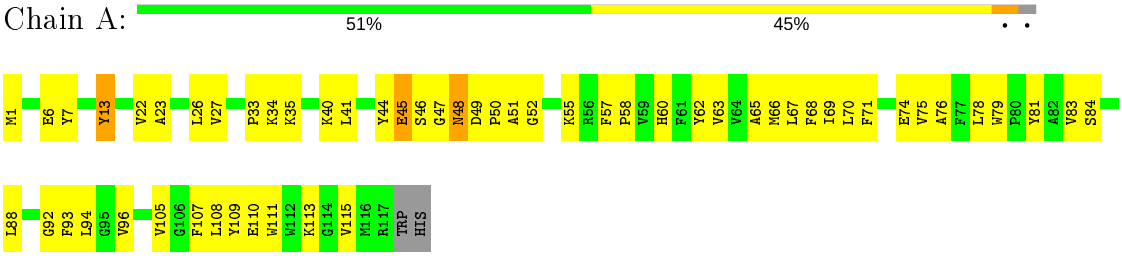
• Molecule 9: Uncharacterized protein

Chain X:



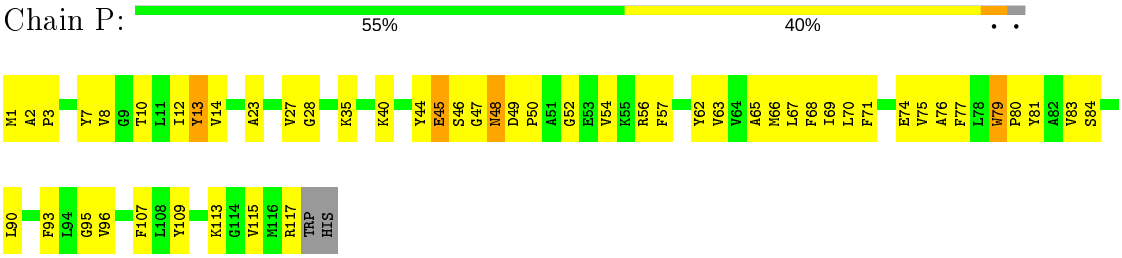
• Molecule 10: NADH-quinone oxidoreductase subunit 7

Chain A:



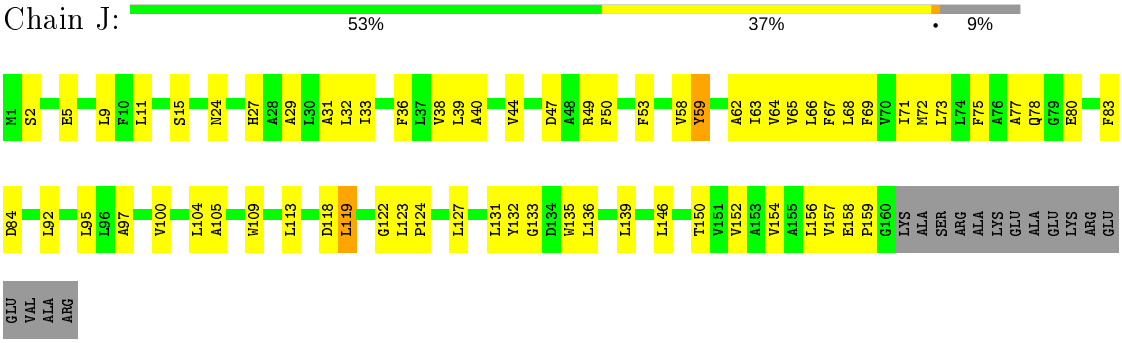
• Molecule 10: NADH-quinone oxidoreductase subunit 7

Chain P:



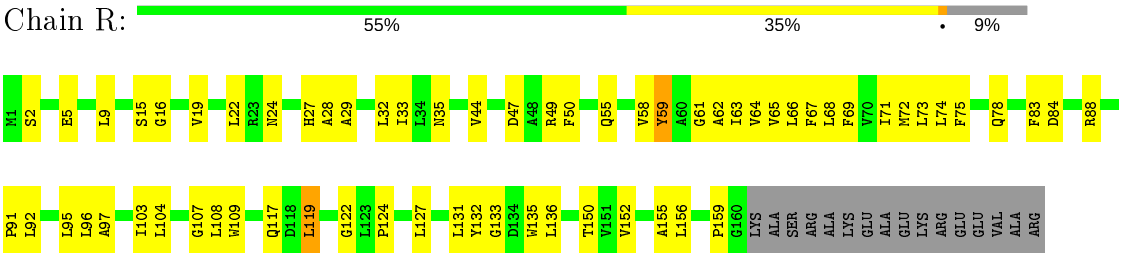
• Molecule 11: NADH-quinone oxidoreductase subunit 10

Chain J:



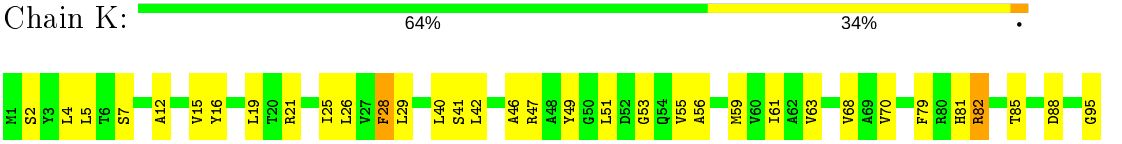
• Molecule 11: NADH-quinone oxidoreductase subunit 10

Chain R:



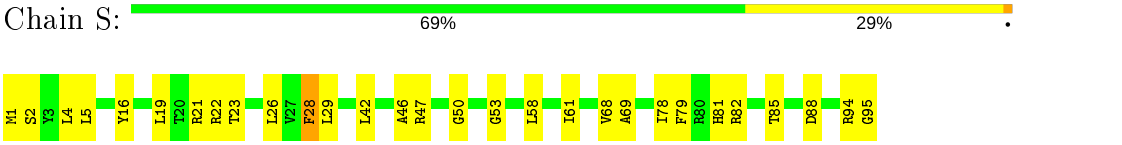
• Molecule 12: NADH-quinone oxidoreductase subunit 11

Chain K:



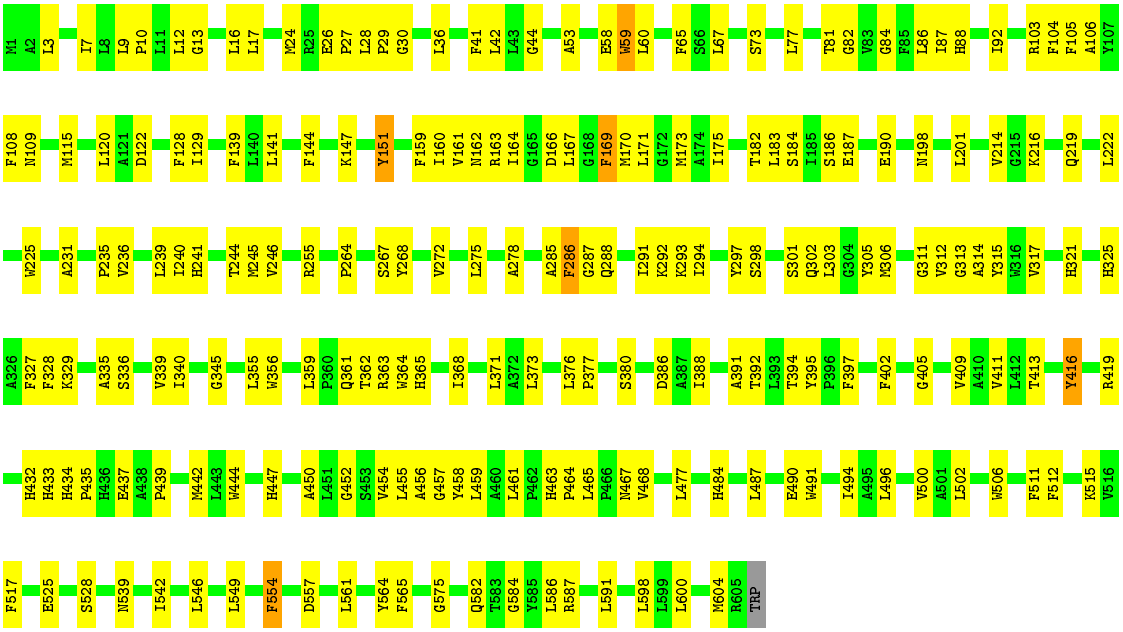
• Molecule 12: NADH-quinone oxidoreductase subunit 11

Chain S:



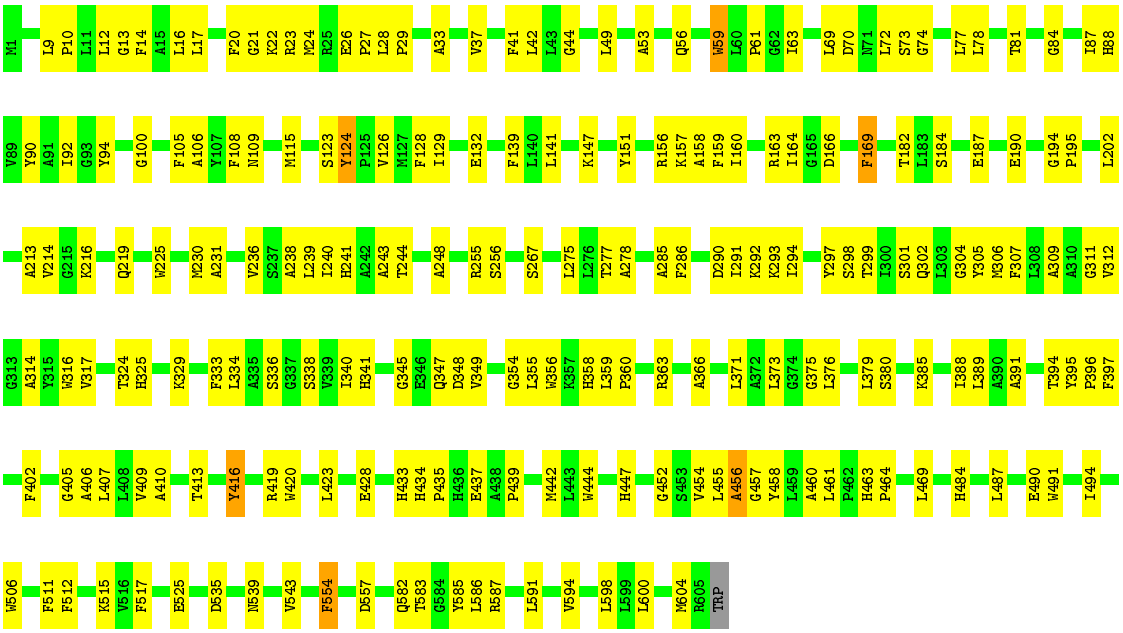
• Molecule 13: NADH-quinone oxidoreductase subunit 12

Chain L:



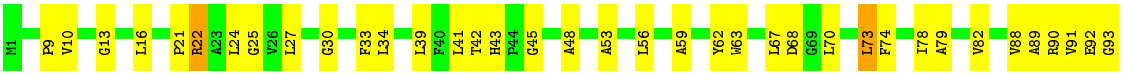
• Molecule 13: NADH-quinone oxidoreductase subunit 12

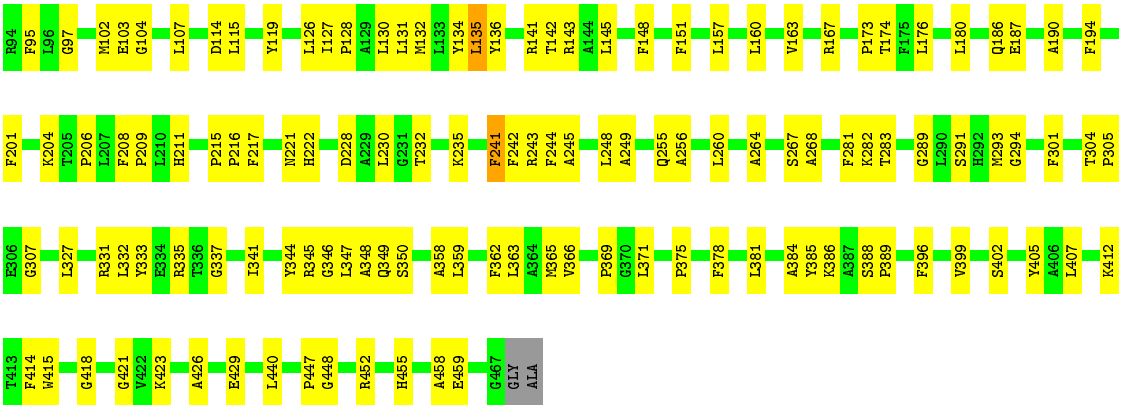
Chain T:



• Molecule 14: NADH-quinone oxidoreductase subunit 13

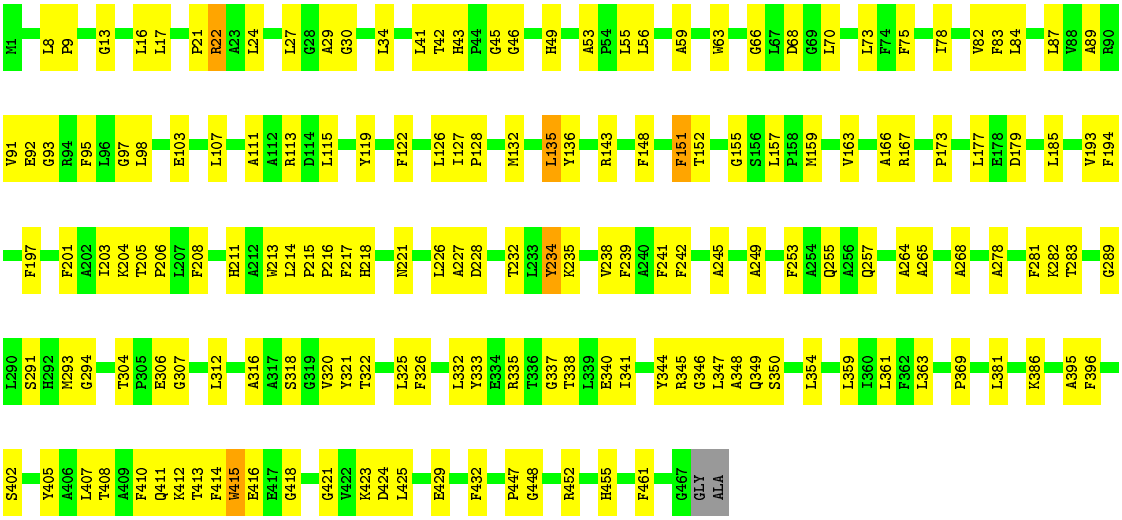
Chain M:





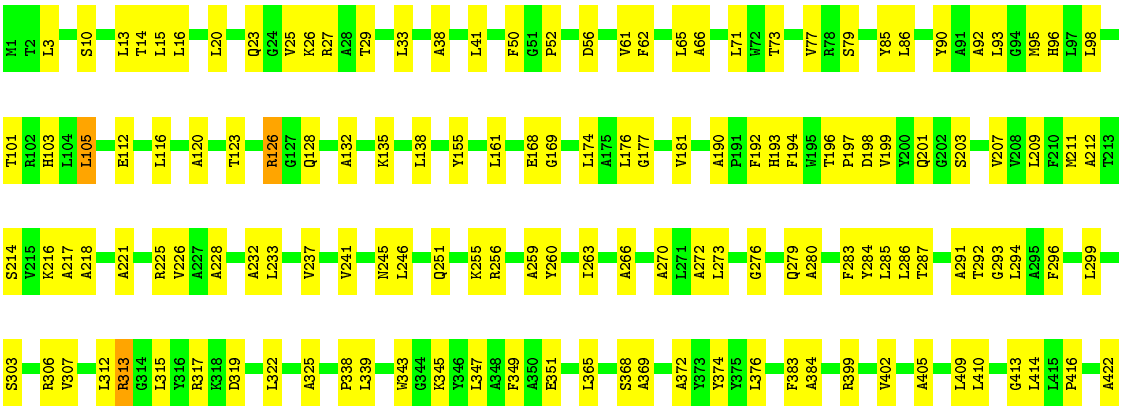
• Molecule 14: NADH-quinone oxidoreductase subunit 13

Chain U:



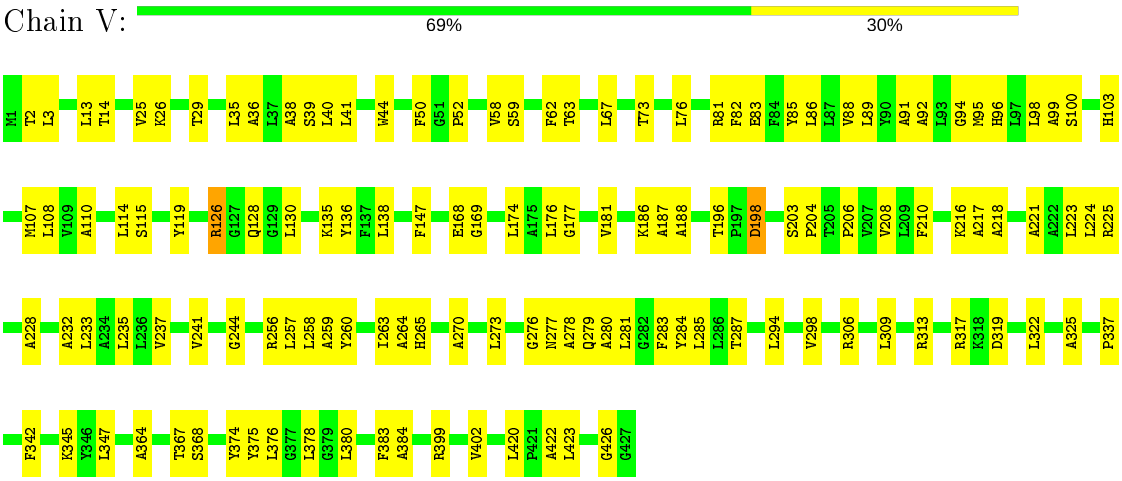
• Molecule 15: NADH-quinone oxidoreductase subunit 14

Chain N:



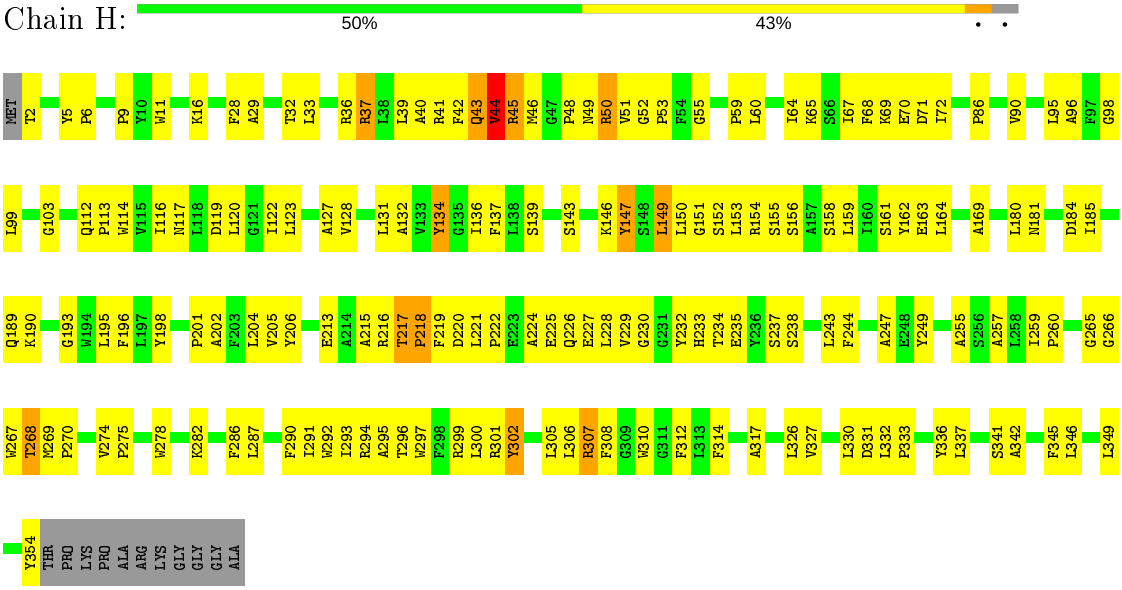
• Molecule 15: NADH-quinone oxidoreductase subunit 14

Chain V:



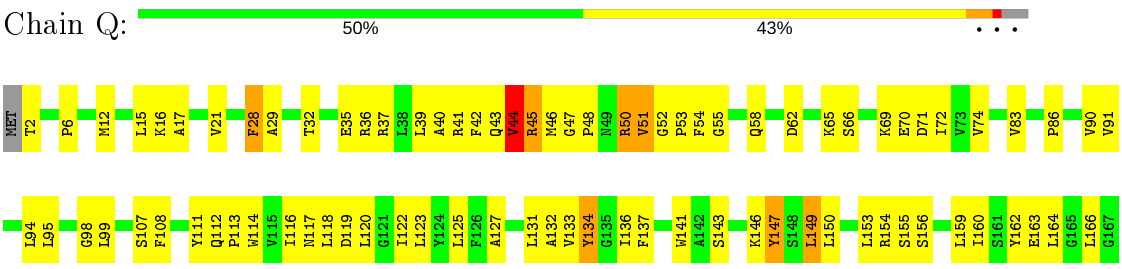
• Molecule 16: NADH-quinone oxidoreductase subunit 8

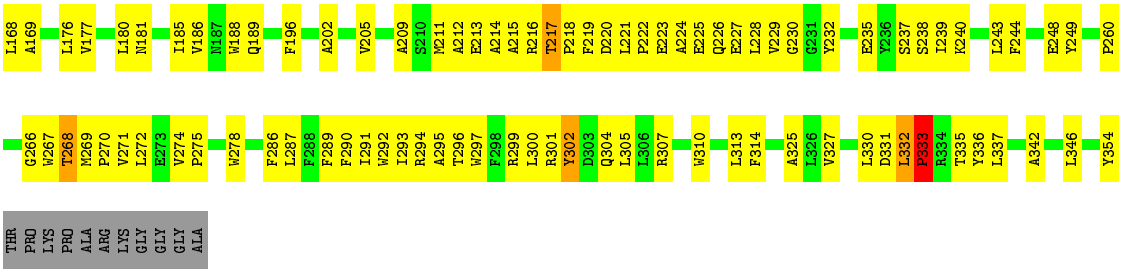
Chain H:



• Molecule 16: NADH-quinone oxidoreductase subunit 8

Chain Q:




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

4 Data and refinement statistics (i)

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

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	95.98Å 340.50Å 264.27Å 90.00° 100.44° 90.00°	Depositor
Resolution (Å)	49.71 – 3.40	Depositor
% Data completeness (in resolution range)	84.1 (49.71-3.40)	Depositor
R_{merge}	0.23	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.40 (at 3.40Å)	Xtriage
Refinement program	PHENIX (dev_3026: ???)	Depositor
R, R_{free}	0.213 , 0.234	Depositor
Wilson B-factor (Å^2)	62.4	Xtriage
Anisotropy	0.027	Xtriage
L-test for twinning[2]	$< \|L\| > = 0.34$, $< L^2 > = 0.17$	Xtriage
Estimated twinning fraction	0.379 for h,-k,-h-l	Xtriage
Reported twinning fraction	0.490 for -H,-K,H+L	Depositor
Outliers	0 of 191608 reflections	Xtriage
Total number of atoms	74144	wwPDB-VP
Average B, all atoms (Å^2)	63.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.17% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

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

5 Model quality

5.1 Standard geometry

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

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

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

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

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

Mol	Chain	#Chirality outliers	#Planarity outliers
7	9	0	1
10	A	0	1
10	P	0	1
13	T	0	2
16	H	0	2
16	Q	0	3
All	All	0	10

All (1) bond length outliers are listed below:

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

All (8) bond angle outliers are listed below:

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

There are no chirality outliers.

All (10) planarity outliers are listed below:

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

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Mol	Chain	Res	Type	Group
10	P	45	GLU	Peptide
16	Q	217	THR	Peptide
16	Q	266	GLY	Peptide
16	Q	333	PRO	Peptide
13	T	434	HIS	Peptide
13	T	456	ALA	Peptide

5.2 Too-close contacts

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	1	3417	0	3389	122	0
1	B	3417	0	3389	155	0
2	2	1406	0	1373	63	0
2	C	1406	0	1373	58	0
3	3	5895	0	5931	235	0
3	D	5895	0	5930	196	0
4	4	3067	0	3049	166	0
4	E	3067	0	3049	166	0
5	5	1607	0	1574	81	0
5	F	1607	0	1574	65	0
6	6	1289	0	1299	104	0
6	G	1289	0	1298	99	0
7	9	1388	0	1383	70	0
7	O	1388	0	1383	65	0
8	7	1031	0	1029	35	0
8	I	1031	0	1029	30	0
9	W	967	0	1010	32	0
9	X	967	0	1010	20	0
10	A	910	0	939	59	0
10	P	910	0	939	56	0
11	J	1183	0	1286	55	0
11	R	1183	0	1286	61	0
12	K	703	0	747	34	0
12	S	703	0	747	29	0
13	L	4604	0	4734	170	0
13	T	4604	0	4734	169	0
14	M	3489	0	3606	127	0

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

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 19.

All (2779) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:W:102:LEU:O	9:W:110:LEU:HD13	1.16	1.26
3:D:283:PRO:HG3	3:D:425:ARG:HH21	1.00	1.13
7:O:20:LYS:N	7:O:21:PRO:HD3	1.64	1.08
3:D:283:PRO:CG	3:D:425:ARG:HH21	1.68	1.04
6:6:56:ALA:HB1	16:H:44:VAL:CG1	1.87	1.02
2:2:3:PHE:HB2	2:2:45:ARG:NH1	1.75	1.01
6:6:144:PRO:O	6:6:148:ILE:HD12	1.59	1.01
3:D:283:PRO:HG3	3:D:425:ARG:NH2	1.74	1.00
7:O:20:LYS:N	7:O:21:PRO:CD	2.24	1.00
6:G:56:ALA:CB	16:Q:44:VAL:CG1	2.38	1.00
3:3:34:CYS:N	3:3:45:CYS:SG	2.36	0.99
9:W:102:LEU:HG	9:W:110:LEU:HD12	1.40	0.98

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

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

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

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

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

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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:K:2:SER:HA	12:K:5:LEU:HD12	1.75	0.68
11:R:68:LEU:HD23	11:R:71:ILE:HD11	1.74	0.68
9:W:11:ARG:NH1	9:W:68:PRO:O	2.27	0.68
13:T:20:PHE:HB3	13:T:23:ARG:HE	1.59	0.68
13:T:340:ILE:O	13:T:345:GLY:N	2.19	0.68
13:T:156:ARG:NH1	14:U:408:THR:OG1	2.26	0.68
4:E:259:THR:O	4:E:296:ARG:NH2	2.27	0.68
15:V:228:ALA:HB1	15:V:233:LEU:CD1	2.24	0.68
15:V:294:LEU:HD11	15:V:325:ALA:HB1	1.73	0.68
1:B:438:ARG:OXT	2:C:146:THR:OG1	2.12	0.68
15:N:128:GLN:OE1	15:N:306:ARG:NH2	2.27	0.68
14:U:115:LEU:HD13	14:U:163:VAL:HG23	1.74	0.68
1:1:79:MET:SD	1:1:217:THR:OG1	2.52	0.68
1:1:361:GLU:OE2	3:3:162:ARG:NH2	2.26	0.68
11:J:15:SER:OG	11:J:31:ALA:O	2.12	0.68
10:A:65:ALA:O	10:A:69:ILE:HG23	1.94	0.68
6:G:21:PHE:HD1	6:G:23:THR:H	1.39	0.68
16:Q:143:SER:HB2	16:Q:235:GLU:HG3	1.74	0.68
4:4:341:GLU:OE1	5:5:91:ARG:NH2	2.27	0.68
15:V:317:ARG:NH1	15:V:384:ALA:O	2.26	0.68
3:3:384:PRO:HG3	3:3:542:ARG:NH1	2.08	0.68
4:4:338:PRO:HG2	5:5:193:ARG:HH11	1.58	0.68
8:I:37:PHE:HE1	8:I:74:PRO:HA	1.59	0.68
3:3:605:PRO:HB2	3:3:609:GLU:HG3	1.76	0.67
16:H:44:VAL:O	16:H:45:ARG:O	2.13	0.67
13:L:105:PHE:O	13:L:109:ASN:ND2	2.25	0.67
1:B:253:GLN:HG2	1:B:327:GLY:HA2	1.76	0.67
8:I:23:TYR:OH	8:I:123:ARG:NH1	2.23	0.67
14:M:208:PHE:O	14:M:211:HIS:ND1	2.28	0.67
13:T:487:LEU:HA	13:T:490:GLU:HG2	1.75	0.67
14:U:89:ALA:HB1	14:U:91:VAL:HG22	1.76	0.67
16:H:265:GLY:O	16:H:282:LYS:NZ	2.20	0.67
13:L:371:LEU:HD22	13:L:376:LEU:HD13	1.77	0.67
3:3:383:PRO:HB3	3:3:679:ARG:HH21	1.59	0.67
7:O:171:GLU:OE2	8:I:43:ARG:NH2	2.28	0.67
1:1:338:VAL:O	1:1:342:TRP:HB2	1.95	0.67
6:6:91:VAL:HG22	10:A:46:SER:HB3	1.77	0.67
4:E:148:TYR:OH	16:Q:42:PHE:O	2.12	0.67
16:Q:327:VAL:O	16:Q:331:ASP:N	2.28	0.67
4:4:409:ARG:NH2	5:5:117:GLU:OE2	2.28	0.67
6:G:30:TRP:CZ3	6:G:34:ASN:ND2	2.63	0.67

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

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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:E:185:GLU:OE2	7:O:165:TYR:OH	2.13	0.65
4:E:27:THR:HA	4:E:46:THR:HA	1.77	0.65
1:1:6:LEU:HD11	1:1:240:GLN:HE21	1.62	0.64
2:2:61:MET:SD	3:3:214:MET:CE	2.85	0.64
11:J:119:LEU:HD23	12:K:51:LEU:HD12	1.79	0.64
16:Q:74:VAL:HG21	16:Q:235:GLU:HB3	1.79	0.64
1:1:312:SER:OG	1:1:315:HIS:ND1	2.25	0.64
16:H:29:ALA:O	16:H:32:THR:OG1	2.16	0.64
5:5:126:PHE:H	5:5:132:LEU:HD11	1.63	0.64
8:7:74:PRO:HG2	8:7:77:ALA:HB2	1.79	0.64
4:E:201:ILE:HA	4:E:204:TYR:HD2	1.61	0.64
13:L:115:MET:HG2	13:L:244:THR:HG22	1.79	0.64
13:T:94:TYR:HE1	13:T:341:HIS:HB2	1.63	0.64
4:4:336:HIS:ND1	5:5:189:ARG:O	2.31	0.64
1:B:75:LYS:NZ	1:B:218:ILE:O	2.27	0.64
1:B:437:TRP:HB3	2:C:92:GLY:HA3	1.78	0.64
11:J:119:LEU:HD11	12:K:47:ARG:HA	1.78	0.64
15:N:92:ALA:HA	15:N:95:MET:HE2	1.79	0.64
7:O:20:LYS:H	7:O:21:PRO:HD3	1.58	0.64
16:Q:43:GLN:O	16:Q:45:ARG:N	2.31	0.64
14:U:348:ALA:HB2	14:U:414:PHE:HB3	1.79	0.64
3:3:694:LEU:HB3	3:3:762:ALA:HB2	1.78	0.64
16:H:267:TRP:CG	16:H:268:THR:N	2.63	0.64
1:1:337:MET:O	1:1:341:MET:HG2	1.96	0.64
10:A:67:LEU:HB3	16:H:310:TRP:CZ2	2.32	0.64
16:H:332:LEU:HB2	16:H:333:PRO:CD	2.27	0.64
16:H:96:ALA:HB2	16:H:128:VAL:HG21	1.80	0.64
5:F:151:PRO:HD3	9:X:112:LYS:HE2	1.80	0.64
3:3:51:ARG:HB3	3:3:94:ASP:HB3	1.79	0.64
1:B:366:PHE:HE2	1:B:390:LEU:HD21	1.61	0.64
4:E:169:HIS:NE2	6:G:45:CYS:SG	2.69	0.64
6:G:56:ALA:HB2	16:Q:44:VAL:HG12	1.79	0.64
11:J:69:PHE:O	11:J:73:LEU:HG	1.98	0.64
13:T:458:TYR:HB3	13:T:461:LEU:HD11	1.80	0.64
1:1:393:LEU:HD23	1:1:397:ARG:NH2	2.12	0.64
3:3:31:PRO:HG3	3:3:137:TYR:CD2	2.33	0.64
14:M:115:LEU:HD13	14:M:163:VAL:HG23	1.80	0.64
7:O:41:HIS:HB3	7:O:113:ILE:HD11	1.79	0.64
16:Q:232:TYR:OH	16:Q:248:GLU:OE1	2.13	0.64
4:4:306:ASN:ND2	5:5:192:TYR:OH	2.23	0.64
3:D:199:VAL:HG11	3:D:219:PRO:HD2	1.80	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:546:ALA:O	3:D:667:ARG:NH1	2.31	0.64
5:F:67:ARG:NH1	5:F:96:GLU:OE2	2.31	0.64
16:H:37:ARG:NH2	16:H:49:ASN:OD1	2.31	0.64
4:4:261:THR:H	4:4:292:GLN:HE22	1.46	0.63
10:A:1:MET:O	16:H:2:THR:N	2.31	0.63
3:D:175:ILE:HG22	3:D:236:LEU:HB2	1.78	0.63
16:H:291:ILE:HA	16:H:294:ARG:HG3	1.79	0.63
13:L:159:PHE:HD2	14:M:407:LEU:HD11	1.62	0.63
13:T:586:LEU:HD13	15:V:138:LEU:HD12	1.81	0.63
4:4:80:THR:O	4:4:84:ARG:NH1	2.31	0.63
3:D:364:LEU:HB2	3:D:650:VAL:HG21	1.79	0.63
16:Q:274:VAL:HG12	16:Q:278:TRP:HD1	1.60	0.63
3:3:405:GLU:OE1	3:3:509:ALA:N	2.27	0.63
3:3:621:VAL:HG23	3:3:672:ALA:HA	1.79	0.63
5:5:66:GLU:HB2	5:5:93:TYR:HB3	1.79	0.63
1:B:30:ASP:OD2	1:B:155:ARG:NH2	2.24	0.63
2:C:110:GLU:OE2	8:I:114:ARG:NE	2.31	0.63
1:B:131:TYR:OH	2:C:17:LYS:O	2.12	0.63
3:D:605:PRO:HB2	3:D:609:GLU:HG3	1.80	0.63
4:E:201:ILE:HG21	4:E:284:ARG:HG3	1.79	0.63
3:3:551:PRO:HB2	3:3:555:GLY:HA2	1.80	0.63
10:P:90:LEU:HD12	16:Q:330:LEU:HD21	1.79	0.63
13:T:419:ARG:NH2	13:T:525:GLU:OE2	2.32	0.63
12:S:88:ASP:OD2	13:T:587:ARG:NH1	2.32	0.63
9:W:90:TYR:HB3	9:W:118:ALA:HB1	1.79	0.63
1:B:243:THR:HG22	1:B:244:GLU:H	1.64	0.63
2:C:6:ASP:HB3	2:C:7:LYS:HE3	1.81	0.63
1:B:38:TYR:HH	1:B:112:HIS:HD1	0.68	0.63
1:B:6:LEU:HB2	1:B:241:MET:HA	1.79	0.63
2:C:146:THR:HG23	2:C:149:ARG:H	1.64	0.63
6:G:59:ASP:OD1	6:G:62:ARG:NH2	2.30	0.63
16:H:151:GLY:HA2	16:H:154:ARG:HD3	1.81	0.63
6:6:63:PHE:HA	16:H:50:ARG:HG2	1.81	0.63
6:G:62:ARG:HB3	16:Q:50:ARG:HB2	1.81	0.63
4:E:26:MET:HG2	10:P:54:VAL:HB	1.81	0.63
1:1:287:ILE:HG12	1:1:330:LEU:HB3	1.81	0.62
4:4:110:PRO:HB3	4:4:301:PRO:HG2	1.81	0.62
1:B:288:GLN:HE21	1:B:331:ILE:HG22	1.62	0.62
4:E:373:PRO:O	4:E:377:ASN:ND2	2.32	0.62
8:I:120:ASP:OD1	8:I:123:ARG:NH1	2.31	0.62
14:M:167:ARG:NH2	14:M:173:PRO:O	2.32	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
14:M:115:LEU:HD12	14:M:180:LEU:HD13	1.82	0.62
15:N:299:LEU:HD22	15:N:307:VAL:HG11	1.81	0.62
14:U:166:ALA:HA	14:U:185:LEU:HD21	1.81	0.62
4:4:201:ILE:HA	4:4:204:TYR:HD2	1.64	0.62
4:4:379:GLN:HE22	5:5:110:SER:HA	1.64	0.62
8:7:37:PHE:HE1	8:7:74:PRO:HA	1.64	0.62
12:S:95:GLY:HA2	15:V:256:ARG:HE	1.63	0.62
3:3:8:ASP:OD2	3:3:28:TYR:OH	2.16	0.62
14:M:130:LEU:HD12	14:M:131:LEU:N	2.14	0.62
7:O:164:PRO:HA	7:O:178:GLU:HB2	1.80	0.62
6:6:90:PRO:O	6:6:93:ARG:HB3	1.99	0.62
4:E:261:THR:H	4:E:292:GLN:NE2	1.96	0.62
15:N:73:THR:HB	15:N:209:LEU:HD22	1.81	0.62
10:A:63:VAL:HG11	10:A:115:VAL:HG21	1.82	0.62
7:9:10:LEU:HA	16:H:296:THR:HG21	1.81	0.62
13:L:380:SER:HB3	13:L:457:GLY:H	1.64	0.62
3:3:199:VAL:HG11	3:3:219:PRO:HD2	1.81	0.62
3:D:35:SER:O	3:D:186:ARG:NH2	2.32	0.62
15:V:187:ALA:O	15:V:216:LYS:NZ	2.32	0.62
15:V:44:TRP:CD1	15:V:426:GLY:HA3	2.34	0.62
16:H:143:SER:HB2	16:H:235:GLU:HG3	1.81	0.62
13:T:87:ILE:HD12	13:T:239:LEU:HD13	1.82	0.62
14:U:333:TYR:O	14:U:337:GLY:N	2.33	0.62
3:3:556:ALA:HB2	3:3:562:GLY:HA3	1.82	0.62
4:E:352:GLU:O	4:E:371:ARG:NE	2.24	0.62
15:N:38:ALA:HA	15:N:41:LEU:HD12	1.82	0.62
11:R:59:TYR:CD1	11:R:63:ILE:HD12	2.35	0.62
1:B:259:LYS:NZ	2:C:180:GLU:HG2	2.15	0.62
1:B:366:PHE:CE2	1:B:390:LEU:HD21	2.34	0.62
13:L:44:GLY:HA3	13:L:77:LEU:HD21	1.81	0.62
14:M:70:LEU:O	14:M:73:LEU:HD23	2.00	0.62
14:U:75:PHE:HZ	14:U:111:ALA:HB2	1.65	0.62
3:3:445:THR:HB	3:3:463:ALA:HB2	1.81	0.62
3:3:468:HIS:ND1	3:3:469:ARG:O	2.33	0.62
13:T:325:HIS:NE2	13:T:329:LYS:HG3	2.15	0.62
1:1:220:ASN:N	18:1:502:FMN:O3P	2.26	0.61
1:B:111:PRO:HB3	1:B:145:LEU:HD23	1.81	0.61
16:H:218:PRO:HB3	16:H:305:LEU:HD13	1.82	0.61
13:L:60:LEU:HD21	14:M:375:PRO:HB3	1.82	0.61
13:T:278:ALA:HA	13:T:301:SER:HA	1.82	0.61
1:B:293:GLY:HA3	1:B:297:THR:HG21	1.82	0.61

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

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

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

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

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

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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:T:124:TYR:HH	13:T:256:SER:HG	1.39	0.56
11:R:96:LEU:HD22	13:T:594:VAL:HG12	1.86	0.56
2:2:162:ARG:NE	2:2:164:GLU:OE2	2.36	0.56
4:4:71:GLU:OE1	5:5:148:LYS:NZ	2.29	0.56
6:6:21:PHE:HD1	6:6:23:THR:H	1.53	0.56
1:B:95:GLU:O	1:B:135:ARG:NH1	2.37	0.56
3:D:227:THR:HG21	3:D:237:ASP:HB2	1.88	0.56
4:E:93:HIS:ND1	4:E:355:TYR:OH	2.24	0.56
13:L:161:VAL:HG13	13:L:222:LEU:HD13	1.86	0.56
14:M:232:THR:HA	14:M:235:LYS:HZ2	1.69	0.56
14:U:59:ALA:O	14:U:167:ARG:NH2	2.38	0.56
3:3:194:VAL:HG12	3:3:411:LEU:HD22	1.88	0.56
5:5:67:ARG:HD3	5:5:96:GLU:HG3	1.87	0.56
5:F:71:VAL:HA	5:F:90:VAL:O	2.05	0.56
6:G:57:ARG:NH2	6:G:143:ARG:HH22	2.04	0.56
11:J:92:LEU:O	11:J:95:LEU:HB3	2.06	0.56
13:T:17:LEU:HA	13:T:21:GLY:HA2	1.86	0.56
1:1:352:SER:HB3	3:3:206:GLY:HA2	1.87	0.56
3:3:367:PRO:O	3:3:552:GLY:N	2.22	0.56
4:4:84:ARG:HG3	4:4:169:HIS:ND1	2.21	0.56
4:E:140:LEU:HD21	4:E:217:ARG:NH1	2.20	0.56
4:E:201:ILE:HA	4:E:204:TYR:CD2	2.40	0.56
10:A:57:PHE:HE2	16:H:149:LEU:HD13	1.70	0.56
1:1:54:ILE:HG12	1:1:76:TRP:HE3	1.70	0.56
4:E:87:TYR:CB	6:G:45:CYS:HB3	2.36	0.56
13:L:314:ALA:HB1	13:L:317:VAL:HB	1.88	0.56
13:T:286:PHE:HD2	13:T:416:TYR:HB3	1.69	0.56
15:V:270:ALA:HA	15:V:273:LEU:HD23	1.88	0.56
1:1:253:GLN:HG2	1:1:327:GLY:HA2	1.87	0.56
3:3:112:LEU:HD23	3:3:130:LEU:HD21	1.88	0.56
5:5:53:VAL:HG22	5:5:55:LEU:CD1	2.36	0.56
8:I:42:TYR:O	8:I:46:ARG:NH2	2.39	0.56
13:L:286:PHE:O	13:L:419:ARG:NH1	2.39	0.56
15:N:201:GLN:OE1	15:N:256:ARG:NH1	2.39	0.56
13:T:151:TYR:HB3	13:T:231:ALA:HB1	1.88	0.56
7:9:101:CYS:N	17:9:201:SF4:S4	2.75	0.56
3:D:351:LEU:HD11	3:D:615:VAL:HG23	1.88	0.56
3:D:494:LYS:O	3:D:498:GLU:HG2	2.06	0.56
6:G:127:VAL:HG12	6:G:131:VAL:HG22	1.88	0.56
16:H:190:LYS:HD3	16:H:268:THR:HG22	1.87	0.56
14:M:157:LEU:HB3	15:N:365:LEU:HB3	1.88	0.56

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

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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:F:38:MET:HE3	5:F:104:VAL:CG1	2.32	0.54
13:L:160:ILE:O	13:L:164:ILE:HG13	2.07	0.54
13:L:59:TRP:O	14:M:452:ARG:NH2	2.39	0.54
11:J:104:LEU:HD23	15:N:174:LEU:HD21	1.89	0.54
3:3:33:PHE:HB2	3:3:45:CYS:SG	2.48	0.54
3:3:715:GLU:OE1	3:3:717:TRP:NE1	2.31	0.54
13:L:255:ARG:HD2	13:L:477:LEU:HD23	1.90	0.54
14:M:448:GLY:O	14:M:452:ARG:HG2	2.07	0.54
15:N:79:SER:O	15:N:85:TYR:OH	2.12	0.54
13:T:359:LEU:O	13:T:363:ARG:NH1	2.39	0.54
15:V:233:LEU:HD21	15:V:273:LEU:HB3	1.90	0.54
3:3:351:LEU:HD11	3:3:615:VAL:HG23	1.89	0.54
3:3:583:VAL:HG23	3:3:598:ALA:HA	1.89	0.54
4:4:163:VAL:HG13	4:4:164:THR:HG23	1.89	0.54
8:I:60:SER:HA	8:I:66:PRO:HA	1.89	0.54
13:L:373:LEU:HD21	13:L:416:TYR:HE1	1.73	0.54
10:P:3:PRO:HD2	16:Q:2:THR:HB	1.89	0.54
16:Q:117:ASN:ND2	16:Q:181:ASN:OD1	2.41	0.54
13:T:94:TYR:CE1	13:T:341:HIS:HB2	2.41	0.54
4:E:338:PRO:HG3	5:F:193:ARG:HB2	1.89	0.54
8:I:34:GLU:OE1	8:I:58:SER:OG	2.18	0.54
13:L:246:VAL:HB	13:L:303:LEU:HD21	1.87	0.54
14:M:13:GLY:HA2	14:M:97:GLY:HA2	1.90	0.54
16:Q:90:VAL:HG21	16:Q:243:LEU:HB3	1.88	0.54
2:2:76:GLY:H	2:2:118:SER:HG	1.52	0.54
3:3:512:LEU:HD21	3:3:534:ALA:HB1	1.88	0.54
4:4:48:SER:HB3	10:A:55:LYS:HE3	1.88	0.54
3:D:201:ASP:OD1	3:D:202:PHE:N	2.38	0.54
4:E:84:ARG:HG2	17:G:201:SF4:S2	2.48	0.54
11:J:47:ASP:O	11:J:122:GLY:N	2.41	0.54
13:T:128:PHE:HD1	13:T:169:PHE:CD2	2.26	0.54
13:T:285:ALA:HA	13:T:297:TYR:HB2	1.90	0.54
5:F:155:THR:HG23	9:X:93:VAL:HB	1.88	0.54
1:1:193:GLU:OE1	1:1:200:ARG:NH2	2.41	0.54
4:4:102:GLU:OE2	4:4:117:ARG:NH2	2.40	0.54
4:4:123:LEU:HD12	4:4:126:LEU:HD12	1.90	0.54
4:4:130:LEU:HD22	4:4:149:ALA:HB1	1.89	0.54
5:5:103:THR:HG23	5:5:127:GLU:O	2.08	0.54
3:D:33:PHE:HZ	3:D:130:LEU:HA	1.72	0.54
3:D:736:VAL:HG22	3:D:775:VAL:HG22	1.90	0.54
11:J:59:TYR:CE2	12:K:61:ILE:HG12	2.42	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:L:286:PHE:HD2	13:L:416:TYR:HB3	1.71	0.54
13:L:87:ILE:HD12	13:L:239:LEU:HD13	1.89	0.54
14:M:126:LEU:HD13	14:M:130:LEU:HD23	1.89	0.54
16:Q:12:MET:HE1	16:Q:15:LEU:HD22	1.88	0.54
16:Q:202:ALA:HA	16:Q:205:VAL:HG22	1.90	0.54
14:U:345:ARG:HG2	14:U:412:LYS:O	2.08	0.54
14:U:84:LEU:HB3	14:U:432:PHE:CE1	2.43	0.54
3:3:370:ASP:OD1	3:3:374:ARG:HD3	2.08	0.54
4:4:42:ARG:HB3	4:4:58:HIS:HB2	1.90	0.54
1:B:250:LYS:NZ	1:B:325:THR:O	2.37	0.54
15:N:299:LEU:HD21	15:N:312:LEU:HD21	1.90	0.54
4:E:50:GLU:CD	16:Q:154:ARG:HH12	2.11	0.54
3:3:378:PRO:HG2	3:3:680:LEU:HD23	1.89	0.54
4:4:143:LEU:HD23	4:4:143:LEU:H	1.73	0.54
1:B:193:GLU:OE1	1:B:200:ARG:NH2	2.26	0.54
3:D:690:GLY:HA3	3:D:770:ARG:NH2	2.23	0.54
13:T:214:VAL:HG22	13:T:219:GLN:HB2	1.90	0.54
1:1:160:LYS:O	1:1:168:SER:OG	2.16	0.54
3:3:693:TYR:O	3:3:760:LEU:N	2.37	0.54
4:4:99:LEU:HD23	4:4:102:GLU:OE1	2.08	0.54
4:4:137:LEU:HD23	4:4:145:PRO:HG2	1.90	0.54
5:F:39:ALA:HA	5:F:107:LEU:HD21	1.91	0.54
16:H:52:GLY:HA3	16:H:55:GLY:H	1.72	0.54
14:M:305:PRO:HB3	14:M:459:GLU:HA	1.89	0.54
13:T:324:THR:HG22	13:T:380:SER:HB2	1.90	0.54
13:T:61:PRO:HD3	14:U:452:ARG:HE	1.72	0.54
14:U:206:PRO:HD3	14:U:235:LYS:HG2	1.88	0.54
1:1:185:GLU:O	1:1:189:MET:HG3	2.08	0.53
1:1:259:LYS:HA	1:1:284:LEU:HD21	1.90	0.53
4:4:34:HIS:HE1	6:6:41:PHE:CE1	2.26	0.53
6:6:101:ASP:OD1	6:6:180:ARG:NH2	2.40	0.53
7:9:121:MET:HB2	7:9:131:TYR:OH	2.09	0.53
7:9:128:ASP:O	7:9:144:LYS:NZ	2.38	0.53
16:H:150:LEU:O	16:H:154:ARG:HG3	2.07	0.53
13:L:104:PHE:CE2	13:L:108:PHE:CZ	2.96	0.53
14:M:130:LEU:C	14:M:130:LEU:HD12	2.29	0.53
10:P:62:TYR:HD2	11:R:66:LEU:HD11	1.73	0.53
13:T:115:MET:HG2	13:T:244:THR:HG22	1.89	0.53
13:T:90:TYR:OH	13:T:338:SER:OG	2.22	0.53
4:4:285:GLU:O	4:4:289:ILE:HG12	2.07	0.53
3:D:283:PRO:HG2	3:D:425:ARG:NH2	2.23	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:51:ARG:HB3	3:D:94:ASP:HB3	1.90	0.53
14:M:335:ARG:NH1	14:M:423:LYS:O	2.40	0.53
14:U:215:PRO:HG2	14:U:216:PRO:HD3	1.90	0.53
3:3:401:ASP:O	3:3:405:GLU:HG3	2.09	0.53
3:3:397:LEU:HD21	3:3:480:LEU:HD13	1.89	0.53
3:3:594:ALA:O	3:3:598:ALA:HB3	2.08	0.53
16:H:147:TYR:HE1	16:H:228:LEU:HA	1.74	0.53
15:N:343:TRP:NE1	15:N:413:GLY:O	2.41	0.53
14:U:346:GLY:O	14:U:349:GLN:HG2	2.08	0.53
2:2:3:PHE:CB	2:2:45:ARG:NH1	2.61	0.53
2:2:27:ILE:HG13	2:2:53:VAL:HG21	1.90	0.53
4:4:224:ILE:HB	4:4:270:GLY:HA3	1.91	0.53
10:A:81:TYR:CE2	10:A:96:VAL:HG11	2.43	0.53
3:D:248:GLU:HG2	5:F:170:PHE:CE1	2.44	0.53
16:H:50:ARG:C	16:H:52:GLY:H	2.11	0.53
6:6:168:GLU:OE1	3:D:520:ARG:NH2	2.42	0.53
3:D:340:GLU:HB3	3:D:564:LEU:HB2	1.89	0.53
3:D:586:HIS:NE2	3:D:640:VAL:HG21	2.23	0.53
16:H:232:TYR:HB2	16:H:244:PHE:CE1	2.42	0.53
8:I:13:TRP:CD2	8:I:72:VAL:HB	2.43	0.53
8:I:74:PRO:HG2	8:I:77:ALA:HB2	1.91	0.53
13:L:413:THR:HA	13:L:416:TYR:CE2	2.43	0.53
14:M:402:SER:HA	14:M:405:TYR:CE2	2.44	0.53
15:N:62:PHE:CE2	15:N:285:LEU:HD22	2.43	0.53
14:U:43:HIS:NE2	14:U:45:GLY:O	2.42	0.53
1:B:275:LEU:HA	1:B:279:TRP:HD1	1.73	0.53
2:C:85:THR:HG22	2:C:86:LEU:H	1.73	0.53
3:D:453:PRO:HA	3:D:468:HIS:O	2.09	0.53
3:D:713:ARG:NE	3:D:746:ARG:HH21	2.07	0.53
14:M:206:PRO:HD2	14:M:293:MET:HG3	1.88	0.53
16:Q:150:LEU:HD21	16:Q:154:ARG:HH11	1.73	0.53
14:U:70:LEU:HD13	14:U:312:LEU:HD13	1.89	0.53
3:3:728:LEU:HB3	3:3:747:VAL:HG11	1.91	0.53
2:C:134:ILE:O	2:C:142:VAL:N	2.41	0.53
6:G:118:PHE:O	6:G:125:GLN:NE2	2.37	0.53
7:O:52:LYS:HB2	7:O:112:ALA:HB2	1.89	0.53
16:Q:35:GLU:OE1	16:Q:249:TYR:OH	2.15	0.53
10:P:56:ARG:HD3	11:R:74:LEU:HA	1.91	0.53
1:1:192:LEU:HD22	1:1:211:LEU:HD21	1.89	0.53
3:3:256:CYS:HB2	3:3:265:ILE:HD13	1.90	0.53
5:5:80:TRP:HA	5:5:80:TRP:CE3	2.44	0.53

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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
15:V:228:ALA:CB	15:V:233:LEU:HD11	2.40	0.52
3:3:614:LEU:O	3:3:621:VAL:HA	2.10	0.52
6:6:127:VAL:HG12	6:6:131:VAL:HG22	1.92	0.52
10:A:13:TYR:CZ	16:H:95:LEU:HA	2.43	0.52
3:D:407:PRO:O	3:D:410:HIS:HB3	2.10	0.52
13:L:386:ASP:OD2	13:L:494:ILE:HA	2.09	0.52
3:D:242:PHE:HD2	7:O:74:GLU:HB2	1.74	0.52
12:S:28:PHE:CZ	12:S:68:VAL:HA	2.44	0.52
1:1:206:PRO:HA	1:1:209:SER:O	2.10	0.52
3:3:309:PRO:HG2	3:3:320:ALA:O	2.09	0.52
7:9:10:LEU:HD12	16:H:296:THR:HG21	1.92	0.52
1:B:424:LEU:HG	1:B:429:ARG:O	2.10	0.52
1:B:393:LEU:HD22	3:D:106:GLY:HA3	1.91	0.52
3:D:124:LYS:HG2	3:D:236:LEU:HD21	1.90	0.52
4:E:370:VAL:HB	4:E:409:ARG:HD2	1.92	0.52
11:J:65:VAL:HG23	16:H:134:TYR:CZ	2.45	0.52
13:L:325:HIS:NE2	13:L:329:LYS:HG3	2.24	0.52
16:Q:224:ALA:HA	16:Q:229:VAL:HA	1.91	0.52
16:Q:36:ARG:NH1	16:Q:58:GLN:HG2	2.23	0.52
11:R:131:LEU:HA	11:R:135:TRP:HB2	1.92	0.52
11:R:29:ALA:O	11:R:33:ILE:HG13	2.09	0.52
15:V:91:ALA:HA	15:V:114:LEU:HA	1.92	0.52
15:V:63:THR:HG22	15:V:96:HIS:HA	1.90	0.52
2:2:24:ARG:HA	2:2:53:VAL:HG21	1.91	0.52
10:A:67:LEU:HD23	16:H:310:TRP:CE2	2.45	0.52
13:L:88:HIS:O	13:L:92:ILE:HG13	2.10	0.52
13:L:129:ILE:HG12	14:M:369:PRO:HB2	1.92	0.52
13:L:600:LEU:HD11	15:N:232:ALA:HB1	1.91	0.52
14:U:30:GLY:O	14:U:34:LEU:HG	2.10	0.52
2:2:87:SER:HB2	19:2:201:FES:S2	2.50	0.52
4:4:281:ARG:HD3	4:4:284:ARG:HH12	1.73	0.52
3:3:115:HIS:HB3	4:4:321:MET:CE	2.39	0.52
1:B:362:GLY:HA3	1:B:394:ILE:HD11	1.91	0.52
2:C:31:LEU:HD22	2:C:41:ILE:HD13	1.91	0.52
3:D:225:ASN:O	3:D:229:ILE:HG13	2.09	0.52
3:D:233:GLY:N	17:D:801:SF4:S2	2.79	0.52
16:H:131:LEU:HA	16:H:134:TYR:HB2	1.91	0.52
15:N:216:LYS:NZ	15:N:266:ALA:HB2	2.24	0.52
15:N:65:LEU:HD22	15:N:286:LEU:HD23	1.91	0.52
6:G:163:TYR:O	7:O:148:ARG:NE	2.43	0.52
11:R:32:LEU:HD13	12:S:29:LEU:HG	1.90	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
15:V:13:LEU:HD22	15:V:25:VAL:HG13	1.92	0.52
15:V:99:ALA:O	15:V:225:ARG:NH1	2.43	0.52
9:W:6:MET:O	9:W:62:ALA:HB2	2.10	0.52
3:3:131:GLN:HG2	4:4:325:ILE:HG23	1.92	0.52
3:3:178:ARG:HH22	8:7:65:GLU:CD	2.13	0.52
4:4:47:LEU:HD12	4:4:48:SER:N	2.24	0.52
7:9:45:ARG:NH2	7:9:139:ASP:OD2	2.41	0.52
3:D:285:VAL:HG13	3:D:286:ASN:H	1.75	0.52
4:E:350:ARG:O	4:E:373:PRO:HB2	2.10	0.52
16:H:147:TYR:CE1	16:H:228:LEU:HD13	2.45	0.52
8:I:43:ARG:HA	8:I:46:ARG:HH21	1.74	0.52
14:M:102:MET:HB3	14:M:230:LEU:HD23	1.91	0.52
14:M:350:SER:OG	14:M:421:GLY:HA2	2.10	0.52
15:N:313:ARG:HB2	15:N:384:ALA:HB3	1.91	0.52
9:X:37:TRP:HE1	9:X:40:LYS:NZ	2.08	0.52
3:3:734:VAL:HG13	3:3:775:VAL:HG13	1.92	0.52
6:6:119:ASN:HA	6:6:125:GLN:NE2	2.23	0.52
4:E:26:MET:HB2	4:E:47:LEU:O	2.10	0.52
12:K:4:LEU:CD1	12:K:41:SER:HA	2.40	0.52
13:L:285:ALA:O	13:L:294:ILE:HG13	2.10	0.52
13:L:405:GLY:O	13:L:409:VAL:HG23	2.10	0.52
10:P:95:GLY:HA3	11:R:136:LEU:HD21	1.92	0.52
13:T:129:ILE:HG12	14:U:369:PRO:HB2	1.90	0.52
15:V:270:ALA:O	15:V:273:LEU:HB2	2.10	0.52
8:7:86:LEU:HB2	8:7:91:ILE:HB	1.92	0.52
4:E:132:PHE:CE2	4:E:279:ARG:HD2	2.45	0.52
6:G:143:ARG:NE	6:G:145:GLU:OE1	2.42	0.52
11:J:131:LEU:HD21	11:J:139:LEU:HD13	1.91	0.52
11:R:47:ASP:O	11:R:122:GLY:N	2.39	0.52
14:U:206:PRO:HG3	14:U:214:LEU:HD22	1.91	0.52
1:B:186:THR:O	1:B:200:ARG:HG3	2.09	0.51
4:E:271:ASP:O	4:E:275:ARG:NE	2.36	0.51
13:L:293:LYS:O	13:L:297:TYR:HD1	1.92	0.51
13:L:458:TYR:HD1	13:L:461:LEU:HD21	1.73	0.51
7:O:59:CYS:HB2	7:O:104:CYS:HB2	1.91	0.51
10:P:77:PHE:O	10:P:80:PRO:HD2	2.10	0.51
16:Q:122:ILE:HA	16:Q:125:LEU:HD12	1.91	0.51
11:R:75:PHE:HZ	11:R:78:GLN:HE21	1.57	0.51
12:S:46:ALA:HB2	12:S:53:GLY:HA3	1.91	0.51
1:1:131:TYR:OH	2:2:17:LYS:O	2.24	0.51
5:5:67:ARG:NH1	5:5:96:GLU:OE2	2.44	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:9:68:ILE:HG12	7:9:93:ILE:HG12	1.91	0.51
16:H:150:LEU:HD23	16:H:154:ARG:HD2	1.92	0.51
11:J:124:PRO:HA	11:J:127:LEU:HB2	1.93	0.51
14:M:119:TYR:CE1	14:M:160:LEU:HD13	2.45	0.51
11:R:119:LEU:HD11	12:S:47:ARG:HA	1.92	0.51
13:T:160:ILE:O	13:T:164:ILE:HG13	2.10	0.51
15:V:188:ALA:HB3	15:V:216:LYS:HZ1	1.74	0.51
1:1:162:LEU:O	1:1:165:THR:HG22	2.11	0.51
1:1:113:LEU:HD12	1:1:228:VAL:HG21	1.92	0.51
2:2:74:PRO:HD3	8:7:125:ALA:HB2	1.91	0.51
1:B:165:THR:HG23	1:B:167:PHE:H	1.75	0.51
4:E:163:VAL:HG13	4:E:164:THR:HG23	1.93	0.51
6:G:72:PRO:O	6:G:99:MET:HG3	2.10	0.51
14:M:43:HIS:NE2	14:M:45:GLY:O	2.43	0.51
15:N:203:SER:O	15:N:255:LYS:NZ	2.43	0.51
16:Q:136:ILE:HG23	16:Q:232:TYR:HD2	1.76	0.51
13:T:17:LEU:HD22	13:T:29:PRO:HB3	1.92	0.51
6:6:153:GLN:HG3	7:9:124:TYR:CZ	2.46	0.51
1:B:243:THR:HG21	1:B:315:HIS:CE1	2.46	0.51
16:H:293:ILE:HG23	16:H:297:TRP:CE3	2.45	0.51
11:J:157:VAL:HG12	11:J:159:PRO:HD3	1.90	0.51
14:M:228:ASP:OD2	14:M:282:LYS:NZ	2.34	0.51
14:U:24:LEU:HD22	14:U:27:LEU:HD21	1.92	0.51
14:U:347:LEU:HB2	14:U:413:THR:O	2.10	0.51
3:3:127:ALA:HB3	3:3:246:ASN:ND2	2.25	0.51
1:B:283:PRO:HB3	1:B:287:ILE:HD13	1.92	0.51
3:D:237:ASP:OD1	3:D:239:THR:HG22	2.11	0.51
3:D:419:ASP:HA	3:D:447:LYS:NZ	2.26	0.51
16:H:217:THR:HG22	16:H:217:THR:O	2.11	0.51
16:H:86:PRO:HG3	16:H:244:PHE:CE2	2.46	0.51
13:L:171:LEU:O	13:L:175:ILE:HG13	2.10	0.51
13:L:433:HIS:O	13:L:433:HIS:ND1	2.42	0.51
15:N:319:ASP:CG	15:N:399:ARG:HH21	2.14	0.51
15:V:228:ALA:CB	15:V:233:LEU:CD1	2.89	0.51
1:1:46:LYS:HE2	1:1:163:PHE:HB3	1.92	0.51
1:1:249:MET:HA	1:1:267:PRO:HA	1.93	0.51
2:2:49:ILE:O	2:2:53:VAL:CG1	2.51	0.51
2:2:85:THR:HG22	2:2:86:LEU:H	1.76	0.51
4:4:333:GLU:O	4:4:363:SER:OG	2.25	0.51
4:4:233:GLY:HA2	5:5:48:PHE:HE1	1.75	0.51
1:B:422:LEU:O	1:B:426:ARG:N	2.26	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:713:ARG:NH2	3:D:715:GLU:OE2	2.44	0.51
3:D:716:LEU:HD21	3:D:758:LEU:HD23	1.93	0.51
16:H:227:GLU:HB2	16:H:299:ARG:HH12	1.76	0.51
13:L:104:PHE:HZ	13:L:235:PRO:HG2	1.76	0.51
13:L:391:ALA:O	13:L:395:TYR:HB2	2.11	0.51
15:N:56:ASP:OD1	15:N:225:ARG:NH1	2.44	0.51
15:N:294:LEU:HD12	15:N:405:ALA:HB3	1.92	0.51
15:N:347:LEU:O	15:N:351:GLU:HG2	2.11	0.51
11:R:69:PHE:O	11:R:73:LEU:HG	2.11	0.51
14:U:155:GLY:HA3	14:U:203:ILE:HG21	1.93	0.51
15:V:279:GLN:HG3	15:V:423:LEU:HB2	1.93	0.51
1:1:132:ILE:HD11	1:1:171:LEU:HD13	1.92	0.51
5:5:155:THR:O	6:6:119:ASN:ND2	2.42	0.51
6:6:113:SER:HB3	7:9:96:LEU:HD13	1.92	0.51
4:E:42:ARG:HB3	4:E:58:HIS:HB2	1.93	0.51
16:H:44:VAL:HG13	16:H:45:ARG:N	2.26	0.51
8:I:61:ASP:HB2	8:I:129:ALA:OXT	2.10	0.51
14:U:264:ALA:HB1	14:U:294:GLY:O	2.10	0.51
15:V:177:GLY:O	15:V:181:VAL:HG23	2.11	0.51
15:V:237:VAL:HG22	15:V:270:ALA:HB3	1.93	0.51
1:1:395:GLU:OE2	1:1:408:TRP:NE1	2.43	0.51
10:A:44:TYR:O	10:A:50:PRO:HG3	2.11	0.51
3:D:3:ARG:HE	3:D:10:ILE:HG21	1.76	0.51
16:H:224:ALA:HA	16:H:229:VAL:HA	1.92	0.51
15:N:372:ALA:O	15:N:376:LEU:HB2	2.10	0.51
11:R:155:ALA:O	15:V:81:ARG:NH1	2.43	0.51
15:V:29:THR:HG21	15:V:85:TYR:HB3	1.92	0.51
10:A:88:LEU:HB3	10:A:92:GLY:HA3	1.93	0.51
3:D:224:GLY:HA3	3:D:295:ARG:HD2	1.92	0.51
3:D:717:TRP:HB2	3:D:759:TYR:HB2	1.92	0.51
4:E:99:LEU:HD23	4:E:102:GLU:OE1	2.11	0.51
6:G:37:TRP:HB3	6:G:75:ALA:HA	1.92	0.51
7:O:17:LEU:HA	16:Q:41:ARG:O	2.11	0.51
13:T:13:GLY:O	13:T:17:LEU:HG	2.10	0.51
1:1:357:THR:HG23	1:1:360:ARG:NH2	2.26	0.51
2:2:61:MET:CE	3:3:214:MET:HG3	2.41	0.51
3:3:237:ASP:OD1	3:3:239:THR:HG22	2.11	0.51
3:3:243:ARG:HB3	3:3:275:LEU:HD22	1.91	0.51
1:B:270:THR:O	1:B:311:MET:HG3	2.11	0.51
16:H:139:SER:OG	16:H:232:TYR:HA	2.11	0.51
16:H:48:PRO:C	16:H:50:ARG:H	2.14	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:L:287:GLY:HA3	13:L:528:SER:HB2	1.93	0.51
15:N:228:ALA:HB1	15:N:233:LEU:CD1	2.40	0.51
13:T:298:SER:O	13:T:302:GLN:HG2	2.11	0.51
13:T:458:TYR:HD1	13:T:461:LEU:HD21	1.76	0.51
1:1:241:MET:SD	1:1:249:MET:HB3	2.51	0.50
3:3:135:VAL:O	5:5:188:SER:HB2	2.10	0.50
3:D:190:TYR:O	3:D:195:PRO:HD2	2.11	0.50
3:D:322:TRP:CH2	3:D:635:GLU:HB2	2.46	0.50
4:E:224:ILE:HD11	4:E:275:ARG:CZ	2.41	0.50
5:F:160:ARG:HB2	5:F:163:ARG:HH21	1.76	0.50
5:F:16:PRO:HD2	5:F:28:VAL:HG13	1.92	0.50
16:H:169:ALA:HB1	16:H:206:TYR:HB2	1.91	0.50
14:M:426:ALA:N	14:M:429:GLU:OE1	2.37	0.50
16:Q:221:LEU:N	16:Q:222:PRO:HA	2.26	0.50
13:T:12:LEU:O	13:T:16:LEU:HG	2.11	0.50
1:1:74:LEU:HD12	1:1:77:SER:OG	2.11	0.50
3:3:370:ASP:OD2	3:3:558:TRP:HD1	1.94	0.50
4:4:42:ARG:HD2	4:4:61:TYR:OH	2.11	0.50
6:6:157:LYS:HA	6:6:162:ALA:HB2	1.93	0.50
1:B:90:ILE:HB	1:B:218:ILE:HG12	1.92	0.50
3:D:688:ARG:HB3	3:D:770:ARG:HB2	1.92	0.50
3:D:2:VAL:HG13	3:D:89:ASP:HA	1.92	0.50
6:G:119:ASN:HA	6:G:125:GLN:NE2	2.26	0.50
6:G:135:VAL:HG21	6:G:154:LEU:HB2	1.93	0.50
14:M:91:VAL:HG23	14:M:92:GLU:H	1.76	0.50
1:1:201:LEU:HD21	3:3:84:VAL:HB	1.93	0.50
5:5:53:VAL:HG13	5:5:71:VAL:HB	1.92	0.50
3:D:192:GLU:HG3	3:D:440:ARG:HH11	1.76	0.50
3:D:305:ARG:HH22	3:D:605:PRO:HA	1.74	0.50
3:D:690:GLY:HA3	3:D:770:ARG:HH21	1.76	0.50
13:L:411:VAL:HG23	13:L:500:VAL:HG13	1.91	0.50
15:N:23:GLN:HB3	15:N:27:ARG:NH2	2.27	0.50
15:N:10:SER:HB3	15:N:90:TYR:HE1	1.75	0.50
15:N:93:LEU:O	15:N:96:HIS:HB3	2.11	0.50
16:Q:227:GLU:HG2	16:Q:228:LEU:N	2.26	0.50
6:G:35:SER:OG	16:Q:62:ASP:HA	2.11	0.50
3:3:136:GLU:HG2	5:5:186:GLY:O	2.10	0.50
3:3:501:LYS:HD2	3:3:501:LYS:H	1.76	0.50
4:4:239:LEU:HG	4:4:244:VAL:HB	1.93	0.50
4:4:32:PRO:HB2	6:6:88:MET:HE1	1.92	0.50
10:A:81:TYR:HB2	11:J:132:TYR:CZ	2.46	0.50

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

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

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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:6:101:ASP:OD2	10:A:35:LYS:HB2	2.12	0.49
1:B:50:PRO:HA	1:B:53:VAL:HG12	1.94	0.49
3:D:34:CYS:SG	3:D:35:SER:N	2.85	0.49
13:L:7:ILE:O	13:L:10:PRO:HD2	2.13	0.49
15:N:343:TRP:NE1	15:N:416:PRO:HG3	2.28	0.49
11:R:59:TYR:CE2	12:S:61:ILE:HG12	2.47	0.49
14:U:316:ALA:O	14:U:320:VAL:HG23	2.12	0.49
3:3:717:TRP:HB3	3:3:753:VAL:HG21	1.95	0.49
4:E:98:ALA:O	4:E:102:GLU:HG3	2.12	0.49
6:G:69:ARG:NH2	16:Q:223:GLU:OE2	2.45	0.49
13:L:173:MET:HB3	14:M:378:PHE:HZ	1.77	0.49
13:T:354:GLY:HA3	13:T:428:GLU:O	2.13	0.49
14:U:335:ARG:NH1	14:U:423:LYS:O	2.45	0.49
15:V:257:LEU:HD23	15:V:258:LEU:HD23	1.94	0.49
3:3:118:ASP:OD2	3:3:166:LYS:NZ	2.26	0.49
5:5:145:PRO:HA	5:5:150:TYR:CD1	2.48	0.49
5:F:55:LEU:HB2	5:F:69:ALA:O	2.13	0.49
13:L:24:MET:SD	13:L:28:LEU:HD23	2.52	0.49
13:L:59:TRP:NE1	14:M:447:PRO:HD2	2.28	0.49
14:M:359:LEU:O	14:M:363:LEU:HG	2.13	0.49
13:T:141:LEU:HB3	13:T:236:VAL:HG11	1.94	0.49
14:U:46:GLY:HA2	14:U:68:ASP:HA	1.95	0.49
2:2:161:LYS:HB3	2:2:166:ILE:HG12	1.94	0.49
1:B:259:LYS:HG3	2:C:179:VAL:O	2.12	0.49
3:D:405:GLU:HG2	3:D:696:PRO:HB2	1.95	0.49
4:E:87:TYR:HB3	6:G:45:CYS:HB3	1.94	0.49
5:F:15:TYR:OH	5:F:37:GLU:HG3	2.13	0.49
6:G:30:TRP:CH2	16:Q:51:VAL:CG1	2.96	0.49
6:G:60:LEU:O	6:G:65:SER:HB2	2.13	0.49
12:K:28:PHE:CZ	12:K:68:VAL:HA	2.48	0.49
6:G:91:VAL:HG13	10:P:46:SER:HB3	1.95	0.49
16:Q:71:ASP:HB2	16:Q:238:SER:HB3	1.94	0.49
11:R:61:GLY:O	11:R:65:VAL:HG21	2.13	0.49
3:3:290:ILE:HB	3:3:295:ARG:HH21	1.78	0.48
3:3:42:ILE:HD12	3:3:42:ILE:O	2.12	0.48
3:D:360:LEU:O	3:D:364:LEU:N	2.40	0.48
11:J:53:PHE:CE2	16:H:120:LEU:HB2	2.48	0.48
16:H:237:SER:OG	16:H:238:SER:N	2.44	0.48
13:L:490:GLU:HG3	13:L:491:TRP:N	2.26	0.48
16:Q:118:LEU:O	16:Q:181:ASN:ND2	2.45	0.48
16:Q:218:PRO:C	16:Q:220:ASP:H	2.17	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:T:187:GLU:O	13:T:190:GLU:HG2	2.13	0.48
14:U:232:THR:HA	14:U:235:LYS:NZ	2.28	0.48
15:V:283:PHE:O	15:V:287:THR:HG23	2.13	0.48
1:1:357:THR:HA	1:1:360:ARG:NH1	2.28	0.48
3:3:557:SER:H	3:3:560:GLU:HB2	1.78	0.48
6:6:163:TYR:HD1	7:9:152:ARG:HD2	1.75	0.48
6:6:35:SER:O	16:H:65:LYS:HD2	2.14	0.48
6:6:91:VAL:O	6:6:95:VAL:HG23	2.13	0.48
3:D:413:LEU:HA	3:D:416:PHE:HB3	1.95	0.48
6:G:163:TYR:CD1	7:O:152:ARG:HD2	2.48	0.48
8:I:86:LEU:HB2	8:I:91:ILE:HB	1.95	0.48
11:J:24:ASN:HB3	11:J:27:HIS:HB2	1.94	0.48
14:M:115:LEU:HD11	14:M:248:LEU:CD2	2.44	0.48
16:Q:41:ARG:NH1	16:Q:47:GLY:H	2.10	0.48
3:3:465:HIS:N	3:3:489:MET:SD	2.82	0.48
4:4:53:LEU:O	4:4:386:LYS:HG3	2.13	0.48
4:4:87:TYR:CB	6:6:45:CYS:HB3	2.44	0.48
7:9:149:GLU:O	7:9:153:THR:OG1	2.17	0.48
3:D:476:ILE:O	3:D:480:LEU:HG	2.13	0.48
6:G:120:ASN:ND2	6:G:122:ALA:H	2.02	0.48
6:G:130:VAL:HG13	9:X:120:PRO:O	2.13	0.48
16:H:224:ALA:HB2	16:H:233:HIS:CE1	2.48	0.48
16:H:40:ALA:HB2	16:H:45:ARG:HH21	1.77	0.48
14:M:93:GLY:O	14:M:136:TYR:OH	2.16	0.48
15:N:233:LEU:HD21	15:N:273:LEU:HB3	1.94	0.48
13:T:267:SER:HB3	13:T:311:GLY:O	2.14	0.48
1:1:394:ILE:HG22	1:1:403:ALA:HB1	1.95	0.48
5:5:68:PHE:HB3	5:5:124:ILE:HD11	1.95	0.48
10:A:22:VAL:O	10:A:26:LEU:HG	2.12	0.48
1:B:292:PRO:HA	1:B:328:VAL:HG13	1.95	0.48
3:D:125:GLY:HA2	3:D:245:ARG:NH2	2.26	0.48
3:D:353:GLU:CD	3:D:637:ALA:HB3	2.34	0.48
13:L:264:PRO:HA	13:L:397:PHE:HE1	1.78	0.48
13:L:58:GLU:HG3	14:M:452:ARG:HH22	1.78	0.48
14:M:327:LEU:O	14:M:331:ARG:HG2	2.13	0.48
13:T:515:LYS:HA	13:T:517:PHE:CE2	2.48	0.48
3:3:165:ASP:HB2	8:7:66:PRO:HG2	1.93	0.48
3:3:688:ARG:HA	3:3:688:ARG:HD3	1.52	0.48
4:4:131:VAL:O	4:4:135:THR:HG23	2.14	0.48
5:5:121:LEU:O	5:5:144:HIS:HB3	2.13	0.48
5:5:138:PRO:HG2	5:5:141:LEU:HD13	1.96	0.48

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

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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:A:83:VAL:HG23	10:A:84:SER:H	1.79	0.47
1:B:365:GLY:O	1:B:369:ASN:ND2	2.47	0.47
3:D:594:ALA:O	3:D:598:ALA:HB3	2.14	0.47
3:D:688:ARG:HA	3:D:688:ARG:HD3	1.52	0.47
6:G:148:ILE:O	6:G:151:VAL:HG22	2.13	0.47
6:G:39:ALA:N	6:G:77:VAL:O	2.34	0.47
3:3:47:MET:HE1	3:3:108:VAL:N	2.30	0.47
3:3:585:MET:HB3	3:3:587:LEU:HD13	1.95	0.47
3:3:550:LEU:HD22	3:3:684:ARG:HH21	1.79	0.47
5:5:102:PRO:HA	5:5:127:GLU:HB2	1.95	0.47
3:D:406:ALA:O	3:D:409:LEU:HB2	2.14	0.47
3:D:587:LEU:O	3:D:604:ALA:N	2.44	0.47
4:E:156:ILE:O	4:E:159:LEU:HB2	2.15	0.47
13:L:166:ASP:O	13:L:170:MET:HG3	2.14	0.47
15:N:61:VAL:O	15:N:65:LEU:HG	2.14	0.47
7:O:94:ASN:OD1	7:O:97:ARG:N	2.47	0.47
13:T:349:VAL:HG13	13:T:423:LEU:HB3	1.97	0.47
15:V:198:ASP:OD1	15:V:256:ARG:NH2	2.47	0.47
1:1:4:PRO:O	1:1:5:ILE:HG13	2.15	0.47
2:2:79:HIS:H	2:2:137:ASN:CG	2.17	0.47
4:4:337:PRO:O	4:4:361:GLY:HA2	2.14	0.47
3:D:32:LEU:HD11	3:D:35:SER:HB2	1.96	0.47
3:D:307:LYS:HE3	3:D:632:GLY:HA2	1.96	0.47
4:E:86:ASP:HB2	4:E:406:ASP:OD2	2.15	0.47
4:E:84:ARG:CZ	4:E:169:HIS:HB3	2.44	0.47
11:J:80:GLU:HB2	11:J:83:PHE:CE2	2.49	0.47
13:L:444:TRP:O	13:L:447:HIS:HB2	2.14	0.47
14:M:186:GLN:HG2	14:M:187:GLU:H	1.79	0.47
15:N:194:PHE:O	15:N:197:PRO:HD2	2.14	0.47
16:Q:133:VAL:HG11	16:Q:160:ILE:HG13	1.96	0.47
14:U:232:THR:HG21	14:U:322:THR:HG21	1.96	0.47
9:W:122:ASP:O	9:W:125:ILE:HG12	2.14	0.47
3:3:193:GLU:HB3	3:3:418:ARG:HH12	1.79	0.47
3:3:347:HIS:HB2	3:3:538:ALA:HB1	1.97	0.47
3:3:505:LEU:O	3:3:532:VAL:HA	2.14	0.47
3:D:734:VAL:HG13	3:D:775:VAL:HG13	1.96	0.47
6:G:153:GLN:HG3	7:O:124:TYR:CZ	2.49	0.47
16:H:39:LEU:O	16:H:43:GLN:CG	2.62	0.47
11:J:63:ILE:HG23	12:K:68:VAL:HG11	1.95	0.47
13:L:26:GLU:O	13:L:29:PRO:HD2	2.13	0.47
13:L:461:LEU:N	13:L:467:ASN:OD1	2.47	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
14:M:232:THR:HA	14:M:235:LYS:NZ	2.30	0.47
14:M:281:PHE:CE1	14:M:341:ILE:HG22	2.48	0.47
14:M:91:VAL:HB	14:M:95:PHE:HE1	1.79	0.47
16:Q:169:ALA:HB2	16:Q:205:VAL:HG23	1.97	0.47
16:Q:40:ALA:HB2	16:Q:45:ARG:HH21	1.79	0.47
16:Q:44:VAL:O	16:Q:45:ARG:O	2.32	0.47
13:T:302:GLN:O	13:T:306:MET:HG3	2.14	0.47
13:T:355:LEU:HB3	13:T:359:LEU:HD12	1.96	0.47
13:T:41:PHE:HD2	13:T:42:LEU:HD12	1.79	0.47
3:3:190:TYR:O	3:3:195:PRO:HD2	2.15	0.47
4:4:115:THR:O	4:4:119:ILE:HG13	2.14	0.47
4:E:310:THR:HG22	4:E:311:PRO:O	2.15	0.47
16:H:189:GLN:O	16:H:193:GLY:HA2	2.14	0.47
16:H:255:ALA:O	16:H:259:ILE:HG13	2.14	0.47
8:I:58:SER:HB3	8:I:69:LEU:HD23	1.96	0.47
6:G:163:TYR:H	7:O:152:ARG:NH1	2.13	0.47
11:R:68:LEU:HD13	16:Q:137:PHE:HZ	1.78	0.47
12:S:28:PHE:CE2	12:S:68:VAL:HA	2.50	0.47
14:U:332:LEU:HA	14:U:335:ARG:HG2	1.96	0.47
1:1:26:SER:HA	1:1:31:TYR:CG	2.49	0.47
3:3:165:ASP:OD2	3:3:168:HIS:HB2	2.14	0.47
3:3:375:THR:HG21	3:3:512:LEU:HB3	1.96	0.47
3:3:689:LYS:H	3:3:689:LYS:HG2	1.52	0.47
4:4:62:LEU:HB2	4:4:408:ASP:OD2	2.15	0.47
4:4:87:TYR:CG	6:6:45:CYS:HB3	2.50	0.47
1:B:195:LEU:HD23	2:C:24:ARG:HH12	1.80	0.47
3:D:191:PHE:HE2	3:D:226:ILE:HD13	1.79	0.47
4:E:38:HIS:CE1	4:E:397:ILE:HG22	2.50	0.47
4:E:47:LEU:HD22	4:E:52:VAL:HA	1.95	0.47
5:F:38:MET:HA	5:F:41:TYR:HD2	1.80	0.47
13:L:355:LEU:HB3	13:L:359:LEU:HD12	1.97	0.47
6:G:56:ALA:HB3	16:Q:44:VAL:HG11	1.95	0.47
10:P:7:TYR:HD2	11:R:44:VAL:HG11	1.79	0.47
13:T:413:THR:HA	13:T:416:TYR:CZ	2.50	0.47
13:T:53:ALA:HB3	13:T:69:LEU:HB3	1.97	0.47
15:V:376:LEU:O	15:V:380:LEU:N	2.37	0.47
9:W:49:LEU:HD12	9:W:57:LEU:O	2.15	0.47
6:6:96:TRP:HZ2	6:6:175:ALA:HB1	1.79	0.47
1:B:250:LYS:HB3	1:B:252:TYR:CE1	2.50	0.47
2:C:24:ARG:NH2	2:C:59:GLU:HB3	2.29	0.47
4:E:372:ALA:HB3	4:E:375:PHE:HB2	1.95	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:L:9:LEU:HB2	13:L:10:PRO:HD3	1.97	0.47
14:M:119:TYR:OH	14:M:160:LEU:HB2	2.14	0.47
15:N:259:ALA:O	15:N:263:ILE:HG13	2.14	0.47
16:Q:260:PRO:HG3	16:Q:286:PHE:CD2	2.50	0.47
11:R:88:ARG:O	11:R:91:PRO:HD2	2.15	0.47
13:T:312:VAL:HA	13:T:397:PHE:CD2	2.50	0.47
1:1:157:TYR:O	1:1:158:LEU:HD23	2.15	0.47
3:3:259:CYS:SG	3:3:261:VAL:HG22	2.55	0.47
3:D:481:LEU:HD11	3:D:520:ARG:HB3	1.97	0.47
3:D:723:ALA:O	3:D:727:ALA:N	2.47	0.47
13:L:10:PRO:HB2	13:L:109:ASN:O	2.15	0.47
13:L:291:ILE:HD12	13:L:336:SER:HB3	1.97	0.47
14:M:127:ILE:O	14:M:130:LEU:HG	2.15	0.47
14:M:33:PHE:HA	14:M:79:ALA:HB1	1.97	0.47
14:M:371:LEU:HD12	14:M:440:LEU:HB3	1.96	0.47
15:N:120:ALA:O	15:N:123:THR:OG1	2.25	0.47
16:Q:333:PRO:HB2	16:Q:335:THR:H	1.79	0.47
4:4:148:TYR:HE2	7:9:16:TYR:CG	2.33	0.47
4:4:379:GLN:NE2	5:5:110:SER:HA	2.29	0.47
7:9:108:CYS:HA	17:9:202:SF4:S3	2.55	0.47
1:B:167:PHE:CE2	1:B:169:PHE:HB2	2.50	0.47
3:D:115:HIS:HB3	4:E:321:MET:CE	2.41	0.47
16:H:326:LEU:HD12	16:H:330:LEU:HD23	1.97	0.47
16:Q:107:SER:OG	16:Q:113:PRO:HG3	2.15	0.47
1:1:343:ASN:HA	1:1:346:ARG:HG2	1.97	0.47
8:7:44:MET:HE2	8:7:46:ARG:HH22	1.80	0.47
10:A:71:PHE:O	10:A:74:GLU:HB3	2.15	0.47
1:B:272:PHE:CZ	1:B:316:LEU:HD21	2.50	0.47
1:B:373:LYS:NZ	1:B:383:ASP:OD1	2.46	0.47
4:E:385:CYS:HB3	4:E:396:ILE:HG21	1.96	0.47
16:H:71:ASP:HB2	16:H:238:SER:HB3	1.97	0.47
12:K:56:ALA:HA	15:N:105:LEU:HD13	1.96	0.47
11:J:59:TYR:HE2	12:K:61:ILE:HG12	1.77	0.47
14:M:148:PHE:HE1	14:M:204:LYS:HZ3	1.62	0.47
14:U:127:ILE:HB	14:U:128:PRO:HD3	1.96	0.47
14:U:159:MET:HG3	14:U:197:PHE:CD1	2.50	0.47
15:V:319:ASP:HB3	15:V:322:LEU:HB2	1.97	0.47
15:V:98:LEU:HD12	15:V:107:MET:HG2	1.96	0.47
9:X:36:ASP:N	9:X:36:ASP:OD1	2.48	0.47
3:3:616:ASN:HD22	3:3:622:LEU:HD11	1.80	0.46
1:B:380:GLU:N	1:B:383:ASP:OD2	2.40	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:728:LEU:O	3:D:749:HIS:NE2	2.35	0.46
4:E:306:ASN:ND2	5:F:192:TYR:OH	2.48	0.46
11:J:113:LEU:HD21	12:K:49:TYR:OH	2.15	0.46
12:K:70:VAL:HG21	15:N:116:LEU:HD22	1.97	0.46
13:L:515:LYS:HA	13:L:517:PHE:CZ	2.49	0.46
13:T:20:PHE:HD1	13:T:23:ARG:HH21	1.62	0.46
13:T:24:MET:HB3	13:T:28:LEU:HD23	1.97	0.46
13:T:405:GLY:O	13:T:409:VAL:HG23	2.14	0.46
1:1:6:LEU:HD21	1:1:12:ARG:HG3	1.97	0.46
1:1:356:CYS:HB3	1:1:358:PRO:HD2	1.96	0.46
2:2:130:THR:HB	2:2:143:GLU:HB3	1.96	0.46
5:5:103:THR:N	5:5:127:GLU:O	2.43	0.46
6:6:102:PRO:HD3	10:A:33:PRO:HG2	1.98	0.46
10:A:41:LEU:HD23	16:H:72:ILE:HD11	1.97	0.46
1:B:135:ARG:NE	1:B:137:GLU:HB2	2.29	0.46
3:D:656:LEU:HD21	9:X:3:ARG:HD3	1.95	0.46
4:E:138:LEU:HD13	4:E:143:LEU:HA	1.97	0.46
15:N:10:SER:HB3	15:N:90:TYR:CE1	2.50	0.46
7:O:108:CYS:HA	17:O:202:SF4:S3	2.55	0.46
11:R:64:VAL:HA	11:R:67:PHE:HB2	1.96	0.46
13:T:70:ASP:OD2	13:T:255:ARG:NH2	2.44	0.46
14:U:70:LEU:O	14:U:73:LEU:HD23	2.15	0.46
1:1:352:SER:O	3:3:205:ARG:HD2	2.15	0.46
3:3:260:PRO:HB2	3:3:617:LEU:HB3	1.96	0.46
5:5:71:VAL:HA	5:5:90:VAL:O	2.15	0.46
10:A:68:PHE:HD2	16:H:164:LEU:HB2	1.79	0.46
1:B:18:TYR:OH	1:B:105:TYR:HB2	2.15	0.46
1:B:186:THR:HB	1:B:200:ARG:H	1.81	0.46
3:D:191:PHE:CE2	3:D:226:ILE:HD13	2.50	0.46
4:E:360:ASP:HB2	5:F:61:PRO:CD	2.45	0.46
13:L:377:PRO:HG2	13:L:502:LEU:HD11	1.97	0.46
6:G:163:TYR:H	7:O:152:ARG:HH12	1.63	0.46
4:E:31:GLY:HA3	10:P:45:GLU:OE2	2.16	0.46
16:Q:6:PRO:HG2	16:Q:112:GLN:HE21	1.80	0.46
16:Q:186:VAL:HG11	16:Q:267:TRP:CZ3	2.50	0.46
14:U:242:PHE:CZ	14:U:461:PHE:HD2	2.34	0.46
1:1:49:THR:OG1	1:1:52:GLU:HG3	2.16	0.46
2:2:40:TRP:CD1	2:2:74:PRO:HA	2.51	0.46
3:3:413:LEU:HA	3:3:416:PHE:HB3	1.97	0.46
4:4:352:GLU:CD	5:5:87:ARG:HH22	2.19	0.46
4:E:125:ARG:HD2	4:E:286:SER:OG	2.15	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:L:286:PHE:HA	13:L:294:ILE:HD11	1.98	0.46
13:L:586:LEU:HD13	15:N:138:LEU:HD12	1.97	0.46
15:N:317:ARG:HH12	15:N:383:PHE:C	2.17	0.46
7:O:149:GLU:O	7:O:153:THR:CB	2.63	0.46
11:R:50:PHE:HB3	11:R:122:GLY:O	2.16	0.46
14:U:218:HIS:HA	14:U:228:ASP:OD1	2.15	0.46
14:U:201:PHE:CD2	14:U:245:ALA:HB2	2.51	0.46
15:V:85:TYR:O	15:V:88:VAL:HB	2.15	0.46
3:3:270:ARG:HB3	3:3:275:LEU:HD11	1.98	0.46
3:3:723:ALA:O	3:3:727:ALA:N	2.49	0.46
4:4:318:GLU:HB2	8:7:39:ASP:CA	2.34	0.46
1:B:103:ASP:OD1	1:B:222:GLU:HB2	2.15	0.46
1:B:18:TYR:CZ	1:B:105:TYR:HB2	2.50	0.46
4:E:226:PRO:HB2	5:F:80:TRP:CH2	2.51	0.46
13:L:41:PHE:HD2	13:L:42:LEU:HD12	1.78	0.46
13:L:554:PHE:HZ	14:M:283:THR:HG21	1.79	0.46
15:N:3:LEU:HD13	15:N:96:HIS:HD2	1.80	0.46
16:Q:176:LEU:HD21	16:Q:337:LEU:HD12	1.97	0.46
13:T:366:ALA:HB1	13:T:420:TRP:HZ3	1.80	0.46
14:U:148:PHE:O	14:U:152:THR:HG23	2.15	0.46
14:U:253:PHE:CZ	14:U:257:GLN:HG3	2.51	0.46
15:V:345:LYS:NZ	15:V:368:SER:OG	2.41	0.46
2:2:34:VAL:HG11	2:2:45:ARG:HG3	1.97	0.46
2:2:45:ARG:O	2:2:49:ILE:HG13	2.15	0.46
2:2:61:MET:SD	3:3:214:MET:HE3	2.55	0.46
3:3:248:GLU:HG2	5:5:170:PHE:CE1	2.50	0.46
7:9:40:ARG:O	7:9:116:GLY:N	2.47	0.46
10:A:23:ALA:O	10:A:27:VAL:HG23	2.16	0.46
3:D:439:GLU:HG2	3:D:440:ARG:HG2	1.98	0.46
4:E:36:SER:HB2	16:Q:226:GLN:HA	1.98	0.46
16:H:221:LEU:N	16:H:222:PRO:HA	2.31	0.46
8:I:19:TRP:CD1	8:I:112:LYS:HE3	2.51	0.46
14:M:128:PRO:O	14:M:132:MET:HG2	2.16	0.46
14:M:167:ARG:HA	14:M:180:LEU:HD21	1.98	0.46
14:M:41:LEU:O	14:M:42:THR:HG22	2.16	0.46
13:T:20:PHE:O	13:T:22:LYS:N	2.48	0.46
14:U:55:LEU:O	14:U:56:LEU:HD12	2.15	0.46
4:4:381:LEU:HB3	4:4:382:PRO:HD3	1.96	0.46
6:6:108:MET:HA	6:6:137:VAL:HG13	1.98	0.46
4:4:28:LEU:HD12	10:A:51:ALA:HA	1.98	0.46
1:B:135:ARG:HH21	1:B:137:GLU:CD	2.19	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:211:LEU:CB	1:B:216:THR:HG21	2.46	0.46
1:B:211:LEU:HB2	1:B:216:THR:HG21	1.98	0.46
2:C:15:PHE:HE1	2:C:53:VAL:HG23	1.80	0.46
4:E:384:ALA:HB1	4:E:396:ILE:HD11	1.98	0.46
10:A:70:LEU:HD13	11:J:150:THR:HG22	1.98	0.46
13:L:419:ARG:HB2	13:L:512:PHE:CD2	2.50	0.46
13:L:459:LEU:O	13:L:468:VAL:N	2.39	0.46
14:M:344:TYR:O	14:M:347:LEU:HD23	2.15	0.46
15:N:62:PHE:CG	15:N:221:ALA:HB2	2.50	0.46
13:T:463:HIS:CE1	13:T:487:LEU:HD22	2.51	0.46
14:U:238:VAL:O	14:U:241:PHE:HB2	2.16	0.46
2:2:61:MET:O	2:2:65:SER:OG	2.26	0.46
3:3:267:ALA:HA	3:3:277:ILE:HD13	1.98	0.46
3:3:83:CYS:SG	3:3:84:VAL:HG13	2.56	0.46
5:5:116:ARG:NH2	5:5:135:ILE:HG12	2.31	0.46
8:7:37:PHE:N	8:7:53:THR:O	2.43	0.46
1:B:162:LEU:O	1:B:165:THR:HG22	2.16	0.46
3:D:459:MET:HG2	3:D:465:HIS:HB2	1.98	0.46
5:F:2:ARG:HG3	5:F:84:ASP:OD2	2.16	0.46
6:G:53:SER:O	6:G:60:LEU:N	2.43	0.46
11:J:105:ALA:O	11:J:109:TRP:HB2	2.16	0.46
14:M:332:LEU:HA	14:M:335:ARG:HG2	1.98	0.46
12:K:46:ALA:HA	15:N:155:TYR:HE2	1.80	0.46
15:N:181:VAL:HA	15:N:192:PHE:CE2	2.51	0.46
15:N:339:LEU:HD23	15:N:410:LEU:HA	1.97	0.46
7:O:105:GLU:CD	7:O:114:VAL:HG13	2.36	0.46
7:O:11:GLY:O	7:O:15:LYS:HG3	2.15	0.46
16:Q:134:TYR:HA	16:Q:137:PHE:CE2	2.50	0.46
13:T:299:THR:HG23	13:T:325:HIS:HE1	1.81	0.46
14:U:289:GLY:O	14:U:293:MET:HG2	2.16	0.46
14:U:281:PHE:HE2	14:U:332:LEU:HD21	1.81	0.46
14:U:306:GLU:OE2	14:U:386:LYS:NZ	2.48	0.46
14:U:70:LEU:HD11	14:U:312:LEU:HD22	1.98	0.46
3:3:310:LEU:HB3	3:3:317:LEU:HB3	1.98	0.46
4:4:115:THR:O	4:4:118:VAL:HG22	2.16	0.46
1:B:39:GLU:O	1:B:43:ARG:HG2	2.16	0.46
3:D:462:ALA:O	3:D:465:HIS:ND1	2.49	0.46
5:F:3:LEU:O	5:F:7:LEU:HG	2.16	0.46
5:F:6:VAL:HG13	5:F:41:TYR:HE1	1.81	0.46
6:G:46:CYS:SG	6:G:109:GLY:HA3	2.55	0.46
16:H:134:TYR:HA	16:H:137:PHE:CE2	2.51	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
16:H:185:ILE:HG22	16:H:189:GLN:OE1	2.15	0.46
16:H:300:LEU:O	16:H:301:ARG:HG2	2.16	0.46
16:H:32:THR:O	16:H:36:ARG:HG3	2.16	0.46
14:M:131:LEU:O	14:M:135:LEU:HD23	2.15	0.46
15:N:101:THR:O	15:N:225:ARG:NH2	2.49	0.46
15:N:270:ALA:O	15:N:273:LEU:HB2	2.16	0.46
6:G:138:PRO:HG2	7:O:121:MET:HG3	1.98	0.46
16:Q:269:MET:HG3	16:Q:270:PRO:HD2	1.98	0.46
13:T:291:ILE:HG13	13:T:292:LYS:N	2.31	0.46
13:T:409:VAL:O	13:T:413:THR:HG23	2.16	0.46
14:U:281:PHE:CE1	14:U:341:ILE:HG22	2.51	0.46
12:S:78:ILE:HG12	15:V:130:LEU:HB3	1.98	0.46
1:1:357:THR:HG23	1:1:360:ARG:HH22	1.81	0.46
3:3:136:GLU:HG2	5:5:189:ARG:HG2	1.98	0.46
3:3:225:ASN:O	3:3:229:ILE:HG13	2.16	0.46
3:3:300:TRP:HZ3	3:3:606:THR:HG21	1.81	0.46
3:3:559:ASP:OD2	3:3:686:LYS:NZ	2.48	0.46
4:4:390:VAL:HB	4:4:391:PRO:HD3	1.98	0.46
2:C:135:GLN:HB2	2:C:141:TYR:HD1	1.81	0.46
3:D:151:LEU:HD12	3:D:152:PRO:HD2	1.98	0.46
3:D:664:LEU:O	3:D:669:VAL:HG12	2.15	0.46
4:E:381:LEU:HB3	4:E:382:PRO:HD3	1.98	0.46
16:H:222:PRO:O	16:H:230:GLY:HA3	2.16	0.46
11:J:59:TYR:O	11:J:64:VAL:HG12	2.16	0.46
7:O:149:GLU:O	7:O:153:THR:OG1	2.27	0.46
10:P:93:PHE:O	10:P:96:VAL:HG12	2.16	0.46
11:R:133:GLY:H	11:R:136:LEU:HB2	1.81	0.46
12:S:94:ARG:NH1	13:T:583:THR:O	2.49	0.46
14:U:335:ARG:NH2	14:U:429:GLU:OE1	2.49	0.46
15:V:244:GLY:O	15:V:260:TYR:HB3	2.16	0.46
3:3:410:HIS:HD2	3:3:411:LEU:HD23	1.81	0.45
3:3:8:ASP:OD1	3:3:9:ARG:HG3	2.14	0.45
3:3:163:HIS:ND1	8:7:71:ASP:HB2	2.32	0.45
3:D:136:GLU:HG2	5:F:189:ARG:HG2	1.98	0.45
4:E:236:GLY:C	4:E:238:SER:H	2.20	0.45
16:H:227:GLU:HG2	16:H:228:LEU:N	2.30	0.45
11:J:69:PHE:HZ	16:H:156:SER:HB3	1.81	0.45
13:L:198:ASN:ND2	13:L:201:LEU:HB2	2.31	0.45
13:L:163:ARG:NE	14:M:399:VAL:HB	2.31	0.45
16:Q:127:ALA:O	16:Q:131:LEU:HG	2.16	0.45
13:T:348:ASP:OD1	13:T:349:VAL:N	2.45	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
15:V:58:VAL:HB	15:V:225:ARG:HH11	1.81	0.45
2:2:110:GLU:OE2	8:7:114:ARG:NE	2.38	0.45
3:3:115:HIS:CG	3:3:116:PRO:HD2	2.50	0.45
3:3:506:ILE:HG12	3:3:533:LEU:HB2	1.99	0.45
4:4:84:ARG:CZ	4:4:169:HIS:HB3	2.46	0.45
6:6:147:LEU:O	6:6:151:VAL:HG13	2.16	0.45
10:A:1:MET:HG3	11:J:123:LEU:HD11	1.97	0.45
1:B:203:PRO:HB2	1:B:204:PRO:HD3	1.98	0.45
3:D:516:VAL:O	3:D:520:ARG:HG3	2.16	0.45
4:E:341:GLU:OE1	5:F:91:ARG:NH2	2.49	0.45
16:H:215:ALA:O	16:H:294:ARG:NH1	2.47	0.45
13:L:388:ILE:O	13:L:392:THR:OG1	2.34	0.45
10:P:67:LEU:HB3	16:Q:310:TRP:HZ2	1.82	0.45
16:Q:149:LEU:O	16:Q:153:LEU:HG	2.16	0.45
13:T:325:HIS:CD2	13:T:329:LYS:HG3	2.51	0.45
1:1:76:TRP:O	1:1:81:LYS:NZ	2.48	0.45
7:9:82:SER:OG	7:9:86:ARG:O	2.23	0.45
1:B:298:PRO:HD2	1:B:321:SER:HA	1.98	0.45
1:B:6:LEU:HD21	1:B:12:ARG:HG3	1.98	0.45
3:D:43:GLY:HA2	19:D:804:FES:S1	2.57	0.45
5:F:28:VAL:HA	5:F:91:ARG:O	2.16	0.45
5:F:99:PRO:HB2	5:F:124:ILE:HA	1.98	0.45
11:J:100:VAL:HA	13:L:598:LEU:HD21	1.96	0.45
15:N:176:LEU:HD22	15:N:226:VAL:HG13	1.98	0.45
16:Q:17:ALA:O	16:Q:21:VAL:HG23	2.16	0.45
13:T:380:SER:HB3	13:T:456:ALA:HB3	1.99	0.45
13:T:463:HIS:CD2	13:T:464:PRO:HD3	2.51	0.45
13:T:90:TYR:CD2	13:T:334:LEU:HD13	2.51	0.45
1:1:259:LYS:NZ	2:2:180:GLU:HG2	2.30	0.45
1:1:195:LEU:CD2	2:2:24:ARG:HH12	2.28	0.45
3:3:417:VAL:HA	3:3:447:LYS:HD3	1.99	0.45
4:4:39:GLY:O	4:4:404:MET:HG3	2.16	0.45
6:6:148:ILE:O	6:6:152:MET:HG3	2.15	0.45
1:B:201:LEU:HG	1:B:203:PRO:HD2	1.99	0.45
4:E:172:TYR:OH	4:E:180:GLU:O	2.24	0.45
4:E:105:LEU:HD13	4:E:309:ILE:HD13	1.98	0.45
5:F:49:LEU:HD21	5:F:52:ILE:HD11	1.99	0.45
13:L:240:ILE:HG22	13:L:241:HIS:HD2	1.81	0.45
14:M:260:LEU:HB3	14:M:301:PHE:CE2	2.52	0.45
16:Q:150:LEU:HD23	16:Q:154:ARG:HD2	1.99	0.45
13:T:219:GLN:OE1	13:T:304:GLY:HA2	2.17	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:T:600:LEU:O	13:T:604:MET:HG3	2.16	0.45
3:3:6:VAL:HG21	3:3:23:VAL:HA	1.99	0.45
4:4:38:HIS:ND1	4:4:139:ASP:OD2	2.48	0.45
6:6:32:ARG:HB3	6:6:104:TRP:HH2	1.82	0.45
7:9:126:TYR:HB3	9:W:39:ASP:CG	2.36	0.45
10:A:66:MET:O	10:A:69:ILE:HG12	2.16	0.45
1:B:98:PRO:HA	2:C:124:CYS:SG	2.57	0.45
4:E:140:LEU:HD11	4:E:217:ARG:HH22	1.82	0.45
4:E:47:LEU:HD12	4:E:48:SER:N	2.31	0.45
6:G:162:ALA:O	6:G:170:LEU:N	2.27	0.45
6:G:53:SER:HB3	6:G:144:PRO:HB3	1.97	0.45
6:G:37:TRP:NE1	6:G:69:ARG:HG3	2.30	0.45
16:H:218:PRO:C	16:H:220:ASP:H	2.20	0.45
16:H:218:PRO:HA	16:H:300:LEU:HB2	1.99	0.45
16:H:67:ILE:HG13	16:H:68:PHE:HD1	1.82	0.45
10:P:71:PHE:O	10:P:74:GLU:HB3	2.16	0.45
7:9:126:TYR:HB3	9:W:39:ASP:OD2	2.17	0.45
4:4:114:GLU:O	4:4:118:VAL:HG13	2.16	0.45
4:4:288:LYS:HA	4:4:288:LYS:HD3	1.72	0.45
6:6:73:ARG:NH2	10:A:40:LYS:O	2.47	0.45
1:B:297:THR:HG22	1:B:322:MET:HG3	1.98	0.45
3:D:468:HIS:CE1	3:D:473:GLU:HG3	2.51	0.45
4:E:281:ARG:HD3	4:E:284:ARG:NH1	2.30	0.45
4:E:32:PRO:HD3	4:E:42:ARG:HG3	1.98	0.45
5:F:55:LEU:HD23	5:F:57:TYR:CE2	2.52	0.45
8:I:70:ALA:HA	8:I:84:LEU:HD23	1.99	0.45
13:L:317:VAL:HG12	13:L:388:ILE:HG12	1.98	0.45
14:M:260:LEU:HB3	14:M:301:PHE:CD2	2.51	0.45
7:O:137:LEU:O	7:O:140:VAL:HG12	2.16	0.45
10:P:1:MET:HG2	10:P:2:ALA:H	1.82	0.45
11:R:109:TRP:CE3	11:R:109:TRP:HA	2.52	0.45
13:T:239:LEU:HD12	13:T:239:LEU:HA	1.79	0.45
13:T:26:GLU:HB3	13:T:27:PRO:HD3	1.97	0.45
13:T:358:HIS:O	13:T:360:PRO:HD3	2.16	0.45
11:R:96:LEU:HD23	13:T:598:LEU:HD12	1.97	0.45
3:3:11:VAL:HG11	3:3:25:HIS:CD2	2.52	0.45
3:3:300:TRP:HE1	3:3:703:GLN:HG2	1.81	0.45
3:3:327:LEU:HA	3:3:327:LEU:HD23	1.78	0.45
3:3:557:SER:N	3:3:560:GLU:HB2	2.32	0.45
4:4:265:PRO:CB	4:4:278:VAL:HG13	2.46	0.45
2:C:15:PHE:CE1	2:C:53:VAL:HG23	2.51	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:722:THR:CG2	3:D:756:GLY:H	2.30	0.45
4:E:115:THR:O	4:E:118:VAL:HG22	2.16	0.45
5:F:80:TRP:HA	5:F:80:TRP:CE3	2.52	0.45
6:G:99:MET:HB3	6:G:103:LYS:HD3	1.97	0.45
16:H:98:GLY:O	16:H:114:TRP:HB2	2.17	0.45
12:K:81:HIS:H	12:K:81:HIS:CD2	2.35	0.45
13:L:13:GLY:O	13:L:17:LEU:HG	2.16	0.45
13:L:554:PHE:CZ	14:M:283:THR:HG21	2.51	0.45
11:J:135:TRP:HZ3	15:N:105:LEU:HD22	1.82	0.45
16:Q:185:ILE:HG22	16:Q:189:GLN:OE1	2.17	0.45
16:Q:333:PRO:HG2	16:Q:336:TYR:CG	2.52	0.45
15:V:294:LEU:HG	15:V:402:VAL:HG13	1.98	0.45
6:G:125:GLN:HB2	9:X:119:ASN:HD21	1.81	0.45
3:3:697:THR:HG21	3:3:761:SER:OG	2.16	0.45
3:3:735:ALA:HA	3:3:744:GLU:HA	1.97	0.45
4:4:211:SER:OG	4:4:215:TYR:CB	2.65	0.45
2:C:79:HIS:ND1	2:C:118:SER:HB2	2.31	0.45
5:F:64:ARG:HA	5:F:64:ARG:HD3	1.64	0.45
13:L:305:TYR:HB3	13:L:321:HIS:CD2	2.52	0.45
13:L:371:LEU:HB3	13:L:376:LEU:HB2	1.99	0.45
13:L:73:SER:HB3	13:L:120:LEU:HD23	1.97	0.45
14:M:130:LEU:HB2	14:M:145:LEU:HD11	1.99	0.45
12:K:63:VAL:HG13	15:N:112:GLU:HG3	1.98	0.45
15:N:207:VAL:O	15:N:211:MET:HG3	2.17	0.45
10:P:10:THR:OG1	16:Q:118:LEU:HD21	2.17	0.45
10:P:66:MET:O	10:P:69:ILE:HG12	2.17	0.45
13:T:371:LEU:HB3	13:T:376:LEU:HB2	1.98	0.45
13:T:139:PHE:CE2	14:U:407:LEU:HD13	2.52	0.45
4:4:236:GLY:C	4:4:238:SER:H	2.19	0.45
4:4:73:ARG:NH2	4:4:81:TYR:OH	2.50	0.45
5:5:33:ARG:O	5:5:37:GLU:HB2	2.17	0.45
1:B:193:GLU:OE1	1:B:211:LEU:HD12	2.16	0.45
18:B:502:FMN:H1'1	18:B:502:FMN:H9	1.73	0.45
1:B:97:GLU:OE1	1:B:180:TYR:OH	2.35	0.45
4:E:144:THR:HG23	16:Q:43:GLN:HB3	1.99	0.45
16:H:202:ALA:O	16:H:205:VAL:HG22	2.17	0.45
11:J:64:VAL:HA	11:J:67:PHE:HB2	1.99	0.45
13:L:325:HIS:HA	13:L:328:PHE:CE2	2.52	0.45
15:N:345:LYS:HB3	15:N:349:PHE:CE2	2.51	0.45
15:V:364:ALA:O	15:V:367:THR:OG1	2.29	0.45
15:V:13:LEU:HB3	15:V:86:LEU:HD11	1.98	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:1:115:ILE:O	1:1:119:ILE:HG13	2.16	0.45
1:1:211:LEU:HB2	1:1:216:THR:HG21	1.98	0.45
3:3:139:LEU:HD12	4:4:326:TYR:CZ	2.52	0.45
3:3:399:LEU:O	3:3:508:GLY:N	2.48	0.45
3:3:503:PRO:HG3	3:3:528:LYS:HD3	1.98	0.45
5:5:1:MET:HB3	5:5:5:ARG:NH2	2.32	0.45
6:6:21:PHE:O	6:6:25:GLU:HG2	2.16	0.45
7:9:137:LEU:O	7:9:140:VAL:HG12	2.17	0.45
10:A:74:GLU:O	10:A:78:LEU:HG	2.17	0.45
2:C:4:PHE:HB3	2:C:11:LEU:HD11	1.99	0.45
3:D:474:ARG:NH2	3:D:516:VAL:HG21	2.32	0.45
11:J:5:GLU:O	11:J:9:LEU:HG	2.17	0.45
13:L:463:HIS:CG	13:L:464:PRO:HD3	2.52	0.45
15:N:228:ALA:HB1	15:N:233:LEU:HD13	1.99	0.45
16:Q:147:TYR:CD1	16:Q:229:VAL:HG22	2.52	0.45
13:T:219:GLN:NE2	13:T:277:THR:HG21	2.31	0.45
13:T:312:VAL:HA	13:T:397:PHE:HD2	1.82	0.45
13:T:394:THR:HB	13:T:484:HIS:O	2.16	0.45
13:T:88:HIS:O	13:T:92:ILE:HG13	2.16	0.45
1:1:6:LEU:HB2	1:1:241:MET:HA	1.99	0.44
3:3:269:THR:HG21	3:3:629:ILE:HG12	1.99	0.44
4:4:219:ARG:HD3	4:4:271:ASP:OD2	2.17	0.44
10:A:76:ALA:HA	10:A:79:TRP:CE3	2.52	0.44
2:C:29:PRO:O	2:C:32:ARG:HB3	2.17	0.44
3:D:381:LEU:HD22	3:D:680:LEU:O	2.17	0.44
4:E:87:TYR:HB3	4:E:169:HIS:HE1	1.82	0.44
14:M:384:ALA:O	14:M:388:SER:N	2.47	0.44
7:O:59:CYS:HB2	7:O:104:CYS:CB	2.47	0.44
7:O:33:LEU:HB2	7:O:163:VAL:HG12	1.99	0.44
14:U:22:ARG:NH1	14:U:92:GLU:CD	2.69	0.44
3:3:46:ARG:NH2	3:3:81:ALA:HB2	2.33	0.44
4:4:101:VAL:O	4:4:105:LEU:HG	2.17	0.44
5:5:103:THR:CG2	5:5:126:PHE:HB3	2.47	0.44
4:4:169:HIS:HE2	6:6:45:CYS:HB2	1.83	0.44
10:A:33:PRO:HD2	16:H:70:GLU:HB2	2.00	0.44
4:E:249:ARG:HB2	4:E:262:PHE:HE2	1.81	0.44
6:G:119:ASN:HA	6:G:125:GLN:HE22	1.82	0.44
4:E:168:PHE:CE1	6:G:141:PRO:HG3	2.52	0.44
13:L:264:PRO:HA	13:L:397:PHE:CE1	2.52	0.44
13:L:26:GLU:HB3	13:L:27:PRO:HD3	1.99	0.44
16:Q:289:PHE:O	16:Q:293:ILE:HG12	2.17	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
16:Q:39:LEU:HD22	16:Q:295:ALA:HB2	1.99	0.44
14:U:13:GLY:HA2	14:U:97:GLY:HA2	1.99	0.44
3:3:293:ALA:HB2	3:3:698:MET:HG2	2.00	0.44
4:4:276:MET:O	4:4:280:ILE:HG13	2.17	0.44
4:4:55:VAL:O	4:4:382:PRO:HG3	2.17	0.44
7:9:9:SER:OG	16:H:296:THR:HG22	2.18	0.44
1:B:275:LEU:HA	1:B:279:TRP:CD1	2.52	0.44
2:C:78:TYR:CZ	2:C:157:LEU:HD22	2.51	0.44
6:G:115:GLY:N	6:G:125:GLN:O	2.50	0.44
6:G:36:LEU:O	6:G:38:PRO:HD3	2.17	0.44
16:H:310:TRP:HA	16:H:314:PHE:CD2	2.51	0.44
13:L:439:PRO:HB2	13:L:442:MET:HB2	1.98	0.44
14:M:95:PHE:HB3	14:M:136:TYR:CZ	2.52	0.44
14:M:30:GLY:O	14:M:34:LEU:HG	2.17	0.44
15:N:14:THR:OG1	15:N:90:TYR:OH	2.31	0.44
14:U:119:TYR:OH	14:U:157:LEU:HD23	2.18	0.44
3:3:34:CYS:CB	3:3:45:CYS:SG	3.05	0.44
3:D:657:HIS:O	3:D:661:GLN:HG2	2.17	0.44
4:E:154:GLU:OE1	4:E:167:ARG:NH1	2.50	0.44
4:E:47:LEU:HD13	4:E:52:VAL:HA	2.00	0.44
6:G:40:THR:HB	6:G:68:PHE:CZ	2.53	0.44
13:L:128:PHE:HD1	13:L:169:PHE:CD2	2.36	0.44
14:M:346:GLY:O	14:M:349:GLN:HG2	2.17	0.44
13:T:202:LEU:HD12	13:T:202:LEU:HA	1.87	0.44
15:V:228:ALA:HB1	15:V:233:LEU:HD13	1.99	0.44
2:2:46:ILE:HD12	3:3:214:MET:HE1	1.99	0.44
3:3:717:TRP:HB2	3:3:759:TYR:HB2	1.99	0.44
4:4:338:PRO:HG2	5:5:193:ARG:NH1	2.28	0.44
1:B:386:ASN:O	1:B:390:LEU:HG	2.18	0.44
3:D:252:THR:OG1	3:D:628:PRO:HD3	2.18	0.44
4:E:114:GLU:O	4:E:118:VAL:HG13	2.18	0.44
5:F:38:MET:HE1	5:F:104:VAL:HG11	1.92	0.44
6:G:37:TRP:HE1	6:G:69:ARG:CG	2.30	0.44
13:L:214:VAL:HG22	13:L:219:GLN:HB2	2.00	0.44
13:L:222:LEU:O	13:L:225:TRP:HD1	2.01	0.44
13:T:128:PHE:CE1	13:T:166:ASP:HB3	2.53	0.44
14:U:335:ARG:NH1	14:U:424:ASP:O	2.43	0.44
15:V:257:LEU:HD11	15:V:374:TYR:HB2	1.98	0.44
3:3:9:ARG:HD2	3:3:26:ALA:O	2.18	0.44
5:5:74:LEU:HD12	5:5:88:PHE:CZ	2.52	0.44
5:5:80:TRP:HA	5:5:80:TRP:HE3	1.82	0.44

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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:T:126:VAL:HA	13:T:129:ILE:HD12	2.00	0.44
14:U:204:LYS:HE3	14:U:234:TYR:O	2.18	0.44
14:U:325:LEU:HG	14:U:361:LEU:HB3	2.00	0.44
9:X:7:ARG:NH2	9:X:100:THR:HG23	2.33	0.44
2:2:40:TRP:CH2	8:7:125:ALA:HA	2.53	0.44
3:3:117:LEU:HA	4:4:321:MET:HE2	2.00	0.44
3:3:722:THR:HG21	3:3:755:LYS:HA	1.98	0.44
4:4:314:ARG:NH1	7:9:106:GLU:O	2.51	0.44
3:D:618:GLU:OE2	3:D:620:ARG:NE	2.42	0.44
4:E:352:GLU:HB3	4:E:371:ARG:CZ	2.48	0.44
4:E:367:ARG:NH1	4:E:369:LYS:HB2	2.32	0.44
11:J:32:LEU:HD13	12:K:29:LEU:HG	2.00	0.44
13:L:3:LEU:HD22	13:L:53:ALA:HB3	1.99	0.44
13:L:82:GLY:O	13:L:86:LEU:HG	2.17	0.44
10:P:44:TYR:CD2	10:P:45:GLU:HB2	2.53	0.44
10:P:71:PHE:O	10:P:75:VAL:HG23	2.17	0.44
13:T:72:LEU:HD23	13:T:255:ARG:HD3	2.00	0.44
13:T:290:ASP:OD1	13:T:291:ILE:N	2.50	0.44
13:T:539:ASN:HA	13:T:543:VAL:HB	1.99	0.44
1:1:111:PRO:HB3	1:1:145:LEU:HD23	1.99	0.43
1:1:214:LYS:O	1:1:216:THR:HG23	2.18	0.43
1:1:410:VAL:HG12	1:1:414:LEU:HD13	2.00	0.43
1:B:137:GLU:HB3	2:C:141:TYR:OH	2.18	0.43
16:H:122:ILE:HG13	16:H:123:LEU:HD12	1.99	0.43
7:9:10:LEU:HD12	16:H:296:THR:CG2	2.47	0.43
16:H:332:LEU:HD12	16:H:332:LEU:H	1.83	0.43
7:O:19:SER:C	7:O:21:PRO:CD	2.73	0.43
16:Q:168:LEU:HD12	16:Q:314:PHE:HB3	1.99	0.43
12:S:79:PHE:CD2	12:S:85:THR:HA	2.53	0.43
13:T:469:LEU:HD12	13:T:469:LEU:HA	1.82	0.43
14:U:113:ARG:O	14:U:177:LEU:HB2	2.19	0.43
15:V:237:VAL:O	15:V:241:VAL:HG23	2.18	0.43
9:X:46:TYR:N	9:X:63:PHE:O	2.50	0.43
1:1:50:PRO:HA	1:1:53:VAL:HG12	2.00	0.43
2:2:171:LYS:O	2:2:177:HIS:HE1	2.01	0.43
2:2:3:PHE:HB2	2:2:45:ARG:HH11	1.75	0.43
1:1:361:GLU:HB3	3:3:113:LEU:HD22	1.99	0.43
4:4:222:GLY:O	4:4:224:ILE:HG13	2.18	0.43
6:6:39:ALA:HB2	6:6:75:ALA:CB	2.48	0.43
1:B:301:PRO:O	1:B:306:VAL:HG11	2.18	0.43
2:C:85:THR:HB	19:C:201:FES:S2	2.59	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:19:VAL:HG23	3:D:85:THR:O	2.18	0.43
3:D:242:PHE:CD2	7:O:74:GLU:HB2	2.53	0.43
3:D:534:ALA:O	3:D:617:LEU:HD12	2.17	0.43
13:L:182:THR:HB	13:L:187:GLU:HG3	2.00	0.43
13:L:463:HIS:NE2	13:L:487:LEU:HD13	2.32	0.43
13:L:65:PHE:CZ	13:L:67:LEU:HD21	2.53	0.43
15:N:190:ALA:HA	15:N:192:PHE:H	1.83	0.43
16:Q:177:VAL:HG22	16:Q:188:TRP:CG	2.54	0.43
13:T:312:VAL:O	13:T:396:PRO:HD2	2.18	0.43
15:V:420:LEU:HA	15:V:423:LEU:HG	1.99	0.43
1:1:424:LEU:HG	1:1:429:ARG:O	2.18	0.43
4:4:166:GLN:OE1	4:4:170:HIS:HA	2.18	0.43
6:6:82:GLY:HA2	17:6:201:SF4:S4	2.58	0.43
1:B:83:ASP:CG	1:B:87:HIS:HE2	2.20	0.43
3:D:312:ARG:NH2	3:D:598:ALA:O	2.51	0.43
4:E:123:LEU:HG	4:E:156:ILE:HG23	2.00	0.43
4:E:231:ASP:O	5:F:110:SER:OG	2.35	0.43
4:E:208:PHE:CE2	4:E:276:MET:HG2	2.54	0.43
13:L:340:ILE:HB	13:L:345:GLY:HA2	1.99	0.43
14:M:9:PRO:HG2	14:M:107:LEU:HD12	2.00	0.43
11:J:104:LEU:HA	15:N:174:LEU:HD21	1.99	0.43
15:N:198:ASP:OD1	15:N:256:ARG:NH2	2.51	0.43
15:N:13:LEU:HD22	15:N:25:VAL:HG13	2.00	0.43
6:G:91:VAL:HG22	10:P:46:SER:HB3	2.00	0.43
16:Q:271:VAL:HG12	16:Q:272:LEU:HG	2.00	0.43
12:S:81:HIS:CD2	12:S:81:HIS:H	2.36	0.43
13:T:33:ALA:O	13:T:37:VAL:HG23	2.19	0.43
14:U:29:ALA:HB1	14:U:83:PHE:HA	1.99	0.43
3:3:409:LEU:HD23	3:3:409:LEU:HA	1.76	0.43
3:3:382:PHE:HB3	3:3:532:VAL:HB	2.00	0.43
4:4:42:ARG:O	4:4:43:LEU:HD23	2.19	0.43
8:7:27:LYS:HD3	8:7:27:LYS:HA	1.86	0.43
2:C:82:VAL:HG22	2:C:134:ILE:HG12	2.01	0.43
3:D:36:GLU:OE1	3:D:37:LYS:N	2.51	0.43
4:E:352:GLU:CD	5:F:87:ARG:HH22	2.21	0.43
16:H:136:ILE:HG23	16:H:232:TYR:HD2	1.83	0.43
11:J:36:PHE:CD2	11:J:59:TYR:HB3	2.54	0.43
13:L:103:ARG:NH2	13:L:144:PHE:O	2.45	0.43
14:M:289:GLY:O	14:M:293:MET:HG2	2.18	0.43
15:N:193:HIS:CD2	15:N:263:ILE:HD13	2.52	0.43
15:N:26:LYS:O	15:N:29:THR:OG1	2.30	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:O:40:ARG:O	7:O:116:GLY:N	2.52	0.43
4:E:26:MET:HE1	10:P:57:PHE:HA	2.01	0.43
11:R:58:VAL:O	11:R:62:ALA:HB3	2.18	0.43
13:T:316:TRP:HZ3	13:T:460:ALA:HB1	1.82	0.43
14:U:159:MET:HG3	14:U:197:PHE:HD1	1.83	0.43
14:U:338:THR:HG22	14:U:340:GLU:H	1.82	0.43
15:V:188:ALA:HB3	15:V:216:LYS:NZ	2.32	0.43
2:2:147:ARG:HB2	2:2:147:ARG:HE	1.72	0.43
3:3:136:GLU:HB3	5:5:187:GLY:HA3	2.01	0.43
4:4:167:ARG:HD3	6:6:143:ARG:HH12	1.83	0.43
8:7:40:PHE:CZ	8:7:53:THR:HG21	2.54	0.43
4:4:73:ARG:NH2	7:9:64:PRO:O	2.50	0.43
1:B:274:GLU:HG2	1:B:279:TRP:CD1	2.54	0.43
1:B:3:GLY:HA2	1:B:4:PRO:HD3	1.89	0.43
4:E:34:HIS:HA	4:E:35:PRO:HA	1.83	0.43
4:E:99:LEU:HA	4:E:102:GLU:OE1	2.18	0.43
16:H:345:PHE:CZ	16:H:349:LEU:HD22	2.53	0.43
8:I:43:ARG:HA	8:I:46:ARG:NH2	2.33	0.43
14:M:90:ARG:HA	14:M:90:ARG:HD2	1.79	0.43
4:E:207:LEU:HD21	7:O:12:ILE:HD11	2.00	0.43
10:P:71:PHE:CE2	10:P:107:PHE:HB2	2.54	0.43
16:Q:214:ALA:HB1	16:Q:248:GLU:HG3	1.99	0.43
16:Q:224:ALA:HA	16:Q:230:GLY:H	1.84	0.43
11:R:44:VAL:HG13	11:R:49:ARG:HG2	1.99	0.43
14:U:359:LEU:HB2	14:U:410:PHE:CE1	2.53	0.43
15:V:58:VAL:HG22	15:V:278:ALA:HB1	2.01	0.43
9:W:31:VAL:HG22	9:W:50:LEU:HD13	2.00	0.43
1:1:272:PHE:HE1	1:1:309:THR:HB	1.83	0.43
4:4:148:TYR:O	4:4:151:ARG:HB3	2.18	0.43
6:6:104:TRP:HE1	6:6:173:VAL:HG22	1.83	0.43
8:7:63:LEU:HD13	8:7:129:ALA:HB3	2.00	0.43
7:9:6:LEU:HD23	16:H:297:TRP:CE2	2.53	0.43
1:B:79:MET:SD	1:B:217:THR:OG1	2.77	0.43
1:B:303:THR:H	1:B:306:VAL:HB	1.84	0.43
4:E:62:LEU:HD11	6:G:43:LEU:O	2.18	0.43
16:H:257:ALA:O	16:H:260:PRO:HD2	2.19	0.43
12:K:46:ALA:HB2	12:K:53:GLY:HA3	2.00	0.43
13:L:268:TYR:O	13:L:272:VAL:HG23	2.17	0.43
13:L:359:LEU:HB3	13:L:362:THR:HB	2.01	0.43
14:M:201:PHE:CE2	14:M:245:ALA:HB2	2.54	0.43
16:Q:181:ASN:O	16:Q:185:ILE:HG13	2.18	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
16:Q:232:TYR:HB2	16:Q:244:PHE:CE1	2.53	0.43
13:T:385:LYS:NZ	13:T:413:THR:OG1	2.52	0.43
14:U:143:ARG:HD3	14:U:143:ARG:HA	1.69	0.43
9:X:14:LEU:HD13	9:X:77:LEU:HB2	2.01	0.43
1:1:45:LEU:HD12	1:1:163:PHE:CE2	2.54	0.43
4:4:240:ARG:HA	4:4:244:VAL:H	1.82	0.43
3:D:141:GLU:HG2	3:D:143:TYR:CZ	2.54	0.43
3:D:351:LEU:HB3	3:D:664:LEU:HD21	2.00	0.43
3:D:719:HIS:NE2	3:D:755:LYS:HE2	2.34	0.43
4:E:38:HIS:CE1	4:E:398:ALA:HA	2.53	0.43
16:H:90:VAL:HG21	16:H:243:LEU:HB3	2.00	0.43
16:H:90:VAL:HA	16:H:247:ALA:HB2	2.00	0.43
16:H:267:TRP:CD1	16:H:275:PRO:HA	2.53	0.43
16:H:216:ARG:NH1	16:H:294:ARG:O	2.50	0.43
11:J:29:ALA:O	11:J:33:ILE:HG13	2.18	0.43
13:L:104:PHE:CZ	13:L:108:PHE:CZ	3.06	0.43
12:K:95:GLY:N	13:L:582:GLN:O	2.40	0.43
16:Q:310:TRP:CE3	16:Q:314:PHE:HE2	2.37	0.43
16:Q:52:GLY:HA3	16:Q:55:GLY:N	2.31	0.43
13:T:41:PHE:HB2	13:T:81:THR:HB	2.00	0.43
13:T:583:THR:HG1	13:T:585:TYR:HD2	1.65	0.43
14:U:173:PRO:HG2	14:U:179:ASP:OD2	2.19	0.43
14:U:91:VAL:HG21	14:U:226:LEU:HD22	2.00	0.43
15:V:98:LEU:HD23	15:V:218:ALA:CB	2.47	0.43
1:1:145:LEU:O	1:1:149:ILE:HG13	2.18	0.43
1:1:357:THR:N	1:1:358:PRO:HD2	2.34	0.43
6:6:163:TYR:HB2	7:9:152:ARG:HH11	1.83	0.43
6:6:69:ARG:HB2	6:6:75:ALA:HB2	2.00	0.43
7:9:71:GLU:HB2	7:9:90:VAL:HB	2.01	0.43
10:A:57:PHE:HB3	10:A:58:PRO:HD2	2.01	0.43
1:B:288:GLN:NE2	1:B:332:PRO:O	2.52	0.43
2:C:130:THR:HB	2:C:143:GLU:HB3	2.00	0.43
3:D:136:GLU:OE1	5:F:186:GLY:N	2.32	0.43
3:D:124:LYS:HG3	3:D:233:GLY:HA2	2.01	0.43
4:E:372:ALA:HB2	4:E:409:ARG:HD3	2.01	0.43
5:F:155:THR:N	6:G:119:ASN:OD1	2.36	0.43
16:H:127:ALA:O	16:H:131:LEU:HG	2.17	0.43
16:H:155:SER:OG	16:H:156:SER:N	2.52	0.43
16:H:330:LEU:HA	16:H:330:LEU:HD13	1.89	0.43
13:L:586:LEU:HD11	15:N:135:LYS:HA	2.00	0.43
10:P:7:TYR:CD1	16:Q:118:LEU:HD22	2.54	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
16:Q:132:ALA:O	16:Q:136:ILE:HG13	2.17	0.43
14:U:347:LEU:HB2	14:U:414:PHE:HA	2.01	0.43
5:5:164:TYR:HB3	9:W:37:TRP:HZ3	1.84	0.43
2:2:40:TRP:CE2	2:2:74:PRO:HG3	2.54	0.43
3:3:468:HIS:ND1	3:3:472:GLU:HB3	2.34	0.43
6:6:78:MET:O	6:6:105:VAL:HA	2.19	0.43
7:9:33:LEU:HD11	7:9:119:PHE:HE2	1.84	0.43
1:B:101:PHE:CE1	1:B:253:GLN:HB2	2.54	0.43
2:C:28:MET:O	2:C:70:TYR:OH	2.34	0.43
3:D:543:GLY:O	3:D:547:MET:HG2	2.19	0.43
3:D:8:ASP:OD1	3:D:9:ARG:HG3	2.18	0.43
5:F:53:VAL:HG13	5:F:71:VAL:HB	1.99	0.43
12:K:15:VAL:O	12:K:19:LEU:HG	2.18	0.43
14:M:103:GLU:O	14:M:107:LEU:HG	2.19	0.43
15:N:294:LEU:HD21	15:N:325:ALA:HB1	1.99	0.43
10:P:49:ASP:CG	10:P:52:GLY:HA3	2.39	0.43
11:R:15:SER:HB3	11:R:35:ASN:OD1	2.19	0.43
13:T:293:LYS:O	13:T:297:TYR:HD1	2.02	0.43
14:U:281:PHE:CE2	14:U:332:LEU:HD21	2.54	0.43
15:V:217:ALA:HA	15:V:285:LEU:CD2	2.49	0.43
9:W:36:ASP:N	9:W:36:ASP:OD1	2.51	0.43
1:1:20:HIS:HB3	1:1:31:TYR:HE1	1.84	0.43
3:3:347:HIS:HB2	3:3:538:ALA:CB	2.48	0.43
3:3:603:PRO:HG2	3:3:634:ALA:HA	2.01	0.43
3:3:732:ALA:O	3:3:747:VAL:HG23	2.18	0.43
5:5:132:LEU:HA	5:5:132:LEU:HD23	1.82	0.43
5:5:134:LYS:NZ	5:5:141:LEU:O	2.52	0.43
6:6:40:THR:HB	6:6:68:PHE:CZ	2.54	0.43
7:9:41:HIS:HB2	7:9:136:MET:SD	2.59	0.43
6:6:163:TYR:H	7:9:152:ARG:NH1	2.17	0.43
10:A:7:TYR:CD1	10:A:7:TYR:N	2.86	0.43
3:D:230:CYS:HA	3:D:231:PRO:HD2	1.93	0.43
4:E:154:GLU:OE2	4:E:157:LEU:HD12	2.19	0.43
4:E:367:ARG:HH12	4:E:369:LYS:HB2	1.83	0.43
6:G:115:GLY:HA2	6:G:125:GLN:HA	2.00	0.43
16:H:342:ALA:O	16:H:346:LEU:HG	2.19	0.43
10:A:1:MET:HG2	11:J:49:ARG:HH12	1.84	0.43
15:N:303:SER:HB3	15:N:307:VAL:HG22	1.99	0.43
15:N:73:THR:O	15:N:77:VAL:HG23	2.18	0.43
7:O:155:LYS:HA	7:O:155:LYS:HD2	1.88	0.43
10:P:28:GLY:HA3	16:Q:239:ILE:HB	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:R:72:MET:HG2	16:Q:141:TRP:CE3	2.53	0.43
16:Q:237:SER:OG	16:Q:238:SER:N	2.51	0.43
16:Q:39:LEU:CD2	16:Q:295:ALA:HB2	2.48	0.43
12:S:23:THR:OG1	12:S:26:LEU:HD13	2.18	0.43
15:V:73:THR:HG21	15:V:210:PHE:HB2	1.99	0.43
15:V:26:LYS:O	15:V:29:THR:OG1	2.30	0.43
15:V:277:ASN:C	15:V:279:GLN:H	2.22	0.43
3:3:33:PHE:HB2	3:3:45:CYS:CB	2.50	0.42
3:3:54:LEU:HD13	3:3:91:MET:HB2	2.00	0.42
4:4:169:HIS:NE2	6:6:45:CYS:SG	2.92	0.42
4:4:172:TYR:O	4:4:179:LYS:HB2	2.19	0.42
7:9:134:GLU:H	7:9:134:GLU:CD	2.23	0.42
1:B:135:ARG:HE	1:B:137:GLU:HB2	1.83	0.42
2:C:42:ARG:HB2	2:C:45:ARG:HG2	2.01	0.42
3:D:118:ASP:O	3:D:122:CYS:HB2	2.19	0.42
3:D:189:ARG:O	3:D:193:GLU:HB2	2.19	0.42
5:F:121:LEU:O	5:F:144:HIS:HB3	2.18	0.42
8:I:13:TRP:CE3	8:I:72:VAL:HB	2.53	0.42
11:J:146:LEU:O	11:J:150:THR:HG23	2.19	0.42
12:K:46:ALA:HB2	12:K:53:GLY:CA	2.49	0.42
13:L:450:ALA:O	13:L:454:VAL:HG23	2.18	0.42
13:L:549:LEU:HA	13:L:549:LEU:HD23	1.89	0.42
13:L:600:LEU:O	13:L:604:MET:HG3	2.19	0.42
16:Q:71:ASP:OD1	16:Q:240:LYS:NZ	2.31	0.42
13:T:340:ILE:HG22	13:T:347:GLN:H	1.84	0.42
14:U:135:LEU:HG	14:U:136:TYR:CD2	2.54	0.42
14:U:359:LEU:O	14:U:363:LEU:HG	2.19	0.42
15:V:115:SER:HB2	15:V:119:TYR:CZ	2.54	0.42
15:V:224:LEU:HD13	15:V:278:ALA:HB2	2.01	0.42
1:1:63:ARG:NH1	1:1:313:TYR:HD2	2.18	0.42
1:1:434:PRO:HG2	1:1:436:LEU:CD1	2.49	0.42
1:1:22:GLY:HA2	2:2:174:HIS:CD2	2.55	0.42
4:4:190:LEU:HD12	4:4:194:LEU:HD13	2.00	0.42
4:4:158:ASP:CG	6:6:57:ARG:HH12	2.18	0.42
6:6:61:ALA:HB1	6:6:66:GLU:OE1	2.18	0.42
3:D:227:THR:CG2	3:D:237:ASP:HB2	2.48	0.42
3:D:395:PHE:HB3	3:D:503:PRO:HB3	2.00	0.42
3:D:567:TYR:HA	3:D:584:VAL:HG23	2.01	0.42
3:D:728:LEU:HD22	3:D:734:VAL:HG21	2.00	0.42
4:E:194:LEU:HD21	4:E:290:ILE:HG22	2.01	0.42
13:L:162:ASN:ND2	13:L:166:ASP:OD2	2.52	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:L:147:LYS:NZ	14:M:349:GLN:OE1	2.43	0.42
15:N:33:LEU:HB2	15:N:71:LEU:HD21	2.01	0.42
13:T:44:GLY:HA3	13:T:77:LEU:HD21	2.01	0.42
15:V:108:LEU:HB2	15:V:147:PHE:CE2	2.51	0.42
3:3:28:TYR:CE2	3:3:96:LEU:HD11	2.54	0.42
4:4:214:PHE:HA	4:4:217:ARG:HB2	2.00	0.42
8:7:67:PHE:O	8:7:86:LEU:HD22	2.19	0.42
7:9:9:SER:O	7:9:12:ILE:HG13	2.18	0.42
1:B:201:LEU:O	1:B:204:PRO:HD2	2.19	0.42
3:D:152:PRO:HD3	4:E:305:PRO:HB2	2.01	0.42
6:G:60:LEU:HG	6:G:65:SER:CB	2.50	0.42
16:H:132:ALA:O	16:H:136:ILE:HG13	2.19	0.42
16:H:216:ARG:NH1	16:H:294:ARG:HB3	2.34	0.42
11:J:53:PHE:HE2	16:H:120:LEU:O	2.02	0.42
13:L:275:LEU:HD13	13:L:402:PHE:HD1	1.84	0.42
14:M:43:HIS:HD2	14:M:48:ALA:HB2	1.84	0.42
15:N:237:VAL:O	15:N:241:VAL:HG23	2.20	0.42
16:Q:217:THR:OG1	16:Q:293:ILE:HG22	2.19	0.42
11:R:103:ILE:O	11:R:107:GLY:N	2.47	0.42
13:T:59:TRP:HE1	14:U:447:PRO:HD2	1.85	0.42
3:3:307:LYS:HB3	3:3:307:LYS:HE2	1.76	0.42
4:4:389:GLN:HG3	4:4:391:PRO:HD2	2.02	0.42
4:4:400:LEU:HD23	4:4:400:LEU:HA	1.90	0.42
4:4:48:SER:CB	10:A:55:LYS:HE3	2.50	0.42
1:B:290:ILE:HG22	1:B:330:LEU:HD22	2.01	0.42
2:C:89:LYS:HA	2:C:93:ALA:H	1.84	0.42
4:E:219:ARG:HD3	4:E:271:ASP:OD2	2.19	0.42
4:E:236:GLY:O	4:E:238:SER:N	2.52	0.42
16:H:233:HIS:ND1	16:H:234:THR:OG1	2.46	0.42
16:H:60:LEU:O	16:H:64:ILE:HG13	2.20	0.42
13:L:419:ARG:NH2	13:L:525:GLU:OE2	2.53	0.42
14:M:160:LEU:O	14:M:163:VAL:HG12	2.19	0.42
15:N:251:GLN:OE1	15:N:256:ARG:HD3	2.19	0.42
3:3:451:PHE:CE1	3:3:466:GLU:HB3	2.55	0.42
4:4:144:THR:HG22	4:4:148:TYR:CE1	2.46	0.42
4:4:248:VAL:HB	4:4:347:GLU:HB2	2.01	0.42
5:5:3:LEU:O	5:5:7:LEU:HG	2.20	0.42
6:6:105:VAL:HB	6:6:132:PRO:O	2.19	0.42
1:B:342:TRP:CE3	1:B:346:ARG:HD2	2.55	0.42
2:C:100:LEU:HD13	2:C:150:LEU:HD21	2.01	0.42
3:D:719:HIS:CD2	3:D:755:LYS:HG2	2.54	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
16:H:189:GLN:HG2	16:H:195:LEU:H	1.85	0.42
16:H:198:TYR:O	16:H:341:SER:OG	2.31	0.42
10:A:111:TRP:HH2	16:H:307:ARG:HG2	1.85	0.42
8:I:120:ASP:O	8:I:124:GLU:HG3	2.19	0.42
13:L:461:LEU:HD13	13:L:465:LEU:HB3	2.02	0.42
14:M:134:TYR:O	14:M:141:ARG:HD3	2.19	0.42
15:N:132:ALA:HB1	15:N:199:VAL:HA	2.01	0.42
15:N:422:ALA:O	15:N:423:LEU:HD23	2.19	0.42
10:P:81:TYR:HE2	16:Q:325:ALA:HB1	1.85	0.42
14:U:17:LEU:HD11	14:U:98:LEU:HD23	2.01	0.42
15:V:204:PRO:O	15:V:208:VAL:HG23	2.19	0.42
15:V:241:VAL:HA	15:V:264:ALA:HA	2.00	0.42
4:4:272:VAL:HG13	4:4:399:SER:HB3	2.00	0.42
4:4:314:ARG:HB3	8:7:44:MET:CE	2.44	0.42
5:5:160:ARG:HH12	7:9:132:GLY:CA	2.31	0.42
5:5:51:ASP:O	5:5:72:TYR:HA	2.19	0.42
2:C:88:CYS:HA	2:C:131:ALA:HB1	2.01	0.42
3:D:32:LEU:CD1	3:D:35:SER:HB2	2.49	0.42
5:F:38:MET:HA	5:F:41:TYR:HB2	2.02	0.42
16:H:151:GLY:HA2	16:H:154:ARG:CD	2.47	0.42
16:H:201:PRO:O	16:H:204:LEU:HB2	2.19	0.42
14:M:148:PHE:HE1	14:M:204:LYS:NZ	2.18	0.42
15:N:66:ALA:HB1	15:N:95:MET:HE3	2.01	0.42
11:R:24:ASN:HB3	11:R:27:HIS:HB2	2.01	0.42
11:R:55:GLN:NE2	11:R:59:TYR:CD2	2.87	0.42
14:U:268:ALA:HA	14:U:291:SER:CA	2.46	0.42
9:W:125:ILE:HD13	9:W:125:ILE:HG21	1.76	0.42
9:X:102:LEU:HG	9:X:110:LEU:HD13	2.01	0.42
3:3:213:THR:OG1	3:3:215:ASP:N	2.49	0.42
3:3:243:ARG:NH1	3:3:275:LEU:HA	2.34	0.42
3:3:470:PRO:HB3	3:3:770:ARG:HD2	2.02	0.42
4:4:112:ARG:O	4:4:116:ILE:HG13	2.20	0.42
4:4:175:ILE:HG13	4:4:335:PHE:HZ	1.84	0.42
4:4:94:ASP:HB3	4:4:173:ILE:HG21	2.01	0.42
4:4:356:TYR:HE1	5:5:26:TRP:HZ2	1.68	0.42
6:6:100:PRO:O	6:6:103:LYS:HD3	2.18	0.42
10:A:49:ASP:CG	10:A:52:GLY:HA3	2.40	0.42
1:B:433:ARG:NH2	2:C:94:GLU:HG3	2.35	0.42
2:C:83:CYS:HA	2:C:122:VAL:O	2.19	0.42
3:D:240:ALA:HB1	3:D:276:ARG:HB2	2.02	0.42
3:D:383:PRO:HG2	3:D:531:LYS:HA	2.02	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:E:234:LEU:HD12	4:E:380:SER:HB2	2.02	0.42
4:E:271:ASP:C	4:E:275:ARG:HH21	2.23	0.42
4:E:136:GLY:HA2	4:E:398:ALA:HB1	2.01	0.42
5:F:129:HIS:HB3	5:F:132:LEU:HG	2.02	0.42
14:M:16:LEU:HD22	14:M:97:GLY:H	1.85	0.42
7:O:40:ARG:HH12	7:O:42:VAL:HG12	1.85	0.42
16:Q:163:GLU:O	16:Q:166:LEU:HB2	2.19	0.42
11:R:16:GLY:HA2	11:R:19:VAL:HG12	2.02	0.42
13:T:194:GLY:HA3	13:T:195:PRO:HD3	1.87	0.42
9:X:48:LEU:HD21	9:X:50:LEU:HB2	2.02	0.42
1:1:203:PRO:HB2	1:1:204:PRO:HD3	2.01	0.42
2:2:26:ALA:O	2:2:30:LEU:HG	2.19	0.42
3:3:203:ILE:HG21	8:7:88:ARG:HG2	2.01	0.42
5:5:74:LEU:HD12	5:5:88:PHE:CE1	2.54	0.42
6:6:29:ALA:HB1	6:6:159:ARG:HA	2.01	0.42
4:4:88:LEU:HD21	6:6:48:ILE:HD13	2.01	0.42
7:9:52:LYS:NZ	7:9:171:GLU:OE2	2.33	0.42
6:6:57:ARG:HA	7:9:23:THR:HA	2.01	0.42
1:B:404:ASP:N	1:B:404:ASP:OD1	2.51	0.42
16:H:147:TYR:HE1	16:H:229:VAL:H	1.68	0.42
11:J:97:ALA:HB2	12:K:16:TYR:HB2	2.01	0.42
13:L:239:LEU:HA	13:L:239:LEU:HD12	1.84	0.42
14:M:194:PHE:HB2	14:M:249:ALA:HB3	2.01	0.42
14:M:215:PRO:CG	14:M:216:PRO:HD3	2.49	0.42
15:N:212:ALA:HB1	15:N:292:THR:HG21	2.01	0.42
16:Q:213:GLU:N	16:Q:213:GLU:OE1	2.53	0.42
1:1:90:ILE:HB	1:1:218:ILE:HG12	2.01	0.42
1:1:273:ARG:HA	1:1:277:TYR:HD2	1.85	0.42
3:3:238:LEU:HG	3:3:707:LYS:HE2	2.02	0.42
6:6:36:LEU:HA	6:6:76:ASP:OD2	2.20	0.42
7:9:6:LEU:O	7:9:10:LEU:HD13	2.20	0.42
1:B:118:MET:HG2	1:B:224:LEU:HD13	2.00	0.42
3:D:194:VAL:HB	3:D:195:PRO:HD3	2.01	0.42
3:D:387:LEU:O	3:D:390:LEU:HB3	2.20	0.42
3:D:469:ARG:HG2	3:D:469:ARG:H	1.54	0.42
3:D:584:VAL:HA	3:D:600:VAL:O	2.20	0.42
4:E:238:SER:HA	4:E:275:ARG:HG2	2.00	0.42
6:G:66:GLU:OE2	16:Q:45:ARG:NH2	2.53	0.42
16:H:149:LEU:HD23	16:H:149:LEU:HA	1.82	0.42
8:I:27:LYS:HD3	8:I:27:LYS:HA	1.87	0.42
13:L:268:TYR:HD1	13:L:397:PHE:HB3	1.84	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:L:454:VAL:HB	13:L:455:LEU:HD22	2.02	0.42
14:M:119:TYR:CZ	14:M:160:LEU:HD13	2.55	0.42
14:M:24:LEU:HD22	14:M:27:LEU:HD21	2.02	0.42
16:Q:287:LEU:O	16:Q:291:ILE:HG13	2.19	0.42
11:R:92:LEU:O	11:R:95:LEU:HB3	2.20	0.42
13:T:444:TRP:O	13:T:447:HIS:HB2	2.20	0.42
1:1:342:TRP:NE1	1:1:372:ALA:HA	2.34	0.42
2:2:79:HIS:H	2:2:137:ASN:ND2	2.18	0.42
3:3:170:LEU:HD23	3:3:170:LEU:HA	1.75	0.42
4:4:149:ALA:HA	4:4:204:TYR:OH	2.20	0.42
4:4:235:THR:HG21	4:4:352:GLU:HB2	2.00	0.42
5:5:101:LEU:HA	5:5:101:LEU:HD12	1.93	0.42
1:B:214:LYS:O	1:B:216:THR:HG23	2.20	0.42
1:B:289:ALA:HB3	1:B:337:MET:HE3	2.02	0.42
2:C:85:THR:OG1	2:C:124:CYS:N	2.52	0.42
3:D:480:LEU:HD23	3:D:480:LEU:HA	1.83	0.42
4:E:260:TYR:HA	4:E:292:GLN:NE2	2.35	0.42
14:M:371:LEU:HD13	14:M:371:LEU:HA	1.91	0.42
15:N:209:LEU:HG	15:N:293:GLY:HA2	2.02	0.42
7:O:9:SER:O	7:O:12:ILE:HG13	2.20	0.42
7:O:178:GLU:O	7:O:178:GLU:HG3	2.20	0.42
16:Q:98:GLY:O	16:Q:114:TRP:HB2	2.19	0.42
11:R:117:GLN:HB2	12:S:47:ARG:O	2.19	0.42
13:T:454:VAL:HB	13:T:455:LEU:HD22	2.02	0.42
14:U:304:THR:HG21	14:U:386:LYS:HB2	2.01	0.42
14:U:344:TYR:O	14:U:347:LEU:HD23	2.20	0.42
1:1:393:LEU:HD23	1:1:397:ARG:HH22	1.81	0.41
2:2:77:LYS:O	2:2:137:ASN:ND2	2.53	0.41
3:3:290:ILE:HB	3:3:295:ARG:NH2	2.35	0.41
3:3:371:PHE:CE1	3:3:374:ARG:HG3	2.55	0.41
3:3:356:LEU:HD22	3:3:654:PHE:HB2	2.02	0.41
5:5:6:VAL:HG13	5:5:41:TYR:HE1	1.85	0.41
7:9:41:HIS:HB3	7:9:113:ILE:CD1	2.42	0.41
10:A:7:TYR:HD1	10:A:7:TYR:N	2.18	0.41
10:A:93:PHE:O	10:A:96:VAL:HG12	2.20	0.41
3:D:551:PRO:HB2	3:D:555:GLY:HA2	2.02	0.41
3:D:5:LYS:HB3	3:D:92:VAL:HA	2.02	0.41
4:E:132:PHE:HE1	4:E:398:ALA:O	2.03	0.41
4:E:276:MET:O	4:E:280:ILE:HG13	2.20	0.41
12:K:42:LEU:HD23	12:K:42:LEU:HA	1.86	0.41
13:L:496:LEU:HD12	13:L:496:LEU:HA	1.93	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:L:604:MET:HG2	15:N:232:ALA:HB2	2.02	0.41
14:M:385:TYR:CE1	14:M:389:PRO:HB3	2.55	0.41
15:N:209:LEU:HB2	15:N:296:PHE:HB3	2.01	0.41
12:S:42:LEU:HA	12:S:42:LEU:HD23	1.94	0.41
12:S:47:ARG:HB3	12:S:47:ARG:HE	1.61	0.41
13:T:309:ALA:HB2	13:T:388:ILE:HD13	2.01	0.41
14:U:452:ARG:HD3	14:U:452:ARG:HA	1.80	0.41
15:V:176:LEU:HA	15:V:176:LEU:HD23	1.91	0.41
15:V:25:VAL:O	15:V:29:THR:HG23	2.19	0.41
1:1:4:PRO:HA	1:1:12:ARG:HH12	1.85	0.41
1:1:149:ILE:HG22	1:1:153:ARG:HE	1.85	0.41
4:4:102:GLU:O	4:4:106:GLY:N	2.53	0.41
4:4:185:GLU:OE1	4:4:185:GLU:N	2.54	0.41
5:5:52:ILE:HG22	5:5:118:VAL:HG21	2.02	0.41
7:9:149:GLU:O	7:9:153:THR:CB	2.67	0.41
1:B:272:PHE:CE2	1:B:292:PRO:HB3	2.55	0.41
1:B:272:PHE:HZ	1:B:316:LEU:HD11	1.85	0.41
1:B:272:PHE:HZ	1:B:316:LEU:HD21	1.85	0.41
3:D:307:LYS:HB3	3:D:307:LYS:HE2	1.84	0.41
15:N:177:GLY:O	15:N:181:VAL:HG23	2.19	0.41
10:P:47:GLY:O	10:P:48:ASN:HB3	2.21	0.41
16:Q:108:PHE:HB2	16:Q:112:GLN:O	2.20	0.41
7:O:25:PRO:HB2	16:Q:50:ARG:HH22	1.84	0.41
13:T:14:PHE:HB2	13:T:109:ASN:HB2	2.02	0.41
13:T:239:LEU:HD12	13:T:243:ALA:HB3	2.02	0.41
14:U:215:PRO:CG	14:U:216:PRO:HD3	2.50	0.41
14:U:354:LEU:HD13	14:U:425:LEU:HG	2.02	0.41
9:X:88:ARG:HB3	9:X:90:TYR:CE1	2.56	0.41
1:1:393:LEU:HA	1:1:397:ARG:CZ	2.50	0.41
2:2:41:ILE:HD12	2:2:70:TYR:HB3	2.02	0.41
3:3:115:HIS:CD2	3:3:116:PRO:HD2	2.55	0.41
1:B:400:CYS:HA	1:B:401:PRO:HD3	1.89	0.41
1:B:356:CYS:N	17:B:501:SF4:S3	2.83	0.41
4:E:137:LEU:HD23	4:E:145:PRO:HB2	2.02	0.41
4:E:302:VAL:HG23	4:E:303:ARG:HG2	2.03	0.41
12:K:47:ARG:HB3	12:K:47:ARG:HE	1.67	0.41
14:M:93:GLY:HA3	14:M:136:TYR:CE1	2.55	0.41
14:M:78:ILE:O	14:M:82:VAL:HG23	2.20	0.41
7:O:102:GLY:HA2	7:O:115:LEU:HD11	2.01	0.41
4:E:28:LEU:HD12	10:P:50:PRO:O	2.19	0.41
10:P:8:VAL:O	10:P:12:ILE:HG13	2.20	0.41

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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:3:368:HIS:HB3	3:3:556:ALA:N	2.35	0.41
4:4:112:ARG:NH1	4:4:299:PRO:HA	2.35	0.41
4:4:62:LEU:HD23	4:4:62:LEU:HA	1.68	0.41
1:B:149:ILE:CG2	1:B:153:ARG:HH21	2.34	0.41
1:B:291:ILE:O	1:B:328:VAL:HA	2.20	0.41
1:B:317:GLN:HA	1:B:321:SER:O	2.21	0.41
3:D:123:ASP:OD2	3:D:241:ARG:HA	2.20	0.41
5:F:159:PHE:HB2	5:F:163:ARG:O	2.20	0.41
13:L:561:LEU:HG	13:L:565:PHE:CE2	2.56	0.41
15:N:181:VAL:HA	15:N:192:PHE:HE2	1.84	0.41
16:Q:162:TYR:CD2	16:Q:209:ALA:HA	2.51	0.41
13:T:433:HIS:CG	13:T:433:HIS:O	2.73	0.41
14:U:265:ALA:HA	14:U:395:ALA:HB2	2.01	0.41
14:U:346:GLY:HA2	14:U:416:GLU:O	2.20	0.41
9:X:34:ILE:HG23	9:X:92:ALA:HB3	2.02	0.41
1:1:394:ILE:HB	1:1:407:VAL:HG11	2.03	0.41
3:D:306:LEU:HD11	3:D:308:THR:O	2.20	0.41
16:H:327:VAL:O	16:H:331:ASP:N	2.49	0.41
11:J:72:MET:HE2	16:H:153:LEU:HD21	2.03	0.41
11:J:97:ALA:O	12:K:12:ALA:HB1	2.20	0.41
13:L:542:ILE:O	13:L:546:LEU:HG	2.20	0.41
14:M:39:LEU:HB3	14:M:67:LEU:HD21	2.02	0.41
14:M:95:PHE:HB3	14:M:136:TYR:CE2	2.56	0.41
15:N:291:ALA:HB2	15:N:409:LEU:HD11	2.02	0.41
7:O:126:TYR:HB3	9:X:39:ASP:CG	2.41	0.41
2:2:101:THR:HG22	8:7:108:ILE:HG12	2.02	0.41
3:3:201:ASP:OD1	3:3:202:PHE:N	2.49	0.41
3:3:387:LEU:O	3:3:390:LEU:HB3	2.20	0.41
3:3:694:LEU:HA	3:3:760:LEU:O	2.21	0.41
10:A:67:LEU:HD21	10:A:110:GLU:OE2	2.21	0.41
1:B:246:SER:HG	1:B:313:TYR:H	1.65	0.41
1:B:245:GLN:HB2	1:B:314:GLU:CD	2.41	0.41
1:B:357:THR:HG21	3:D:111:THR:OG1	2.21	0.41
4:E:38:HIS:HE1	4:E:398:ALA:HA	1.85	0.41
4:E:73:ARG:NE	4:E:81:TYR:OH	2.54	0.41
11:J:58:VAL:O	11:J:62:ALA:HB3	2.20	0.41
13:L:582:GLN:OE1	15:N:260:TYR:OH	2.36	0.41
14:M:143:ARG:HA	14:M:143:ARG:HD3	1.68	0.41
10:P:67:LEU:HD23	16:Q:310:TRP:CZ2	2.56	0.41
16:Q:293:ILE:HD12	16:Q:297:TRP:CZ3	2.56	0.41
2:2:154:LEU:HD23	2:2:154:LEU:HA	1.78	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:3:355:LEU:HB2	3:3:547:MET:SD	2.61	0.41
7:9:70:VAL:HG22	7:9:91:TYR:CD2	2.56	0.41
10:A:48:ASN:OD1	10:A:49:ASP:HB2	2.20	0.41
1:B:352:SER:OG	1:B:359:CYS:SG	2.72	0.41
1:B:63:ARG:HD3	1:B:313:TYR:CD2	2.56	0.41
2:C:78:TYR:HD2	2:C:116:LEU:HD12	1.86	0.41
3:D:256:CYS:O	3:D:262:GLY:HA2	2.21	0.41
3:D:284:GLU:HG2	3:D:284:GLU:H	1.68	0.41
3:D:341:VAL:HG22	3:D:565:TYR:HB2	2.03	0.41
4:E:185:GLU:N	4:E:185:GLU:OE1	2.52	0.41
11:J:154:VAL:O	11:J:158:GLU:HB2	2.21	0.41
13:L:587:ARG:O	13:L:591:LEU:HD13	2.21	0.41
15:N:155:TYR:HB2	15:N:161:LEU:HD21	2.03	0.41
7:O:37:PHE:HB3	7:O:117:TYR:HD1	1.86	0.41
12:S:94:ARG:HG2	13:T:583:THR:O	2.21	0.41
13:T:59:TRP:HB3	13:T:63:ILE:O	2.20	0.41
15:V:280:ALA:HA	15:V:347:LEU:HD13	2.03	0.41
1:1:342:TRP:CZ2	1:1:372:ALA:HA	2.56	0.41
3:3:116:PRO:O	3:3:117:LEU:HB2	2.21	0.41
3:3:168:HIS:O	3:3:176:LEU:N	2.51	0.41
3:3:473:GLU:O	3:3:476:ILE:N	2.53	0.41
4:4:202:ASP:OD1	4:4:284:ARG:NE	2.54	0.41
4:4:27:THR:HG22	4:4:44:MET:HE3	2.03	0.41
5:5:120:ASP:OD1	5:5:137:THR:OG1	2.29	0.41
5:5:47:ASN:O	5:5:108:TRP:NE1	2.43	0.41
5:5:53:VAL:HG22	5:5:55:LEU:HD11	2.03	0.41
6:6:165:GLU:OE2	7:9:148:ARG:NH1	2.53	0.41
7:9:118:ASP:HB3	7:9:143:THR:CG2	2.51	0.41
7:9:41:HIS:O	7:9:136:MET:HB3	2.20	0.41
4:E:330:HIS:O	4:E:334:GLY:HA2	2.20	0.41
4:E:34:HIS:HB2	10:P:45:GLU:OE2	2.21	0.41
4:E:353:LEU:HD12	4:E:354:GLY:H	1.86	0.41
6:G:177:LYS:HB2	6:G:177:LYS:HE3	1.78	0.41
13:L:327:PHE:CE1	13:L:452:GLY:HA3	2.56	0.41
14:M:141:ARG:HG3	14:M:142:THR:H	1.85	0.41
16:Q:122:ILE:HG13	16:Q:123:LEU:HD12	2.03	0.41
16:Q:65:LYS:NZ	16:Q:69:LYS:HE2	2.35	0.41
13:T:379:LEU:HD23	13:T:379:LEU:HA	1.88	0.41
14:U:381:LEU:HB2	14:U:396:PHE:CZ	2.55	0.41
14:U:8:LEU:HB3	14:U:9:PRO:HD3	2.03	0.41
1:1:100:SER:HA	1:1:253:GLN:HE21	1.86	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:3:180:ARG:O	3:3:232:VAL:HG21	2.20	0.41
1:B:102:LYS:HB3	1:B:253:GLN:OE1	2.21	0.41
1:B:433:ARG:HH12	2:C:89:LYS:CE	2.30	0.41
2:C:47:GLU:HB3	2:C:51:ARG:HH12	1.86	0.41
1:B:197:ALA:HB3	2:C:66:PHE:CE2	2.56	0.41
3:D:251:GLU:HG2	3:D:268:ASP:OD1	2.21	0.41
6:G:33:SER:O	6:G:36:LEU:HG	2.21	0.41
6:G:37:TRP:HB2	16:Q:65:LYS:HE2	2.03	0.41
16:H:269:MET:HG3	16:H:270:PRO:HD2	2.02	0.41
7:9:22:VAL:HB	16:H:44:VAL:CG2	2.51	0.41
13:L:491:TRP:HA	13:L:494:ILE:HG12	2.01	0.41
14:M:264:ALA:HB1	14:M:294:GLY:O	2.20	0.41
14:M:73:LEU:HD23	14:M:74:PHE:N	2.36	0.41
16:Q:91:VAL:O	16:Q:95:LEU:HG	2.20	0.41
13:T:293:LYS:HE2	13:T:297:TYR:HE1	1.86	0.41
13:T:90:TYR:CE1	13:T:334:LEU:HD22	2.56	0.41
13:T:49:LEU:HD23	13:T:49:LEU:HA	1.94	0.41
14:U:49:HIS:O	14:U:66:GLY:HA2	2.21	0.41
14:U:78:ILE:O	14:U:82:VAL:HG23	2.21	0.41
2:2:7:LYS:O	2:2:11:LEU:HG	2.22	0.40
3:3:192:GLU:O	3:3:443:ARG:NH1	2.54	0.40
3:3:256:CYS:O	3:3:262:GLY:HA2	2.21	0.40
3:3:349:ALA:HB3	3:3:544:LEU:HD21	2.04	0.40
3:3:455:ARG:NH2	3:3:750:ARG:NH2	2.69	0.40
4:4:193:LEU:HA	4:4:196:VAL:HG12	2.02	0.40
4:4:197:LEU:N	4:4:198:PRO:HD2	2.36	0.40
5:5:168:ALA:HA	5:5:171:ARG:HH11	1.86	0.40
4:4:64:THR:OG1	6:6:123:ILE:HD11	2.20	0.40
6:6:39:ALA:N	6:6:77:VAL:O	2.35	0.40
6:6:78:MET:HB3	6:6:105:VAL:HG22	2.03	0.40
1:B:259:LYS:HB3	1:B:281:GLY:HA3	2.02	0.40
3:D:307:LYS:HE3	3:D:632:GLY:CA	2.51	0.40
3:D:290:ILE:HG23	17:D:803:SF4:S4	2.61	0.40
4:E:156:ILE:HG12	4:E:193:LEU:HD11	2.03	0.40
5:F:101:LEU:HA	5:F:101:LEU:HD12	1.99	0.40
5:F:113:PHE:O	5:F:116:ARG:HB2	2.21	0.40
13:L:216:LYS:HD3	13:L:245:MET:SD	2.61	0.40
14:M:141:ARG:HG3	14:M:142:THR:N	2.36	0.40
14:M:242:PHE:HZ	14:M:458:ALA:HA	1.85	0.40
14:M:244:PHE:O	14:M:248:LEU:HB2	2.21	0.40
15:N:16:LEU:O	15:N:20:LEU:N	2.55	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:P:83:VAL:HG23	10:P:84:SER:H	1.86	0.40
10:P:68:PHE:CD2	16:Q:164:LEU:HB2	2.56	0.40
16:Q:216:ARG:HD2	16:Q:294:ARG:HA	2.02	0.40
13:T:385:LYS:NZ	13:T:410:ALA:HA	2.36	0.40
13:T:600:LEU:HD12	15:V:235:LEU:HD23	2.03	0.40
9:W:46:TYR:O	9:W:61:ASP:HA	2.21	0.40
1:1:211:LEU:HA	1:1:211:LEU:HD12	1.91	0.40
3:3:503:PRO:CG	3:3:528:LYS:HD3	2.51	0.40
7:9:17:LEU:HA	16:H:41:ARG:O	2.21	0.40
2:C:147:ARG:HE	2:C:147:ARG:HB2	1.72	0.40
3:D:464:ILE:HA	3:D:489:MET:SD	2.61	0.40
4:E:240:ARG:O	4:E:267:GLY:N	2.47	0.40
4:E:245:ASN:HA	4:E:266:LEU:HD21	2.03	0.40
4:E:352:GLU:OE2	5:F:87:ARG:NH2	2.53	0.40
4:E:73:ARG:O	4:E:365:PRO:HD2	2.22	0.40
16:H:103:GLY:O	16:H:113:PRO:HG2	2.21	0.40
16:H:2:THR:HA	16:H:5:TYR:CD2	2.51	0.40
10:A:60:HIS:CE1	16:H:306:LEU:HD12	2.55	0.40
13:L:141:LEU:HB3	13:L:236:VAL:HG11	2.02	0.40
13:L:598:LEU:HA	13:L:598:LEU:HD23	1.90	0.40
14:M:88:VAL:HG22	14:M:331:ARG:HE	1.86	0.40
14:M:362:PHE:O	14:M:365:MET:HB3	2.20	0.40
15:N:345:LYS:O	15:N:349:PHE:CD2	2.74	0.40
15:N:294:LEU:CG	15:N:402:VAL:HG13	2.49	0.40
7:O:20:LYS:HG3	7:O:20:LYS:H	1.74	0.40
16:Q:267:TRP:O	16:Q:269:MET:N	2.54	0.40
16:Q:301:ARG:O	16:Q:302:TYR:HB3	2.21	0.40
16:Q:21:VAL:HG13	16:Q:94:LEU:HD13	2.03	0.40
12:S:21:ARG:NE	12:S:26:LEU:HD23	2.37	0.40
13:T:74:GLY:O	13:T:78:LEU:HG	2.21	0.40
14:U:103:GLU:O	14:U:107:LEU:HG	2.21	0.40
14:U:381:LEU:HB2	14:U:396:PHE:CE2	2.57	0.40
1:1:20:HIS:HB3	1:1:31:TYR:CE1	2.55	0.40
1:1:435:SER:HA	2:2:95:GLU:OE2	2.21	0.40
3:3:133:ARG:HA	3:3:136:GLU:OE2	2.21	0.40
3:3:438:LYS:O	3:3:441:MET:HG3	2.21	0.40
3:3:715:GLU:HA	3:3:746:ARG:O	2.21	0.40
4:4:236:GLY:O	4:4:238:SER:N	2.54	0.40
4:4:396:ILE:HA	4:4:399:SER:OG	2.20	0.40
5:5:116:ARG:HB3	5:5:135:ILE:HG13	2.03	0.40
4:E:246:TYR:OH	4:E:352:GLU:OE1	2.39	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:F:55:LEU:O	5:F:68:PHE:HA	2.21	0.40
10:A:107:PHE:HE1	16:H:310:TRP:HD1	1.68	0.40
16:H:33:LEU:HD11	16:H:55:GLY:O	2.21	0.40
11:J:11:LEU:HB3	11:J:38:VAL:HG21	2.02	0.40
13:L:356:TRP:CZ3	13:L:363:ARG:HD2	2.55	0.40
14:M:348:ALA:HB2	14:M:414:PHE:HB3	2.02	0.40
16:Q:155:SER:OG	16:Q:156:SER:N	2.55	0.40
16:Q:291:ILE:HA	16:Q:294:ARG:CG	2.45	0.40
13:T:22:LYS:HZ1	13:T:100:GLY:HA2	1.86	0.40
14:U:148:PHE:HA	14:U:213:TRP:HB2	2.04	0.40
1:1:201:LEU:HD11	3:3:84:VAL:HG21	2.03	0.40
2:2:3:PHE:CE2	2:2:34:VAL:HG22	2.55	0.40
3:3:136:GLU:HA	5:5:188:SER:H	1.86	0.40
3:3:243:ARG:HD2	3:3:275:LEU:HD22	2.02	0.40
3:3:307:LYS:HE3	3:3:632:GLY:HA2	2.03	0.40
5:5:54:GLY:O	5:5:55:LEU:HD12	2.21	0.40
8:7:44:MET:CE	8:7:46:ARG:HH22	2.34	0.40
10:A:47:GLY:O	10:A:48:ASN:HB3	2.21	0.40
3:D:180:ARG:O	3:D:232:VAL:HG21	2.22	0.40
3:D:202:PHE:HB3	3:D:209:THR:CG2	2.52	0.40
3:D:478:LEU:HG	3:D:483:ASP:HB2	2.03	0.40
4:E:26:MET:N	4:E:48:SER:OG	2.48	0.40
16:H:5:TYR:OH	16:H:184:ASP:OD1	2.25	0.40
16:H:274:VAL:CG2	16:H:275:PRO:HD2	2.52	0.40
16:H:44:VAL:C	16:H:45:ARG:O	2.59	0.40
13:L:183:LEU:HA	13:L:183:LEU:HD23	1.74	0.40
13:L:122:ASP:OD1	13:L:186:SER:HB3	2.22	0.40
13:L:539:ASN:OD1	13:L:539:ASN:N	2.54	0.40
14:M:127:ILE:O	14:M:131:LEU:HG	2.22	0.40
15:N:255:LYS:HE2	15:N:306:ARG:HA	2.03	0.40
13:T:389:LEU:HD21	13:T:407:LEU:HD13	2.03	0.40
13:T:554:PHE:HZ	14:U:283:THR:HG21	1.84	0.40
15:V:256:ARG:HG2	15:V:260:TYR:HE2	1.86	0.40
15:V:294:LEU:O	15:V:298:VAL:HG23	2.21	0.40
15:V:337:PRO:HG3	15:V:342:PHE:CD2	2.56	0.40
15:V:35:LEU:HA	15:V:35:LEU:HD23	1.93	0.40
15:V:40:LEU:HD12	15:V:67:LEU:HD12	2.02	0.40
15:V:89:LEU:HD23	15:V:89:LEU:HA	1.87	0.40
1:1:135:ARG:HE	1:1:137:GLU:HB2	1.86	0.40
1:1:45:LEU:HD12	1:1:163:PHE:CD2	2.56	0.40
3:3:196:GLY:HA3	3:3:461:TRP:CZ2	2.56	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:3:40:SER:HA	3:3:437:ILE:O	2.21	0.40
3:3:451:PHE:HE1	3:3:466:GLU:HB3	1.87	0.40
6:6:106:ILE:HG12	6:6:135:VAL:HB	2.03	0.40
1:B:357:THR:N	1:B:358:PRO:HD2	2.36	0.40
2:C:110:GLU:HA	8:I:121:ARG:NH1	2.25	0.40
3:D:293:ALA:HB2	3:D:698:MET:HG2	2.04	0.40
4:E:169:HIS:HE2	6:G:45:CYS:CB	2.35	0.40
5:F:74:LEU:O	5:F:87:ARG:HA	2.20	0.40
16:H:213:GLU:N	16:H:213:GLU:OE1	2.55	0.40
11:J:75:PHE:CZ	11:J:77:ALA:HB3	2.57	0.40
14:M:304:THR:HG21	14:M:386:LYS:HB2	2.04	0.40
14:M:358:ALA:O	14:M:362:PHE:HD2	2.04	0.40
15:N:98:LEU:HD23	15:N:218:ALA:HB1	2.03	0.40
16:Q:28:PHE:HB2	16:Q:249:TYR:HB3	2.04	0.40
13:T:184:SER:HB3	13:T:187:GLU:HG2	2.02	0.40
13:T:371:LEU:O	13:T:375:GLY:N	2.55	0.40
14:U:128:PRO:O	14:U:132:MET:HG2	2.21	0.40
11:R:155:ALA:HB2	15:V:83:GLU:HG2	2.03	0.40
9:W:113:ARG:O	9:W:117:ILE:HG12	2.21	0.40
9:W:51:HIS:HA	9:W:56:ASP:OD1	2.22	0.40

There are no symmetry-related clashes.

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

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

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	1	435/438 (99%)	403 (93%)	32 (7%)	0	100	100
1	B	435/438 (99%)	399 (92%)	36 (8%)	0	100	100
2	2	176/181 (97%)	170 (97%)	6 (3%)	0	100	100
2	C	176/181 (97%)	169 (96%)	7 (4%)	0	100	100

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

All (17) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
16	H	45	ARG
16	H	51	VAL
7	O	21	PRO
16	Q	51	VAL
16	H	44	VAL
16	Q	44	VAL
16	Q	45	ARG
16	H	50	ARG
16	H	218	PRO
16	H	268	THR
16	Q	50	ARG
13	L	435	PRO
16	Q	268	THR
13	T	435	PRO
16	Q	333	PRO
16	H	53	PRO
16	Q	53	PRO

5.3.2 Protein sidechains

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

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	1	355/356 (100%)	344 (97%)	11 (3%)	40	68
1	B	355/356 (100%)	345 (97%)	10 (3%)	43	70
2	2	150/152 (99%)	144 (96%)	6 (4%)	31	60
2	C	150/152 (99%)	144 (96%)	6 (4%)	31	60
3	3	609/628 (97%)	599 (98%)	10 (2%)	62	81
3	D	609/628 (97%)	598 (98%)	11 (2%)	59	79
4	4	332/355 (94%)	328 (99%)	4 (1%)	71	85
4	E	332/355 (94%)	326 (98%)	6 (2%)	59	79
5	5	167/175 (95%)	163 (98%)	4 (2%)	49	74
5	F	167/175 (95%)	164 (98%)	3 (2%)	59	79
6	6	135/149 (91%)	125 (93%)	10 (7%)	13	42

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
6	G	135/149 (91%)	126 (93%)	9 (7%)	16 46
7	9	148/150 (99%)	147 (99%)	1 (1%)	84 92
7	O	148/150 (99%)	146 (99%)	2 (1%)	67 83
8	7	104/106 (98%)	103 (99%)	1 (1%)	76 88
8	I	104/106 (98%)	103 (99%)	1 (1%)	76 88
9	W	99/101 (98%)	98 (99%)	1 (1%)	76 88
9	X	99/101 (98%)	98 (99%)	1 (1%)	76 88
10	A	90/92 (98%)	88 (98%)	2 (2%)	52 75
10	P	90/92 (98%)	87 (97%)	3 (3%)	38 66
11	J	118/130 (91%)	114 (97%)	4 (3%)	37 65
11	R	118/130 (91%)	115 (98%)	3 (2%)	47 72
12	K	71/71 (100%)	69 (97%)	2 (3%)	43 70
12	S	71/71 (100%)	69 (97%)	2 (3%)	43 70
13	L	453/454 (100%)	445 (98%)	8 (2%)	59 79
13	T	453/454 (100%)	445 (98%)	8 (2%)	59 79
14	M	332/332 (100%)	324 (98%)	8 (2%)	49 74
14	U	332/332 (100%)	323 (97%)	9 (3%)	44 70
15	N	302/302 (100%)	297 (98%)	5 (2%)	60 80
15	V	302/302 (100%)	297 (98%)	5 (2%)	60 80
16	H	293/300 (98%)	280 (96%)	13 (4%)	28 58
16	Q	293/300 (98%)	282 (96%)	11 (4%)	33 61
All	All	7516/7706 (98%)	7336 (98%)	180 (2%)	49 74

All (180) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	1	18	TYR
1	1	81	LYS
1	1	249	MET
1	1	337	MET
1	1	342	TRP
1	1	353	CYS
1	1	359	CYS
1	1	366	PHE
1	1	397	ARG

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

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

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Mol	Chain	Res	Type
1	B	342	TRP
1	B	353	CYS
1	B	355	LYS
1	B	359	CYS
1	B	366	PHE
1	B	397	ARG
1	B	437	TRP
2	C	7	LYS
2	C	33	ARG
2	C	35	GLN
2	C	45	ARG
2	C	116	LEU
2	C	147	ARG
3	D	3	ARG
3	D	132	ASP
3	D	184	CYS
3	D	259	CYS
3	D	337	ARG
3	D	369	LEU
3	D	469	ARG
3	D	617	LEU
3	D	655	ARG
3	D	761	SER
3	D	774	ARG
4	E	87	TYR
4	E	129	HIS
4	E	143	LEU
4	E	152	GLU
4	E	208	PHE
4	E	262	PHE
5	F	31	ARG
5	F	147	ARG
5	F	178	ASP
6	G	37	TRP
6	G	49	GLU
6	G	55	ASP
6	G	68	PHE
6	G	83	ARG
6	G	88	MET
6	G	120	ASN
6	G	156	LYS
6	G	176	TRP

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

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

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

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

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

5.3.3 RNA

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains

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

5.5 Carbohydrates

There are no monosaccharides in this entry.

5.6 Ligand geometry

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	6	201	6	0,12,12	0.00	-	-		
19	FES	D	804	3	0,4,4	0.00	-	-		
17	SF4	O	201	7	0,12,12	0.00	-	-		
17	SF4	1	501	1	0,12,12	0.00	-	-		
17	SF4	D	803	3	0,12,12	0.00	-	-		
17	SF4	3	802	3	0,12,12	0.00	-	-		
17	SF4	G	201	6	0,12,12	0.00	-	-		
17	SF4	D	801	3	0,12,12	0.00	-	-		
18	FMN	1	502	-	31,33,33	1.48	4 (12%)	40,50,50	1.60	5 (12%)
20	HQW	E	501	-	29,31,31	1.63	6 (20%)	25,44,44	2.14	7 (28%)
17	SF4	3	803	3	0,12,12	0.00	-	-		
19	FES	C	201	2	0,4,4	0.00	-	-		
17	SF4	9	201	7	0,12,12	0.00	-	-		
19	FES	2	201	2	0,4,4	0.00	-	-		
20	HQW	4	501	-	29,31,31	2.02	7 (24%)	25,44,44	1.92	8 (32%)
17	SF4	B	501	1	0,12,12	0.00	-	-		
18	FMN	B	502	-	31,33,33	1.42	4 (12%)	40,50,50	1.64	5 (12%)
17	SF4	3	801	3	0,12,12	0.00	-	-		
17	SF4	D	802	3	0,12,12	0.00	-	-		
17	SF4	O	202	7	0,12,12	0.00	-	-		
19	FES	3	804	3	0,4,4	0.00	-	-		
17	SF4	9	202	7	0,12,12	0.00	-	-		

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	6	201	6	-	-	0/6/5/5
19	FES	D	804	3	-	-	0/1/1/1
17	SF4	O	201	7	-	-	0/6/5/5
17	SF4	1	501	1	-	-	0/6/5/5
17	SF4	D	803	3	-	-	0/6/5/5
17	SF4	3	802	3	-	-	0/6/5/5
17	SF4	G	201	6	-	-	0/6/5/5
17	SF4	D	801	3	-	-	0/6/5/5
18	FMN	1	502	-	-	8/18/18/18	0/3/3/3

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
20	HQW	E	501	-	-	6/12/27/27	0/3/3/3
17	SF4	3	803	3	-	-	0/6/5/5
19	FES	C	201	2	-	-	0/1/1/1
17	SF4	9	201	7	-	-	0/6/5/5
19	FES	2	201	2	-	-	0/1/1/1
20	HQW	4	501	-	-	6/12/27/27	0/3/3/3
17	SF4	B	501	1	-	-	0/6/5/5
18	FMN	B	502	-	-	8/18/18/18	0/3/3/3
17	SF4	3	801	3	-	-	0/6/5/5
17	SF4	D	802	3	-	-	0/6/5/5
17	SF4	O	202	7	-	-	0/6/5/5
19	FES	3	804	3	-	-	0/1/1/1
17	SF4	9	202	7	-	-	0/6/5/5

All (21) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
20	4	501	HQW	C7-C6	-5.42	1.32	1.39
20	4	501	HQW	C9-C11	4.44	1.54	1.41
18	1	502	FMN	C10-N1	4.16	1.38	1.33
18	B	502	FMN	C10-N1	4.11	1.38	1.33
20	E	501	HQW	C7-C6	-4.03	1.34	1.39
18	1	502	FMN	C4A-N5	3.94	1.39	1.33
20	4	501	HQW	O25-C13	3.89	1.40	1.35
20	E	501	HQW	C9-C7	3.56	1.51	1.41
18	B	502	FMN	C4A-N5	3.49	1.38	1.33
20	4	501	HQW	O25-C6	3.24	1.39	1.35
18	B	502	FMN	C4-N3	3.16	1.38	1.33
18	1	502	FMN	C4-N3	3.13	1.38	1.33
20	E	501	HQW	C9-C11	3.11	1.50	1.41
20	4	501	HQW	O24-C2	-3.01	1.40	1.44
20	E	501	HQW	C23-N1	2.87	1.51	1.45
18	1	502	FMN	C1'-N10	2.76	1.51	1.48
20	4	501	HQW	C23-N1	2.72	1.51	1.45
18	B	502	FMN	C1'-N10	2.60	1.50	1.48
20	E	501	HQW	O24-C2	-2.42	1.40	1.44
20	4	501	HQW	O26-C13	2.36	1.39	1.36
20	E	501	HQW	O25-C6	2.09	1.37	1.35

All (25) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
18	B	502	FMN	C4-N3-C2	5.95	120.17	115.14
18	1	502	FMN	C4-N3-C2	5.92	120.14	115.14
20	E	501	HQW	C11-C9-C7	-5.44	114.78	122.88
18	B	502	FMN	C5A-C9A-N10	4.30	120.83	117.72
20	E	501	HQW	C17-C14-C10	-4.13	123.70	130.74
18	B	502	FMN	C1'-N10-C10	4.04	122.03	118.41
20	4	501	HQW	C11-C9-C7	-3.99	116.93	122.88
20	E	501	HQW	O26-C13-C11	3.88	124.27	118.82
20	4	501	HQW	C12-C7-C9	-3.79	113.62	120.40
20	E	501	HQW	C3-C2-C6	-3.71	110.27	116.10
18	1	502	FMN	C5A-C9A-N10	3.53	120.27	117.72
20	4	501	HQW	O26-C13-C11	3.53	123.78	118.82
18	1	502	FMN	C4A-N5-C5A	3.51	120.28	116.77
20	E	501	HQW	O24-C5-C4	3.26	109.16	105.58
20	4	501	HQW	C17-C14-C10	-3.06	125.53	130.74
18	1	502	FMN	C1'-N10-C9A	2.98	120.64	118.29
20	4	501	HQW	O24-C5-C4	2.83	108.69	105.58
18	B	502	FMN	C4A-N5-C5A	2.77	119.54	116.77
18	B	502	FMN	C4A-C4-N3	-2.52	119.98	123.43
20	E	501	HQW	C15-C10-C14	-2.39	119.63	124.64
20	4	501	HQW	C3-C2-C6	-2.35	112.40	116.10
20	4	501	HQW	C15-C10-C14	-2.22	119.99	124.64
18	1	502	FMN	C4A-C4-N3	-2.07	120.60	123.43
20	E	501	HQW	C14-C10-C8	2.04	122.61	116.96
20	4	501	HQW	C14-C10-C8	2.01	122.54	116.96

There are no chirality outliers.

All (28) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
18	1	502	FMN	N10-C1'-C2'-O2'
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'
20	E	501	HQW	C14-C10-C8-C4
20	E	501	HQW	C15-C10-C8-C4
20	4	501	HQW	C14-C10-C8-C4
20	4	501	HQW	C15-C10-C8-C4
18	B	502	FMN	N10-C1'-C2'-O2'
18	B	502	FMN	C1'-C2'-C3'-O3'
18	B	502	FMN	C1'-C2'-C3'-C4'

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Mol	Chain	Res	Type	Atoms
18	B	502	FMN	O2'-C2'-C3'-O3'
18	B	502	FMN	O2'-C2'-C3'-C4'
18	B	502	FMN	O4'-C4'-C5'-O5'
20	E	501	HQW	C10-C14-C17-C19
20	E	501	HQW	C10-C14-C17-C18
20	4	501	HQW	C10-C14-C17-C18
20	4	501	HQW	C10-C14-C17-C19
18	B	502	FMN	C3'-C4'-C5'-O5'
18	1	502	FMN	N10-C1'-C2'-C3'
20	E	501	HQW	O24-C2-C6-C7
20	4	501	HQW	O24-C2-C6-C7
18	B	502	FMN	N10-C1'-C2'-C3'
20	E	501	HQW	C3-C2-C6-C7
20	4	501	HQW	C3-C2-C6-C7
18	1	502	FMN	C3'-C4'-C5'-O5'

There are no ring outliers.

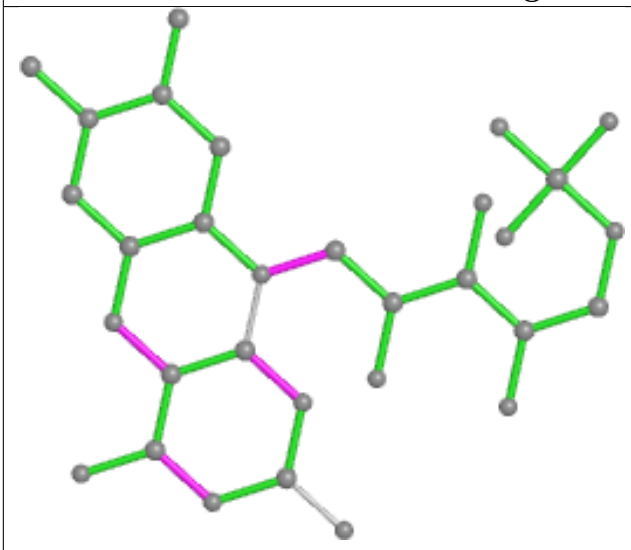
17 monomers are involved in 24 short contacts:

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

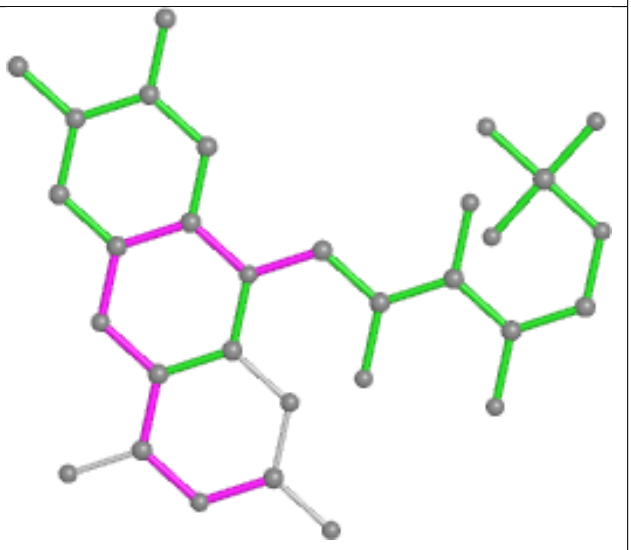
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

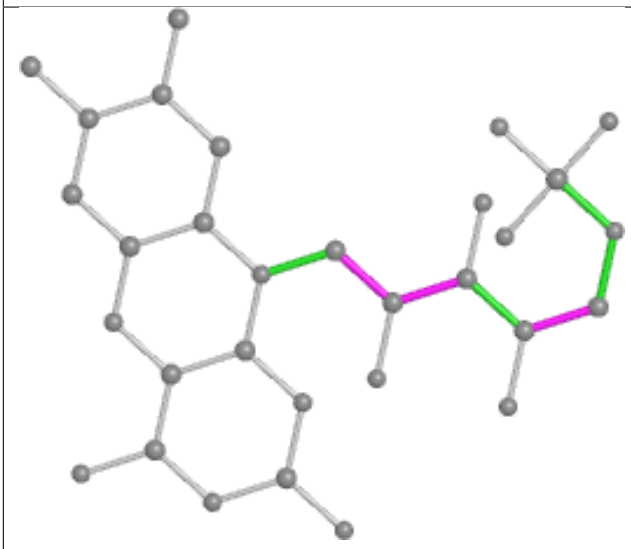
Ligand FMN 1 502



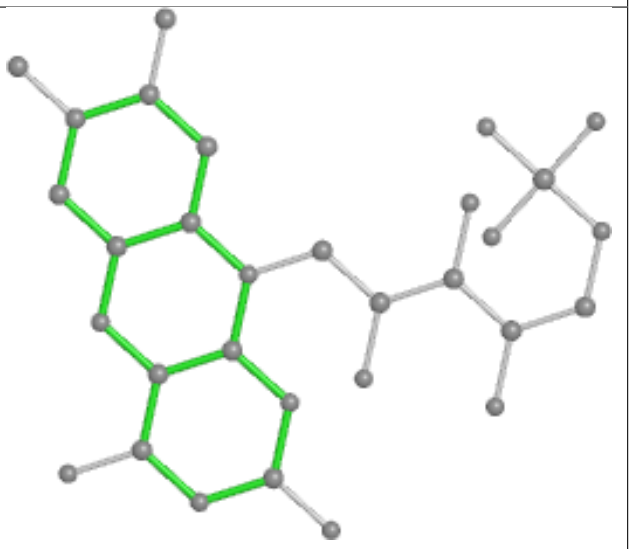
Bond lengths



Bond angles

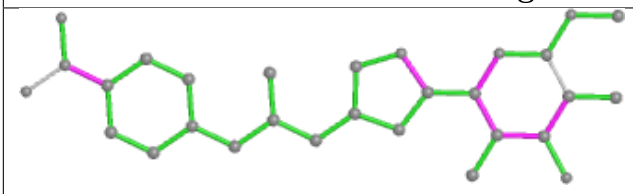


Torsions

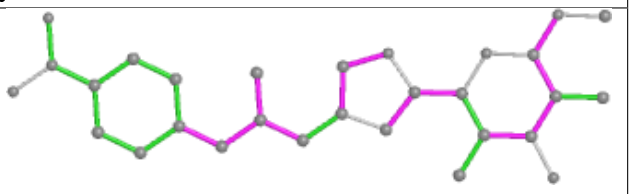


Rings

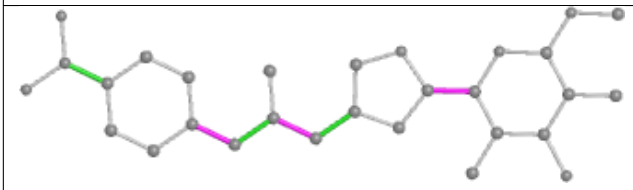
Ligand HQW E 501



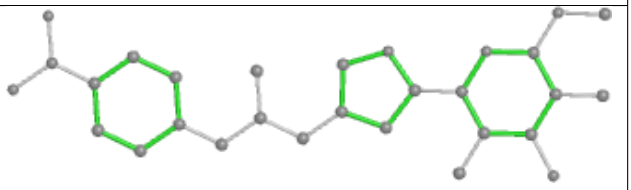
Bond lengths



Bond angles

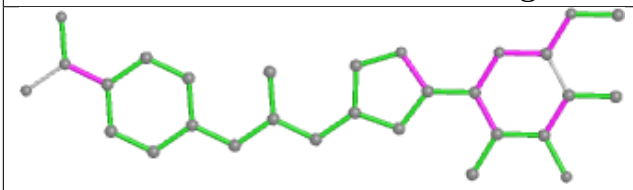


Torsions

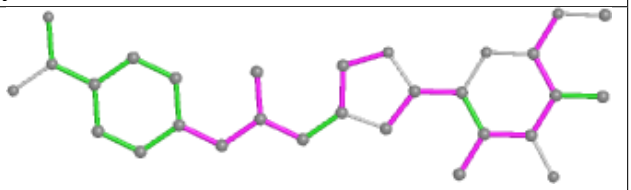


Rings

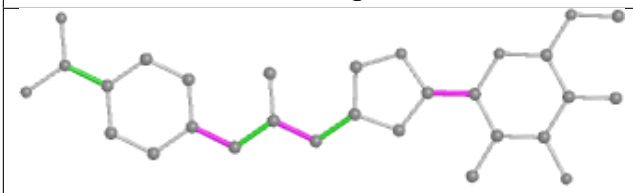
Ligand HQW 4 501



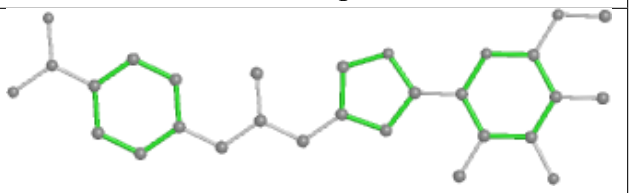
Bond lengths



Bond angles

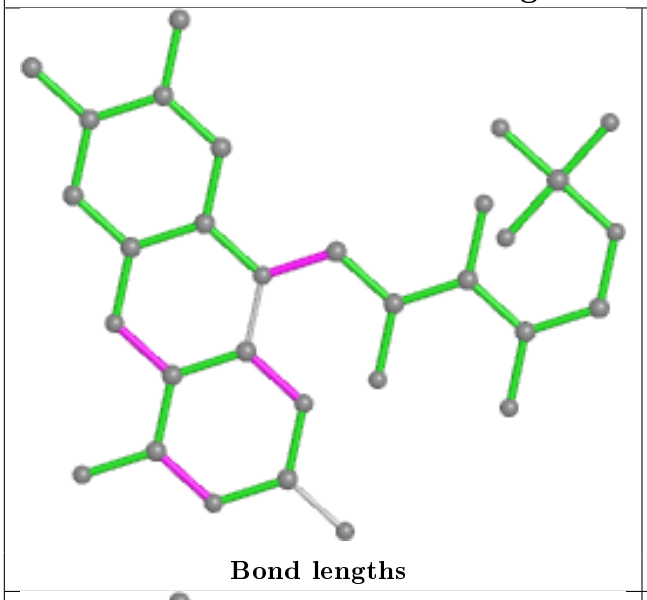


Torsions

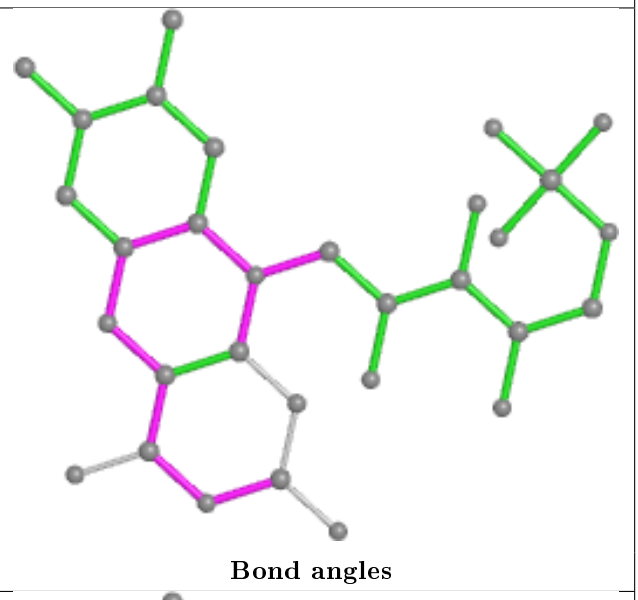


Rings

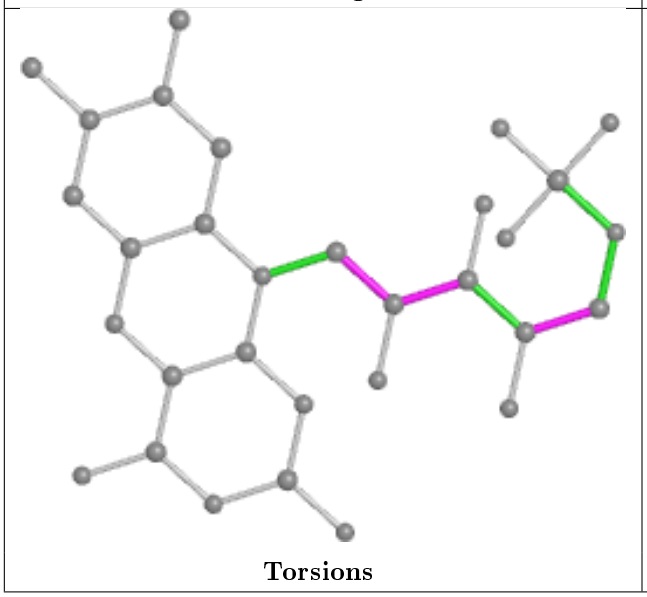
Ligand FMN B 502



Bond lengths



Bond angles



Torsions

Rings

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

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

6.2 Non-standard residues in protein, DNA, RNA chains

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

6.3 Carbohydrates

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

6.4 Ligands

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

6.5 Other polymers

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