



# Full wwPDB/EMDataBank EM Map/Model Validation Report ⓘ

Nov 28, 2017 – 12:53 PM EST

PDB ID : 5XTB  
EMDB ID: : EMD-6771  
Title : Cryo-EM structure of human respiratory complex I matrix arm  
Authors : Gu, J.; Wu, M.; Yang, M.  
Deposited on : unknown  
Resolution : 3.40 Å(reported)

This is a Full wwPDB/EMDataBank EM Map/Model Validation Report  
for a publicly released PDB/EMDB entry.

We welcome your comments at [validation@mail.wwpdb.org](mailto:validation@mail.wwpdb.org)  
A user guide is available at  
<http://wwpdb.org/validation/2016/EMValidationReportHelp>  
with specific help available everywhere you see the ⓘ symbol.

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MolProbity : 4.02b-467  
Mogul : 1.7.2 (RC1), CSD as538be (2017)  
Percentile statistics : 20161228.v01 (using entries in the PDB archive December 28th 2016)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et. al. (1996)  
Validation Pipeline (wwPDB-VP) : rb-20030345

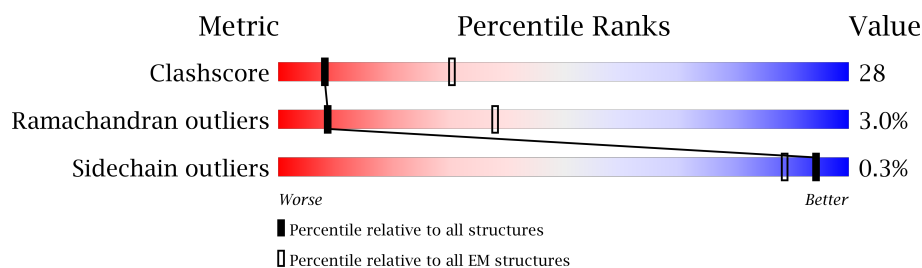
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*ELECTRON MICROSCOPY*

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.



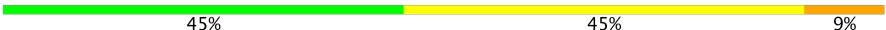



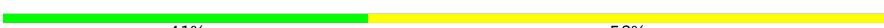




Metric	Whole archive (#Entries)	EM structures (#Entries)
Clashscore	125131	1336
Ramachandran outliers	121729	1120
Sidechain outliers	121581	1026

The table below summarises the geometric issues observed across the polymeric chains. The red, orange, yellow and green segments on the bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria. 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  $\leq 5\%$ .

Mol	Chain	Length	Quality of chain
1	A	431	48% 50% .
2	B	176	51% 48% .
3	C	156	56% 43% .
4	E	113	49% 49% .
5	F	83	49% 51%
6	G	85	46% 52% .
7	H	112	54% 45% .
8	I	110	46% 36% . 14%
9	J	337	48% 50% .

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Mol	Chain	Length	Quality of chain
10	K	33	 45% 45% 9%
11	L	118	 43% 56% 1%
12	M	687	 47% 52% 1%
13	N	143	 59% 38% 3%
14	O	212	 41% 58% 1%
15	P	208	 49% 47% 4%
16	Q	385	 46% 53% 1%
17	T	95	 58% 39% 3%
18	W	22	 64% 32% 4%

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 criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
19	SF4	A	501	-	-	X	-
19	SF4	B	302	-	-	X	-
19	SF4	M	801	-	-	X	-
20	FMN	A	502	-	-	X	-
22	NDP	J	401	-	-	X	-
23	FES	O	301	-	-	X	-

## 2 Entry composition

There are 23 unique types of molecules in this entry. The entry contains 27962 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, 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 dehydrogenase [ubiquinone] flavoprotein 1, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	431	Total	C	N	O	S	0	0
			3322	2096	594	612	20		

- Molecule 2 is a protein called NADH dehydrogenase [ubiquinone] iron-sulfur protein 8, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	B	176	Total	C	N	O	S	0	0
			1420	893	243	271	13		

- Molecule 3 is a protein called NADH dehydrogenase [ubiquinone] iron-sulfur protein 7, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	C	156	Total	C	N	O	S	0	0
			1249	794	227	214	14		

- Molecule 4 is a protein called NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 6.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	E	113	Total	C	N	O	S	0	0
			968	623	178	162	5		

- Molecule 5 is a protein called NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 2.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	F	83	Total	C	N	O	S	0	0
			670	422	124	122	2		

- Molecule 6 is a protein called Acyl carrier protein, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	G	85	Total	C	N	O	S	0	0
			672	434	99	134	5		

- Molecule 7 is a protein called NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 5.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	H	112	Total	C	N	O	S	0	0
			922	593	157	169	3		

- Molecule 8 is a protein called NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 7.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	I	95	Total	C	N	O	S	0	0
			769	483	146	138	2		

- Molecule 9 is a protein called NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 9, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	J	337	Total	C	N	O	S	0	0
			2712	1759	482	463	8		

- Molecule 10 is a protein called NADH dehydrogenase [ubiquinone] flavoprotein 3, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
10	K	33	Total	C	N	O	S	0	0
			274	173	47	53	1		

- Molecule 11 is a protein called NADH dehydrogenase [ubiquinone] iron-sulfur protein 4, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
11	L	118	Total	C	N	O	S	0	0
			964	608	173	179	4		

- Molecule 12 is a protein called NADH-ubiquinone oxidoreductase 75 kDa subunit, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
12	M	687	Total	C	N	O	S	0	0
			5274	3310	917	1009	38		

- Molecule 13 is a protein called NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 12.

Mol	Chain	Residues	Atoms					AltConf	Trace
13	N	143	Total	C	N	O	S	0	0
			1195	770	210	212	3		

- Molecule 14 is a protein called NADH dehydrogenase [ubiquinone] flavoprotein 2, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
14	O	212	Total	C	N	O	S	0	0
			1643	1047	276	310	10		

- Molecule 15 is a protein called NADH dehydrogenase [ubiquinone] iron-sulfur protein 3, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
15	P	208	Total	C	N	O	S	0	0
			1730	1117	297	313	3		

- Molecule 16 is a protein called NADH dehydrogenase [ubiquinone] iron-sulfur protein 2, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
16	Q	385	Total	C	N	O	S	0	0
			3087	1971	536	558	22		

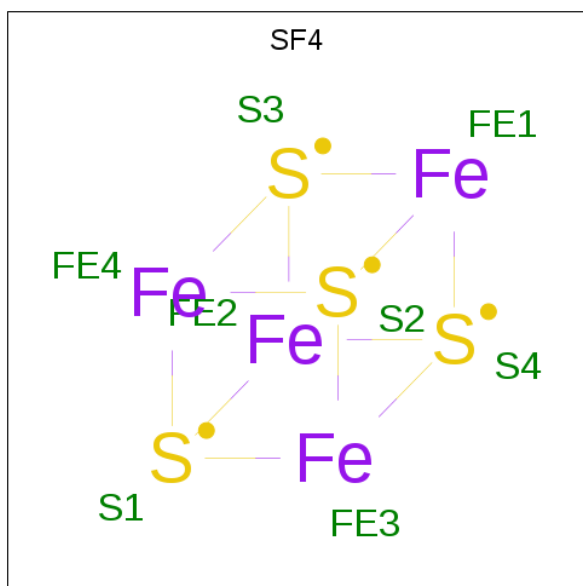
- Molecule 17 is a protein called NADH dehydrogenase [ubiquinone] iron-sulfur protein 6, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
17	T	95	Total	C	N	O	S	0	0
			742	459	138	142	3		

- Molecule 18 is a protein called NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 13.

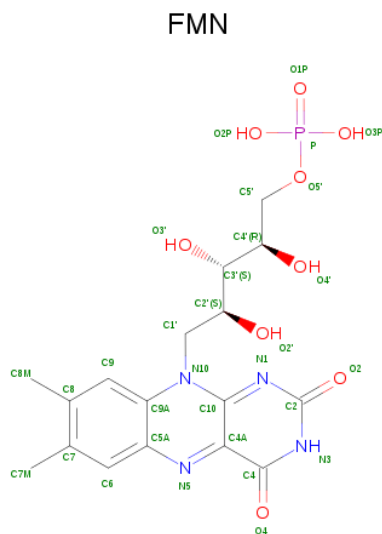
Mol	Chain	Residues	Atoms					AltConf	Trace
18	W	22	Total	C	N	O	S	0	0
			179	113	35	30	1		

- Molecule 19 is IRON/SULFUR CLUSTER (three-letter code: SF4) (formula:  $\text{Fe}_4\text{S}_4$ ).



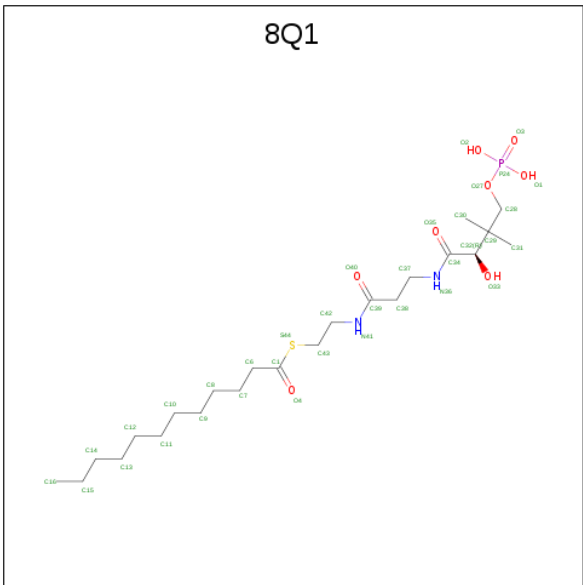
Mol	Chain	Residues	Atoms			AltConf
19	A	1	Total	Fe	S	0
			8	4	4	
19	B	1	Total	Fe	S	0
			16	8	8	
19	B	1	Total	Fe	S	0
			16	8	8	
19	C	1	Total	Fe	S	0
			8	4	4	
19	M	1	Total	Fe	S	0
			16	8	8	
19	M	1	Total	Fe	S	0
			16	8	8	

- Molecule 20 is FLAVIN MONONUCLEOTIDE (three-letter code: FMN) (formula:  $\text{C}_{17}\text{H}_{21}\text{N}_4\text{O}_9\text{P}$ ).



Mol	Chain	Residues	Atoms					AltConf
20	A	1	Total	C	N	O	P	0
			31	17	4	9	1	

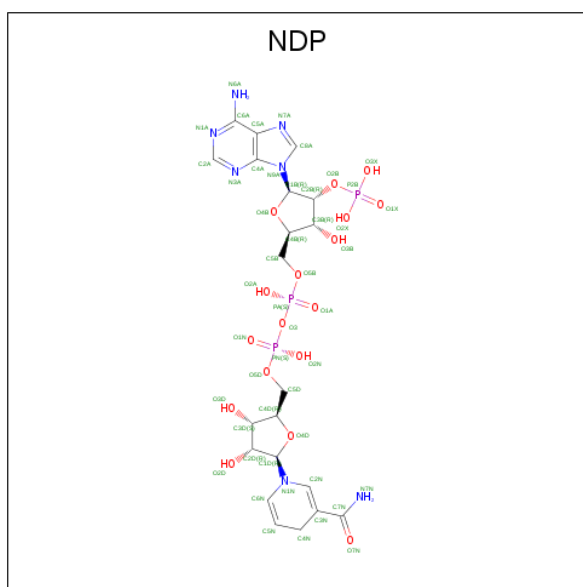
- Molecule 21 is S-[2-({N-[(2R)-2-hydroxy-3,3-dimethyl-4-(phosphonooxy)butanoyl]-beta-alanyl}amino)ethyl] dodecanethioate (three-letter code: 8Q1) (formula:  $C_{23}H_{45}N_2O_8PS$ ).



Mol	Chain	Residues	Atoms						AltConf
21	E	1	Total 35	C 23	N 2	O 8	P 1	S 1	0

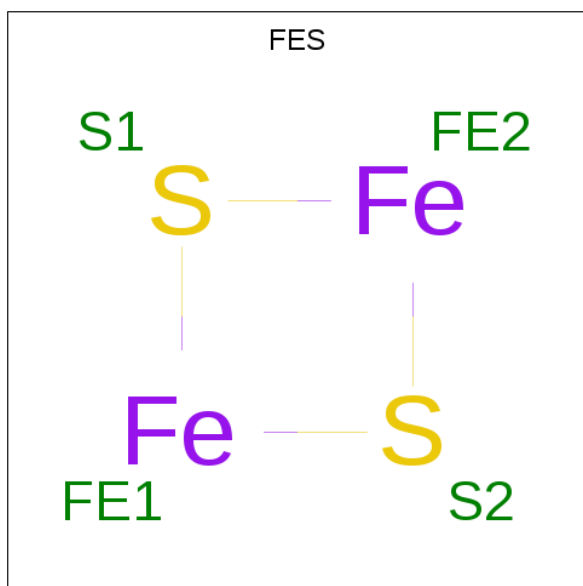
- Molecule 22 is NADPH DIHYDRO-NICOTINAMIDE-ADENINE-DINUCLEOTIDE PHOSPHATE (three-letter code: NDP) (formula:  $C_{21}H_{30}N_7O_{17}P_3$ ).





Mol	Chain	Residues	Atoms					AltConf
22	J	1	Total	C	N	O	P	0
			48	21	7	17	3	

- Molecule 23 is FE2/S2 (INORGANIC) CLUSTER (three-letter code: FES) (formula:  $\text{Fe}_2\text{S}_2$ ).

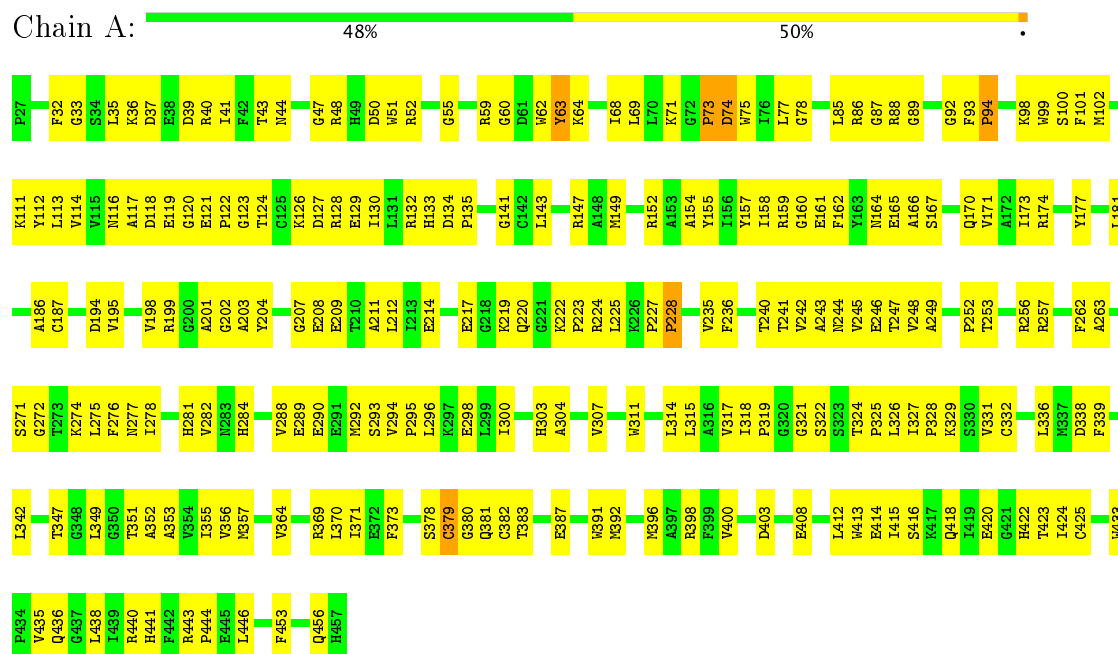


Mol	Chain	Residues	Atoms			AltConf
23	M	1	Total 4	Fe 2	S 2	0
23	O	1	Total 4	Fe 2	S 2	0

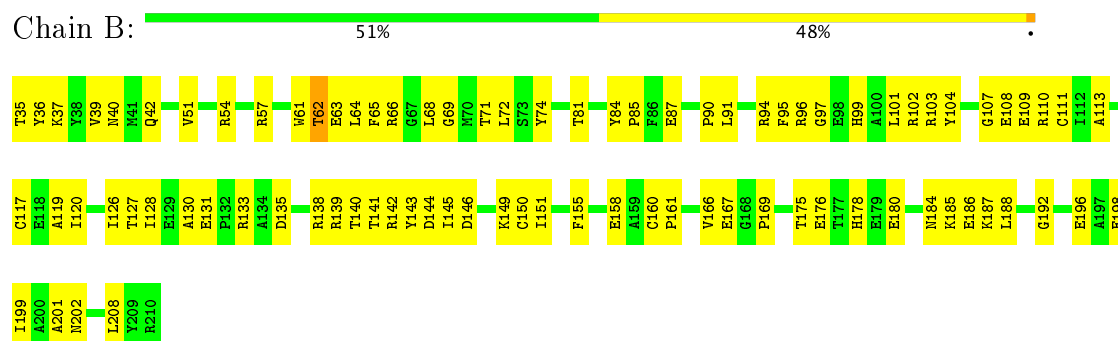
### 3 Residue-property plots

These plots are drawn for all protein, RNA and DNA 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.

- Molecule 1: NADH dehydrogenase [ubiquinone] flavoprotein 1, mitochondrial

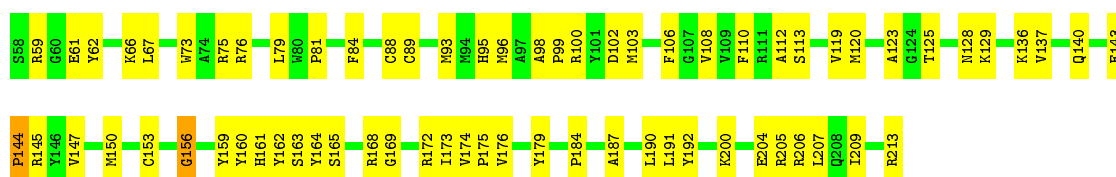


- Molecule 2: NADH dehydrogenase [ubiquinone] iron-sulfur protein 8, mitochondrial



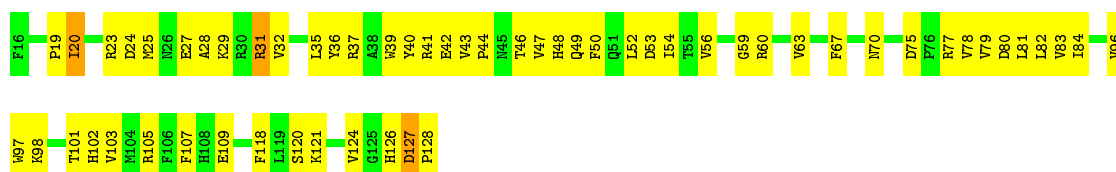
- Molecule 3: NADH dehydrogenase [ubiquinone] iron-sulfur protein 7, mitochondrial





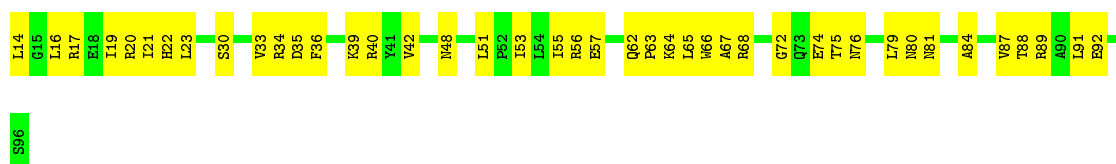
- Molecule 4: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 6

Chain E: 49% 49%



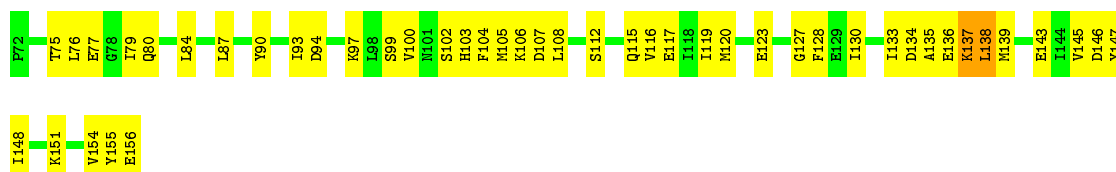
- Molecule 5: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 2

Chain F: 49% 51%



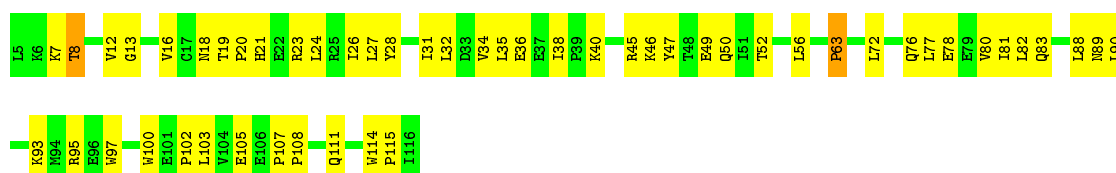
- Molecule 6: Acyl carrier protein, mitochondrial

Chain G: 46% 52%



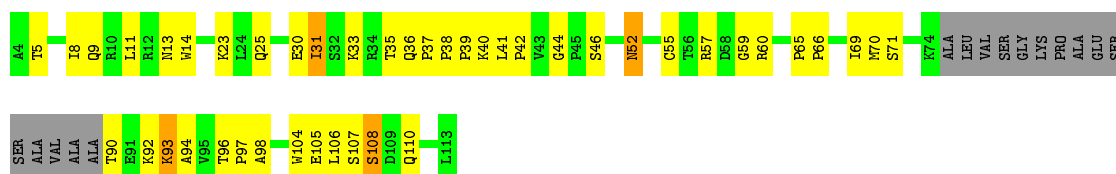
- Molecule 7: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 5

Chain H: 54% 45%



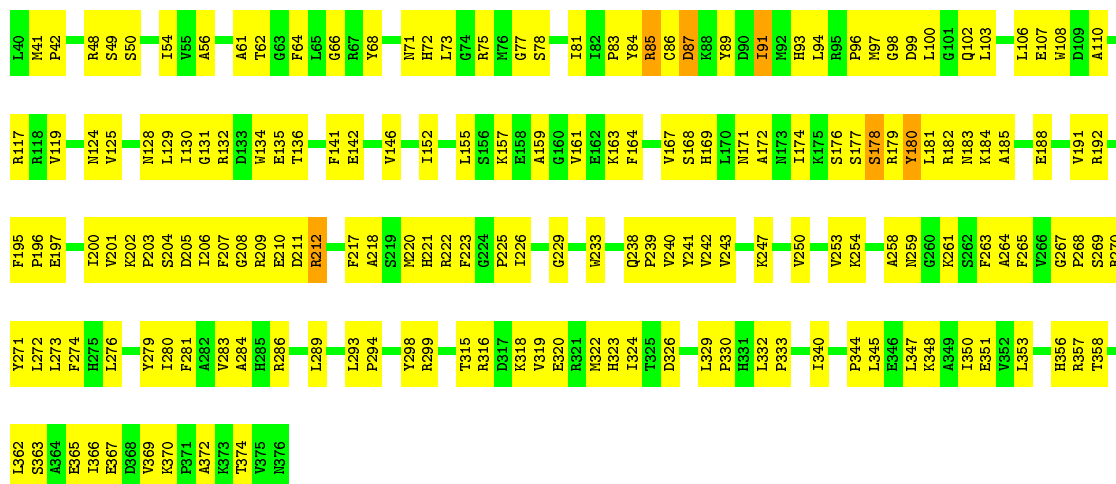
- Molecule 8: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 7

Chain I: 46% 36% 14%



- Molecule 9: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 9, mitochondrial

Chain J: 48% 50%



- Molecule 10: NADH dehydrogenase [ubiquinone] flavoprotein 3, mitochondrial

Chain K: 45% 45% 9%



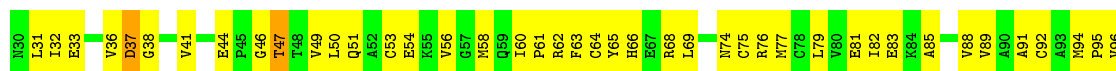
- Molecule 11: NADH dehydrogenase [ubiquinone] iron-sulfur protein 4, mitochondrial

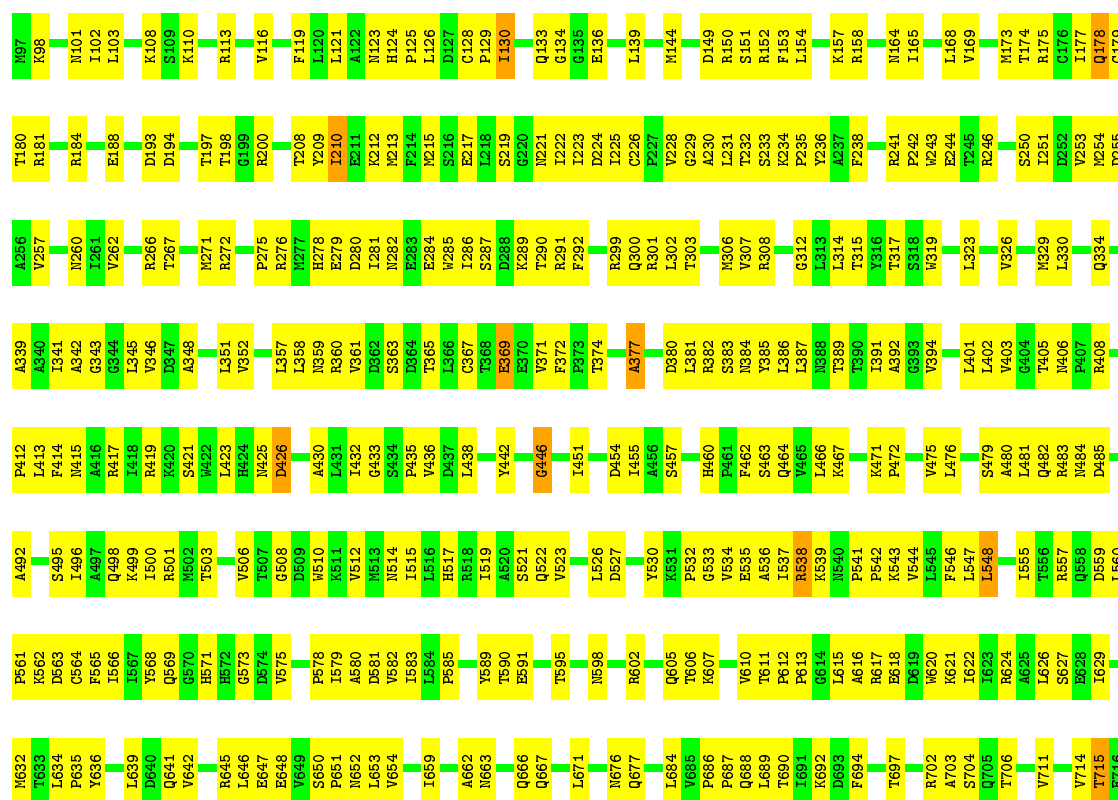
Chain L: 43% 56%



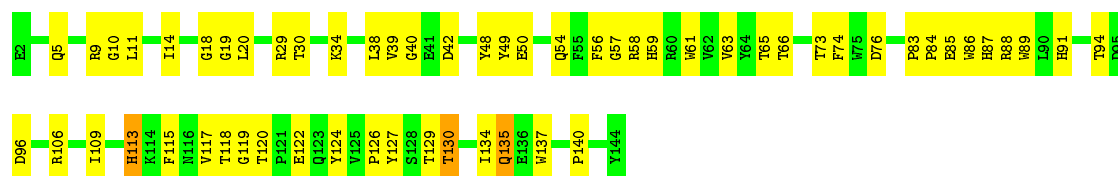
- Molecule 12: NADH-ubiquinone oxidoreductase 75 kDa subunit, mitochondrial

Chain M: 47% 52%

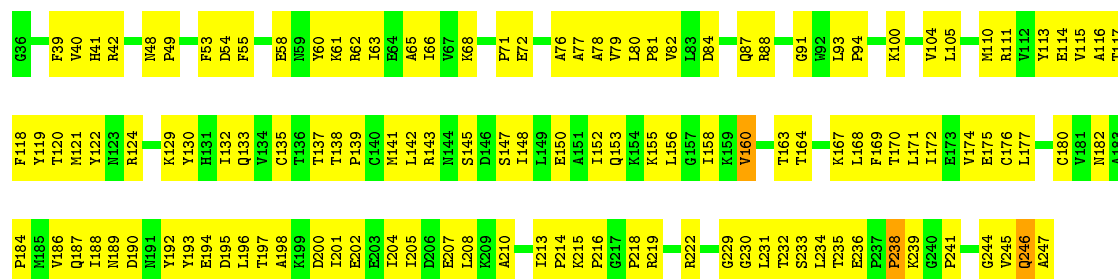




- Molecule 13: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 12

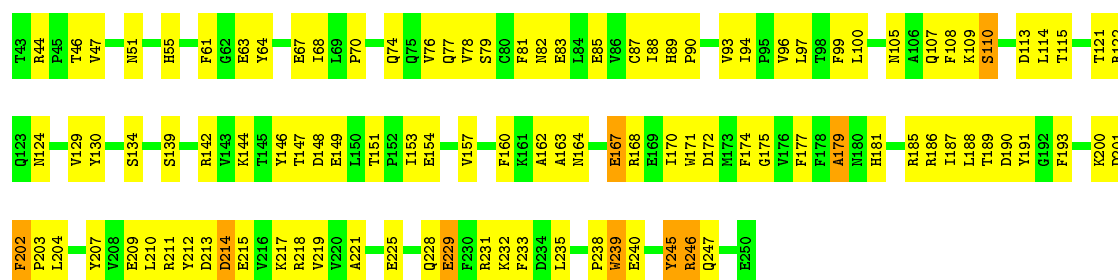


- Molecule 14: NADH dehydrogenase [ubiquinone] flavoprotein 2, mitochondrial

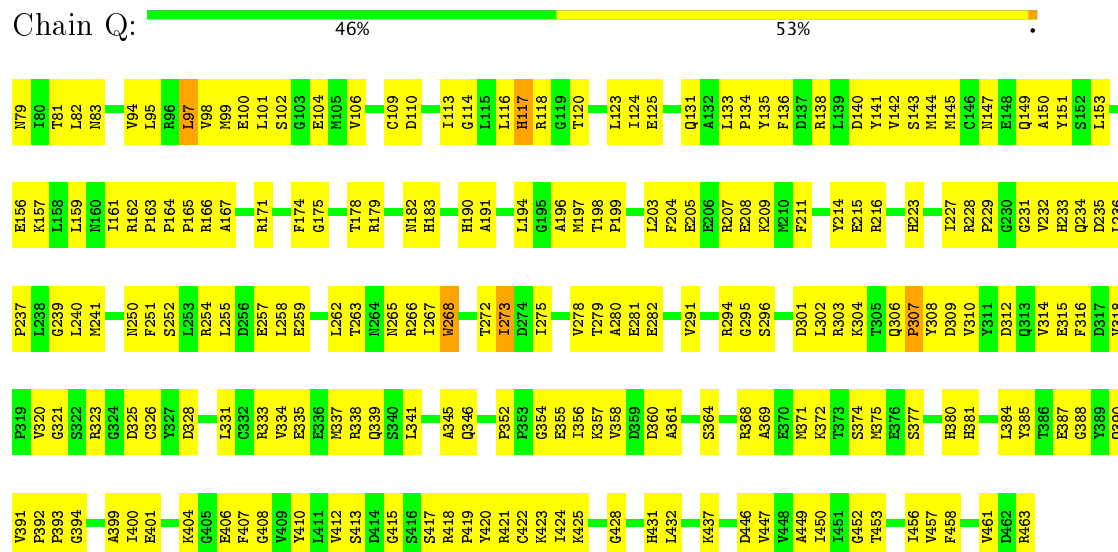


- Molecule 15: NADH dehydrogenase [ubiquinone] iron-sulfur protein 3, mitochondrial

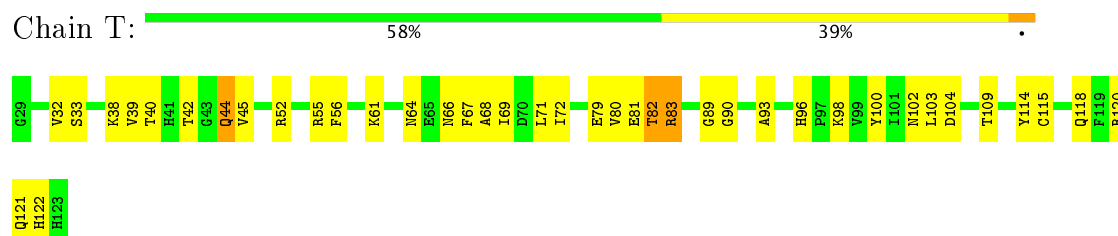




- Molecule 16: NADH dehydrogenase [ubiquinone] iron-sulfur protein 2, mitochondrial



- Molecule 17: NADH dehydrogenase [ubiquinone] iron-sulfur protein 6, mitochondrial



- Molecule 18: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 13



## 4 Experimental information

Property	Value	Source
Reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	167761	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	NONE	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ( $e^-/\text{\AA}^2$ )	1.25	Depositor
Minimum defocus (nm)	Not provided	Depositor
Maximum defocus (nm)	Not provided	Depositor
Magnification	Not provided	Depositor
Image detector	FEI FALCON II (4k x 4k)	Depositor

## 5 Model quality

### 5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: FMN, 8Q1, SF4, FES, NDP

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	$\# Z  > 2$	RMSZ	$\# Z  > 2$
1	A	0.30	0/3398	0.49	0/4590
10	K	0.27	0/282	0.47	0/381
11	L	0.33	0/987	0.53	0/1331
12	M	0.32	0/5362	0.53	0/7266
13	N	0.37	0/1236	0.55	0/1681
14	O	0.29	0/1682	0.51	0/2289
15	P	0.38	0/1780	0.59	0/2424
16	Q	0.44	0/3161	0.60	1/4275 (0.0%)
17	T	0.31	0/755	0.47	0/1017
18	W	0.34	0/185	0.65	0/249
2	B	0.50	0/1452	0.57	0/1964
3	C	0.58	0/1280	0.57	0/1732
4	E	0.34	0/993	0.53	0/1335
5	F	0.28	0/682	0.52	0/922
6	G	0.33	0/684	0.53	0/926
7	H	0.33	0/941	0.59	0/1275
8	I	0.29	0/788	0.54	0/1066
9	J	0.34	0/2785	0.52	0/3771
All	All	0.36	0/28433	0.54	1/38494 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
16	Q	97	LEU	CA-CB-CG	5.67	128.34	115.30

There are no chirality outliers.

There are no planarity outliers.



## 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	A	3322	0	3289	209	0
2	B	1420	0	1371	99	0
3	C	1249	0	1253	65	0
4	E	968	0	982	62	0
5	F	670	0	679	37	0
6	G	672	0	650	32	0
7	H	922	0	950	58	0
8	I	769	0	788	45	0
9	J	2712	0	2757	227	0
10	K	274	0	257	24	0
11	L	964	0	962	65	0
12	M	5274	0	5312	329	0
13	N	1195	0	1155	47	0
14	O	1643	0	1646	111	0
15	P	1730	0	1685	114	0
16	Q	3087	0	3069	223	0
17	T	742	0	723	37	0
18	W	179	0	179	11	0
19	A	8	0	0	6	0
19	B	16	0	0	3	0
19	C	8	0	0	1	0
19	M	16	0	0	4	0
20	A	31	0	19	17	0
21	E	35	0	0	4	0
22	J	48	0	26	26	0
23	M	4	0	0	1	0
23	O	4	0	0	2	0
All	All	27962	0	27752	1536	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 28.

All (1536) 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:J:130:ILE:HG23	22:J:401:NDP:C8A	1.45	1.46
12:M:134:GLY:HA2	19:M:801:SF4:S3	1.57	1.42
16:Q:262:LEU:HD22	16:Q:268:TRP:CD1	1.64	1.32
9:J:206:ILE:HA	9:J:240:VAL:O	1.35	1.26
9:J:171:ASN:O	9:J:181:LEU:HD21	1.23	1.24
9:J:130:ILE:HG23	22:J:401:NDP:N7A	1.52	1.24
9:J:206:ILE:O	9:J:211:ASP:OD2	1.61	1.19
9:J:171:ASN:O	9:J:181:LEU:CD2	1.92	1.18
16:Q:268:TRP:CZ3	16:Q:272:THR:HG21	1.79	1.16
1:A:93:PHE:CE2	1:A:98:LYS:HD3	1.80	1.14
9:J:171:ASN:C	9:J:181:LEU:HD21	1.69	1.13
4:E:25:MET:HB3	4:E:29:LYS:CE	1.77	1.12
12:M:134:GLY:CA	19:M:801:SF4:S3	2.42	1.08
4:E:25:MET:HB3	4:E:29:LYS:HE3	1.32	1.07
9:J:130:ILE:HG23	22:J:401:NDP:H8A	1.28	1.06
9:J:221:HIS:CE1	9:J:222:ARG:HG3	1.91	1.04
4:E:25:MET:CB	4:E:29:LYS:HE3	1.89	1.02
9:J:130:ILE:CG2	22:J:401:NDP:N7A	2.24	1.01
9:J:141:PHE:CE2	9:J:180:TYR:HA	1.98	0.99
9:J:130:ILE:CG2	22:J:401:NDP:C8A	2.41	0.99
9:J:176:SER:HA	9:J:182:ARG:HH21	1.24	0.99
1:A:116:ASN:ND2	20:A:502:FMN:C8	2.25	0.98
9:J:171:ASN:HB3	9:J:181:LEU:HD11	1.46	0.97
3:C:204:GLU:OE2	3:C:206:ARG:NH1	1.98	0.97
9:J:206:ILE:HB	9:J:242:VAL:HG22	1.47	0.96
16:Q:262:LEU:HD22	16:Q:268:TRP:HD1	1.23	0.95
1:A:116:ASN:HD22	20:A:502:FMN:C8M	1.78	0.95
14:O:177:LEU:N	23:O:301:FES:S1	2.39	0.94
1:A:116:ASN:HD22	20:A:502:FMN:C8	1.82	0.91
4:E:25:MET:O	4:E:29:LYS:HG3	1.69	0.91
7:H:45:ARG:NH1	7:H:49:GLU:OE2	2.04	0.91
1:A:93:PHE:HE2	1:A:98:LYS:HD3	1.17	0.90
9:J:169:HIS:HD2	22:J:401:NDP:H5N	1.34	0.90
9:J:141:PHE:CZ	9:J:180:TYR:HA	2.07	0.90
15:P:134:SER:HG	15:P:139:SER:HG	1.19	0.90
9:J:171:ASN:CB	9:J:181:LEU:HD11	2.02	0.89
9:J:83:PRO:HB2	9:J:108:TRP:NE1	1.88	0.89
9:J:206:ILE:HB	9:J:242:VAL:CG2	2.04	0.88
16:Q:400:ILE:HB	16:Q:407:PHE:HB3	1.54	0.87
16:Q:194:LEU:HD12	16:Q:268:TRP:CZ2	2.09	0.87
9:J:169:HIS:HD2	22:J:401:NDP:C5N	1.87	0.86
7:H:36:GLU:HA	7:H:45:ARG:HH21	1.38	0.86

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:M:130:ILE:HD13	17:T:114:TYR:CE1	2.11	0.86
2:B:81:THR:O	13:N:58:ARG:NH2	2.09	0.86
1:A:126:LYS:HB3	1:A:277:ASN:HD21	1.40	0.86
9:J:212:ARG:HH11	9:J:212:ARG:HG2	1.37	0.85
9:J:206:ILE:CA	9:J:240:VAL:O	2.24	0.85
4:E:25:MET:HB3	4:E:29:LYS:HE2	1.55	0.84
3:C:100:ARG:HH21	16:Q:208:GLU:HB3	1.39	0.84
16:Q:273:ILE:CD1	16:Q:325:ASP:OD2	2.25	0.84
9:J:176:SER:CA	9:J:182:ARG:HH21	1.88	0.84
7:H:102:PRO:HA	15:P:70:PRO:HB2	1.57	0.84
1:A:244:ASN:N	20:A:502:FMN:O2P	2.09	0.84
4:E:70:ASN:OD1	21:E:201:8Q1:O4	1.95	0.83
9:J:85:ARG:HH11	9:J:85:ARG:HG3	1.41	0.83
12:M:299:ARG:HG2	12:M:300:GLN:H	1.41	0.83
3:C:156:GLY:HA2	3:C:169:GLY:HA2	1.62	0.82
9:J:169:HIS:CD2	22:J:401:NDP:H5N	2.15	0.82
4:E:101:THR:HG22	15:P:218:ARG:HB2	1.60	0.81
9:J:226:ILE:HD12	9:J:289:LEU:H	1.45	0.81
5:F:57:GLU:HB3	12:M:662:ALA:H	1.45	0.80
16:Q:273:ILE:HD13	16:Q:325:ASP:OD2	1.81	0.80
3:C:120:MET:HB3	3:C:147:VAL:HG12	1.64	0.80
9:J:177:SER:HB2	9:J:320:GLU:HB3	1.64	0.79
9:J:207:PHE:HA	9:J:211:ASP:OD2	1.82	0.79
9:J:217:PHE:HZ	9:J:322:MET:CE	1.95	0.79
12:M:223:ILE:HD13	12:M:233:SER:HB3	1.64	0.79
9:J:270:ARG:NH2	9:J:326:ASP:O	2.16	0.79
2:B:133:ARG:HG3	2:B:135:ASP:H	1.47	0.79
16:Q:294:ARG:O	16:Q:321:GLY:N	2.11	0.78
3:C:59:ARG:HH22	3:C:61:GLU:HB3	1.48	0.78
9:J:206:ILE:HG12	22:J:401:NDP:N7N	1.99	0.78
16:Q:140:ASP:OD2	16:Q:143:SER:OG	2.02	0.78
9:J:176:SER:HA	9:J:182:ARG:NH2	1.99	0.78
3:C:59:ARG:NH2	3:C:61:GLU:HB3	1.98	0.78
12:M:647:GLU:HB2	12:M:654:VAL:HG11	1.65	0.78
9:J:86:CYS:O	9:J:87:ASP:HB2	1.83	0.77
16:Q:268:TRP:CZ3	16:Q:272:THR:CG2	2.66	0.77
8:I:33:LYS:NZ	8:I:35:THR:O	2.17	0.77
9:J:130:ILE:CG2	22:J:401:NDP:H8A	2.10	0.77
5:F:63:PRO:HB2	5:F:79:LEU:HB2	1.65	0.77
16:Q:194:LEU:CD1	16:Q:268:TRP:CZ2	2.67	0.77
15:P:187:ILE:HG22	15:P:188:LEU:HG	1.66	0.77

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
16:Q:125:GLU:HA	16:Q:419:PRO:HG2	1.67	0.77
9:J:217:PHE:CB	9:J:280:ILE:HD13	2.15	0.77
3:C:143:GLU:OE1	9:J:89:TYR:OH	2.03	0.76
1:A:64:LYS:NZ	14:O:244:GLY:O	2.18	0.76
12:M:68:ARG:HD2	12:M:285:TRP:HE1	1.48	0.76
5:F:42:VAL:HG21	12:M:671:LEU:HD12	1.66	0.76
15:P:85:GLU:OE2	15:P:142:ARG:NH1	2.19	0.76
7:H:50:GLN:HE22	8:I:93:LYS:HA	1.50	0.76
9:J:217:PHE:HZ	9:J:322:MET:HE2	1.50	0.76
4:E:37:ARG:NH2	6:G:123:GLU:OE2	2.19	0.75
14:O:182:ASN:ND2	14:O:194:GLU:OE1	2.19	0.75
4:E:79:VAL:HG22	21:E:201:8Q1:C38	2.16	0.75
1:A:174:ARG:HG3	10:K:91:LEU:HD21	1.69	0.75
9:J:221:HIS:ND1	9:J:222:ARG:N	2.35	0.75
11:L:75:ARG:NH1	11:L:119:ASP:OD2	2.16	0.75
12:M:406:ASN:HB2	12:M:438:LEU:HD21	1.68	0.75
12:M:54:GLU:OE2	12:M:62:ARG:NH2	2.19	0.75
16:Q:118:ARG:NH2	16:Q:138:ARG:O	2.20	0.74
16:Q:384:LEU:HA	16:Q:388:GLY:HA2	1.67	0.74
12:M:128:CYS:HB2	12:M:129:PRO:HD3	1.68	0.74
9:J:77:GLY:O	9:J:102:GLN:NE2	2.19	0.74
9:J:54:ILE:HB	9:J:78:SER:HB2	1.68	0.74
3:C:88:CYS:SG	16:Q:223:HIS:NE2	2.60	0.74
6:G:79:ILE:HG21	6:G:148:ILE:HG21	1.70	0.74
12:M:543:LYS:HG3	12:M:565:PHE:HD2	1.51	0.74
12:M:50:LEU:HB2	12:M:92:CYS:HA	1.68	0.74
12:M:506:VAL:HG12	12:M:508:GLY:H	1.52	0.74
9:J:174:ILE:HG13	9:J:182:ARG:HG3	1.70	0.73
12:M:128:CYS:HB2	12:M:129:PRO:CD	2.18	0.73
12:M:307:VAL:HG13	12:M:582:VAL:HG22	1.69	0.73
1:A:98:LYS:HD2	1:A:101:PHE:CE2	2.24	0.73
9:J:201:VAL:HG12	9:J:203:PRO:HD3	1.71	0.73
16:Q:345:ALA:HB2	18:W:19:ILE:HD11	1.70	0.73
15:P:233:PHE:O	16:Q:418:ARG:NH2	2.22	0.73
3:C:67:LEU:HD22	3:C:207:LEU:HD21	1.70	0.73
9:J:132:ARG:NH2	22:J:401:NDP:C2B	2.52	0.73
16:Q:333:ARG:NH2	16:Q:453:THR:O	2.22	0.73
12:M:58:MET:SD	15:P:246:ARG:NH1	2.55	0.73
9:J:132:ARG:NH2	22:J:401:NDP:O2B	2.22	0.73
14:O:116:ALA:O	14:O:124:ARG:NH1	2.22	0.73
1:A:158:ILE:HG21	1:A:166:ALA:HB2	1.70	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
16:Q:232:VAL:HG12	16:Q:234:GLN:H	1.54	0.72
16:Q:268:TRP:HZ3	16:Q:272:THR:HG21	1.52	0.72
16:Q:282:GLU:OE2	16:Q:437:LYS:NZ	2.22	0.72
8:I:106:LEU:O	8:I:108:SER:N	2.19	0.72
1:A:219:LYS:HA	11:L:174:THR:HG22	1.71	0.72
11:L:92:ASN:HB3	15:P:238:PRO:HA	1.70	0.72
12:M:198:THR:HG22	14:O:39:PHE:HB3	1.70	0.72
17:T:83:ARG:NH1	17:T:102:ASN:OD1	2.22	0.72
12:M:121:LEU:HD21	12:M:139:LEU:HD21	1.72	0.72
3:C:143:GLU:OE2	3:C:145:ARG:NH2	2.23	0.72
12:M:543:LYS:NZ	12:M:563:ASP:OD2	2.23	0.72
5:F:17:ARG:HB2	5:F:68:ARG:HE	1.54	0.72
9:J:212:ARG:NH2	22:J:401:NDP:O2N	2.22	0.72
14:O:129:LYS:H	14:O:168:LEU:HA	1.53	0.72
3:C:129:LYS:NZ	16:Q:113:ILE:O	2.23	0.72
16:Q:281:GLU:N	16:Q:281:GLU:OE1	2.22	0.72
1:A:381:GLN:HG2	19:A:501:SF4:S2	2.29	0.72
5:F:68:ARG:NH1	12:M:359:ASN:OD1	2.23	0.72
9:J:83:PRO:HB2	9:J:108:TRP:HE1	1.53	0.72
16:Q:241:MET:HG3	18:W:11:PRO:HB2	1.72	0.72
1:A:391:TRP:HH2	12:M:153:PHE:HA	1.55	0.71
12:M:63:PHE:O	12:M:181:ARG:NH2	2.23	0.71
12:M:566:ILE:HG13	12:M:580:ALA:HA	1.72	0.71
15:P:55:HIS:NE2	15:P:78:VAL:O	2.24	0.71
16:Q:95:LEU:HD13	16:Q:97:LEU:HD23	1.73	0.71
1:A:116:ASN:ND2	20:A:502:FMN:C8M	2.52	0.71
1:A:124:THR:HG23	1:A:126:LYS:HG2	1.72	0.71
12:M:557:ARG:NH1	12:M:579:ILE:O	2.24	0.71
16:Q:432:LEU:HD12	16:Q:461:VAL:HG11	1.73	0.71
1:A:327:ILE:HG23	1:A:331:VAL:HG13	1.72	0.71
9:J:350:ILE:HD13	9:J:366:ILE:HG12	1.72	0.71
11:L:137:PHE:O	11:L:141:ASN:ND2	2.15	0.71
12:M:374:THR:HB	12:M:377:ALA:HA	1.72	0.71
16:Q:262:LEU:CD2	16:Q:268:TRP:CD1	2.60	0.71
11:L:82:PRO:HG3	11:L:98:LYS:HE3	1.72	0.71
14:O:187:GLN:HE21	14:O:190:ASP:HA	1.56	0.70
1:A:158:ILE:HB	1:A:199:ARG:HG2	1.73	0.70
9:J:176:SER:O	9:J:182:ARG:NH2	2.24	0.70
9:J:279:TYR:HB2	9:J:372:ALA:HB2	1.71	0.70
1:A:381:GLN:NE2	19:A:501:SF4:S3	2.63	0.70
4:E:70:ASN:O	21:E:201:8Q1:O40	2.10	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
15:P:46:THR:O	16:Q:162:ARG:N	2.16	0.70
9:J:221:HIS:CE1	9:J:222:ARG:CG	2.72	0.70
12:M:144:MET:SD	16:Q:380:HIS:ND1	2.63	0.70
1:A:211:ALA:HB2	1:A:223:PRO:HG3	1.74	0.70
7:H:12:VAL:HG13	16:Q:280:ALA:H	1.57	0.69
9:J:85:ARG:HD2	9:J:85:ARG:O	1.92	0.69
12:M:299:ARG:HD3	12:M:703:ALA:HB1	1.74	0.69
1:A:116:ASN:O	1:A:245:VAL:HG23	1.91	0.69
9:J:210:GLU:HG2	9:J:210:GLU:O	1.92	0.69
5:F:39:LYS:HG3	5:F:40:ARG:H	1.56	0.69
9:J:233:TRP:HA	9:J:272:LEU:HD21	1.74	0.69
12:M:225:ILE:HD12	12:M:285:TRP:HH2	1.57	0.69
12:M:472:PRO:O	12:M:510:TRP:NE1	2.25	0.69
12:M:613:PRO:HB2	13:N:134:ILE:HD13	1.73	0.69
1:A:383:THR:HG22	12:M:75:CYS:HA	1.72	0.69
4:E:25:MET:O	4:E:29:LYS:CG	2.38	0.69
15:P:93:VAL:HB	15:P:154:GLU:HB2	1.72	0.69
7:H:12:VAL:HG13	16:Q:280:ALA:N	2.07	0.69
1:A:60:GLY:HA3	14:O:241:PRO:HB3	1.75	0.69
12:M:595:THR:HA	12:M:605:GLN:HA	1.74	0.69
4:E:25:MET:C	4:E:29:LYS:HG3	2.13	0.69
2:B:184:ASN:HD21	13:N:127:TYR:H	1.39	0.69
12:M:381:LEU:O	12:M:383:SER:N	2.24	0.69
16:Q:262:LEU:HD13	16:Q:268:TRP:NE1	2.08	0.68
3:C:159:TYR:HE1	16:Q:135:TYR:CZ	2.12	0.68
14:O:137:THR:HG21	14:O:176:CYS:HB2	1.74	0.68
16:Q:190:HIS:HD2	16:Q:452:GLY:HA3	1.58	0.68
1:A:318:ILE:HG22	1:A:326:LEU:HA	1.74	0.68
2:B:126:ILE:O	15:P:231:ARG:NH2	2.23	0.68
12:M:466:LEU:HD23	12:M:500:ILE:HD11	1.75	0.68
9:J:202:LYS:HB2	9:J:264:ALA:HA	1.75	0.68
1:A:379:CYS:HA	12:M:200:ARG:HB2	1.74	0.68
15:P:157:VAL:HG21	15:P:181:HIS:HD2	1.59	0.68
16:Q:450:ILE:O	16:Q:453:THR:OG1	2.07	0.68
9:J:171:ASN:O	9:J:181:LEU:CG	2.41	0.68
12:M:476:LEU:HB3	12:M:515:ILE:HG22	1.74	0.68
17:T:79:GLU:HG2	17:T:120:ARG:HB3	1.76	0.68
9:J:247:LYS:HD2	9:J:340:ILE:HD12	1.74	0.68
12:M:173:MET:O	12:M:175:ARG:N	2.24	0.68
1:A:381:GLN:HG3	1:A:382:CYS:H	1.59	0.68
12:M:500:ILE:O	12:M:503:THR:OG1	2.12	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:G:105:MET:HG3	6:G:106:LYS:HG3	1.76	0.67
2:B:120:ILE:HD11	16:Q:385:TYR:HB3	1.74	0.67
6:G:145:VAL:HA	6:G:148:ILE:HD12	1.77	0.67
9:J:203:PRO:HA	9:J:265:PHE:HB2	1.75	0.67
22:J:401:NDP:H1B	22:J:401:NDP:O2X	1.94	0.67
1:A:118:ASP:O	1:A:159:ARG:HD2	1.95	0.67
1:A:295:PRO:HG2	1:A:298:GLU:HB2	1.77	0.67
20:A:502:FMN:O4'	20:A:502:FMN:H9	1.94	0.67
2:B:119:ALA:HA	15:P:233:PHE:HE2	1.60	0.67
4:E:25:MET:HB2	4:E:29:LYS:HE3	1.75	0.67
3:C:128:ASN:ND2	3:C:164:TYR:O	2.24	0.67
12:M:194:ASP:O	12:M:208:THR:OG1	2.10	0.67
1:A:89:GLY:HA2	1:A:244:ASN:HD22	1.59	0.67
3:C:136:LYS:O	3:C:140:GLN:HG3	1.94	0.67
14:O:133:GLN:HB2	14:O:174:VAL:HG21	1.75	0.67
1:A:43:THR:HG21	14:O:239:LYS:HB2	1.76	0.67
7:H:114:TRP:HE1	16:Q:394:GLY:HA2	1.59	0.67
11:L:58:LYS:NZ	11:L:139:GLU:OE1	2.27	0.67
7:H:32:LEU:HD23	7:H:35:LEU:HD21	1.77	0.67
10:K:100:SER:HA	14:O:72:GLU:HB3	1.77	0.66
2:B:111:CYS:O	2:B:139:ARG:NH2	2.28	0.66
16:Q:338:ARG:HH22	18:W:23:ARG:HB3	1.58	0.66
9:J:258:ALA:HA	9:J:261:LYS:HD2	1.78	0.66
10:K:99:PRO:HG2	14:O:71:PRO:HB3	1.76	0.66
1:A:379:CYS:SG	1:A:380:GLY:N	2.68	0.66
4:E:107:PHE:HB3	4:E:109:GLU:HG3	1.78	0.66
12:M:254:MET:HB2	12:M:290:THR:HG22	1.78	0.66
16:Q:251:PHE:HB2	16:Q:254:ARG:HH21	1.59	0.66
12:M:180:THR:OG1	12:M:184:ARG:NH1	2.29	0.66
1:A:116:ASN:ND2	20:A:502:FMN:C9	2.59	0.66
12:M:300:GLN:HB2	13:N:137:TRP:HA	1.77	0.66
1:A:74:ASP:O	1:A:78:GLY:N	2.27	0.66
3:C:125:THR:HG21	16:Q:118:ARG:HG2	1.76	0.66
14:O:54:ASP:OD1	14:O:60:TYR:OH	2.11	0.66
7:H:12:VAL:HG11	16:Q:278:VAL:O	1.96	0.65
1:A:214:GLU:OE2	1:A:224:ARG:NH1	2.24	0.65
3:C:161:HIS:O	3:C:168:ARG:NH2	2.28	0.65
7:H:72:LEU:HD22	7:H:77:LEU:HD13	1.78	0.65
11:L:81:VAL:HG11	11:L:150:ARG:HA	1.78	0.65
9:J:132:ARG:NH2	22:J:401:NDP:H2B	2.11	0.65
9:J:205:ASP:HB2	9:J:239:PRO:HA	1.79	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:J:48:ARG:NH1	9:J:98:GLY:O	2.29	0.65
5:F:56:ARG:NH2	12:M:527:ASP:O	2.29	0.65
12:M:65:TYR:O	12:M:181:ARG:NH2	2.29	0.65
1:A:424:ILE:HG22	19:A:501:SF4:S4	2.36	0.65
4:E:23:ARG:N	4:E:27:GLU:OE1	2.24	0.65
17:T:40:THR:OG1	17:T:42:THR:O	2.14	0.65
1:A:364:VAL:HG12	1:A:400:VAL:HG12	1.78	0.65
12:M:36:VAL:O	12:M:38:GLY:N	2.29	0.65
10:K:81:THR:HB	14:O:88:ARG:HD2	1.78	0.65
1:A:398:ARG:NH1	1:A:408:GLU:OE1	2.25	0.64
11:L:89:SER:OG	15:P:239:TRP:NE1	2.26	0.64
8:I:66:PRO:HB3	15:P:79:SER:HB3	1.77	0.64
1:A:98:LYS:HD2	1:A:101:PHE:HE2	1.61	0.64
1:A:244:ASN:OD1	1:A:245:VAL:N	2.29	0.64
5:F:33:VAL:HG22	5:F:87:VAL:HG21	1.78	0.64
9:J:206:ILE:CB	9:J:242:VAL:HG22	2.25	0.64
11:L:111:LEU:HG	11:L:112:MET:HG2	1.80	0.64
17:T:39:VAL:HG12	17:T:45:VAL:HB	1.79	0.64
16:Q:171:ARG:HH21	16:Q:231:GLY:HA2	1.61	0.64
3:C:93:MET:HG2	3:C:110:PHE:HZ	1.62	0.64
12:M:169:VAL:HG12	12:M:223:ILE:HD11	1.79	0.64
2:B:51:VAL:HG22	2:B:54:ARG:HH11	1.62	0.64
1:A:414:GLU:OE1	12:M:152:ARG:NH1	2.30	0.64
16:Q:136:PHE:HB3	16:Q:147:ASN:HB3	1.79	0.64
16:Q:81:THR:HG22	16:Q:100:GLU:HG2	1.78	0.64
2:B:151:ILE:HG21	3:C:159:TYR:HD2	1.62	0.63
12:M:591:GLU:N	12:M:591:GLU:OE1	2.30	0.63
12:M:326:VAL:HG23	12:M:626:LEU:HD13	1.80	0.63
12:M:618:GLU:OE2	12:M:620:TRP:NE1	2.30	0.63
16:Q:145:MET:H	16:Q:178:THR:HG21	1.63	0.63
8:I:23:LYS:NZ	16:Q:252:SER:OG	2.31	0.63
1:A:85:LEU:HD21	1:A:247:THR:HG23	1.80	0.63
1:A:416:SER:HB3	1:A:436:GLN:HE21	1.63	0.63
14:O:87:GLN:O	14:O:91:GLY:N	2.22	0.63
6:G:120:MET:HA	6:G:123:GLU:HG2	1.78	0.63
12:M:467:LYS:HG3	12:M:503:THR:HB	1.80	0.63
12:M:692:LYS:HD2	12:M:715:THR:HG22	1.80	0.63
1:A:207:GLY:O	20:A:502:FMN:C5A	2.47	0.63
11:L:75:ARG:HH21	11:L:101:PHE:HB3	1.63	0.63
12:M:266:ARG:HG2	12:M:267:THR:HG23	1.79	0.63
1:A:391:TRP:CH2	12:M:153:PHE:HA	2.34	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:57:ARG:O	16:Q:266:ARG:NH2	2.30	0.63
1:A:116:ASN:HD22	20:A:502:FMN:HM83	1.63	0.62
14:O:245:VAL:O	14:O:247:ALA:N	2.31	0.62
10:K:82:TYR:HD2	14:O:62:ARG:HH12	1.46	0.62
2:B:99:HIS:NE2	19:B:302:SF4:S1	2.70	0.62
9:J:141:PHE:CZ	9:J:180:TYR:HD1	2.17	0.62
14:O:40:VAL:HG13	14:O:42:ARG:H	1.64	0.62
16:Q:357:LYS:HE3	16:Q:364:SER:HB2	1.81	0.62
16:Q:412:VAL:HB	16:Q:421:ARG:HB3	1.81	0.62
9:J:241:TYR:CE2	9:J:243:VAL:HB	2.35	0.62
14:O:158:ILE:HD11	14:O:164:THR:HB	1.81	0.62
16:Q:150:ALA:HB1	16:Q:400:ILE:HG13	1.80	0.62
16:Q:432:LEU:HG	16:Q:456:ILE:HD13	1.81	0.62
6:G:80:GLN:HE22	6:G:100:VAL:HG13	1.63	0.62
9:J:83:PRO:HB3	9:J:119:VAL:HG21	1.81	0.62
12:M:282:ASN:HA	12:M:413:LEU:HD23	1.81	0.62
1:A:325:PRO:HG3	1:A:433:TRP:HB3	1.81	0.62
9:J:83:PRO:HB2	9:J:108:TRP:CD1	2.33	0.62
10:K:98:GLN:HB3	14:O:71:PRO:HA	1.80	0.62
14:O:143:ARG:HB3	14:O:184:PRO:HD3	1.82	0.62
15:P:83:GLU:HB3	15:P:142:ARG:HH12	1.65	0.62
12:M:546:PHE:HB2	12:M:568:TYR:HA	1.81	0.62
1:A:282:VAL:HG21	1:A:304:ALA:HB1	1.83	0.61
6:G:76:LEU:HD21	6:G:155:TYR:HA	1.82	0.61
2:B:36:TYR:HB3	8:I:104:TRP:CE3	2.34	0.61
9:J:319:VAL:O	9:J:323:HIS:ND1	2.28	0.61
11:L:109:ASN:ND2	11:L:111:LEU:O	2.33	0.61
3:C:184:PRO:HD3	16:Q:223:HIS:HD2	1.65	0.61
1:A:88:ARG:O	1:A:244:ASN:ND2	2.32	0.61
7:H:89:ASN:O	7:H:93:LYS:HG2	2.00	0.61
12:M:387:LEU:HA	12:M:514:ASN:HB2	1.82	0.61
9:J:272:LEU:HD23	9:J:274:PHE:H	1.65	0.61
9:J:48:ARG:HH21	15:P:211:ARG:HD2	1.64	0.61
12:M:537:ILE:O	12:M:539:LYS:N	2.33	0.61
15:P:154:GLU:HA	15:P:179:ALA:HB2	1.81	0.61
16:Q:428:GLY:HA2	16:Q:431:HIS:HD2	1.66	0.61
12:M:534:VAL:HG12	12:M:536:ALA:H	1.66	0.61
12:M:627:SER:OG	12:M:632:MET:O	2.17	0.61
9:J:226:ILE:HD12	9:J:289:LEU:N	2.16	0.61
9:J:286:ARG:NH2	9:J:356:HIS:O	2.34	0.61
13:N:130:THR:N	17:T:44:GLN:OE1	2.34	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:M:177:ILE:HG13	12:M:179:CYS:SG	2.40	0.61
12:M:346:VAL:HB	12:M:548:LEU:HD13	1.82	0.61
13:N:29:ARG:NH2	13:N:65:THR:O	2.23	0.61
1:A:37:ASP:OD2	14:O:236:GLU:N	2.30	0.61
11:L:128:PHE:HA	15:P:121:THR:HG22	1.82	0.61
15:P:94:ILE:HG13	15:P:154:GLU:HB3	1.82	0.61
8:I:52:ASN:OD1	8:I:57:ARG:NE	2.34	0.60
14:O:137:THR:OG1	14:O:176:CYS:N	2.34	0.60
11:L:75:ARG:HH11	11:L:104:ARG:HE	1.49	0.60
12:M:385:TYR:OH	12:M:527:ASP:OD1	2.17	0.60
12:M:31:LEU:HD22	12:M:44:GLU:HA	1.83	0.60
1:A:164:ASN:ND2	14:O:190:ASP:O	2.34	0.60
1:A:339:PHE:HB3	1:A:349:LEU:HD13	1.81	0.60
12:M:352:VAL:HG21	12:M:646:LEU:HD21	1.82	0.60
2:B:103:ARG:NH2	17:T:66:ASN:O	2.35	0.60
2:B:64:LEU:O	2:B:68:LEU:N	2.30	0.60
9:J:188:GLU:HG3	9:J:200:ILE:HG21	1.83	0.60
1:A:161:GLU:O	14:O:192:TYR:OH	2.18	0.60
1:A:203:ALA:HA	12:M:200:ARG:HH12	1.65	0.60
4:E:37:ARG:HH21	4:E:41:ARG:NH2	2.00	0.60
7:H:77:LEU:O	7:H:80:VAL:HG12	2.01	0.60
12:M:483:ARG:O	12:M:485:ASP:N	2.34	0.60
15:P:212:TYR:HA	15:P:219:VAL:HA	1.83	0.60
3:C:205:ARG:HG3	3:C:205:ARG:O	2.02	0.60
4:E:97:TRP:HH2	15:P:185:ARG:HH11	1.49	0.60
16:Q:166:ARG:NH1	16:Q:352:PRO:O	2.30	0.60
2:B:187:LYS:HB2	13:N:124:TYR:CE1	2.36	0.60
12:M:339:ALA:HB3	12:M:544:VAL:HG12	1.82	0.60
1:A:263:ALA:HA	1:A:271:SER:HB3	1.83	0.60
9:J:141:PHE:CZ	9:J:180:TYR:CA	2.84	0.60
12:M:387:LEU:HD12	12:M:514:ASN:HB2	1.83	0.60
13:N:129:THR:HA	17:T:44:GLN:HE22	1.67	0.60
16:Q:140:ASP:HB3	16:Q:147:ASN:HD21	1.67	0.60
12:M:168:LEU:HD23	12:M:292:PHE:HD2	1.66	0.60
13:N:137:TRP:CH2	13:N:140:PRO:HD3	2.36	0.60
16:Q:338:ARG:HH12	18:W:23:ARG:HB3	1.65	0.60
12:M:69:LEU:HD21	12:M:184:ARG:HB2	1.83	0.60
1:A:35:LEU:HD22	1:A:290:GLU:HA	1.83	0.59
1:A:412:LEU:HA	1:A:415:ILE:HD12	1.84	0.59
9:J:217:PHE:HB2	9:J:280:ILE:HD13	1.83	0.59
12:M:228:VAL:HG23	12:M:230:ALA:H	1.66	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:M:345:LEU:HB2	12:M:548:LEU:HD21	1.84	0.59
16:Q:179:ARG:CZ	16:Q:303:ARG:HH21	2.14	0.59
9:J:221:HIS:HE1	9:J:222:ARG:HG3	1.61	0.59
9:J:207:PHE:HE2	9:J:348:LYS:HB2	1.68	0.59
9:J:85:ARG:HH11	9:J:85:ARG:CG	2.09	0.59
1:A:288:VAL:HG11	1:A:303:HIS:CD2	2.38	0.59
2:B:208:LEU:HD22	8:I:39:PRO:HD2	1.85	0.59
9:J:208:GLY:H	9:J:211:ASP:HB2	1.66	0.59
12:M:602:ARG:HE	12:M:659:ILE:HD11	1.67	0.59
1:A:123:GLY:HA3	1:A:355:ILE:HD11	1.83	0.59
12:M:460:HIS:CD2	12:M:462:PHE:HB3	2.38	0.59
16:Q:142:VAL:HG11	16:Q:182:ASN:HA	1.84	0.59
1:A:93:PHE:HE2	1:A:98:LYS:CD	2.05	0.59
12:M:334:GLN:HB2	12:M:361:VAL:HB	1.85	0.59
4:E:127:ASP:HB3	4:E:128:PRO:HD2	1.84	0.59
12:M:519:ILE:HG12	12:M:521:SER:H	1.68	0.59
15:P:204:LEU:HD11	16:Q:123:LEU:HD23	1.83	0.59
9:J:212:ARG:NH1	9:J:212:ARG:HG2	2.15	0.59
4:E:32:VAL:O	4:E:35:LEU:HB3	2.03	0.59
7:H:40:LYS:HD3	7:H:45:ARG:NH1	2.18	0.59
9:J:172:ALA:O	9:J:185:ALA:HB2	2.03	0.59
14:O:48:ASN:HD22	14:O:94:PRO:HA	1.68	0.59
2:B:186:GLU:OE2	17:T:64:ASN:N	2.36	0.59
1:A:118:ASP:OD1	1:A:120:GLY:N	2.35	0.58
3:C:173:ILE:HG22	3:C:174:VAL:HG13	1.84	0.58
9:J:315:THR:HG23	9:J:318:LYS:H	1.66	0.58
12:M:543:LYS:HG3	12:M:565:PHE:CD2	2.33	0.58
12:M:624:ARG:NE	12:M:636:TYR:O	2.36	0.58
1:A:220:GLN:NE2	14:O:114:GLU:O	2.35	0.58
9:J:181:LEU:HD23	9:J:181:LEU:O	2.03	0.58
9:J:73:LEU:O	9:J:78:SER:OG	2.21	0.58
16:Q:182:ASN:HD21	16:Q:404:LYS:HE3	1.68	0.58
9:J:192:ARG:O	9:J:196:PRO:HA	2.02	0.58
12:M:126:LEU:HD12	17:T:98:LYS:O	2.04	0.58
2:B:74:TYR:OH	16:Q:257:GLU:OE1	2.20	0.58
15:P:147:THR:HG21	15:P:153:ILE:HB	1.84	0.58
2:B:198:GLU:OE1	13:N:88:ARG:HB2	2.04	0.58
3:C:89:CYS:HB2	3:C:123:ALA:HB1	1.86	0.58
4:E:126:HIS:NE2	12:M:612:PRO:O	2.37	0.58
9:J:358:THR:O	9:J:362:LEU:N	2.36	0.58
9:J:75:ARG:NH1	15:P:215:GLU:OE2	2.34	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
16:Q:251:PHE:HA	16:Q:254:ARG:HE	1.69	0.58
16:Q:273:ILE:HD13	16:Q:325:ASP:CG	2.23	0.58
2:B:39:VAL:HG22	16:Q:321:GLY:HA2	1.86	0.58
12:M:330:LEU:HD22	12:M:626:LEU:HD21	1.84	0.58
8:I:23:LYS:HD3	16:Q:250:ASN:HA	1.85	0.58
12:M:308:ARG:HA	12:M:314:LEU:HA	1.86	0.58
14:O:138:THR:HA	14:O:141:MET:HB3	1.85	0.58
10:K:89:LEU:HD11	14:O:61:LYS:HE3	1.86	0.58
5:F:88:THR:HA	5:F:91:LEU:HD12	1.85	0.58
12:M:306:MET:HB3	12:M:314:LEU:HD13	1.86	0.58
12:M:36:VAL:HG11	12:M:56:VAL:HG11	1.84	0.58
16:Q:412:VAL:HG12	16:Q:420:TYR:HB3	1.86	0.58
1:A:307:VAL:HG11	1:A:314:LEU:HD21	1.86	0.58
12:M:226:CYS:HB2	12:M:231:LEU:HD12	1.85	0.58
12:M:251:ILE:HG22	12:M:260:ASN:HA	1.85	0.58
12:M:222:ILE:O	12:M:225:ILE:HG22	2.04	0.58
12:M:385:TYR:HB2	12:M:517:HIS:HE2	1.69	0.58
8:I:69:ILE:HB	15:P:76:VAL:HB	1.85	0.58
5:F:63:PRO:HB2	5:F:79:LEU:CB	2.31	0.57
9:J:329:LEU:HD13	9:J:332:LEU:HB2	1.84	0.57
12:M:177:ILE:O	12:M:177:ILE:HG13	2.04	0.57
1:A:48:ARG:HH12	14:O:231:LEU:HD11	1.69	0.57
11:L:89:SER:HG	15:P:239:TRP:HE1	1.41	0.57
1:A:438:LEU:HD21	1:A:446:LEU:HD21	1.86	0.57
3:C:67:LEU:HD22	3:C:207:LEU:CD2	2.34	0.57
12:M:173:MET:C	12:M:175:ARG:H	2.05	0.57
16:Q:251:PHE:HD2	16:Q:341:LEU:HD21	1.69	0.57
1:A:201:ALA:HB1	14:O:121:MET:HB2	1.86	0.57
12:M:210:ILE:HG23	12:M:212:LYS:H	1.69	0.57
12:M:217:GLU:HB2	12:M:408:ARG:HH21	1.69	0.57
12:M:358:LEU:O	12:M:363:SER:N	2.35	0.57
14:O:160:VAL:HA	14:O:171:LEU:HD23	1.86	0.57
16:Q:326:CYS:SG	16:Q:453:THR:HG22	2.44	0.57
9:J:204:SER:O	9:J:240:VAL:HG23	2.04	0.57
9:J:212:ARG:HH11	9:J:212:ARG:CG	2.12	0.57
9:J:293:LEU:HD12	9:J:294:PRO:HD2	1.86	0.57
12:M:257:VAL:HG11	12:M:413:LEU:HD22	1.85	0.57
2:B:66:ARG:NH2	18:W:26:PRO:O	2.38	0.57
14:O:148:ILE:HG23	14:O:201:ILE:HD11	1.87	0.57
1:A:235:VAL:HG22	1:A:240:THR:HG21	1.87	0.57
4:E:118:PHE:HA	4:E:121:LYS:HD3	1.86	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:J:64:PHE:HD1	9:J:210:GLU:HB3	1.69	0.57
2:B:87:GLU:HG2	13:N:61:TRP:HB3	1.87	0.57
1:A:159:ARG:HH22	14:O:177:LEU:HA	1.70	0.57
2:B:97:GLY:H	2:B:167:GLU:HG3	1.70	0.57
6:G:134:ASP:O	6:G:138:LEU:N	2.38	0.57
9:J:220:MET:HB2	9:J:281:PHE:HZ	1.68	0.57
12:M:501:ARG:NH1	12:M:666:GLN:HB2	2.18	0.57
12:M:636:TYR:CE1	12:M:642:VAL:HB	2.39	0.57
12:M:650:SER:OG	12:M:652:ASN:OD1	2.22	0.57
16:Q:123:LEU:HB3	16:Q:135:TYR:OH	2.05	0.57
16:Q:251:PHE:CD2	16:Q:341:LEU:HD21	2.40	0.57
1:A:382:CYS:SG	19:A:501:SF4:S4	3.03	0.57
2:B:36:TYR:HB3	8:I:104:TRP:HE3	1.68	0.57
1:A:126:LYS:HB2	1:A:275:LEU:HD22	1.85	0.57
9:J:283:VAL:HG12	9:J:369:VAL:HG21	1.86	0.57
12:M:225:ILE:HD12	12:M:285:TRP:CH2	2.39	0.57
1:A:209:GLU:HB3	20:A:502:FMN:H3'	1.85	0.57
5:F:16:LEU:HD11	5:F:19:ILE:HB	1.87	0.57
8:I:39:PRO:HB2	8:I:41:LEU:HD12	1.87	0.57
9:J:84:TYR:CB	9:J:91:ILE:HD11	2.34	0.57
1:A:159:ARG:NH1	14:O:177:LEU:O	2.33	0.57
1:A:243:ALA:HA	20:A:502:FMN:O2P	2.04	0.56
8:I:36:GLN:HE22	16:Q:239:GLY:HA2	1.68	0.56
9:J:141:PHE:CZ	9:J:180:TYR:CD1	2.92	0.56
12:M:391:ILE:O	12:M:417:ARG:NH2	2.38	0.56
12:M:454:ASP:HB3	12:M:460:HIS:HB2	1.85	0.56
16:Q:390:GLN:HE22	16:Q:417:SER:HB3	1.68	0.56
1:A:227:PRO:HB3	12:M:95:PRO:HD3	1.87	0.56
16:Q:306:GLN:O	16:Q:308:TYR:N	2.38	0.56
3:C:147:VAL:HG23	3:C:176:VAL:HA	1.86	0.56
2:B:151:ILE:HG21	3:C:159:TYR:CD2	2.41	0.56
6:G:97:LYS:HD3	6:G:108:LEU:HG	1.86	0.56
12:M:193:ASP:OD2	14:O:111:ARG:NH2	2.39	0.56
15:P:190:ASP:CG	15:P:191:TYR:H	2.08	0.56
1:A:116:ASN:ND2	20:A:502:FMN:HM83	2.20	0.56
9:J:217:PHE:HB3	9:J:280:ILE:HD13	1.87	0.56
12:M:591:GLU:HB3	12:M:612:PRO:HD3	1.87	0.56
1:A:123:GLY:N	14:O:180:CYS:SG	2.71	0.56
12:M:221:ASN:HB3	12:M:285:TRP:CE3	2.40	0.56
13:N:84:PRO:HD3	13:N:113:HIS:CD2	2.41	0.56
1:A:222:LYS:HE2	1:A:379:CYS:HB2	1.88	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
15:P:213:ASP:OD1	15:P:214:ASP:N	2.38	0.56
1:A:319:PRO:O	1:A:324:THR:OG1	2.23	0.56
1:A:86:ARG:HA	1:A:94:PRO:HA	1.88	0.56
5:F:80:ASN:OD1	5:F:81:ASN:ND2	2.39	0.56
16:Q:390:GLN:OE1	16:Q:417:SER:N	2.38	0.56
5:F:16:LEU:HB3	5:F:51:LEU:HD13	1.88	0.56
9:J:117:ARG:HG2	9:J:155:LEU:HD22	1.86	0.56
11:L:82:PRO:HD3	11:L:98:LYS:HG2	1.87	0.56
12:M:492:ALA:O	12:M:495:SER:OG	2.21	0.56
12:M:50:LEU:N	12:M:91:ALA:O	2.38	0.56
16:Q:94:VAL:HG11	16:Q:458:PHE:HB3	1.87	0.56
2:B:103:ARG:HH12	17:T:68:ALA:HB2	1.69	0.56
1:A:342:LEU:HB3	1:A:347:THR:HB	1.87	0.56
9:J:84:TYR:O	9:J:107:GLU:HA	2.06	0.56
9:J:132:ARG:HD2	9:J:134:TRP:NE1	2.20	0.56
8:I:46:SER:OG	12:M:150:ARG:NH2	2.38	0.56
12:M:476:LEU:HD11	12:M:480:ALA:HB3	1.87	0.56
12:M:620:TRP:HE1	12:M:639:LEU:HD13	1.71	0.55
5:F:17:ARG:HB3	5:F:68:ARG:HH21	1.72	0.55
12:M:124:HIS:ND1	12:M:125:PRO:HD2	2.22	0.55
12:M:408:ARG:HB3	12:M:415:ASN:ND2	2.21	0.55
14:O:41:HIS:ND1	14:O:41:HIS:O	2.40	0.55
16:Q:316:PHE:HB2	16:Q:339:GLN:HE21	1.70	0.55
1:A:149:MET:HG3	1:A:241:THR:HG21	1.89	0.55
9:J:134:TRP:CZ3	9:J:136:THR:HA	2.42	0.55
9:J:181:LEU:HD13	9:J:324:ILE:HD13	1.88	0.55
12:M:481:LEU:HD11	12:M:515:ILE:HD12	1.88	0.55
13:N:57:GLY:H	13:N:59:HIS:CE1	2.24	0.55
15:P:235:LEU:HD22	16:Q:387:GLU:HG2	1.87	0.55
4:E:75:ASP:HB3	4:E:78:VAL:HG23	1.89	0.55
7:H:16:VAL:HA	7:H:78:GLU:OE2	2.06	0.55
9:J:171:ASN:HB2	9:J:181:LEU:HD11	1.84	0.55
12:M:598:ASN:HB3	12:M:602:ARG:HB3	1.89	0.55
15:P:51:ASN:HB2	15:P:82:ASN:HD21	1.72	0.55
12:M:128:CYS:N	12:M:129:PRO:HD2	2.21	0.55
2:B:145:ILE:HG22	2:B:188:LEU:HD11	1.89	0.55
16:Q:273:ILE:HD11	16:Q:325:ASP:OD2	2.04	0.55
1:A:119:GLU:HB3	1:A:162:PHE:HE2	1.70	0.55
5:F:68:ARG:HD2	5:F:72:GLY:HA2	1.87	0.55
12:M:329:MET:HG3	12:M:565:PHE:CE2	2.41	0.55
12:M:697:THR:O	12:M:702:ARG:NH2	2.40	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
16:Q:291:VAL:HA	16:Q:294:ARG:HB2	1.89	0.55
16:Q:232:VAL:HB	16:Q:356:ILE:HG22	1.88	0.55
1:A:33:GLY:H	1:A:294:VAL:HG12	1.72	0.55
4:E:56:VAL:HG23	9:J:367:GLU:OE2	2.07	0.55
11:L:61:ILE:HB	11:L:64:LEU:HB2	1.89	0.55
12:M:341:ILE:HD12	12:M:555:ILE:HG13	1.89	0.55
12:M:510:TRP:CD1	12:M:512:VAL:HG22	2.42	0.55
13:N:48:TYR:HB3	13:N:89:TRP:CZ3	2.41	0.55
11:L:61:ILE:HG21	15:P:149:GLU:OE1	2.07	0.55
9:J:49:SER:HB2	15:P:225:GLU:HB3	1.87	0.55
16:Q:83:ASN:HA	16:Q:98:VAL:HG22	1.89	0.55
9:J:164:PHE:HE2	9:J:191:VAL:HG13	1.72	0.54
9:J:94:LEU:HG	9:J:97:MET:SD	2.46	0.54
11:L:162:ALA:HA	11:L:168:LYS:NZ	2.22	0.54
15:P:55:HIS:CD2	15:P:78:VAL:HG12	2.42	0.54
4:E:80:ASP:HA	4:E:83:VAL:HG22	1.90	0.54
9:J:141:PHE:HZ	9:J:180:TYR:CD1	2.26	0.54
9:J:344:PRO:HG2	9:J:347:LEU:HD13	1.89	0.54
12:M:241:ARG:HG2	12:M:243:TRP:CZ2	2.42	0.54
12:M:308:ARG:HD2	12:M:312:GLY:O	2.08	0.54
12:M:380:ASP:OD1	12:M:381:LEU:N	2.40	0.54
15:P:107:GLN:HB3	15:P:109:LYS:HE3	1.89	0.54
16:Q:191:ALA:HB1	16:Q:196:ALA:HB3	1.89	0.54
2:B:37:LYS:N	16:Q:318:VAL:O	2.37	0.54
1:A:418:GLN:O	1:A:422:HIS:ND1	2.39	0.54
1:A:381:GLN:CG	19:A:501:SF4:S2	2.94	0.54
12:M:173:MET:C	12:M:175:ARG:N	2.60	0.54
12:M:47:THR:OG1	12:M:51:GLN:OE1	2.23	0.54
7:H:111:GLN:NE2	15:P:124:ASN:HB2	2.22	0.54
1:A:278:ILE:HG12	1:A:304:ALA:HB2	1.89	0.54
9:J:168:SER:O	22:J:401:NDP:H6N	2.08	0.54
12:M:402:LEU:HA	12:M:475:VAL:HB	1.88	0.54
1:A:328:PRO:HG2	1:A:441:HIS:CD2	2.43	0.54
4:E:36:TYR:HD1	4:E:67:PHE:CE2	2.25	0.54
9:J:172:ALA:HA	9:J:181:LEU:CD2	2.38	0.54
1:A:207:GLY:O	20:A:502:FMN:C9A	2.56	0.54
9:J:203:PRO:HG2	22:J:401:NDP:C5N	2.37	0.54
12:M:405:THR:HA	12:M:686:PRO:HG3	1.90	0.54
10:K:92:SER:HB2	14:O:68:LYS:HD2	1.90	0.54
15:P:172:ASP:OD2	15:P:189:THR:OG1	2.23	0.54
2:B:68:LEU:O	2:B:71:THR:HG22	2.08	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:H:12:VAL:HG11	16:Q:296:SER:HB2	1.90	0.54
8:I:59:GLY:HA2	15:P:47:VAL:HG22	1.90	0.54
12:M:53:CYS:HB2	12:M:60:ILE:HD11	1.90	0.54
7:H:31:ILE:HA	7:H:34:VAL:HG12	1.90	0.54
12:M:358:LEU:HB3	12:M:363:SER:O	2.07	0.54
1:A:63:TYR:HE2	1:A:64:LYS:HZ2	1.56	0.54
15:P:85:GLU:HG3	15:P:142:ARG:HB2	1.88	0.54
16:Q:136:PHE:HE2	16:Q:151:TYR:CD1	2.26	0.54
1:A:225:LEU:HG	1:A:227:PRO:HD3	1.90	0.53
1:A:141:GLY:HA2	1:A:252:PRO:HD3	1.90	0.53
9:J:141:PHE:CE1	9:J:180:TYR:HD1	2.25	0.53
9:J:178:SER:OG	9:J:181:LEU:CB	2.57	0.53
9:J:167:VAL:HA	9:J:201:VAL:HB	1.88	0.53
11:L:85:ASN:OD1	11:L:87:MET:N	2.36	0.53
15:P:235:LEU:HB3	16:Q:387:GLU:HG2	1.91	0.53
2:B:104:TYR:CE2	2:B:110:ARG:HA	2.43	0.53
2:B:61:TRP:O	2:B:63:GLU:N	2.41	0.53
9:J:207:PHE:CZ	9:J:345:LEU:HA	2.44	0.53
12:M:389:THR:OG1	12:M:514:ASN:ND2	2.40	0.53
16:Q:391:VAL:HG12	16:Q:392:PRO:O	2.09	0.53
16:Q:196:ALA:O	16:Q:198:THR:N	2.41	0.53
12:M:149:ASP:HB2	16:Q:361:ALA:HB3	1.90	0.53
1:A:117:ALA:HB3	1:A:157:TYR:O	2.08	0.53
4:E:50:PHE:HB2	4:E:52:LEU:HD12	1.89	0.53
9:J:298:TYR:CE2	9:J:319:VAL:HG22	2.44	0.53
12:M:351:LEU:HD23	12:M:530:TYR:HE2	1.73	0.53
12:M:343:GLY:HA3	12:M:548:LEU:HB2	1.90	0.53
13:N:84:PRO:HA	13:N:87:HIS:HB3	1.90	0.53
1:A:41:ILE:HG23	1:A:253:THR:HG21	1.90	0.53
1:A:357:MET:HG2	14:O:142:LEU:HD21	1.91	0.53
3:C:75:ARG:NH2	3:C:144:PRO:HG3	2.24	0.53
12:M:308:ARG:NH1	12:M:578:PRO:O	2.42	0.53
15:P:238:PRO:O	15:P:239:TRP:HB2	2.08	0.53
15:P:88:ILE:HG22	15:P:89:HIS:O	2.09	0.53
3:C:62:TYR:OH	3:C:66:LYS:NZ	2.29	0.53
12:M:53:CYS:SG	12:M:102:ILE:HD12	2.48	0.53
12:M:82:ILE:HB	12:M:85:ALA:HB2	1.91	0.53
13:N:94:THR:HG22	13:N:96:ASP:H	1.73	0.53
14:O:129:LYS:HB3	14:O:168:LEU:HG	1.91	0.53
2:B:66:ARG:HH22	18:W:28:ARG:HB2	1.73	0.53
1:A:121:GLU:HA	1:A:204:TYR:HE1	1.74	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:65:PHE:O	2:B:69:GLY:N	2.41	0.53
9:J:141:PHE:HE2	9:J:183:ASN:HB2	1.74	0.53
9:J:172:ALA:HA	9:J:181:LEU:HD23	1.90	0.53
9:J:223:PHE:O	9:J:225:PRO:HD2	2.09	0.53
9:J:64:PHE:CE1	9:J:68:TYR:HE2	2.27	0.53
1:A:217:GLU:HB3	11:L:171:ARG:HH22	1.72	0.53
1:A:382:CYS:HA	12:M:74:ASN:HA	1.91	0.53
9:J:141:PHE:CZ	9:J:180:TYR:CB	2.92	0.53
4:E:128:PRO:HB3	11:L:104:ARG:HH22	1.73	0.53
12:M:46:GLY:O	12:M:96:VAL:HG22	2.09	0.53
14:O:204:ILE:O	14:O:208:LEU:HG	2.09	0.53
3:C:172:ARG:NH1	15:P:209:GLU:OE2	2.36	0.53
16:Q:265:ASN:OD1	16:Q:266:ARG:N	2.42	0.53
1:A:86:ARG:NE	1:A:92:GLY:O	2.40	0.53
4:E:81:LEU:HD23	11:L:64:LEU:HD22	1.90	0.53
9:J:64:PHE:CD1	9:J:210:GLU:HB3	2.44	0.53
11:L:120:PRO:HB2	15:P:203:PRO:HG3	1.91	0.53
12:M:168:LEU:HB3	12:M:292:PHE:HE2	1.74	0.53
12:M:565:PHE:HA	12:M:581:ASP:OD2	2.08	0.53
12:M:68:ARG:HD2	12:M:285:TRP:NE1	2.20	0.53
2:B:90:PRO:HD2	3:C:100:ARG:HH11	1.74	0.53
6:G:75:THR:O	6:G:79:ILE:HG12	2.09	0.53
1:A:236:PHE:HZ	14:O:77:ALA:HB2	1.73	0.53
16:Q:262:LEU:HD22	16:Q:268:TRP:NE1	2.18	0.53
1:A:293:SER:HB2	1:A:336:LEU:HD23	1.91	0.52
1:A:164:ASN:HB3	10:K:77:HIS:HB2	1.91	0.52
17:T:52:ARG:HB3	17:T:55:ARG:HH12	1.74	0.52
4:E:25:MET:CB	4:E:29:LYS:CE	2.59	0.52
7:H:97:TRP:HB3	7:H:100:TRP:CH2	2.43	0.52
12:M:613:PRO:HB3	13:N:134:ILE:HG21	1.91	0.52
2:B:66:ARG:HH12	18:W:28:ARG:HB3	1.74	0.52
1:A:77:LEU:HD21	1:A:100:SER:HA	1.90	0.52
4:E:24:ASP:OD1	4:E:25:MET:N	2.42	0.52
7:H:7:LYS:HG2	7:H:8:THR:HG23	1.92	0.52
11:L:61:ILE:HG22	11:L:64:LEU:HD12	1.92	0.52
12:M:460:HIS:O	12:M:463:SER:OG	2.13	0.52
15:P:113:ASP:HB3	15:P:115:THR:HG23	1.91	0.52
16:Q:159:LEU:HD21	16:Q:391:VAL:HA	1.90	0.52
1:A:116:ASN:HD22	20:A:502:FMN:C9	2.22	0.52
1:A:154:ALA:HB3	1:A:195:VAL:HG12	1.91	0.52
9:J:176:SER:C	9:J:182:ARG:HH21	2.13	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:M:385:TYR:HB2	12:M:517:HIS:NE2	2.25	0.52
16:Q:428:GLY:HA2	16:Q:431:HIS:CD2	2.45	0.52
16:Q:449:ALA:O	16:Q:453:THR:HG23	2.08	0.52
8:I:41:LEU:C	18:W:8:GLN:HE22	2.13	0.52
1:A:317:VAL:HG13	1:A:356:VAL:HA	1.91	0.52
2:B:140:THR:HG1	2:B:185:LYS:HZ2	1.51	0.52
6:G:123:GLU:HB2	6:G:128:PHE:O	2.09	0.52
6:G:137:LYS:O	6:G:139:MET:N	2.42	0.52
7:H:32:LEU:O	7:H:36:GLU:HG3	2.10	0.52
15:P:115:THR:HG22	16:Q:423:LYS:HD3	1.92	0.52
21:E:201:8Q1:C30	21:E:201:8Q1:N36	2.73	0.52
9:J:168:SER:HA	9:J:184:LYS:CE	2.40	0.52
9:J:168:SER:N	9:J:201:VAL:O	2.40	0.52
12:M:319:TRP:HZ2	12:M:615:LEU:O	1.92	0.52
1:A:181:LEU:HA	1:A:187:CYS:HB3	1.92	0.52
6:G:143:GLU:HA	6:G:146:ASP:HB3	1.92	0.52
11:L:170:THR:O	11:L:172:VAL:N	2.35	0.52
12:M:61:PRO:HG2	12:M:113:ARG:HE	1.74	0.52
3:C:184:PRO:HD3	16:Q:223:HIS:CD2	2.43	0.52
16:Q:338:ARG:NH2	18:W:23:ARG:HB3	2.24	0.52
1:A:170:GLN:HE21	10:K:91:LEU:HD12	1.74	0.52
12:M:253:VAL:HG23	12:M:345:LEU:HD22	1.90	0.52
12:M:314:LEU:HD11	13:N:140:PRO:HD2	1.92	0.52
10:K:77:HIS:CD2	14:O:215:LYS:HE2	2.44	0.52
16:Q:394:GLY:O	16:Q:413:SER:OG	2.23	0.52
17:T:56:PHE:CD1	17:T:61:LYS:HB2	2.45	0.52
2:B:107:GLY:HA3	17:T:71:LEU:HD23	1.91	0.52
12:M:634:LEU:HD23	12:M:636:TYR:CZ	2.45	0.52
5:F:65:LEU:HB2	5:F:79:LEU:HD11	1.92	0.52
12:M:394:VAL:HG21	12:M:414:PHE:HE1	1.73	0.52
12:M:464:GLN:HE22	12:M:467:LYS:HE2	1.75	0.52
12:M:519:ILE:HD13	12:M:522:GLN:HB2	1.90	0.52
12:M:645:ARG:O	12:M:648:GLU:HG2	2.10	0.52
1:A:62:TRP:CE2	1:A:181:LEU:HD13	2.45	0.51
2:B:99:HIS:HE1	2:B:150:CYS:SG	2.33	0.51
4:E:50:PHE:HB2	4:E:52:LEU:CD1	2.40	0.51
12:M:188:GLU:O	12:M:419:ARG:NE	2.40	0.51
5:F:72:GLY:HA3	12:M:359:ASN:HB3	1.92	0.51
12:M:573:GLY:HA3	13:N:137:TRP:NE1	2.25	0.51
12:M:89:VAL:HB	12:M:94:MET:HG3	1.91	0.51
13:N:30:THR:HG21	13:N:63:VAL:HG22	1.91	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:423:THR:OG1	19:A:501:SF4:S4	2.68	0.51
11:L:169:ARG:NH1	12:M:426:ASP:HA	2.25	0.51
11:L:84:ARG:HG3	11:L:90:GLY:O	2.10	0.51
12:M:50:LEU:HA	12:M:60:ILE:HD13	1.93	0.51
1:A:68:ILE:HD11	1:A:256:ARG:HG2	1.91	0.51
3:C:162:TYR:O	16:Q:123:LEU:HD21	2.10	0.51
7:H:24:LEU:HD21	7:H:81:ILE:HG22	1.92	0.51
8:I:25:GLN:OE1	16:Q:254:ARG:HD3	2.10	0.51
15:P:94:ILE:N	15:P:154:GLU:OE1	2.27	0.51
3:C:209:ILE:HG21	9:J:86:CYS:O	2.11	0.51
13:N:34:LYS:NZ	13:N:58:ARG:HG2	2.25	0.51
3:C:112:ALA:O	3:C:113:SER:OG	2.29	0.51
14:O:152:ILE:HG21	14:O:171:LEU:HD13	1.92	0.51
15:P:186:ARG:NH2	15:P:193:PHE:O	2.40	0.51
16:Q:203:LEU:HD11	16:Q:258:LEU:HD11	1.93	0.51
6:G:147:TYR:O	6:G:151:LYS:N	2.43	0.51
13:N:137:TRP:HH2	13:N:140:PRO:HD3	1.75	0.51
12:M:278:HIS:CD2	12:M:280:ASP:HB2	2.44	0.51
12:M:385:TYR:O	12:M:517:HIS:NE2	2.43	0.51
13:N:40:GLY:HA3	13:N:48:TYR:HB2	1.92	0.51
2:B:201:ALA:HB1	13:N:88:ARG:NH1	2.26	0.51
16:Q:304:LYS:HE3	16:Q:316:PHE:CE1	2.46	0.51
5:F:36:PHE:HB2	5:F:84:ALA:HB1	1.92	0.51
11:L:107:TRP:HZ3	11:L:118:ALA:HB2	1.76	0.51
12:M:308:ARG:HD3	12:M:314:LEU:HB3	1.92	0.51
12:M:532:PRO:HB2	12:M:534:VAL:HG23	1.93	0.51
16:Q:228:ARG:CZ	16:Q:233:HIS:HB2	2.40	0.51
16:Q:381:HIS:O	16:Q:385:TYR:HD2	1.93	0.51
1:A:300:ILE:HA	1:A:304:ALA:HB3	1.93	0.51
9:J:221:HIS:HE1	9:J:222:ARG:CG	2.20	0.51
11:L:61:ILE:HG12	11:L:140:LYS:O	2.10	0.51
16:Q:145:MET:HB3	16:Q:227:ILE:HD12	1.92	0.51
17:T:80:VAL:HG12	17:T:82:THR:H	1.76	0.51
1:A:342:LEU:O	1:A:347:THR:N	2.42	0.51
4:E:19:PRO:HA	4:E:77:ARG:HD3	1.93	0.51
7:H:107:PRO:HB2	7:H:111:GLN:HB2	1.93	0.51
9:J:142:GLU:OE2	9:J:146:VAL:HG21	2.11	0.51
9:J:217:PHE:CZ	9:J:322:MET:CE	2.86	0.51
12:M:151:SER:OG	16:Q:374:SER:HB2	2.11	0.51
12:M:430:ALA:HA	12:M:442:TYR:HB2	1.93	0.51
12:M:302:LEU:HB3	12:M:585:PRO:HB3	1.93	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:N:18:GLY:O	13:N:20:LEU:N	2.44	0.51
14:O:130:TYR:HA	14:O:189:ASN:HD21	1.76	0.51
14:O:63:ILE:HA	14:O:66:ILE:HD12	1.92	0.51
15:P:168:ARG:NH1	15:P:185:ARG:HG3	2.26	0.51
2:B:37:LYS:O	16:Q:320:VAL:N	2.37	0.50
5:F:30:SER:OG	5:F:63:PRO:HG3	2.11	0.50
12:M:307:VAL:HB	12:M:317:THR:HG21	1.93	0.50
12:M:76:ARG:HE	12:M:79:LEU:HD21	1.74	0.50
1:A:118:ASP:O	1:A:159:ARG:CD	2.59	0.50
2:B:127:THR:HB	2:B:144:ASP:OD1	2.10	0.50
9:J:168:SER:C	9:J:184:LYS:HE2	2.31	0.50
9:J:178:SER:OG	9:J:181:LEU:HB3	2.11	0.50
12:M:610:VAL:O	12:M:611:THR:OG1	2.25	0.50
16:Q:143:SER:HB2	16:Q:178:THR:HB	1.93	0.50
16:Q:291:VAL:N	16:Q:294:ARG:HH21	2.09	0.50
1:A:63:TYR:CE2	1:A:64:LYS:HG3	2.47	0.50
2:B:113:ALA:HB1	2:B:130:ALA:HB2	1.94	0.50
2:B:138:ARG:NH1	12:M:238:PHE:HA	2.26	0.50
2:B:109:GLU:OE2	2:B:139:ARG:HD2	2.11	0.50
4:E:50:PHE:HE1	4:E:96:VAL:HG13	1.76	0.50
6:G:112:SER:O	6:G:115:GLN:HB3	2.11	0.50
1:A:152:ARG:HH12	10:K:99:PRO:HB3	1.76	0.50
12:M:372:PHE:CD1	12:M:481:LEU:HD13	2.46	0.50
13:N:119:GLY:O	13:N:120:THR:OG1	2.27	0.50
1:A:281:HIS:NE2	14:O:142:LEU:O	2.38	0.50
17:T:83:ARG:NH1	17:T:103:LEU:H	2.08	0.50
7:H:83:GLN:HG2	15:P:107:GLN:NE2	2.26	0.50
7:H:111:GLN:NE2	15:P:122:ARG:HB3	2.26	0.50
7:H:114:TRP:NE1	16:Q:394:GLY:HA2	2.25	0.50
1:A:87:GLY:N	1:A:93:PHE:O	2.44	0.50
12:M:506:VAL:HG12	12:M:508:GLY:N	2.25	0.50
12:M:77:MET:HA	12:M:116:VAL:HG21	1.92	0.50
12:M:92:CYS:SG	23:M:803:FES:S2	3.10	0.50
15:P:74:GLN:HB2	15:P:87:CYS:HB2	1.93	0.50
7:H:90:LEU:HD11	15:P:99:PHE:HD1	1.76	0.50
9:J:85:ARG:NH1	9:J:85:ARG:CG	2.72	0.50
15:P:202:PHE:HB2	15:P:203:PRO:HD2	1.92	0.50
1:A:63:TYR:HD2	1:A:256:ARG:HD2	1.76	0.50
2:B:108:GLU:OE1	17:T:68:ALA:HB1	2.12	0.50
2:B:37:LYS:HE2	8:I:110:GLN:O	2.11	0.50
8:I:9:GLN:O	8:I:13:ASN:ND2	2.40	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:J:159:ALA:HB3	9:J:161:VAL:HG23	1.93	0.50
9:J:161:VAL:HG12	9:J:163:LYS:H	1.76	0.50
9:J:62:THR:HB	22:J:401:NDP:HO3A	1.77	0.50
12:M:61:PRO:HG2	12:M:113:ARG:NE	2.26	0.50
16:Q:334:VAL:O	16:Q:338:ARG:HG2	2.12	0.50
17:T:89:GLY:HA2	17:T:115:CYS:SG	2.52	0.50
1:A:443:ARG:HB3	1:A:444:PRO:HD3	1.94	0.50
9:J:54:ILE:HA	9:J:124:ASN:HD21	1.76	0.50
9:J:84:TYR:HB2	9:J:91:ILE:HD11	1.92	0.50
12:M:88:VAL:HG13	12:M:108:LYS:HE2	1.94	0.50
12:M:213:MET:HG3	12:M:215:MET:HG3	1.93	0.50
12:M:32:ILE:HG23	12:M:98:LYS:HB2	1.93	0.50
12:M:381:LEU:HB2	12:M:384:ASN:OD1	2.12	0.50
16:Q:133:LEU:HD12	16:Q:229:PRO:HD3	1.93	0.50
12:M:168:LEU:HD23	12:M:292:PHE:CD2	2.47	0.50
12:M:569:GLN:NE2	12:M:622:ILE:HD12	2.26	0.50
7:H:115:PRO:O	15:P:247:GLN:NE2	2.45	0.50
15:P:74:GLN:HB2	15:P:87:CYS:SG	2.52	0.50
16:Q:424:ILE:O	16:Q:463:ARG:NE	2.45	0.50
16:Q:404:LYS:HZ3	16:Q:457:VAL:HB	1.75	0.50
1:A:102:MET:SD	1:A:149:MET:HB3	2.52	0.49
3:C:73:TRP:HD1	3:C:76:ARG:NH2	2.10	0.49
9:J:141:PHE:CZ	9:J:180:TYR:HB2	2.47	0.49
9:J:176:SER:C	9:J:182:ARG:NH2	2.65	0.49
9:J:365:GLU:N	9:J:365:GLU:OE1	2.45	0.49
11:L:75:ARG:HH11	11:L:104:ARG:NE	2.10	0.49
14:O:193:TYR:HB3	14:O:196:LEU:HD11	1.94	0.49
2:B:175:THR:HA	13:N:118:THR:HG21	1.94	0.49
9:J:62:THR:HB	22:J:401:NDP:O2X	2.12	0.49
15:P:190:ASP:OD1	15:P:191:TYR:N	2.45	0.49
2:B:51:VAL:HG22	2:B:54:ARG:NH1	2.26	0.49
4:E:49:GLN:HE21	4:E:96:VAL:HG21	1.78	0.49
10:K:104:GLU:N	10:K:104:GLU:OE1	2.46	0.49
11:L:115:ALA:O	15:P:228:GLN:N	2.44	0.49
12:M:464:GLN:NE2	12:M:467:LYS:HE2	2.27	0.49
13:N:87:HIS:O	13:N:91:HIS:HD2	1.95	0.49
11:L:92:ASN:HB2	15:P:239:TRP:H	1.77	0.49
1:A:112:TYR:CD1	1:A:155:TYR:HE2	2.29	0.49
7:H:115:PRO:HG3	16:Q:393:PRO:HB2	1.94	0.49
9:J:268:PRO:HG3	9:J:344:PRO:HA	1.94	0.49
16:Q:149:GLN:CD	16:Q:171:ARG:HB3	2.33	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
15:P:113:ASP:OD1	16:Q:425:LYS:HD2	2.13	0.49
1:A:111:LYS:O	1:A:152:ARG:N	2.34	0.49
1:A:378:SER:O	1:A:380:GLY:N	2.45	0.49
2:B:36:TYR:HD2	8:I:104:TRP:HB2	1.76	0.49
5:F:21:ILE:HG12	5:F:55:ILE:HG12	1.93	0.49
1:A:208:GLU:OE1	1:A:211:ALA:N	2.39	0.49
1:A:71:LYS:HA	1:A:147:ARG:HH21	1.77	0.49
2:B:36:TYR:CD2	8:I:104:TRP:HB2	2.48	0.49
9:J:209:ARG:HD2	15:P:217:LYS:HE2	1.93	0.49
9:J:64:PHE:HE2	9:J:242:VAL:HG21	1.77	0.49
12:M:300:GLN:HA	13:N:135:GLN:O	2.12	0.49
7:H:107:PRO:HD3	15:P:74:GLN:HE22	1.76	0.49
16:Q:323:ARG:N	16:Q:328:ASP:OD2	2.46	0.49
1:A:130:ILE:HD11	1:A:275:LEU:HD21	1.94	0.49
3:C:79:LEU:HB2	3:C:108:VAL:HG12	1.95	0.49
9:J:201:VAL:HG13	9:J:265:PHE:CE2	2.47	0.49
9:J:350:ILE:HG21	9:J:366:ILE:HG12	1.95	0.49
12:M:66:HIS:HE1	12:M:68:ARG:HG2	1.78	0.49
16:Q:360:ASP:O	16:Q:364:SER:OG	2.29	0.49
1:A:160:GLY:HA2	1:A:199:ARG:NH1	2.27	0.49
9:J:179:ARG:HB3	9:J:179:ARG:NH1	2.27	0.49
12:M:123:ASN:HA	12:M:157:LYS:HG2	1.94	0.49
12:M:348:ALA:O	12:M:352:VAL:HG23	2.12	0.49
12:M:64:CYS:O	12:M:184:ARG:NH2	2.46	0.49
7:H:111:GLN:HE22	15:P:122:ARG:HB3	1.77	0.49
16:Q:194:LEU:HD12	16:Q:268:TRP:CE2	2.45	0.49
1:A:274:LYS:HB2	1:A:292:MET:SD	2.53	0.49
12:M:372:PHE:CE1	12:M:481:LEU:HD13	2.48	0.49
1:A:274:LYS:HZ2	1:A:352:ALA:HB3	1.77	0.49
11:L:95:LYS:NZ	15:P:240:GLU:OE2	2.45	0.49
12:M:136:GLU:N	12:M:136:GLU:OE1	2.46	0.49
12:M:209:TYR:O	12:M:210:ILE:HG22	2.12	0.49
12:M:392:ALA:HA	12:M:417:ARG:HH22	1.78	0.49
13:N:11:LEU:HA	13:N:14:ILE:HD12	1.94	0.49
16:Q:358:VAL:HG12	16:Q:360:ASP:H	1.78	0.49
1:A:132:ARG:HG2	1:A:165:GLU:OE1	2.13	0.48
4:E:47:VAL:HG11	4:E:56:VAL:HG22	1.95	0.48
7:H:18:ASN:O	7:H:19:THR:OG1	2.31	0.48
7:H:35:LEU:O	7:H:45:ARG:NE	2.43	0.48
9:J:64:PHE:CE2	9:J:242:VAL:HG21	2.48	0.48
14:O:155:LYS:HZ3	14:O:205:ILE:HB	1.77	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
16:Q:179:ARG:HG2	16:Q:183:HIS:CD2	2.48	0.48
4:E:128:PRO:HG3	11:L:74:THR:OG1	2.14	0.48
9:J:152:ILE:HG22	9:J:164:PHE:HE1	1.78	0.48
12:M:636:TYR:HB2	12:M:641:GLN:HB3	1.95	0.48
16:Q:140:ASP:HB3	16:Q:147:ASN:ND2	2.28	0.48
13:N:129:THR:HA	17:T:44:GLN:NE2	2.28	0.48
9:J:89:TYR:CD1	9:J:89:TYR:C	2.85	0.48
12:M:36:VAL:HG23	12:M:41:VAL:HG21	1.95	0.48
12:M:711:VAL:HA	12:M:714:VAL:HG12	1.94	0.48
16:Q:136:PHE:CE2	16:Q:151:TYR:HB2	2.49	0.48
16:Q:175:GLY:O	16:Q:178:THR:OG1	2.29	0.48
2:B:94:ARG:CZ	16:Q:237:PRO:HG3	2.44	0.48
9:J:197:GLU:OE1	9:J:197:GLU:N	2.45	0.48
12:M:365:THR:HG22	12:M:537:ILE:HD11	1.95	0.48
14:O:197:THR:H	14:O:200:ASP:HB3	1.77	0.48
16:Q:149:GLN:HG3	16:Q:171:ARG:HD3	1.94	0.48
1:A:158:ILE:N	1:A:198:VAL:O	2.47	0.48
1:A:318:ILE:HD11	1:A:355:ILE:HD13	1.95	0.48
7:H:46:LYS:HE3	8:I:90:THR:OG1	2.13	0.48
9:J:206:ILE:HB	9:J:242:VAL:HG23	1.90	0.48
12:M:126:LEU:HD23	16:Q:375:MET:SD	2.52	0.48
14:O:115:VAL:O	14:O:119:TYR:HD2	1.96	0.48
16:Q:301:ASP:OD1	16:Q:302:LEU:N	2.47	0.48
4:E:20:ILE:H	4:E:77:ARG:HG2	1.78	0.48
9:J:217:PHE:HZ	9:J:322:MET:HE1	1.77	0.48
9:J:93:HIS:O	9:J:96:PRO:HD2	2.14	0.48
11:L:98:LYS:HA	11:L:126:LEU:O	2.13	0.48
12:M:124:HIS:CG	12:M:125:PRO:HD2	2.48	0.48
12:M:704:SER:OG	12:M:706:THR:HG22	2.14	0.48
15:P:160:PHE:C	15:P:162:ALA:H	2.16	0.48
5:F:68:ARG:HA	5:F:74:GLU:HG2	1.95	0.48
2:B:142:ARG:NH2	11:L:112:MET:O	2.47	0.48
12:M:564:CYS:O	12:M:566:ILE:HG12	2.14	0.48
4:E:36:TYR:HD1	4:E:67:PHE:HE2	1.62	0.48
8:I:38:PRO:HA	8:I:39:PRO:HD3	1.58	0.48
14:O:207:GLU:HA	14:O:210:ALA:HB3	1.96	0.48
14:O:233:SER:OG	14:O:234:LEU:N	2.47	0.48
16:Q:194:LEU:CD1	16:Q:268:TRP:CE2	2.97	0.48
2:B:40:ASN:O	2:B:42:GLN:N	2.43	0.48
4:E:52:LEU:HB3	4:E:54:ILE:HG13	1.96	0.48
8:I:96:THR:OG1	8:I:98:ALA:O	2.19	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:J:212:ARG:CG	9:J:212:ARG:NH1	2.72	0.48
12:M:200:ARG:HH21	14:O:120:THR:HG23	1.79	0.48
12:M:262:VAL:HG23	12:M:276:ARG:HB2	1.95	0.48
12:M:383:SER:HA	12:M:386:LEU:HD12	1.95	0.48
13:N:38:LEU:HD22	13:N:50:GLU:HB2	1.96	0.48
16:Q:124:ILE:HG22	16:Q:419:PRO:HG3	1.96	0.48
4:E:98:LYS:HG2	15:P:191:TYR:HB3	1.96	0.48
5:F:48:ASN:HD21	5:F:53:ILE:HD11	1.78	0.48
9:J:218:ALA:HB2	9:J:353:LEU:HD22	1.96	0.48
9:J:250:VAL:O	9:J:254:LYS:HG2	2.13	0.48
9:J:357:ARG:HG3	9:J:362:LEU:HA	1.95	0.48
12:M:302:LEU:N	12:M:571:HIS:O	2.33	0.48
12:M:360:ARG:NH1	12:M:635:PRO:HD3	2.29	0.48
1:A:256:ARG:O	14:O:246:GLN:HB3	2.13	0.48
1:A:119:GLU:OE1	1:A:127:ASP:HB2	2.14	0.47
1:A:370:LEU:O	1:A:373:PHE:HB3	2.14	0.47
5:F:35:ASP:O	5:F:39:LYS:HG2	2.14	0.47
6:G:77:GLU:N	6:G:77:GLU:OE1	2.38	0.47
8:I:11:LEU:O	8:I:14:TRP:HB3	2.13	0.47
11:L:75:ARG:NH2	11:L:101:PHE:HB3	2.29	0.47
11:L:162:ALA:HA	11:L:168:LYS:HZ2	1.79	0.47
8:I:44:GLY:HA2	16:Q:355:GLU:HG3	1.95	0.47
16:Q:412:VAL:O	16:Q:420:TYR:N	2.43	0.47
1:A:99:TRP:HH2	1:A:248:VAL:HA	1.78	0.47
2:B:151:ILE:HD13	3:C:159:TYR:CD2	2.50	0.47
6:G:123:GLU:OE1	6:G:130:ILE:N	2.39	0.47
7:H:40:LYS:HA	7:H:45:ARG:HD3	1.94	0.47
9:J:203:PRO:O	22:J:401:NDP:H5N	2.14	0.47
12:M:287:SER:HB3	12:M:290:THR:HG23	1.97	0.47
1:A:114:VAL:O	1:A:242:VAL:HA	2.13	0.47
7:H:32:LEU:HG	7:H:52:THR:HG21	1.96	0.47
9:J:141:PHE:HE2	9:J:183:ASN:HD22	1.62	0.47
9:J:91:ILE:HA	9:J:93:HIS:CE1	2.49	0.47
2:B:138:ARG:HG2	12:M:238:PHE:CG	2.48	0.47
13:N:85:GLU:HG2	13:N:86:TRP:N	2.29	0.47
16:Q:97:LEU:HA	16:Q:110:ASP:O	2.15	0.47
16:Q:205:GLU:HG3	16:Q:209:LYS:NZ	2.29	0.47
1:A:126:LYS:HZ3	1:A:246:GLU:HG3	1.79	0.47
7:H:34:VAL:HG23	7:H:95:ARG:CZ	2.44	0.47
10:K:89:LEU:HD13	14:O:65:ALA:HB2	1.95	0.47
10:K:91:LEU:HA	10:K:94:PHE:HD2	1.79	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
17:T:109:THR:HB	17:T:118:GLN:HB3	1.95	0.47
9:J:220:MET:SD	9:J:223:PHE:CD2	3.08	0.47
9:J:238:GLN:NE2	9:J:267:GLY:O	2.43	0.47
3:C:95:HIS:HE1	16:Q:211:PHE:CE2	2.32	0.47
16:Q:390:GLN:NE2	16:Q:417:SER:HB3	2.29	0.47
1:A:119:GLU:O	1:A:159:ARG:NH1	2.45	0.47
2:B:198:GLU:OE2	2:B:202:ASN:ND2	2.46	0.47
2:B:84:TYR:CE2	2:B:85:PRO:HB3	2.49	0.47
6:G:84:LEU:HD23	6:G:87:LEU:HD12	1.96	0.47
8:I:97:PRO:HG3	15:P:61:PHE:CG	2.49	0.47
9:J:99:ASP:O	9:J:102:GLN:HG2	2.14	0.47
11:L:121:LEU:HA	15:P:203:PRO:HB3	1.97	0.47
6:G:104:PHE:CD1	6:G:108:LEU:HD22	2.50	0.47
7:H:28:TYR:HD1	7:H:52:THR:HG23	1.80	0.47
1:A:276:PHE:CE2	1:A:290:GLU:HB3	2.50	0.47
2:B:133:ARG:NH1	2:B:139:ARG:HG3	2.29	0.47
3:C:96:MET:HG2	3:C:103:MET:HB3	1.96	0.47
9:J:141:PHE:CE2	9:J:183:ASN:ND2	2.83	0.47
1:A:51:TRP:HE1	10:K:76:HIS:HD1	1.62	0.47
11:L:92:ASN:O	11:L:95:LYS:HG2	2.15	0.47
12:M:69:LEU:HD22	12:M:181:ARG:HG3	1.95	0.47
14:O:54:ASP:OD1	14:O:55:PHE:N	2.47	0.47
1:A:69:LEU:HD11	1:A:143:LEU:HD21	1.96	0.47
7:H:108:PRO:HG2	7:H:111:GLN:HG2	1.97	0.47
9:J:130:ILE:HG21	22:J:401:NDP:N7A	2.23	0.47
12:M:198:THR:HG23	14:O:117:THR:HG21	1.97	0.47
16:Q:156:GLU:OE2	16:Q:163:PRO:HG3	2.15	0.47
2:B:91:LEU:HG	16:Q:215:GLU:OE2	2.15	0.47
8:I:69:ILE:O	8:I:71:SER:N	2.48	0.47
11:L:77:VAL:HG22	11:L:78:ARG:H	1.80	0.47
12:M:303:THR:O	12:M:615:LEU:HB2	2.15	0.47
12:M:535:GLU:O	12:M:538:ARG:HG2	2.15	0.47
16:Q:79:ASN:ND2	16:Q:100:GLU:HB3	2.30	0.47
16:Q:338:ARG:NH1	18:W:23:ARG:HB3	2.29	0.47
1:A:113:LEU:HD23	1:A:113:LEU:C	2.35	0.47
1:A:311:TRP:CD1	1:A:314:LEU:HD12	2.50	0.47
9:J:229:GLY:HA2	9:J:293:LEU:O	2.15	0.47
9:J:41:MET:HB3	9:J:42:PRO:HD2	1.97	0.47
12:M:236:TYR:CZ	12:M:272:ARG:HD3	2.49	0.47
15:P:186:ARG:NH2	15:P:193:PHE:HB3	2.29	0.47
16:Q:408:GLY:HA3	16:Q:425:LYS:HB3	1.98	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:M:292:PHE:HB3	12:M:706:THR:HG21	1.96	0.46
12:M:546:PHE:CE2	12:M:566:ILE:HD12	2.50	0.46
14:O:182:ASN:HD21	14:O:218:PRO:HB3	1.79	0.46
3:C:100:ARG:NH2	16:Q:208:GLU:HB3	2.18	0.46
1:A:177:TYR:CE2	10:K:91:LEU:HD13	2.50	0.46
3:C:147:VAL:CG2	3:C:176:VAL:HA	2.46	0.46
3:C:106:PHE:CE2	3:C:191:LEU:HD11	2.51	0.46
14:O:138:THR:OG1	14:O:139:PRO:HD3	2.15	0.46
2:B:192:GLY:O	2:B:196:GLU:HB2	2.15	0.46
12:M:616:ALA:O	12:M:617:ARG:NH1	2.44	0.46
12:M:645:ARG:HG3	12:M:648:GLU:OE2	2.16	0.46
13:N:49:TYR:HD2	13:N:61:TRP:CZ3	2.33	0.46
14:O:200:ASP:O	14:O:204:ILE:HG12	2.16	0.46
16:Q:159:LEU:O	16:Q:161:ILE:HG13	2.16	0.46
2:B:94:ARG:NH2	16:Q:237:PRO:HG3	2.30	0.46
16:Q:315:GLU:HB2	16:Q:346:GLN:HE22	1.80	0.46
3:C:137:VAL:HA	3:C:140:GLN:CD	2.36	0.46
9:J:176:SER:CA	9:J:182:ARG:NH2	2.67	0.46
9:J:238:GLN:HG3	9:J:269:SER:O	2.15	0.46
12:M:692:LYS:HG3	12:M:714:VAL:HG13	1.98	0.46
12:M:81:GLU:CD	12:M:108:LYS:HB3	2.36	0.46
16:Q:131:GLN:O	16:Q:134:PRO:HD2	2.16	0.46
1:A:129:GLU:OE1	1:A:132:ARG:NH1	2.49	0.46
3:C:81:PRO:HA	3:C:119:VAL:O	2.15	0.46
9:J:281:PHE:HA	9:J:284:ALA:HB3	1.97	0.46
13:N:83:PRO:HG2	13:N:86:TRP:HB2	1.98	0.46
1:A:174:ARG:HB2	10:K:91:LEU:HD11	1.96	0.46
4:E:40:TYR:OH	6:G:117:GLU:OE2	2.28	0.46
7:H:114:TRP:CD2	7:H:115:PRO:HA	2.51	0.46
11:L:107:TRP:O	11:L:116:SER:HB2	2.16	0.46
11:L:69:GLU:HB2	11:L:73:LYS:HZ2	1.80	0.46
12:M:266:ARG:NE	12:M:271:MET:HE3	2.30	0.46
12:M:37:ASP:OD1	12:M:38:GLY:N	2.41	0.46
12:M:457:SER:O	12:M:499:LYS:NZ	2.49	0.46
12:M:620:TRP:NE1	12:M:639:LEU:HD13	2.30	0.46
15:P:201:ASP:OD1	15:P:202:PHE:N	2.48	0.46
15:P:64:TYR:CE2	15:P:68:ILE:HD11	2.50	0.46
7:H:35:LEU:HA	7:H:38:ILE:HD12	1.96	0.46
11:L:78:ARG:HA	11:L:146:ASP:OD1	2.16	0.46
2:B:138:ARG:HD3	12:M:130:ILE:HG22	1.98	0.46
12:M:323:LEU:HG	12:M:629:ILE:HD12	1.98	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
16:Q:113:ILE:HG12	16:Q:114:GLY:H	1.80	0.46
16:Q:216:ARG:HE	16:Q:240:LEU:HD23	1.80	0.46
16:Q:446:ASP:O	16:Q:450:ILE:HG13	2.16	0.46
1:A:86:ARG:HB3	1:A:92:GLY:O	2.16	0.46
12:M:128:CYS:CB	12:M:129:PRO:CD	2.86	0.46
12:M:299:ARG:O	12:M:301:ARG:HG2	2.15	0.46
14:O:196:LEU:HD21	14:O:204:ILE:HG13	1.98	0.46
15:P:124:ASN:HB3	15:P:146:TYR:HB2	1.98	0.46
16:Q:255:LEU:HD11	16:Q:337:MET:HG2	1.98	0.46
1:A:275:LEU:HA	1:A:289:GLU:HA	1.97	0.46
3:C:163:SER:H	3:C:168:ARG:HH22	1.64	0.46
5:F:14:LEU:N	5:F:17:ARG:HH22	2.13	0.46
11:L:109:ASN:OD1	11:L:110:PRO:HD2	2.16	0.46
11:L:69:GLU:HB2	11:L:73:LYS:NZ	2.30	0.46
14:O:135:CYS:O	14:O:145:SER:OG	2.25	0.46
14:O:78:ALA:O	14:O:82:VAL:HG23	2.15	0.46
16:Q:97:LEU:O	16:Q:97:LEU:HD12	2.15	0.46
4:E:40:TYR:CE1	4:E:60:ARG:HD3	2.51	0.46
9:J:168:SER:HA	9:J:184:LYS:HE3	1.97	0.46
12:M:589:TYR:CE2	12:M:590:THR:HG23	2.50	0.46
15:P:97:LEU:HA	15:P:100:LEU:HD12	1.97	0.46
15:P:83:GLU:HB3	15:P:142:ARG:NH1	2.29	0.46
16:Q:205:GLU:O	16:Q:209:LYS:HG3	2.16	0.46
16:Q:316:PHE:HD1	16:Q:339:GLN:NE2	2.14	0.46
17:T:68:ALA:O	17:T:72:ILE:HG13	2.16	0.46
1:A:128:ARG:O	1:A:132:ARG:HG3	2.15	0.45
5:F:36:PHE:CE1	5:F:40:ARG:HB2	2.51	0.45
8:I:33:LYS:NZ	8:I:36:GLN:HA	2.30	0.45
9:J:220:MET:SD	9:J:223:PHE:HD2	2.39	0.45
12:M:221:ASN:OD1	12:M:291:ARG:NH2	2.35	0.45
12:M:382:ARG:O	12:M:386:LEU:HG	2.16	0.45
12:M:421:SER:O	12:M:425:ASN:N	2.49	0.45
12:M:64:CYS:SG	12:M:75:CYS:HB3	2.56	0.45
1:A:203:ALA:HB2	14:O:119:TYR:CE1	2.50	0.45
1:A:89:GLY:HA2	1:A:244:ASN:ND2	2.28	0.45
2:B:151:ILE:HD13	3:C:159:TYR:CE2	2.51	0.45
16:Q:94:VAL:HG21	16:Q:458:PHE:HB2	1.99	0.45
17:T:52:ARG:HB3	17:T:55:ARG:NH1	2.31	0.45
1:A:73:PRO:HB2	1:A:74:ASP:H	1.58	0.45
6:G:133:ILE:O	6:G:136:GLU:HB2	2.15	0.45
9:J:220:MET:O	9:J:223:PHE:HB2	2.16	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:M:68:ARG:NH2	12:M:284:GLU:OE1	2.33	0.45
12:M:546:PHE:HD2	12:M:568:TYR:HD1	1.63	0.45
15:P:97:LEU:HD23	15:P:100:LEU:HD12	1.97	0.45
7:H:36:GLU:HA	7:H:45:ARG:NH2	2.19	0.45
9:J:207:PHE:CE2	9:J:348:LYS:HB2	2.49	0.45
14:O:153:GLN:HG3	14:O:158:ILE:O	2.15	0.45
1:A:321:GLY:HA2	1:A:353:ALA:HB3	1.97	0.45
1:A:371:ILE:HD11	1:A:435:VAL:HB	1.97	0.45
7:H:28:TYR:CD2	7:H:56:LEU:HD13	2.51	0.45
8:I:55:CYS:HB3	12:M:110:LYS:HE3	1.98	0.45
12:M:197:THR:O	14:O:114:GLU:HG2	2.17	0.45
14:O:218:PRO:HG2	14:O:222:ARG:O	2.16	0.45
14:O:58:GLU:O	14:O:62:ARG:HG3	2.15	0.45
14:O:76:ALA:HA	14:O:79:VAL:HG23	1.98	0.45
15:P:170:ILE:HG23	15:P:174:PHE:CD2	2.52	0.45
16:Q:136:PHE:CD2	16:Q:151:TYR:HB2	2.52	0.45
1:A:392:MET:O	1:A:396:MET:HG2	2.16	0.45
1:A:440:ARG:HE	1:A:441:HIS:CE1	2.35	0.45
3:C:59:ARG:HH22	3:C:61:GLU:CB	2.25	0.45
4:E:59:GLY:O	4:E:63:VAL:HG23	2.16	0.45
6:G:123:GLU:O	6:G:127:GLY:N	2.50	0.45
8:I:30:GLU:HG2	8:I:31:ILE:N	2.32	0.45
9:J:299:ARG:HE	9:J:316:ARG:HH11	1.62	0.45
9:J:99:ASP:H	9:J:102:GLN:HB2	1.82	0.45
12:M:602:ARG:NE	12:M:659:ILE:HD11	2.30	0.45
12:M:688:GLN:O	12:M:690:THR:N	2.50	0.45
14:O:80:LEU:HB2	14:O:81:PRO:HD3	1.99	0.45
1:A:44:ASN:HD22	1:A:59:ARG:NH2	2.14	0.45
2:B:160:CYS:O	16:Q:368:ARG:NH1	2.41	0.45
2:B:94:ARG:HE	16:Q:234:GLN:NE2	2.15	0.45
3:C:161:HIS:CE1	3:C:168:ARG:HD2	2.51	0.45
3:C:153:CYS:SG	19:C:301:SF4:S2	3.07	0.45
4:E:43:VAL:HB	4:E:44:PRO:HD3	1.98	0.45
5:F:22:HIS:HB2	5:F:64:LYS:HB3	1.97	0.45
7:H:31:ILE:HG12	7:H:88:LEU:HA	1.99	0.45
12:M:164:ASN:OD1	12:M:165:ILE:N	2.49	0.45
12:M:158:ARG:HH21	12:M:178:GLN:HE22	1.64	0.45
1:A:201:ALA:O	14:O:119:TYR:HB3	2.17	0.45
7:H:32:LEU:HA	7:H:35:LEU:HG	1.97	0.45
9:J:108:TRP:HZ3	9:J:110:ALA:HA	1.82	0.45
12:M:446:GLY:N	12:M:451:ILE:HD11	2.32	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
15:P:167:GLU:HG2	15:P:181:HIS:CD2	2.52	0.45
2:B:127:THR:HA	15:P:231:ARG:HH12	1.81	0.45
16:Q:399:ALA:HB1	16:Q:406:GLU:HG3	1.98	0.45
1:A:157:TYR:HB2	1:A:212:LEU:HD21	1.99	0.45
4:E:120:SER:O	4:E:124:VAL:HG23	2.17	0.45
9:J:178:SER:OG	9:J:181:LEU:HB2	2.17	0.45
9:J:273:LEU:O	9:J:276:LEU:HB3	2.17	0.45
11:L:102:ASP:N	11:L:102:ASP:OD1	2.50	0.45
13:N:48:TYR:HB3	13:N:89:TRP:HZ3	1.81	0.45
2:B:90:PRO:HG2	13:N:56:PHE:CE2	2.52	0.45
14:O:198:ALA:HA	14:O:201:ILE:HD12	1.99	0.45
14:O:207:GLU:HG2	14:O:213:ILE:HG13	1.99	0.45
14:O:84:ASP:O	14:O:88:ARG:N	2.47	0.45
15:P:164:ASN:HA	15:P:181:HIS:HE2	1.82	0.45
16:Q:145:MET:HG3	16:Q:174:PHE:HB3	1.99	0.45
16:Q:190:HIS:HD2	16:Q:452:GLY:CA	2.26	0.45
16:Q:304:LYS:HE3	16:Q:316:PHE:CZ	2.52	0.45
6:G:99:SER:HG	6:G:102:SER:HG	1.61	0.45
12:M:498:GLN:HE22	12:M:501:ARG:HD2	1.82	0.45
12:M:471:LYS:HB3	12:M:510:TRP:CH2	2.52	0.45
14:O:205:ILE:HA	14:O:208:LEU:HD12	1.98	0.45
16:Q:369:ALA:HA	17:T:93:ALA:HB2	1.99	0.45
17:T:67:PHE:O	17:T:71:LEU:HD13	2.17	0.45
2:B:91:LEU:HD23	2:B:95:PHE:CD2	2.52	0.44
3:C:160:TYR:HE1	16:Q:120:THR:HG22	1.81	0.44
7:H:23:ARG:HH22	7:H:27:LEU:HD21	1.83	0.44
12:M:299:ARG:HG2	12:M:300:GLN:N	2.19	0.44
12:M:381:LEU:C	12:M:383:SER:H	2.16	0.44
12:M:307:VAL:HG22	12:M:582:VAL:HG13	2.00	0.44
12:M:612:PRO:HB3	12:M:616:ALA:HB3	1.99	0.44
15:P:214:ASP:O	15:P:217:LYS:HD2	2.16	0.44
15:P:63:GLU:O	15:P:67:GLU:HG3	2.17	0.44
16:Q:235:ASP:OD1	16:Q:356:ILE:HD12	2.17	0.44
1:A:225:LEU:HB2	1:A:424:ILE:HD11	1.99	0.44
3:C:88:CYS:SG	16:Q:223:HIS:CE1	3.10	0.44
9:J:329:LEU:HD12	9:J:329:LEU:O	2.17	0.44
12:M:219:SER:O	12:M:222:ILE:HG12	2.16	0.44
12:M:275:PRO:HB3	12:M:286:ILE:HB	1.98	0.44
14:O:145:SER:O	14:O:148:ILE:HB	2.18	0.44
16:Q:259:GLU:O	16:Q:263:THR:OG1	2.34	0.44
12:M:157:LYS:HB2	17:T:100:TYR:CD2	2.52	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:69:GLY:O	2:B:72:LEU:HB3	2.17	0.44
3:C:168:ARG:HG3	3:C:172:ARG:NH1	2.31	0.44
6:G:99:SER:OG	6:G:102:SER:OG	2.29	0.44
4:E:53:ASP:OD2	9:J:351:GLU:HB3	2.17	0.44
12:M:546:PHE:CZ	12:M:566:ILE:HD12	2.52	0.44
1:A:369:ARG:NH2	14:O:175:GLU:OE2	2.33	0.44
14:O:195:ASP:HB2	14:O:219:ARG:H	1.83	0.44
1:A:63:TYR:HE2	1:A:64:LYS:NZ	2.15	0.44
8:I:37:PRO:HA	8:I:38:PRO:HD3	1.81	0.44
12:M:306:MET:HA	12:M:315:THR:O	2.18	0.44
12:M:455:ILE:HG12	12:M:463:SER:HB3	1.99	0.44
1:A:317:VAL:HG22	1:A:356:VAL:HA	1.99	0.44
1:A:319:PRO:HB2	1:A:347:THR:HG21	1.98	0.44
9:J:141:PHE:CD2	9:J:183:ASN:ND2	2.86	0.44
9:J:163:LYS:HE2	9:J:253:VAL:HA	1.98	0.44
11:L:136:SER:O	11:L:140:LYS:HG3	2.16	0.44
12:M:229:GLY:O	12:M:232:THR:HG23	2.18	0.44
12:M:566:ILE:HD11	12:M:579:ILE:HG22	1.99	0.44
16:Q:149:GLN:NE2	16:Q:309:ASP:OD2	2.49	0.44
1:A:173:ILE:HG22	1:A:177:TYR:CE2	2.52	0.44
1:A:116:ASN:HD21	20:A:502:FMN:C8	2.22	0.44
7:H:13:GLY:HA2	16:Q:279:THR:HG22	2.00	0.44
9:J:72:HIS:O	9:J:75:ARG:HG2	2.18	0.44
11:L:62:THR:HG23	11:L:72:ILE:HD13	1.99	0.44
12:M:37:ASP:HA	12:M:103:LEU:HD23	1.98	0.44
12:M:385:TYR:HB2	12:M:517:HIS:CE1	2.53	0.44
12:M:510:TRP:HD1	12:M:512:VAL:HG22	1.82	0.44
12:M:371:VAL:HG12	12:M:533:GLY:O	2.17	0.44
12:M:639:LEU:O	12:M:642:VAL:HG12	2.18	0.44
15:P:188:LEU:HD22	16:Q:117:HIS:HB2	2.00	0.44
16:Q:164:PRO:HA	16:Q:165:PRO:HD3	1.83	0.44
17:T:96:HIS:NE2	17:T:115:CYS:SG	2.90	0.44
2:B:131:GLU:OE1	2:B:141:THR:HG21	2.18	0.44
4:E:35:LEU:HD11	4:E:39:TRP:HE1	1.81	0.44
7:H:23:ARG:O	7:H:26:ILE:HB	2.18	0.44
12:M:255:ASP:HB3	12:M:257:VAL:HG23	1.98	0.44
8:I:97:PRO:HG3	15:P:61:PHE:CD1	2.52	0.44
16:Q:307:PRO:HB2	16:Q:312:ASP:HB3	2.00	0.44
1:A:167:SER:O	1:A:171:VAL:HG23	2.18	0.44
1:A:123:GLY:CA	1:A:355:ILE:HD11	2.48	0.44
5:F:39:LYS:HG3	5:F:40:ARG:N	2.29	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:H:12:VAL:HG13	7:H:13:GLY:N	2.33	0.44
14:O:236:GLU:HB3	14:O:238:PRO:HD2	2.00	0.44
9:J:168:SER:O	9:J:203:PRO:HD2	2.18	0.44
1:A:152:ARG:NH1	10:K:99:PRO:HB3	2.33	0.44
12:M:221:ASN:HB3	12:M:285:TRP:HE3	1.82	0.44
15:P:163:ALA:O	15:P:167:GLU:HB2	2.17	0.44
15:P:188:LEU:HA	16:Q:114:GLY:HA3	2.00	0.44
9:J:71:ASN:ND2	15:P:214:ASP:HB3	2.33	0.44
16:Q:106:VAL:HG11	16:Q:109:CYS:HB2	2.00	0.44
16:Q:174:PHE:HD1	16:Q:214:TYR:HE1	1.66	0.44
16:Q:265:ASN:OD1	16:Q:267:ILE:HD12	2.17	0.44
16:Q:358:VAL:O	16:Q:364:SER:OG	2.24	0.44
1:A:118:ASP:O	1:A:119:GLU:C	2.55	0.43
2:B:178:HIS:HB2	3:C:179:TYR:CZ	2.53	0.43
8:I:60:ARG:HD3	16:Q:159:LEU:HD22	1.99	0.43
9:J:83:PRO:HA	9:J:106:LEU:O	2.18	0.43
11:L:133:ASP:O	11:L:136:SER:OG	2.21	0.43
11:L:72:ILE:HA	11:L:143:TRP:CD1	2.53	0.43
12:M:136:GLU:HB3	12:M:242:PRO:HG2	2.00	0.43
12:M:278:HIS:NE2	12:M:280:ASP:HB2	2.33	0.43
12:M:358:LEU:HD22	12:M:363:SER:HB2	1.99	0.43
13:N:5:GLN:O	13:N:9:ARG:HG2	2.17	0.43
14:O:132:ILE:O	14:O:172:ILE:HG22	2.18	0.43
15:P:55:HIS:NE2	15:P:78:VAL:HG12	2.33	0.43
17:T:81:GLU:HA	17:T:122:HIS:O	2.17	0.43
1:A:36:LYS:HB2	1:A:39:ASP:CG	2.38	0.43
2:B:128:ILE:HG12	2:B:143:TYR:HD1	1.83	0.43
2:B:61:TRP:HB2	2:B:65:PHE:HE2	1.82	0.43
4:E:50:PHE:CD2	4:E:103:VAL:HG21	2.52	0.43
4:E:39:TRP:O	4:E:43:VAL:HG23	2.18	0.43
6:G:138:LEU:O	6:G:143:GLU:HB2	2.18	0.43
9:J:283:VAL:O	9:J:357:ARG:NH2	2.51	0.43
11:L:72:ILE:HA	11:L:143:TRP:NE1	2.33	0.43
12:M:385:TYR:HE1	12:M:523:VAL:HG23	1.82	0.43
9:J:168:SER:CA	9:J:184:LYS:HE3	2.47	0.43
4:E:53:ASP:HA	9:J:366:ILE:HD11	2.00	0.43
3:C:163:SER:HB3	16:Q:123:LEU:HD11	2.00	0.43
3:C:88:CYS:HB3	16:Q:141:TYR:CG	2.54	0.43
1:A:37:ASP:OD2	14:O:235:THR:N	2.49	0.43
2:B:169:PRO:HG3	2:B:198:GLU:HG2	2.00	0.43
2:B:35:THR:N	8:I:105:GLU:O	2.51	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:H:50:GLN:NE2	8:I:93:LYS:HD2	2.32	0.43
9:J:125:VAL:HG12	9:J:163:LYS:HB2	2.00	0.43
9:J:220:MET:HA	9:J:223:PHE:CD2	2.53	0.43
9:J:204:SER:OG	9:J:240:VAL:HG23	2.18	0.43
9:J:81:ILE:HG22	9:J:83:PRO:HD3	2.00	0.43
4:E:126:HIS:HD2	12:M:612:PRO:HD2	1.84	0.43
12:M:501:ARG:HH12	12:M:666:GLN:HB2	1.82	0.43
12:M:200:ARG:HB3	14:O:118:PHE:CD1	2.54	0.43
14:O:147:SER:HA	14:O:150:GLU:OE1	2.18	0.43
15:P:157:VAL:HG21	15:P:181:HIS:CD2	2.46	0.43
16:Q:150:ALA:CB	16:Q:400:ILE:HG13	2.49	0.43
12:M:133:GLN:HA	12:M:136:GLU:OE2	2.17	0.43
12:M:646:LEU:HD13	12:M:653:LEU:HB3	2.00	0.43
13:N:73:THR:HG22	13:N:74:PHE:N	2.34	0.43
1:A:274:LYS:NZ	1:A:351:THR:O	2.51	0.43
2:B:166:VAL:HG11	2:B:199:ILE:HG23	2.00	0.43
3:C:156:GLY:O	3:C:161:HIS:ND1	2.52	0.43
5:F:67:ALA:HB3	5:F:75:THR:OG1	2.18	0.43
5:F:65:LEU:O	5:F:76:ASN:HA	2.18	0.43
6:G:115:GLN:NE2	6:G:135:ALA:HB1	2.34	0.43
10:K:86:ASP:O	10:K:90:GLU:HG3	2.18	0.43
12:M:341:ILE:HD13	12:M:367:CYS:SG	2.59	0.43
12:M:342:ALA:O	12:M:369:GLU:HG2	2.18	0.43
14:O:104:VAL:HG12	14:O:105:LEU:HD12	2.00	0.43
14:O:143:ARG:CB	14:O:184:PRO:HD3	2.47	0.43
15:P:55:HIS:HD2	15:P:79:SER:O	2.01	0.43
4:E:43:VAL:O	4:E:47:VAL:HG23	2.19	0.43
9:J:56:ALA:HA	9:J:125:VAL:HG23	2.01	0.43
9:J:131:GLY:HA3	22:J:401:NDP:O3D	2.19	0.43
9:J:167:VAL:HG22	9:J:201:VAL:HB	2.00	0.43
11:L:77:VAL:HG22	11:L:78:ARG:N	2.33	0.43
4:E:118:PHE:HZ	12:M:621:LYS:HG3	1.83	0.43
14:O:163:THR:HG22	14:O:170:THR:HG22	2.01	0.43
1:A:194:ASP:OD2	10:K:96:MET:N	2.41	0.43
2:B:158:GLU:O	16:Q:368:ARG:NH2	2.52	0.43
4:E:28:ALA:HA	4:E:31:ARG:HG3	1.99	0.43
5:F:87:VAL:O	5:F:91:LEU:HG	2.18	0.43
4:E:48:HIS:HE1	9:J:363:SER:O	2.02	0.43
10:K:78:ASP:HA	14:O:215:LYS:HD3	2.00	0.43
12:M:243:TRP:CD1	12:M:244:GLU:HG3	2.54	0.43
12:M:221:ASN:HB3	12:M:285:TRP:CZ3	2.53	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:M:651:PRO:O	12:M:654:VAL:HG22	2.19	0.43
14:O:93:LEU:HA	14:O:94:PRO:HD2	1.86	0.43
15:P:129:VAL:HG22	15:P:144:LYS:HB3	2.01	0.43
15:P:90:PRO:O	15:P:93:VAL:HG23	2.18	0.43
16:Q:144:MET:HA	16:Q:147:ASN:HD22	1.84	0.43
16:Q:410:TYR:O	16:Q:422:CYS:HA	2.19	0.43
16:Q:372:LYS:HD2	17:T:93:ALA:HA	2.00	0.43
2:B:84:TYR:OH	3:C:192:TYR:HB2	2.19	0.43
9:J:124:ASN:OD1	9:J:125:VAL:N	2.52	0.43
12:M:289:LYS:NZ	12:M:694:PHE:O	2.25	0.43
16:Q:147:ASN:O	16:Q:150:ALA:HB3	2.17	0.43
16:Q:391:VAL:O	16:Q:415:GLY:HA2	2.18	0.43
1:A:282:VAL:HA	1:A:307:VAL:HA	2.01	0.43
2:B:133:ARG:NH2	17:T:69:ILE:HG13	2.34	0.43
2:B:175:THR:HB	2:B:180:GLU:OE1	2.19	0.43
9:J:293:LEU:HD23	9:J:298:TYR:HD1	1.84	0.43
12:M:323:LEU:HA	12:M:326:VAL:HG22	1.99	0.43
10:K:82:TYR:HB3	14:O:62:ARG:HH22	1.84	0.43
15:P:171:TRP:CZ3	15:P:177:PHE:HA	2.54	0.43
16:Q:295:GLY:HA2	16:Q:321:GLY:HA3	2.01	0.43
8:I:42:PRO:HG3	16:Q:354:GLY:O	2.19	0.43
17:T:79:GLU:OE1	17:T:122:HIS:HB3	2.19	0.43
1:A:403:ASP:HA	1:A:453:PHE:CE2	2.54	0.42
9:J:169:HIS:CD2	22:J:401:NDP:C5N	2.79	0.42
12:M:134:GLY:HA3	19:M:801:SF4:S3	2.52	0.42
14:O:164:THR:HG23	14:O:167:LYS:N	2.34	0.42
15:P:97:LEU:HD11	15:P:130:TYR:CE2	2.54	0.42
16:Q:116:LEU:O	16:Q:118:ARG:HG3	2.19	0.42
17:T:102:ASN:HD21	17:T:104:ASP:HB2	1.84	0.42
1:A:134:ASP:N	1:A:135:PRO:HD3	2.34	0.42
1:A:314:LEU:O	1:A:315:LEU:HD12	2.19	0.42
2:B:104:TYR:N	2:B:108:GLU:O	2.32	0.42
7:H:21:HIS:NE2	7:H:63:PRO:O	2.52	0.42
7:H:7:LYS:O	7:H:8:THR:OG1	2.29	0.42
7:H:83:GLN:HG2	15:P:107:GLN:HE21	1.84	0.42
9:J:180:TYR:O	9:J:184:LYS:HG3	2.20	0.42
3:C:175:PRO:HB3	9:J:96:PRO:HD3	2.01	0.42
11:L:131:LYS:HD2	11:L:147:ILE:CG2	2.49	0.42
12:M:153:PHE:O	12:M:154:LEU:HD12	2.19	0.42
11:L:154:LYS:HG2	12:M:279:GLU:HG3	2.02	0.42
13:N:66:THR:HG23	13:N:74:PHE:H	1.85	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
16:Q:167:ALA:O	16:Q:171:ARG:HG3	2.18	0.42
12:M:124:HIS:HD2	16:Q:375:MET:HE2	1.84	0.42
2:B:117:CYS:HB2	19:B:301:SF4:S1	2.60	0.42
4:E:80:ASP:OD1	4:E:81:LEU:N	2.52	0.42
6:G:93:ILE:HG12	6:G:94:ASP:O	2.19	0.42
9:J:221:HIS:ND1	9:J:221:HIS:C	2.73	0.42
9:J:61:ALA:HA	9:J:66:GLY:HA3	2.00	0.42
11:L:170:THR:HG22	12:M:423:LEU:O	2.19	0.42
12:M:542:PRO:HB2	12:M:543:LYS:HD3	2.01	0.42
12:M:573:GLY:HA3	13:N:137:TRP:CD1	2.55	0.42
17:T:52:ARG:O	17:T:55:ARG:HG2	2.20	0.42
1:A:40:ARG:NH1	1:A:289:GLU:O	2.40	0.42
2:B:166:VAL:HG11	2:B:199:ILE:CG2	2.49	0.42
13:N:106:ARG:O	13:N:109:ILE:HG12	2.18	0.42
1:A:47:GLY:HA2	1:A:133:HIS:HB3	2.00	0.42
2:B:40:ASN:C	2:B:42:GLN:H	2.21	0.42
2:B:176:GLU:OE1	3:C:200:LYS:HD2	2.20	0.42
16:Q:281:GLU:CD	16:Q:281:GLU:N	2.73	0.42
17:T:83:ARG:HH12	17:T:103:LEU:H	1.68	0.42
1:A:227:PRO:HB2	1:A:228:PRO:HD3	2.00	0.42
6:G:87:LEU:HA	6:G:90:TYR:HB3	2.00	0.42
8:I:5:THR:HB	8:I:8:ILE:HD12	2.00	0.42
7:H:47:TYR:OH	8:I:92:LYS:HG3	2.20	0.42
8:I:94:ALA:HB1	15:P:105:ASN:HD21	1.84	0.42
9:J:128:ASN:O	9:J:129:LEU:HD12	2.19	0.42
11:L:130:THR:O	11:L:133:ASP:HB3	2.19	0.42
12:M:543:LYS:N	12:M:543:LYS:HD2	2.35	0.42
12:M:559:ASP:OD1	12:M:560:LEU:N	2.51	0.42
12:M:319:TRP:HH2	12:M:617:ARG:NE	2.18	0.42
12:M:49:VAL:HG23	12:M:94:MET:O	2.20	0.42
15:P:109:LYS:O	15:P:110:SER:OG	2.31	0.42
16:Q:338:ARG:O	16:Q:341:LEU:HB2	2.19	0.42
1:A:32:PHE:HB3	1:A:294:VAL:HA	2.02	0.42
1:A:122:PRO:HB2	1:A:322:SER:HB2	2.01	0.42
5:F:57:GLU:HB3	12:M:662:ALA:N	2.24	0.42
7:H:50:GLN:HE22	8:I:93:LYS:HD2	1.85	0.42
9:J:171:ASN:O	9:J:181:LEU:HG	2.18	0.42
12:M:560:LEU:HD12	12:M:561:PRO:HD2	2.02	0.42
15:P:200:LYS:HE2	16:Q:420:TYR:CE1	2.55	0.42
15:P:202:PHE:HB2	15:P:207:TYR:CE2	2.55	0.42
16:Q:371:MET:HA	16:Q:377:SER:OG	2.20	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:159:ARG:HD3	1:A:162:PHE:CE2	2.55	0.42
3:C:150:MET:SD	3:C:190:LEU:HD13	2.60	0.42
7:H:81:ILE:HG13	7:H:82:LEU:N	2.34	0.42
9:J:283:VAL:HG13	9:J:369:VAL:HG11	2.02	0.42
10:K:101:SER:OG	10:K:102:GLY:N	2.53	0.42
11:L:79:ILE:HD12	11:L:145:TYR:CD2	2.54	0.42
12:M:357:LEU:O	12:M:361:VAL:HG22	2.20	0.42
12:M:711:VAL:O	12:M:715:THR:HG23	2.19	0.42
16:Q:82:LEU:HD12	16:Q:101:LEU:HD12	2.00	0.42
16:Q:199:PRO:HB3	16:Q:258:LEU:HD21	2.01	0.42
16:Q:275:ILE:HD13	16:Q:446:ASP:OD1	2.20	0.42
16:Q:99:MET:HE2	16:Q:447:VAL:HG21	2.02	0.42
17:T:40:THR:OG1	17:T:44:GLN:HG2	2.20	0.42
8:I:40:LYS:HG2	18:W:8:GLN:HA	2.00	0.42
1:A:262:PHE:CZ	1:A:272:GLY:HA3	2.54	0.42
4:E:25:MET:O	4:E:29:LYS:N	2.44	0.42
9:J:152:ILE:HG22	9:J:164:PHE:CE1	2.55	0.42
12:M:314:LEU:HD22	12:M:583:ILE:HD12	2.02	0.42
12:M:307:VAL:HA	12:M:582:VAL:HA	2.01	0.42
12:M:66:HIS:CE1	12:M:68:ARG:HG2	2.53	0.42
14:O:213:ILE:HG22	14:O:214:PRO:O	2.20	0.42
1:A:257:ARG:HH12	14:O:239:LYS:NZ	2.17	0.42
16:Q:116:LEU:HD11	16:Q:141:TYR:OH	2.20	0.42
1:A:202:GLY:O	12:M:200:ARG:NH2	2.42	0.42
1:A:223:PRO:HB2	1:A:425:CYS:SG	2.60	0.42
3:C:187:ALA:O	3:C:190:LEU:HB3	2.20	0.42
4:E:102:HIS:HA	4:E:105:ARG:HG3	2.02	0.42
5:F:62:GLN:HE21	5:F:64:LYS:NZ	2.17	0.42
11:L:86:ASN:ND2	12:M:224:ASP:OD2	2.53	0.42
12:M:541:PRO:HA	12:M:542:PRO:HD2	1.77	0.42
12:M:342:ALA:HA	12:M:547:LEU:HB2	2.00	0.42
14:O:176:CYS:HA	23:O:301:FES:S1	2.60	0.42
14:O:53:PHE:HE2	14:O:55:PHE:CE1	2.38	0.42
9:J:209:ARG:HD2	15:P:217:LYS:CE	2.50	0.42
16:Q:235:ASP:HA	16:Q:356:ILE:HD12	2.02	0.42
16:Q:368:ARG:HA	16:Q:371:MET:HG2	2.01	0.42
2:B:96:ARG:HB3	2:B:167:GLU:HG2	2.01	0.41
4:E:78:VAL:O	4:E:82:LEU:HD13	2.20	0.41
11:L:131:LYS:HD2	11:L:147:ILE:HG23	2.02	0.41
12:M:83:GLU:HB2	12:M:101:ASN:HB3	2.02	0.41
12:M:33:GLU:O	12:M:98:LYS:HA	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:N:117:VAL:HG11	13:N:122:GLU:HB2	2.02	0.41
2:B:184:ASN:ND2	13:N:126:PRO:HA	2.35	0.41
14:O:100:LYS:O	14:O:104:VAL:HG23	2.20	0.41
6:G:116:VAL:HA	6:G:119:ILE:HG22	2.01	0.41
12:M:598:ASN:HD22	12:M:602:ARG:NH1	2.19	0.41
13:N:10:GLY:O	13:N:14:ILE:HG13	2.20	0.41
1:A:220:GLN:NE2	14:O:114:GLU:HB3	2.34	0.41
15:P:96:VAL:O	15:P:100:LEU:HG	2.20	0.41
16:Q:149:GLN:OE1	16:Q:171:ARG:HB3	2.20	0.41
16:Q:190:HIS:CE1	16:Q:268:TRP:CH2	3.08	0.41
16:Q:316:PHE:HD1	16:Q:339:GLN:HE21	1.67	0.41
1:A:52:ARG:O	1:A:55:GLY:N	2.51	0.41
6:G:103:HIS:N	6:G:107:ASP:HB2	2.35	0.41
9:J:157:LYS:HA	9:J:195:PHE:HE1	1.85	0.41
9:J:50:SER:O	9:J:77:GLY:HA3	2.20	0.41
12:M:234:LYS:N	12:M:235:PRO:HD2	2.36	0.41
12:M:557:ARG:HE	12:M:579:ILE:HG23	1.86	0.41
15:P:210:LEU:HA	15:P:221:ALA:HA	2.01	0.41
16:Q:233:HIS:CD2	16:Q:234:GLN:HB2	2.55	0.41
8:I:60:ARG:HD2	16:Q:390:GLN:O	2.19	0.41
1:A:413:TRP:HZ3	1:A:436:GLN:HB3	1.84	0.41
1:A:453:PHE:O	1:A:456:GLN:HG2	2.20	0.41
9:J:130:ILE:HA	22:J:401:NDP:H8A	2.02	0.41
9:J:221:HIS:ND1	9:J:222:ARG:HG3	2.31	0.41
9:J:263:PHE:CE1	9:J:333:PRO:HG2	2.55	0.41
4:E:84:ILE:HD13	15:P:177:PHE:CE1	2.56	0.41
16:Q:341:LEU:HA	16:Q:341:LEU:HD23	1.88	0.41
17:T:32:VAL:HG22	17:T:38:LYS:HE3	2.03	0.41
1:A:296:LEU:HD22	1:A:332:CYS:SG	2.61	0.41
12:M:266:ARG:HB3	12:M:271:MET:HE3	2.03	0.41
12:M:236:TYR:CE1	12:M:272:ARG:HB3	2.55	0.41
12:M:492:ALA:O	12:M:496:ILE:HG13	2.19	0.41
12:M:433:GLY:HA3	12:M:684:LEU:HD23	2.01	0.41
13:N:34:LYS:NZ	13:N:54:GLN:HG2	2.36	0.41
15:P:240:GLU:OE1	15:P:246:ARG:NE	2.51	0.41
16:Q:236:LEU:HA	16:Q:237:PRO:HD3	1.93	0.41
1:A:387:GLU:HG2	12:M:119:PHE:O	2.20	0.41
9:J:62:THR:HG21	22:J:401:NDP:O1X	2.21	0.41
12:M:254:MET:CB	12:M:290:THR:HG22	2.46	0.41
12:M:589:TYR:O	12:M:606:THR:HG21	2.20	0.41
14:O:156:LEU:HD13	14:O:158:ILE:HD12	2.03	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
17:T:80:VAL:O	17:T:121:GLN:HA	2.20	0.41
2:B:57:ARG:HG2	2:B:62:THR:OG1	2.21	0.41
8:I:23:LYS:NZ	16:Q:252:SER:HG	2.18	0.41
9:J:98:GLY:HA3	9:J:103:LEU:HG	2.01	0.41
22:J:401:NDP:P2B	22:J:401:NDP:O3B	2.79	0.41
12:M:479:SER:HG	12:M:687:PRO:HD3	1.86	0.41
11:L:117:THR:OG1	15:P:229:GLU:OE1	2.39	0.41
1:A:116:ASN:HB3	20:A:502:FMN:HM83	2.01	0.41
1:A:222:LYS:NZ	12:M:197:THR:HG21	2.35	0.41
1:A:339:PHE:HA	1:A:342:LEU:HD12	2.03	0.41
1:A:382:CYS:HA	12:M:75:CYS:H	1.85	0.41
5:F:23:LEU:HD21	5:F:34:ARG:HG2	2.03	0.41
5:F:89:ARG:HD2	5:F:92:GLU:OE2	2.21	0.41
9:J:329:LEU:HD22	9:J:332:LEU:HD12	2.01	0.41
12:M:382:ARG:NE	12:M:527:ASP:OD1	2.54	0.41
12:M:436:VAL:HG21	12:M:686:PRO:HG2	2.02	0.41
1:A:122:PRO:HA	14:O:176:CYS:SG	2.61	0.41
14:O:236:GLU:C	14:O:238:PRO:HD2	2.41	0.41
17:T:33:SER:HB3	17:T:45:VAL:HG21	2.03	0.41
1:A:113:LEU:HD23	1:A:114:VAL:N	2.35	0.41
1:A:329:LYS:HA	1:A:332:CYS:HB3	2.02	0.41
20:A:502:FMN:H9	20:A:502:FMN:H1'2	1.76	0.41
2:B:128:ILE:HG12	2:B:143:TYR:CD1	2.56	0.41
2:B:146:ASP:OD2	2:B:149:LYS:HE2	2.21	0.41
14:O:148:ILE:O	14:O:152:ILE:HG13	2.21	0.41
16:Q:310:VAL:O	16:Q:314:VAL:HG23	2.21	0.41
16:Q:331:LEU:O	16:Q:335:GLU:HG3	2.21	0.41
3:C:213:ARG:O	3:C:213:ARG:HG2	2.19	0.41
3:C:98:ALA:HB1	3:C:99:PRO:HD2	2.03	0.41
7:H:19:THR:N	7:H:20:PRO:HD3	2.35	0.41
9:J:179:ARG:HH11	9:J:179:ARG:HB3	1.84	0.41
11:L:123:ASN:HB3	15:P:232:LYS:HD2	2.02	0.41
12:M:246:ARG:NH2	15:P:229:GLU:OE2	2.54	0.41
14:O:87:GLN:OE1	14:O:122:TYR:HA	2.21	0.41
15:P:77:GLN:HB2	15:P:85:GLU:HB2	2.03	0.41
15:P:81:PHE:HE1	16:Q:157:LYS:O	2.03	0.41
1:A:284:HIS:CE1	14:O:229:GLY:HA3	2.56	0.41
2:B:101:LEU:O	2:B:192:GLY:HA3	2.21	0.41
2:B:62:THR:OG1	2:B:63:GLU:N	2.53	0.41
3:C:137:VAL:HA	3:C:140:GLN:OE1	2.20	0.41
3:C:81:PRO:HA	3:C:119:VAL:HG13	2.03	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:J:201:VAL:HG13	9:J:265:PHE:CD2	2.55	0.41
9:J:329:LEU:HD13	9:J:332:LEU:HD12	2.03	0.41
12:M:483:ARG:HG3	12:M:483:ARG:O	2.21	0.41
14:O:198:ALA:O	14:O:202:GLU:HG2	2.21	0.41
16:Q:204:PHE:CE1	16:Q:207:ARG:HD3	2.56	0.41
1:A:63:TYR:CD2	1:A:64:LYS:HG3	2.55	0.40
2:B:102:ARG:HB2	2:B:196:GLU:OE2	2.21	0.40
2:B:90:PRO:O	2:B:91:LEU:HD12	2.22	0.40
6:G:123:GLU:HB3	6:G:130:ILE:HG12	2.04	0.40
9:J:157:LYS:HB2	9:J:195:PHE:HD1	1.86	0.40
9:J:168:SER:CA	9:J:184:LYS:CE	2.99	0.40
9:J:271:TYR:HE1	9:J:374:THR:HB	1.85	0.40
11:L:78:ARG:HD2	12:M:607:LYS:HE2	2.02	0.40
12:M:401:LEU:HD13	12:M:462:PHE:CE2	2.56	0.40
14:O:168:LEU:HD22	14:O:169:PHE:CE2	2.56	0.40
15:P:148:ASP:HB2	15:P:151:THR:HG23	2.02	0.40
16:Q:316:PHE:HB2	16:Q:339:GLN:CG	2.51	0.40
2:B:160:CYS:HA	2:B:161:PRO:HD2	1.83	0.40
3:C:79:LEU:O	3:C:108:VAL:HA	2.21	0.40
4:E:37:ARG:HH21	4:E:41:ARG:HH22	1.68	0.40
6:G:154:VAL:O	6:G:156:GLU:HG3	2.22	0.40
13:N:39:VAL:HG12	13:N:40:GLY:O	2.21	0.40
14:O:186:VAL:HG12	14:O:188:ILE:HG13	2.03	0.40
12:M:198:THR:CG2	14:O:39:PHE:HB3	2.47	0.40
16:Q:120:THR:O	16:Q:124:ILE:HG13	2.22	0.40
16:Q:153:LEU:O	16:Q:157:LYS:HG3	2.21	0.40
16:Q:331:LEU:HA	16:Q:331:LEU:HD23	1.84	0.40
1:A:314:LEU:O	1:A:329:LYS:HD2	2.21	0.40
2:B:155:PHE:HB2	19:B:302:SF4:S2	2.61	0.40
2:B:169:PRO:HG3	2:B:198:GLU:CG	2.51	0.40
2:B:84:TYR:CD1	2:B:85:PRO:HA	2.56	0.40
7:H:45:ARG:O	7:H:49:GLU:HG3	2.21	0.40
9:J:202:LYS:N	9:J:263:PHE:O	2.54	0.40
12:M:403:VAL:HG22	12:M:432:ILE:HD12	2.03	0.40
12:M:522:GLN:HE21	12:M:526:LEU:HG	1.85	0.40
12:M:646:LEU:O	12:M:651:PRO:HA	2.20	0.40
14:O:110:MET:HA	14:O:113:TYR:CD2	2.56	0.40
15:P:61:PHE:O	15:P:64:TYR:HB3	2.20	0.40
16:Q:303:ARG:HG3	16:Q:401:GLU:HG3	2.03	0.40
16:Q:314:VAL:HG12	16:Q:316:PHE:HD2	1.87	0.40
1:A:249:ALA:O	1:A:252:PRO:HD2	2.21	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:E:42:GLU:OE2	4:E:46:THR:OG1	2.40	0.40
5:F:22:HIS:ND1	5:F:64:LYS:HD2	2.36	0.40
12:M:128:CYS:HA	19:M:801:SF4:S4	2.61	0.40
12:M:198:THR:CG2	14:O:117:THR:HG21	2.52	0.40
15:P:100:LEU:O	15:P:108:PHE:HD2	2.05	0.40
7:H:12:VAL:CG1	16:Q:280:ALA:N	2.81	0.40
1:A:288:VAL:HG21	1:A:303:HIS:CD2	2.57	0.40
1:A:292:MET:O	1:A:338:ASP:N	2.55	0.40
1:A:73:PRO:O	1:A:75:TRP:N	2.55	0.40
2:B:143:TYR:HB3	2:B:185:LYS:HB2	2.03	0.40
5:F:14:LEU:N	5:F:17:ARG:HH12	2.20	0.40
5:F:20:ARG:CG	5:F:66:TRP:HB2	2.51	0.40
8:I:65:PRO:HD3	15:P:245:TYR:CE2	2.56	0.40
11:L:163:ASN:O	11:L:171:ARG:N	2.55	0.40
1:A:222:LYS:HB2	11:L:175:LYS:O	2.22	0.40
12:M:408:ARG:O	12:M:412:PRO:HG3	2.22	0.40
12:M:568:TYR:HB2	12:M:580:ALA:CB	2.51	0.40
15:P:114:LEU:HG	15:P:130:TYR:CE1	2.56	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 PDB entries followed by that with respect to all EM entries.

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	429/431 (100%)	396 (92%)	24 (6%)	9 (2%)	8	43
2	B	174/176 (99%)	163 (94%)	10 (6%)	1 (1%)	28	68
3	C	154/156 (99%)	137 (89%)	12 (8%)	5 (3%)	5	34
4	E	111/113 (98%)	101 (91%)	8 (7%)	2 (2%)	10	46
5	F	81/83 (98%)	74 (91%)	7 (9%)	0	100	100
6	G	83/85 (98%)	78 (94%)	3 (4%)	2 (2%)	7	40

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
7	H	110/112 (98%)	100 (91%)	5 (4%)	5 (4%)	3	24
8	I	91/110 (83%)	79 (87%)	6 (7%)	6 (7%)	1	15
9	J	335/337 (99%)	314 (94%)	14 (4%)	7 (2%)	8	43
10	K	31/33 (94%)	27 (87%)	1 (3%)	3 (10%)	1	7
11	L	116/118 (98%)	104 (90%)	8 (7%)	4 (3%)	4	32
12	M	685/687 (100%)	608 (89%)	54 (8%)	23 (3%)	4	32
13	N	141/143 (99%)	119 (84%)	15 (11%)	7 (5%)	2	22
14	O	210/212 (99%)	188 (90%)	15 (7%)	7 (3%)	4	33
15	P	206/208 (99%)	173 (84%)	22 (11%)	11 (5%)	2	20
16	Q	383/385 (100%)	355 (93%)	23 (6%)	5 (1%)	14	53
17	T	93/95 (98%)	87 (94%)	2 (2%)	4 (4%)	3	26
18	W	20/22 (91%)	16 (80%)	1 (5%)	3 (15%)	0	2
All	All	3453/3506 (98%)	3119 (90%)	230 (7%)	104 (3%)	9	35

All (104) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	63	TYR
1	A	73	PRO
1	A	379	CYS
2	B	62	THR
12	M	37	ASP
12	M	47	THR
12	M	178	GLN
12	M	210	ILE
12	M	369	GLU
13	N	115	PHE
14	O	232	THR
14	O	246	GLN
15	P	167	GLU
17	T	82	THR
3	C	84	PHE
3	C	165	SER
4	E	20	ILE
4	E	127	ASP
6	G	138	LEU
7	H	105	GLU
8	I	31	ILE

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Mol	Chain	Res	Type
8	I	93	LYS
8	I	107	SER
9	J	87	ASP
11	L	173	SER
12	M	250	SER
12	M	482	GLN
12	M	484	ASN
12	M	562	LYS
12	M	663	ASN
12	M	676	ASN
13	N	19	GLY
13	N	76	ASP
14	O	49	PRO
14	O	160	VAL
16	Q	104	GLU
16	Q	117	HIS
17	T	44	GLN
18	W	11	PRO
1	A	74	ASP
7	H	8	THR
7	H	63	PRO
8	I	52	ASN
9	J	135	GLU
9	J	178	SER
10	K	101	SER
11	L	165	SER
12	M	538	ARG
12	M	677	GLN
12	M	689	LEU
12	M	715	THR
13	N	113	HIS
14	O	238	PRO
15	P	44	ARG
15	P	179	ALA
15	P	214	ASP
15	P	229	GLU
16	Q	197	MET
17	T	83	ARG
1	A	50	ASP
1	A	186	ALA
3	C	156	GLY
7	H	76	GLN

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Mol	Chain	Res	Type
8	I	108	SER
9	J	100	LEU
9	J	330	PRO
9	J	370	LYS
10	K	78	ASP
11	L	172	VAL
12	M	377	ALA
12	M	426	ASP
13	N	42	ASP
13	N	130	THR
14	O	216	PRO
14	O	230	GLY
15	P	175	GLY
15	P	246	ARG
18	W	16	TYR
1	A	228	PRO
1	A	420	GLU
7	H	103	LEU
9	J	259	ASN
12	M	281	ILE
12	M	548	LEU
12	M	667	GLN
15	P	110	SER
15	P	202	PHE
15	P	239	TRP
15	P	245	TYR
16	Q	102	SER
3	C	102	ASP
6	G	137	LYS
8	I	70	MET
11	L	96	LYS
12	M	446	GLY
13	N	135	GLN
12	M	435	PRO
17	T	90	GLY
18	W	10	MET
1	A	94	PRO
12	M	575	VAL
3	C	144	PRO
16	Q	307	PRO
10	K	102	GLY

### 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 PDB entries followed by that with respect to all EM entries.

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	346/346 (100%)	346 (100%)	0	100	100
2	B	151/151 (100%)	151 (100%)	0	100	100
3	C	132/132 (100%)	132 (100%)	0	100	100
4	E	106/106 (100%)	105 (99%)	1 (1%)	82	92
5	F	74/74 (100%)	74 (100%)	0	100	100
6	G	74/79 (94%)	74 (100%)	0	100	100
7	H	100/100 (100%)	100 (100%)	0	100	100
8	I	87/96 (91%)	87 (100%)	0	100	100
9	J	292/292 (100%)	288 (99%)	4 (1%)	71	88
10	K	32/32 (100%)	32 (100%)	0	100	100
11	L	107/107 (100%)	107 (100%)	0	100	100
12	M	576/577 (100%)	574 (100%)	2 (0%)	94	98
13	N	129/129 (100%)	129 (100%)	0	100	100
14	O	181/181 (100%)	181 (100%)	0	100	100
15	P	190/190 (100%)	190 (100%)	0	100	100
16	Q	331/331 (100%)	329 (99%)	2 (1%)	89	95
17	T	79/79 (100%)	79 (100%)	0	100	100
18	W	19/19 (100%)	19 (100%)	0	100	100
All	All	3006/3021 (100%)	2997 (100%)	9 (0%)	94	98

All (9) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
4	E	31	ARG
9	J	85	ARG
9	J	91	ILE
9	J	180	TYR
9	J	212	ARG
12	M	130	ILE

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Mol	Chain	Res	Type
12	M	174	THR
16	Q	268	TRP
16	Q	273	ILE

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (64) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	44	ASN
1	A	116	ASN
1	A	164	ASN
1	A	170	GLN
1	A	284	HIS
1	A	313	ASN
1	A	441	HIS
2	B	184	ASN
3	C	95	HIS
4	E	48	HIS
4	E	49	GLN
4	E	51	GLN
4	E	70	ASN
5	F	62	GLN
5	F	81	ASN
6	G	80	GLN
6	G	101	ASN
7	H	50	GLN
7	H	73	GLN
7	H	76	GLN
7	H	83	GLN
7	H	111	GLN
8	I	73	GLN
9	J	71	ASN
9	J	102	GLN
9	J	183	ASN
10	K	77	HIS
11	L	71	HIS
11	L	86	ASN
12	M	384	ASN
12	M	425	ASN
12	M	444	HIS
12	M	460	HIS
12	M	464	GLN
12	M	498	GLN

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Mol	Chain	Res	Type
12	M	514	ASN
12	M	688	GLN
13	N	91	HIS
13	N	113	HIS
13	N	135	GLN
14	O	59	ASN
14	O	69	ASN
14	O	189	ASN
14	O	191	ASN
15	P	74	GLN
15	P	82	ASN
15	P	105	ASN
15	P	124	ASN
15	P	247	GLN
16	Q	79	ASN
16	Q	87	GLN
16	Q	88	HIS
16	Q	147	ASN
16	Q	182	ASN
16	Q	183	HIS
16	Q	190	HIS
16	Q	233	HIS
16	Q	234	GLN
16	Q	339	GLN
16	Q	431	HIS
16	Q	442	HIS
16	Q	454	GLN
17	T	64	ASN
18	W	8	GLN

### 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 carbohydrates in this entry.

## 5.6 Ligand geometry

11 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
19	SF4	A	501	1	0,12,12	0.00	-	0,24,24	0.00	-
20	FMN	A	502	-	31,33,33	1.47	5 (16%)	38,50,50	1.96	7 (18%)
19	SF4	B	301	2	0,12,12	0.00	-	0,24,24	0.00	-
19	SF4	B	302	2	0,12,12	0.00	-	0,24,24	0.00	-
19	SF4	C	301	3	0,12,12	0.00	-	0,24,24	0.00	-
21	8Q1	E	201	-	32,34,34	1.65	6 (18%)	39,43,43	1.53	8 (20%)
22	NDP	J	401	-	43,52,52	0.98	2 (4%)	49,80,80	1.41	3 (6%)
19	SF4	M	801	12	0,12,12	0.00	-	0,24,24	0.00	-
19	SF4	M	802	12	0,12,12	0.00	-	0,24,24	0.00	-
23	FES	M	803	-	0,4,4	0.00	-	0,4,4	0.00	-
23	FES	O	301	14	0,4,4	0.00	-	0,4,4	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
19	SF4	A	501	1	-	0/0/48/48	0/6/5/5
20	FMN	A	502	-	-	0/16/18/18	0/3/3/3
19	SF4	B	301	2	-	0/0/48/48	0/6/5/5
19	SF4	B	302	2	-	0/0/48/48	0/6/5/5
19	SF4	C	301	3	-	0/0/48/48	0/6/5/5
21	8Q1	E	201	-	-	2/41/41/41	0/0/0/0
22	NDP	J	401	-	-	0/30/77/77	0/5/5/5
19	SF4	M	801	12	-	0/0/48/48	0/6/5/5
19	SF4	M	802	12	-	0/0/48/48	0/6/5/5
23	FES	M	803	-	-	0/0/4/4	0/1/1/1
23	FES	O	301	14	-	0/0/4/4	0/1/1/1

All (13) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
21	E	201	8Q1	O35-C34	-2.50	1.18	1.23
21	E	201	8Q1	O40-C39	-2.27	1.18	1.23
20	A	502	FMN	C6-C5A	-2.04	1.38	1.41
21	E	201	8Q1	C6-C1	2.11	1.53	1.50
22	J	401	NDP	C5A-C4A	2.59	1.46	1.40
21	E	201	8Q1	C1-S44	2.61	1.81	1.76
20	A	502	FMN	C9A-C5A	2.93	1.48	1.42
20	A	502	FMN	C8-C7	3.00	1.48	1.41
22	J	401	NDP	C6N-C5N	3.01	1.38	1.33
20	A	502	FMN	C4-C4A	3.81	1.48	1.41
20	A	502	FMN	C4A-C10	3.82	1.47	1.41
21	E	201	8Q1	C39-N41	4.77	1.44	1.33
21	E	201	8Q1	C34-N36	5.61	1.45	1.33

All (18) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	J	401	NDP	N3A-C2A-N1A	-7.00	122.77	128.86
20	A	502	FMN	C4-C4A-C10	-3.98	116.74	119.96
20	A	502	FMN	C4A-C4-N3	-3.38	118.67	123.48
21	E	201	8Q1	O4-C1-C6	-3.38	120.99	123.95
22	J	401	NDP	C4A-C5A-N7A	-2.66	106.84	109.41
21	E	201	8Q1	O4-C1-S44	-2.44	120.28	122.84
21	E	201	8Q1	O35-C34-N36	-2.39	118.46	123.07
21	E	201	8Q1	C42-N41-C39	-2.35	118.33	122.84
21	E	201	8Q1	C37-N36-C34	-2.30	118.30	122.59
22	J	401	NDP	C3D-C2D-C1D	2.19	105.64	101.43
21	E	201	8Q1	C32-C34-N36	2.61	122.02	116.58
21	E	201	8Q1	C43-S44-C1	2.62	110.57	101.90
20	A	502	FMN	C5A-C9A-N10	2.94	119.84	117.66
20	A	502	FMN	C1'-N10-C10	3.27	121.86	118.50
20	A	502	FMN	C4-C4A-N5	3.28	122.27	118.68
20	A	502	FMN	C4A-N5-C5A	3.45	120.41	116.76
21	E	201	8Q1	C6-C1-S44	5.40	118.72	113.28
20	A	502	FMN	C4-N3-C2	7.27	121.52	115.16

There are no chirality outliers.

All (2) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
21	E	201	8Q1	C29-C32-C34-N36
21	E	201	8Q1	O35-C34-C32-C29

There are no ring outliers.

10 monomers are involved in 64 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
19	A	501	SF4	6	0
20	A	502	FMN	17	0
19	B	301	SF4	1	0
19	B	302	SF4	2	0
19	C	301	SF4	1	0
21	E	201	8Q1	4	0
22	J	401	NDP	26	0
19	M	801	SF4	4	0
23	M	803	FES	1	0
23	O	301	FES	2	0

## 5.7 Other polymers [i](#)

There are no such residues in this entry.

## 5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.