



Full wwPDB EM Validation Report ⓘ

Aug 5, 2026 – 08:44 AM JST

PDB ID : 5XTB / pdb_00005xtb
EMDB ID : EMD-6771
Title : Cryo-EM structure of human respiratory complex I matrix arm
Authors : Gu, J.; Wu, M.; Yang, M.
Deposited on : 2017-06-18
Resolution : 3.40 Å(reported)

This is a Full wwPDB EM Validation Report for a publicly released PDB entry.

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A user guide is available at

<https://www.wwpdb.org/validation/2017/EMValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

EMDB validation analysis : 0.0.1.dev133
Mogul : 1.8.5 (274361), CSD as541be (2020)
MolProbity : 4-5-2 with Phenix2.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data in the EMDB archive up until May 2025)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.50

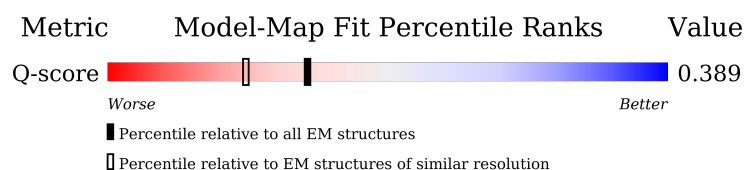
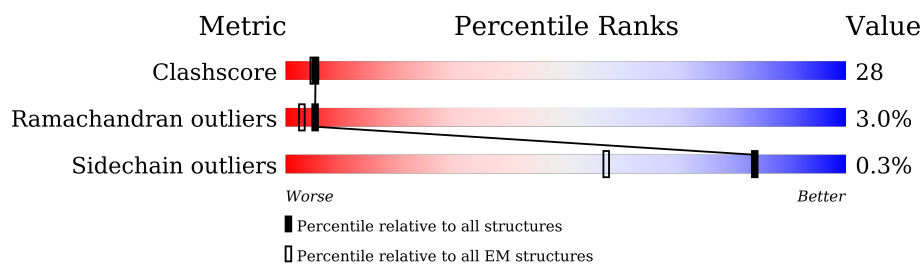
1 Overall quality at a glance

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)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
Q-score	-	25397	14717 (2.90 - 3.90)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the map. The red, orange, yellow and green segments of the bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the EM map (all-atom inclusion $< 40\%$). The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	431	
2	B	176	
3	C	156	
4	E	113	

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Mol	Chain	Length	Quality of chain
5	F	83	
6	G	85	
7	H	112	
8	I	110	
9	J	337	
10	K	33	
11	L	118	
12	M	687	
13	N	143	
14	O	212	
15	P	208	
16	Q	385	
17	T	95	
18	W	22	

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		

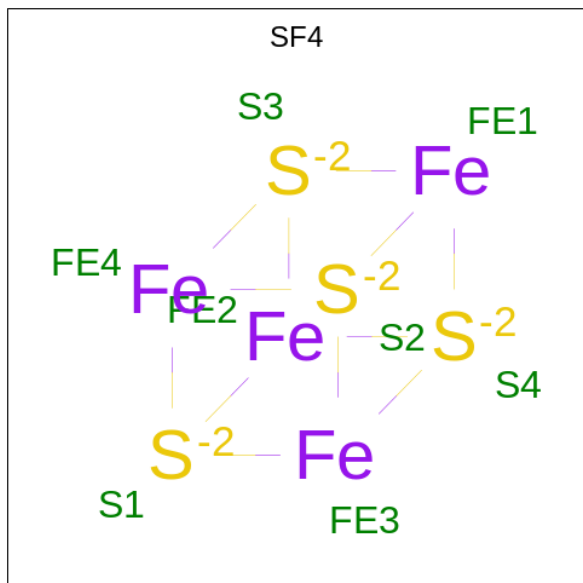
- Molecule 17 is a protein called NADH dehydrogenase [ubiquinone] iron-sulfur protein 6, mitochondrial.

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.

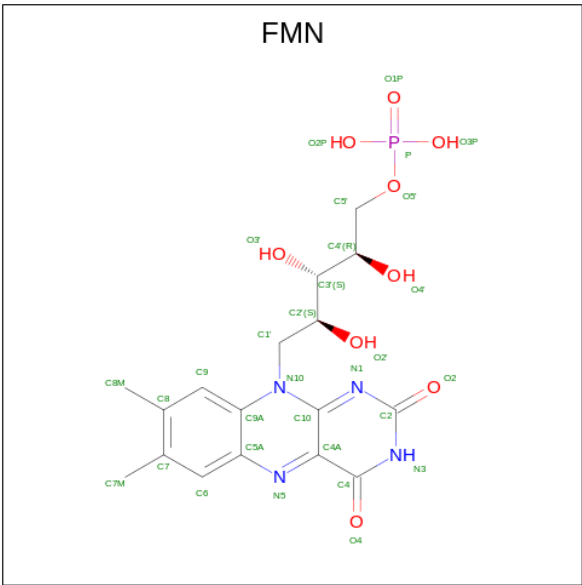
Mol	Chain	Residues	Atoms					AltConf	Trace
18	W	22	Total	C	N	O	S	0	0
			179	113	35	30	1		

- Molecule 19 is IRON/SULFUR CLUSTER (CCD ID: SF4) (formula: Fe_4S_4).



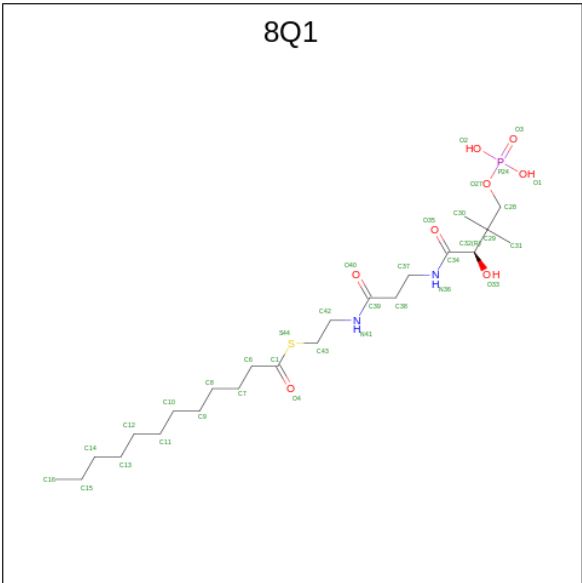
Mol	Chain	Residues	Atoms			AltConf
19	A	1	Total	Fe	S	0
			8	4	4	
19	B	1	Total	Fe	S	0
			8	4	4	
19	B	1	Total	Fe	S	0
			8	4	4	
19	C	1	Total	Fe	S	0
			8	4	4	
19	M	1	Total	Fe	S	0
			8	4	4	
19	M	1	Total	Fe	S	0
			8	4	4	

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



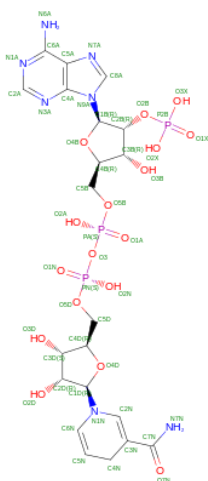
Mol	Chain	Residues	Atoms					AltConf
20	A	1	Total	C	N	O	P	0
			31	17	4	9	1	

- Molecule 21 is S-[2-({N-[(2R)-2-hydroxy-3,3-dimethyl-4-(phosphonooxy)butanoyl]-beta-alanyl}amino)ethyl] dodecanethioate (CCD ID: 8Q1) (formula: C₂₃H₄₅N₂O₈PS).



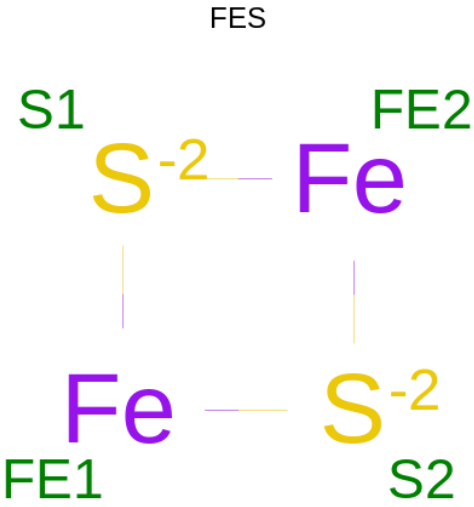
Mol	Chain	Residues	Atoms					AltConf	
21	E	1	Total	C	N	O	P	S	0
			35	23	2	8	1	1	

- Molecule 22 is NADPH DIHYDRO-NICOTINAMIDE-ADENINE-DINUCLEOTIDE PHOSPHATE (CCD ID: NDP) (formula: C₂₁H₃₀N₇O₁₇P₃).



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

- Molecule 23 is FE2/S2 (INORGANIC) CLUSTER (CCD ID: FES) (formula: Fe_2S_2).

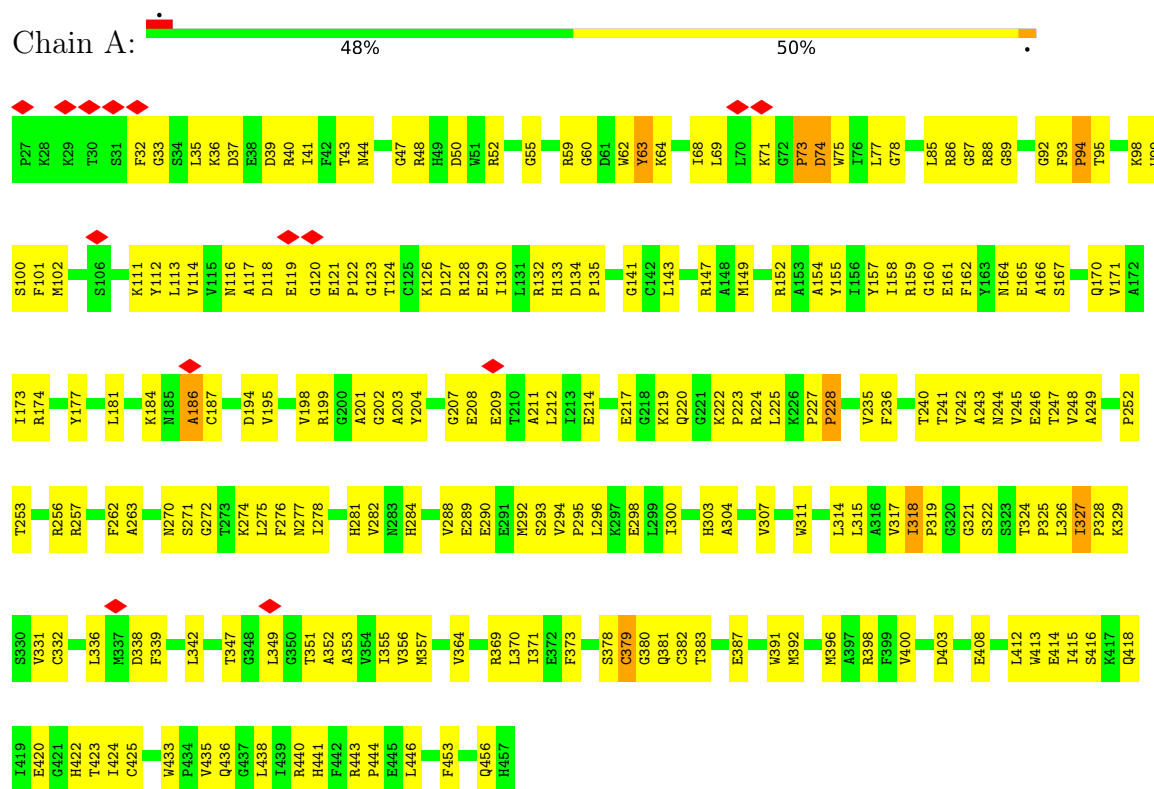


Mol	Chain	Residues	Atoms			AltConf
23	M	1	Total 4	Fe 2	S 2	0
23	O	1	Total 4	Fe 2	S 2	0

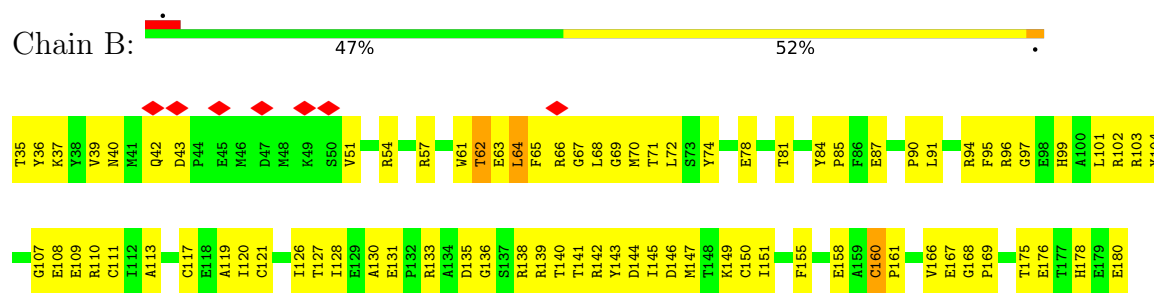
3 Residue-property plots

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion in map density. 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. A red diamond above a residue indicates a poor fit to the EM map for this residue (all-atom inclusion < 40%). 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

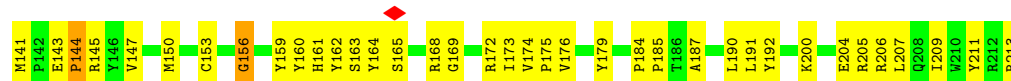
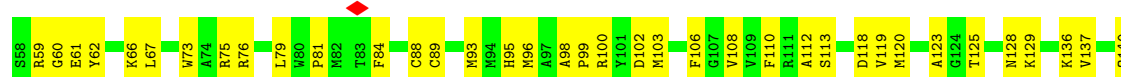


- Molecule 2: NADH dehydrogenase [ubiquinone] iron-sulfur protein 8, mitochondrial

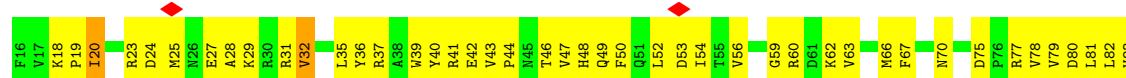




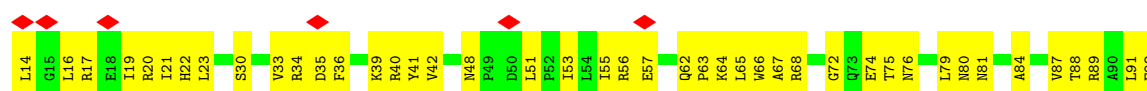
- Molecule 3: NADH dehydrogenase [ubiquinone] iron-sulfur protein 7, mitochondrial



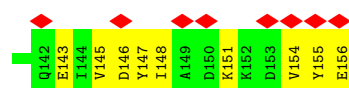
- Molecule 4: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 6



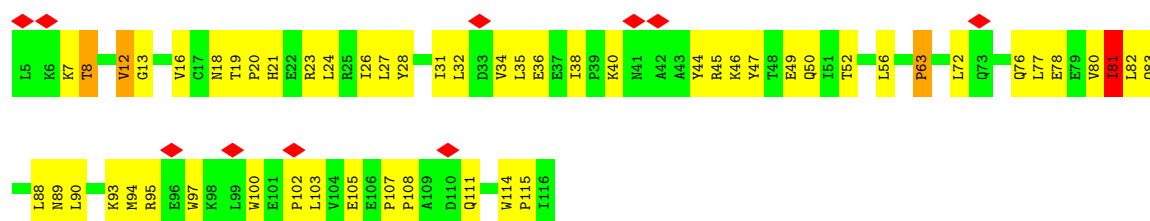
- Molecule 5: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 2



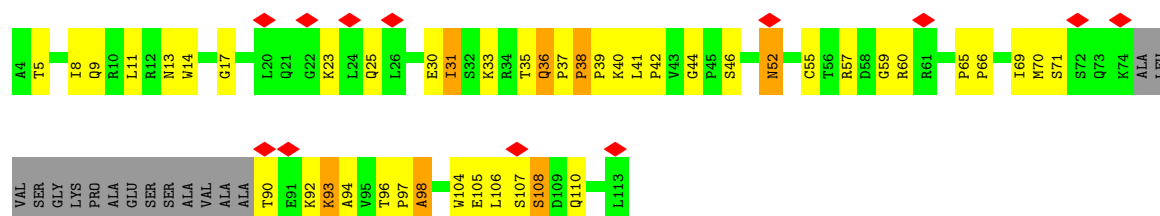
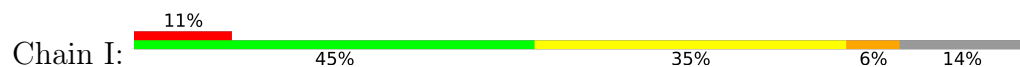
- Molecule 6: Acyl carrier protein, mitochondrial



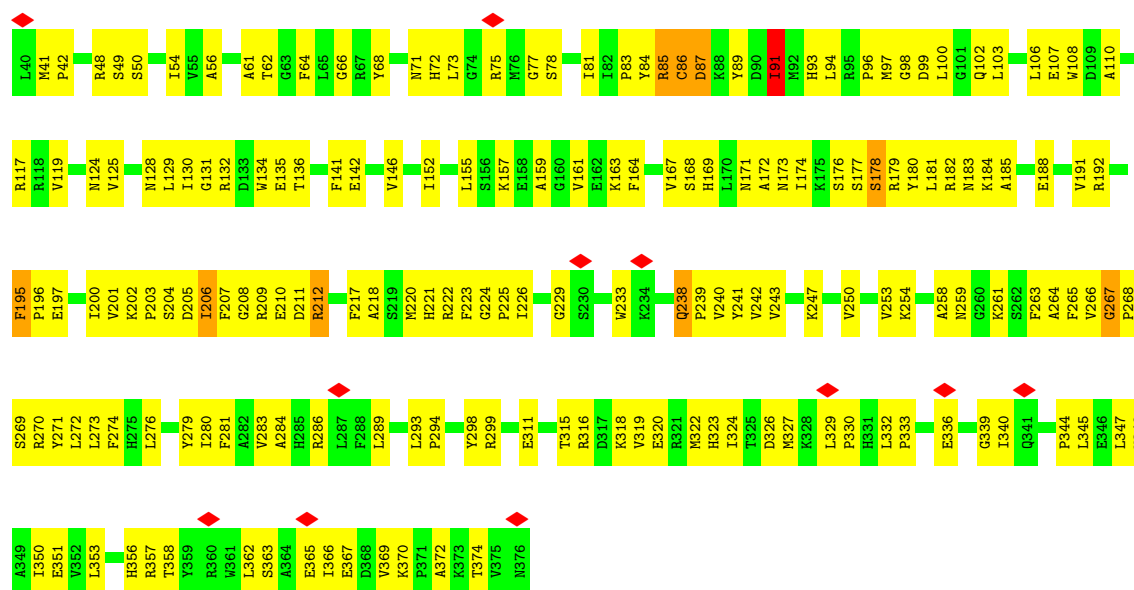
- Molecule 7: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 5



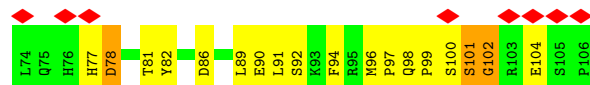
- Molecule 8: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 7



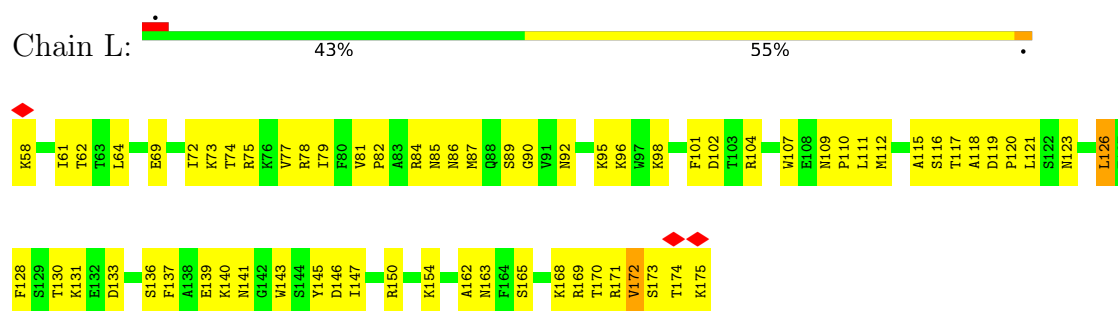
- Molecule 9: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 9, mitochondrial



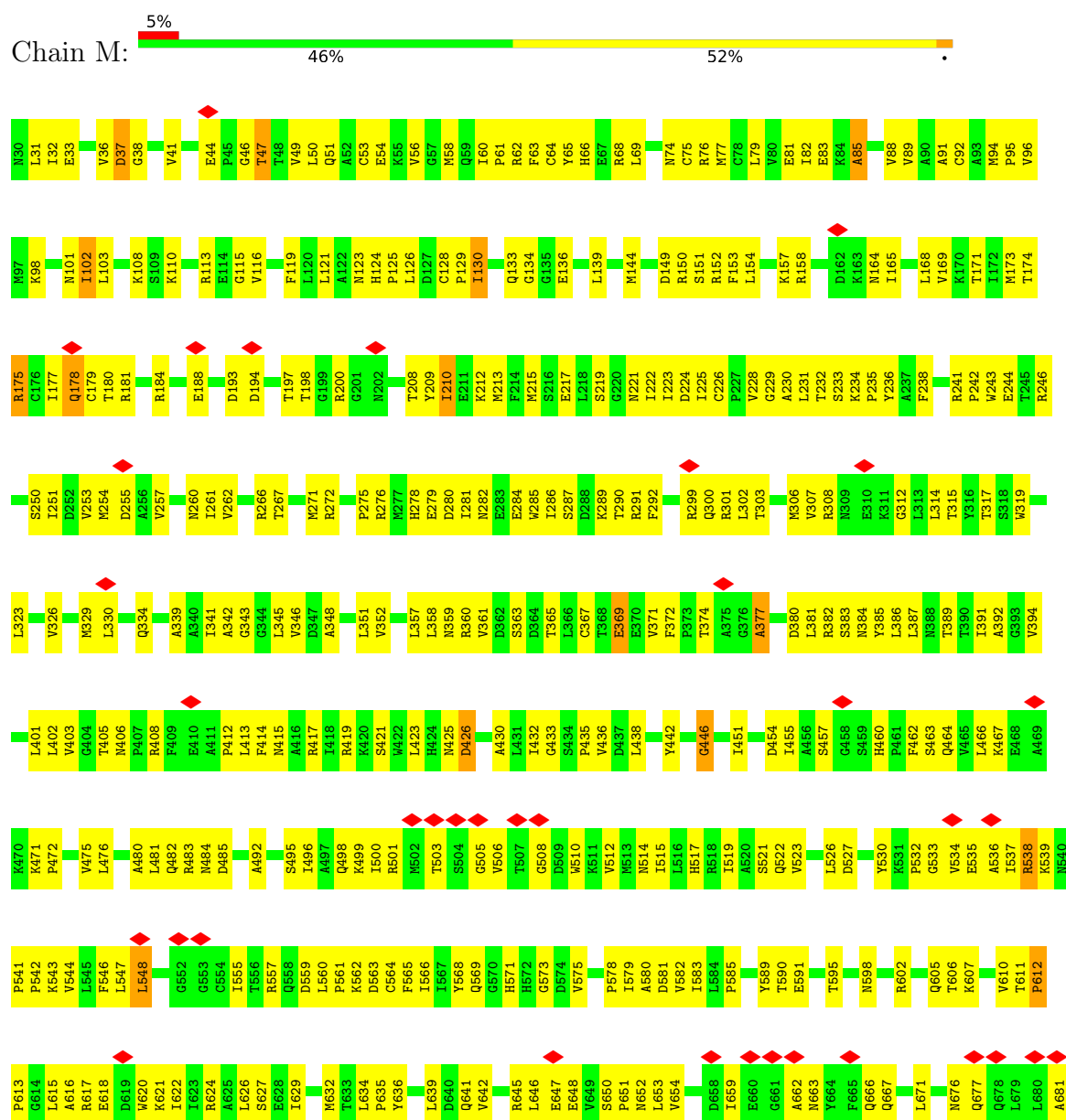
- Molecule 10: NADH dehydrogenase [ubiquinone] flavoprotein 3, mitochondrial



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

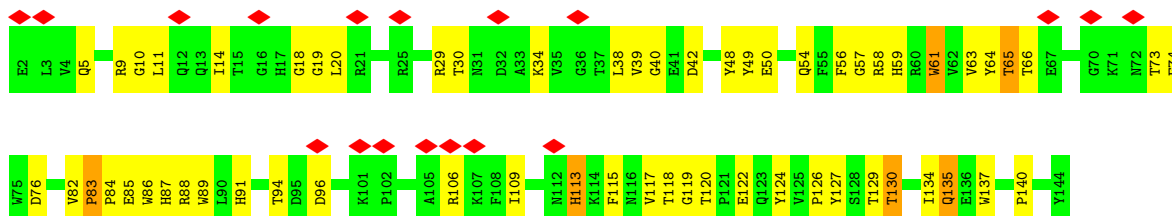


- Molecule 12: NADH-ubiquinone oxidoreductase 75 kDa subunit, mitochondrial

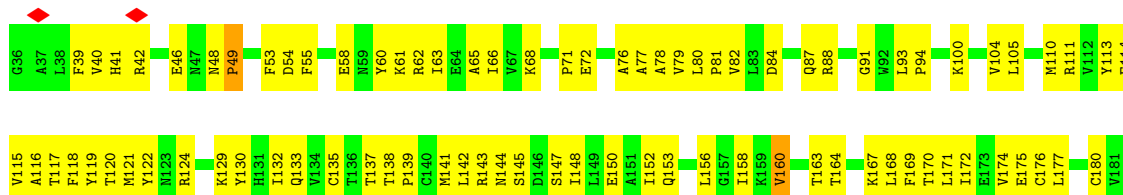




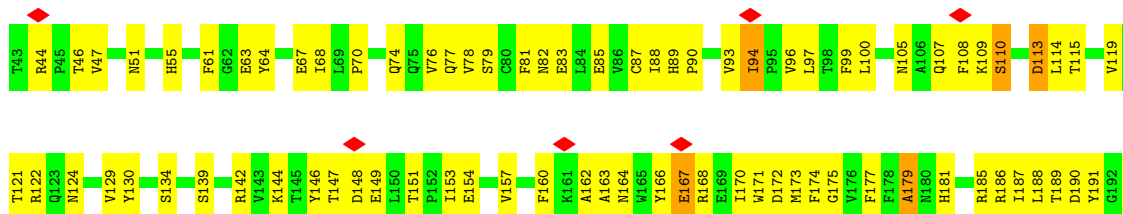
- Molecule 13: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 12



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

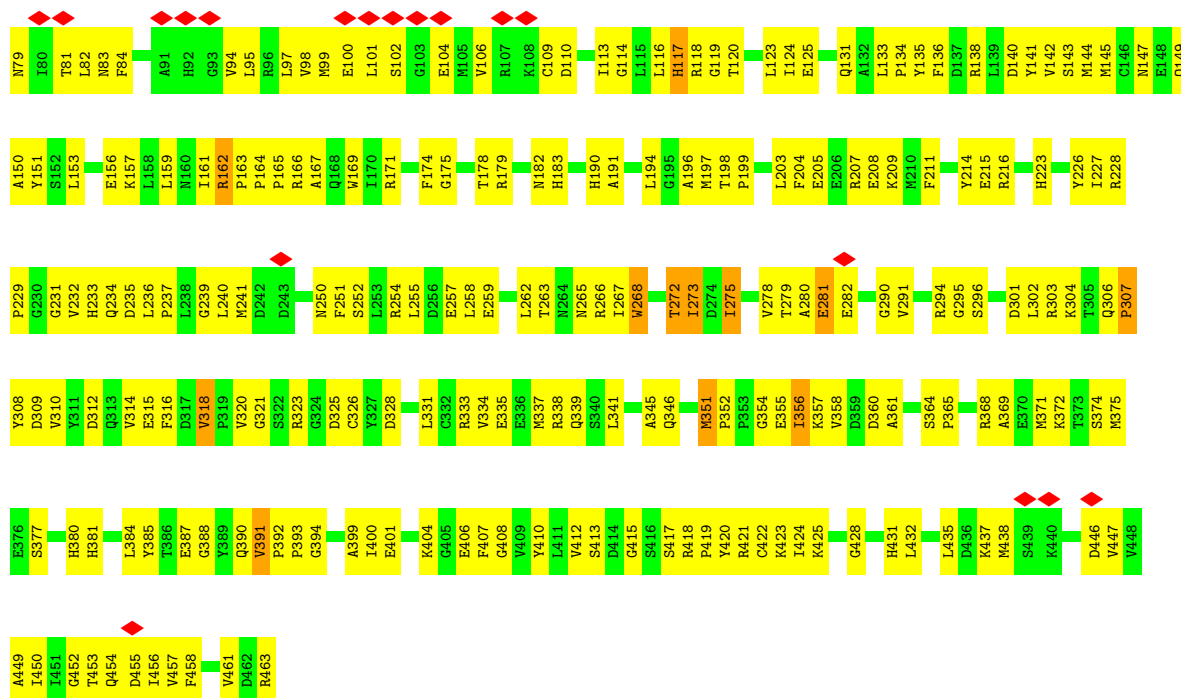


- Molecule 15: NADH dehydrogenase [ubiquinone] iron-sulfur protein 3, mitochondrial

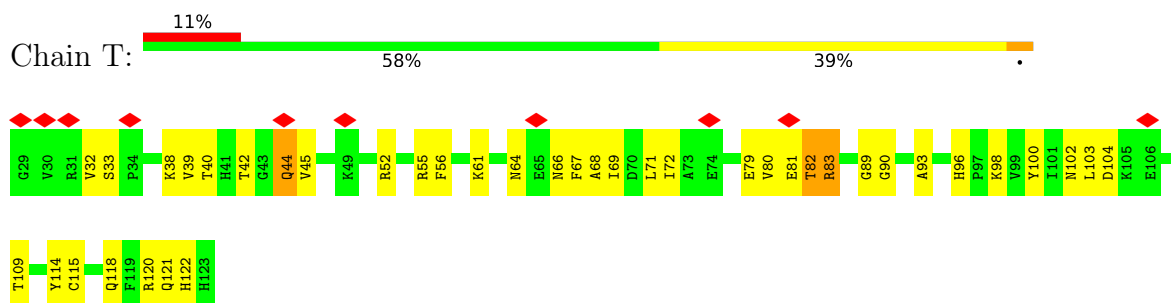


- Molecule 16: NADH dehydrogenase [ubiquinone] iron-sulfur protein 2, mitochondrial

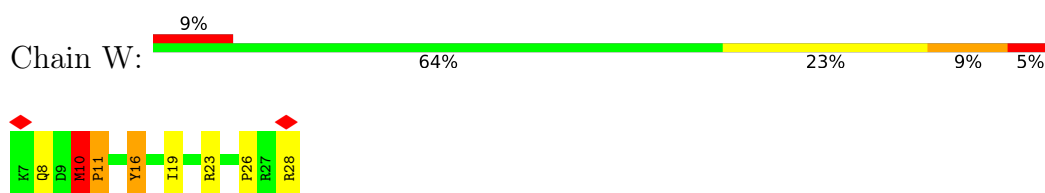




- Molecule 17: NADH dehydrogenase [ubiquinone] iron-sulfur protein 6, mitochondrial



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



4 Experimental information

Property	Value	Source
EM 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	
Maximum defocus (nm)	Not provided	
Magnification	Not provided	
Image detector	FEI FALCON II (4k x 4k)	Depositor
Maximum map value	0.616	Depositor
Minimum map value	-0.193	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.005	Depositor
Recommended contour level	0.0516	Depositor
Map size ($\text{\AA}$)	519.83997, 519.83997, 519.83997	wwPDB
Map dimensions	480, 480, 480	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing ($\text{\AA}$)	1.083, 1.083, 1.083	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, NDP, FES

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
1	A	0.39	0/3398	0.87	5/4590 (0.1%)
2	B	0.59	0/1452	0.96	10/1964 (0.5%)
3	C	0.74	0/1280	0.93	3/1732 (0.2%)
4	E	0.44	0/993	0.92	3/1335 (0.2%)
5	F	0.36	0/682	0.87	0/922
6	G	0.40	0/684	0.83	0/926
7	H	0.45	0/941	0.86	2/1275 (0.2%)
8	I	0.45	0/788	1.10	7/1066 (0.7%)
9	J	0.44	0/2785	0.91	12/3771 (0.3%)
10	K	0.30	0/282	0.73	0/381
11	L	0.42	0/987	0.83	1/1331 (0.1%)
12	M	0.43	0/5362	0.87	9/7266 (0.1%)
13	N	0.44	0/1236	0.91	7/1681 (0.4%)
14	O	0.39	0/1682	0.87	4/2289 (0.2%)
15	P	0.48	0/1780	0.94	5/2424 (0.2%)
16	Q	0.56	0/3161	1.00	12/4275 (0.3%)
17	T	0.38	0/755	0.79	0/1017
18	W	0.43	0/185	1.43	2/249 (0.8%)
All	All	0.47	0/28433	0.91	82/38494 (0.2%)

There are no bond length outliers.

All (82) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
18	W	10	MET	CA-C-N	-10.87	109.19	120.38
18	W	10	MET	C-N-CA	-10.87	109.19	120.38
8	I	38	PRO	CA-C-N	10.33	130.64	119.28
8	I	38	PRO	C-N-CA	10.33	130.64	119.28
16	Q	162	ARG	CA-C-N	10.24	127.03	119.66
16	Q	162	ARG	C-N-CA	10.24	127.03	119.66

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
16	Q	365	PRO	CA-C-N	9.97	129.92	119.85
16	Q	365	PRO	C-N-CA	9.97	129.92	119.85
4	E	18	LYS	CA-C-N	9.27	129.21	119.85
4	E	18	LYS	C-N-CA	9.27	129.21	119.85
3	C	60	GLY	N-CA-C	8.57	122.86	112.49
13	N	82	VAL	CA-C-N	8.17	125.62	119.66
13	N	82	VAL	C-N-CA	8.17	125.62	119.66
9	J	311	GLU	CA-C-N	8.06	127.99	119.85
9	J	311	GLU	C-N-CA	8.06	127.99	119.85
16	Q	318	VAL	N-CA-C	7.44	115.28	107.76
3	C	141	MET	CA-C-N	7.37	127.29	119.85
3	C	141	MET	C-N-CA	7.37	127.29	119.85
16	Q	351	MET	CA-C-N	7.09	124.83	119.66
16	Q	351	MET	C-N-CA	7.09	124.83	119.66
14	O	237	PRO	N-CA-C	7.00	119.24	110.70
16	Q	356	ILE	N-CA-C	-6.92	105.78	112.29
9	J	224	GLY	CA-C-N	6.91	126.87	120.03
9	J	224	GLY	C-N-CA	6.91	126.87	120.03
1	A	318	ILE	CA-C-N	6.85	126.84	119.78
1	A	318	ILE	C-N-CA	6.85	126.84	119.78
1	A	327	ILE	CA-C-N	6.80	126.78	119.78
1	A	327	ILE	C-N-CA	6.80	126.78	119.78
15	P	166	TYR	N-CA-C	-6.64	104.05	111.28
2	B	168	GLY	CA-C-N	6.63	126.57	119.28
2	B	168	GLY	C-N-CA	6.63	126.57	119.28
9	J	91	ILE	CB-CA-C	-6.37	104.86	112.19
8	I	98	ALA	CA-C-N	-6.25	113.94	120.38
8	I	98	ALA	C-N-CA	-6.25	113.94	120.38
12	M	505	GLY	N-CA-C	-6.25	107.08	115.21
15	P	119	VAL	CA-C-N	6.22	126.13	119.28
15	P	119	VAL	C-N-CA	6.22	126.13	119.28
9	J	238	GLN	CA-C-N	6.21	126.18	119.78
9	J	238	GLN	C-N-CA	6.21	126.18	119.78
12	M	175	ARG	N-CA-C	6.05	117.88	111.28
13	N	64	TYR	N-CA-C	6.04	120.49	113.18
9	J	86	CYS	N-CA-C	6.00	117.49	111.07
2	B	160	CYS	CA-C-N	5.96	125.84	119.28
2	B	160	CYS	C-N-CA	5.96	125.84	119.28
16	Q	391	VAL	CA-C-N	-5.96	115.31	119.66
16	Q	391	VAL	C-N-CA	-5.96	115.31	119.66
15	P	113	ASP	N-CA-C	5.81	117.94	108.76
2	B	64	LEU	N-CA-C	-5.80	104.86	111.07

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
13	N	65	THR	CB-CA-C	-5.76	108.94	115.79
8	I	36	GLN	CA-C-N	5.75	123.85	119.66
8	I	36	GLN	C-N-CA	5.75	123.85	119.66
1	A	318	ILE	N-CA-C	5.71	114.17	107.77
7	H	81	ILE	N-CA-C	-5.67	105.00	110.72
12	M	612	PRO	CA-C-N	5.65	125.50	119.28
12	M	612	PRO	C-N-CA	5.65	125.50	119.28
8	I	17	GLY	N-CA-C	-5.64	107.86	115.36
14	O	236	GLU	CA-C-N	5.58	126.12	120.38
14	O	236	GLU	C-N-CA	5.58	126.12	120.38
16	Q	272	THR	N-CA-C	5.56	120.34	113.50
12	M	261	ILE	N-CA-C	5.56	116.68	108.45
14	O	233	SER	CB-CA-C	-5.48	109.78	117.23
9	J	267	GLY	CA-C-N	5.43	125.25	119.28
9	J	267	GLY	C-N-CA	5.43	125.25	119.28
16	Q	281	GLU	N-CA-C	5.39	117.15	111.28
12	M	85	ALA	CA-C-N	5.38	125.19	119.28
12	M	85	ALA	C-N-CA	5.38	125.19	119.28
2	B	78	GLU	CA-C-N	5.35	125.29	119.78
2	B	78	GLU	C-N-CA	5.35	125.29	119.78
2	B	43	ASP	CA-C-N	5.28	125.22	119.78
2	B	43	ASP	C-N-CA	5.28	125.22	119.78
13	N	83	PRO	CA-C-N	5.26	125.07	119.28
13	N	83	PRO	C-N-CA	5.26	125.07	119.28
7	H	12	VAL	N-CA-C	5.24	115.90	110.82
12	M	102	ILE	N-CA-C	5.20	114.28	106.42
11	L	126	LEU	N-CA-C	5.12	116.53	107.61
4	E	32	VAL	N-CA-C	5.12	115.33	110.42
9	J	195	PHE	CA-C-N	5.09	124.88	119.28
9	J	195	PHE	C-N-CA	5.09	124.88	119.28
12	M	681	ALA	N-CA-C	5.06	114.83	108.45
2	B	67	GLY	N-CA-C	-5.04	106.68	112.73
15	P	94	ILE	CB-CA-C	-5.04	107.40	114.00
13	N	61	TRP	N-CA-C	5.01	115.92	108.60

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	212	0
2	B	1420	0	1371	104	0
3	C	1249	0	1253	68	0
4	E	968	0	982	65	0
5	F	670	0	679	38	0
6	G	672	0	650	32	0
7	H	922	0	950	59	0
8	I	769	0	788	46	0
9	J	2712	0	2757	231	0
10	K	274	0	257	24	0
11	L	964	0	962	64	0
12	M	5274	0	5312	334	0
13	N	1195	0	1155	49	0
14	O	1643	0	1646	112	0
15	P	1730	0	1685	115	0
16	Q	3087	0	3069	239	0
17	T	742	0	723	37	0
18	W	179	0	179	13	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	16	0
21	E	35	0	0	4	0
22	J	48	0	26	27	0
23	M	4	0	0	1	0
23	O	4	0	0	2	0
All	All	27962	0	27752	1579	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 (1579) 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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:C	9:J:181:LEU:HD21	1.69	1.18
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
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:217:PHE:HZ	9:J:322:MET:HE2	1.25	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:141:PHE:CZ	9:J:180:TYR:HA	2.07	0.90
9:J:169:HIS:HD2	22:J:401:NDP:H5N	1.34	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
15:P:134:SER:HG	15:P:139:SER:HG	1.20	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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:126:LYS:HB3	1:A:277:ASN:HD21	1.40	0.86
9:J:212:ARG:HG2	9:J:212:ARG:HH11	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:HG3	9:J:85:ARG:HH11	1.41	0.83
12:M:299:ARG:HG2	12:M:300:GLN:H	1.41	0.83
16:Q:145:MET:HE1	16:Q:226:TYR:HB3	1.61	0.82
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
9:J:217:PHE:CZ	9:J:322:MET:HE2	2.17	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
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:116:ASN:HD22	20:A:502:FMN:HM81	1.51	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:54:GLU:OE2	12:M:62:ARG:NH2	2.19	0.75
12:M:406:ASN:HB2	12:M:438:LEU:HD21	1.68	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:54:ILE:HB	9:J:78:SER:HB2	1.68	0.74
9:J:77:GLY:O	9:J:102:GLN:NE2	2.19	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
4:E:25:MET:C	4:E:29:LYS:HG3	2.13	0.73
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:158:ILE:HG21	1:A:166:ALA:HB2	1.70	0.72
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
16:Q:450:ILE:O	16:Q:453:THR:OG1	2.07	0.72
1:A:219:LYS:HA	11:L:174:THR:HG22	1.71	0.72
8:I:106:LEU:O	8:I:108:SER:N	2.19	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
3:C:129:LYS:NZ	16:Q:113:ILE:O	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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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:O	9:J:210:GLU:HG2	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
12:M:124:HIS:HD2	16:Q:375:MET:HE2	1.58	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
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
1:A:379:CYS:HA	12:M:200:ARG:HB2	1.74	0.68
9:J:202:LYS:HB2	9:J:264:ALA:HA	1.75	0.68
15:P:157:VAL:HG21	15:P:181:HIS:HD2	1.59	0.68
9:J:171:ASN:O	9:J:181:LEU:CG	2.41	0.68
11:L:89:SER:OG	15:P:239:TRP:NE1	2.26	0.68
12:M:289:LYS:NZ	12:M:694:PHE:O	2.25	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:173:ASN:HB2	9:J:327:MET:HE1	1.76	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
2:B:120:ILE:HD11	16:Q:385:TYR:HB3	1.74	0.67
6:G:105:MET:HG3	6:G:106:LYS:HG3	1.76	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:H9	20:A:502:FMN:O4'	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
1:A:43:THR:HG21	14:O:239:LYS:HB2	1.76	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
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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:L:81:VAL:HG11	11:L:150:ARG:HA	1.78	0.65
12:M:460:HIS:O	12:M:463:SER:OG	2.13	0.65
9:J:132:ARG:NH2	22:J:401:NDP:H2B	2.11	0.65
15:P:173:MET:HE1	15:P:189:THR:HG23	1.78	0.65
5:F:56:ARG:NH2	12:M:527:ASP:O	2.29	0.65
9:J:48:ARG:NH1	9:J:98:GLY:O	2.29	0.65
9:J:205:ASP:HB2	9:J:239:PRO:HA	1.79	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
10:K:81:THR:HB	14:O:88:ARG:HD2	1.78	0.65
12:M:36:VAL:O	12:M:38:GLY:N	2.29	0.65
1:A:398:ARG:NH1	1:A:408:GLU:OE1	2.25	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
8:I:23:LYS:NZ	16:Q:252:SER:OG	2.31	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
1:A:85:LEU:HD21	1:A:247:THR:HG23	1.80	0.63
1:A:379:CYS:SG	1:A:380:GLY:N	2.68	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:M:692:LYS:HD2	12:M:715:THR:HG22	1.80	0.63
16:Q:273:ILE:HD13	16:Q:325:ASP:CG	2.23	0.63
1:A:207:GLY:O	20:A:502:FMN:C5A	2.47	0.63
2:B:70:MET:HE2	16:Q:257:GLU:HG2	1.79	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
2:B:57:ARG:O	16:Q:266:ARG:NH2	2.30	0.63
10:K:82:TYR:HD2	14:O:62:ARG:HH12	1.46	0.62
14:O:245:VAL:O	14:O:247:ALA:N	2.31	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
12:M:173:MET:C	12:M:175:ARG:H	2.05	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
2:B:36:TYR:HB3	8:I:104:TRP:CE3	2.34	0.61
6:G:76:LEU:HD21	6:G:155:TYR:HA	1.82	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:48:ARG:HH21	15:P:211:ARG:HD2	1.64	0.61
9:J:272:LEU:HD23	9:J:274:PHE:H	1.65	0.61
12:M:537:ILE:O	12:M:539:LYS:N	2.33	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
15:P:190:ASP:CG	15:P:191:TYR:H	2.08	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
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:31:LEU:HD22	12:M:44:GLU:HA	1.83	0.60
12:M:385:TYR:OH	12:M:527:ASP:OD1	2.17	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
2:B:103:ARG:NH2	17:T:66:ASN:O	2.35	0.60
12:M:352:VAL:HG21	12:M:646:LEU:HD21	1.82	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:O	3:C:205:ARG:HG3	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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:85:ARG:HH11	9:J:85:ARG:CG	2.09	0.59
9:J:207:PHE:HE2	9:J:348:LYS:HB2	1.68	0.59
9:J:221:HIS:HE1	9:J:222:ARG:HG3	1.61	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:HG2	9:J:212:ARG:NH1	2.15	0.59
12:M:173:MET:C	12:M:175:ARG:N	2.60	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
2:B:186:GLU:OE2	17:T:64:ASN:N	2.36	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
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:73:LEU:O	9:J:78:SER:OG	2.21	0.58
9:J:181:LEU:HD23	9:J:181:LEU:O	2.03	0.58
16:Q:182:ASN:HD21	16:Q:404:LYS:HE3	1.68	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:74:TYR:OH	16:Q:257:GLU:OE1	2.20	0.58
5:F:41:TYR:OH	12:M:380:ASP:OD2	2.20	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
15:P:147:THR:HG21	15:P:153:ILE:HB	1.84	0.58
2:B:39:VAL:HG22	16:Q:321:GLY:HA2	1.86	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:75:ARG:NH1	15:P:215:GLU:OE2	2.34	0.58
9:J:358:THR:O	9:J:362:LEU:N	2.36	0.58
16:Q:251:PHE:HA	16:Q:254:ARG:HE	1.69	0.58
16:Q:438:MET:HE1	16:Q:454:GLN:NE2	2.18	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
10:K:89:LEU:HD11	14:O:61:LYS:HE3	1.86	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
5:F:88:THR:HA	5:F:91:LEU:HD12	1.85	0.58
12:M:36:VAL:HG11	12:M:56:VAL:HG11	1.84	0.58
12:M:306:MET:HB3	12:M:314:LEU:HD13	1.86	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
8:I:69:ILE:HB	15:P:76:VAL:HB	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
1:A:48:ARG:HH12	14:O:231:LEU:HD11	1.69	0.57
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:HG13	12:M:177:ILE:O	2.04	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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
2:B:87:GLU:HG2	13:N:61:TRP:HB3	1.87	0.57
4:E:118:PHE:HA	4:E:121:LYS:HD3	1.86	0.57
9:J:64:PHE:HD1	9:J:210:GLU:HB3	1.69	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
8:I:41:LEU:C	18:W:8:GLN:HE22	2.13	0.57
9:J:176:SER:C	9:J:182:ARG:HH21	2.13	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:159:ARG:NH1	14:O:177:LEU:O	2.33	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: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
2:B:151:ILE:HG21	3:C:159:TYR:CD2	2.41	0.56
3:C:147:VAL:HG23	3:C:176:VAL:HA	1.86	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:G:97:LYS:HD3	6:G:108:LEU:HG	1.86	0.56
9:J:217:PHE:HB3	9:J:280:ILE:HD13	1.87	0.56
12:M:193:ASP:OD2	14:O:111:ARG:NH2	2.39	0.56
1:A:123:GLY:N	14:O:180:CYS:SG	2.71	0.56
12:M:591:GLU:HB3	12:M:612:PRO:HD3	1.87	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
15:P:213:ASP:OD1	15:P:214:ASP:N	2.38	0.56
1:A:86:ARG:HA	1:A:94:PRO:HA	1.88	0.56
1:A:319:PRO:O	1:A:324:THR:OG1	2.23	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
2:B:103:ARG:HH12	17:T:68:ALA:HB2	1.69	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:50:LEU:N	12:M:91:ALA:O	2.38	0.56
12:M:492:ALA:O	12:M:495:SER:OG	2.21	0.56
16:Q:94:VAL:HG11	16:Q:458:PHE:HB3	1.87	0.56
1:A:342:LEU:HB3	1:A:347:THR:HB	1.87	0.56
8:I:46:SER:OG	12:M:150:ARG:NH2	2.38	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
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
3:C:62:TYR:OH	3:C:66:LYS:NZ	2.29	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:O	14:O:41:HIS:ND1	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:25:MET:HE3	4:E:29:LYS:HE2	1.88	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:J:168:SER:C	9:J:184:LYS:HE2	2.31	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
4:E:66:MET:HE3	4:E:106:PHE:HD1	1.71	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
16:Q:232:VAL:HB	16:Q:356:ILE:HG22	1.88	0.55
16:Q:291:VAL:HA	16:Q:294:ARG:HB2	1.89	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
9:J:49:SER:HB2	15:P:225:GLU:HB3	1.87	0.55
11:L:61:ILE:HB	11:L:64:LEU:HB2	1.89	0.55
11:L:61:ILE:HG21	15:P:149:GLU:OE1	2.07	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
16:Q:83:ASN:HA	16:Q:98:VAL:HG22	1.89	0.55
9:J:94:LEU:HG	9:J:97:MET:SD	2.46	0.54
9:J:164:PHE:HE2	9:J:191:VAL:HG13	1.72	0.54
11:L:162:ALA:HA	11:L:168:LYS:NZ	2.22	0.54
13:N:34:LYS:HZ1	13:N:58:ARG:HG2	1.72	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
2:B:37:LYS:N	16:Q:318:VAL:O	2.37	0.54
9:J:176:SER:C	9:J:182:ARG:NH2	2.65	0.54
16:Q:191:ALA:HB1	16:Q:196:ALA:HB3	1.89	0.54
1:A:381:GLN:CG	19:A:501:SF4:S2	2.94	0.54
1:A:418:GLN:O	1:A:422:HIS:ND1	2.39	0.54
7:H:111:GLN:NE2	15:P:124:ASN:HB2	2.22	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:M:47:THR:OG1	12:M:51:GLN:OE1	2.23	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
8:I:42:PRO:HB3	18:W:10:MET:HE1	1.90	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
10:K:92:SER:HB2	14:O:68:LYS:HD2	1.90	0.54
12:M:405:THR:HA	12:M:686:PRO:HG3	1.90	0.54
15:P:160:PHE:C	15:P:162:ALA:H	2.16	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
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:215:MET:HE1	12:M:714:VAL:HG23	1.90	0.54
12:M:358:LEU:HB3	12:M:363:SER:O	2.07	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:141:GLY:HA2	1:A:252:PRO:HD3	1.90	0.53
1:A:225:LEU:HG	1:A:227:PRO:HD3	1.90	0.53
9:J:141:PHE:CE1	9:J:180:TYR:HD1	2.25	0.53
9:J:167:VAL:HA	9:J:201:VAL:HB	1.88	0.53
9:J:178:SER:OG	9:J:181:LEU:CB	2.57	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:61:TRP:O	2:B:63:GLU:N	2.41	0.53
2:B:104:TYR:CE2	2:B:110:ARG:HA	2.43	0.53
6:G:105:MET:HE2	6:G:138:LEU:HD23	1.89	0.53
9:J:207:PHE:CZ	9:J:345:LEU:HA	2.44	0.53
12:M:124:HIS:CD2	16:Q:375:MET:HE2	2.43	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
12:M:149:ASP:HB2	16:Q:361:ALA:HB3	1.90	0.53
16:Q:196:ALA:O	16:Q:198:THR:N	2.41	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:J:298:TYR:CE2	9:J:319:VAL:HG22	2.44	0.53
12:M:343:GLY:HA3	12:M:548:LEU:HB2	1.90	0.53
12:M:351:LEU:HD23	12:M:530:TYR:HE2	1.73	0.53
13:N:84:PRO:HA	13:N:87:HIS:HB3	1.90	0.53
16:Q:149:GLN:CD	16:Q:171:ARG:HB3	2.33	0.53
16:Q:435:LEU:HA	16:Q:438:MET:HE3	1.91	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
2:B:61:TRP:CD1	16:Q:266:ARG:HH12	2.26	0.53
3:C:75:ARG:NH2	3:C:144:PRO:HG3	2.24	0.53
9:J:89:TYR:C	9:J:89:TYR:CD1	2.85	0.53
12:M:308:ARG:NH1	12:M:578:PRO:O	2.42	0.53
15:P:88:ILE:HG22	15:P:89:HIS:O	2.09	0.53
15:P:238:PRO:O	15:P:239:TRP:HB2	2.08	0.53
2:B:66:ARG:HH22	18:W:28:ARG:HB2	1.73	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
1:A:121:GLU:HA	1:A:204:TYR:HE1	1.74	0.53
1:A:217:GLU:HB3	11:L:171:ARG:HH22	1.72	0.53
2:B:65:PHE:O	2:B:69:GLY:N	2.41	0.53
9:J:64:PHE:CE1	9:J:68:TYR:HE2	2.27	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
1:A:382:CYS:HA	12:M:74:ASN:HA	1.91	0.53
3:C:172:ARG:NH1	15:P:209:GLU:OE2	2.36	0.53
4:E:128:PRO:HB3	11:L:104:ARG:HH22	1.73	0.53
9:J:141:PHE:CZ	9:J:180:TYR:CB	2.92	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
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:68:ARG:HD2	12:M:285:TRP:NE1	2.20	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
1:A:236:PHE:HZ	14:O:77:ALA:HB2	1.73	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
16:Q:262:LEU:HD22	16:Q:268:TRP:NE1	2.18	0.53
1:A:164:ASN:HB3	10:K:77:HIS:HB2	1.91	0.52
1:A:293:SER:HB2	1:A:336:LEU:HD23	1.91	0.52
17:T:52:ARG:HB3	17:T:55:ARG:HH12	1.74	0.52
2:B:66:ARG:HH12	18:W:28:ARG:HB3	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
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
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
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
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
3:C:184:PRO:HD3	16:Q:223:HIS:CD2	2.43	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
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
2:B:107:GLY:HA3	17:T:71:LEU:HD23	1.91	0.52
10:K:77:HIS:CD2	14:O:215:LYS:HE2	2.44	0.52
12:M:253:VAL:HG23	12:M:345:LEU:HD22	1.90	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:M:314:LEU:HD11	13:N:140:PRO:HD2	1.92	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
12:M:634:LEU:HD23	12:M:636:TYR:CZ	2.45	0.52
1:A:423:THR:OG1	19:A:501:SF4:S4	2.68	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
5:F:72:GLY:HA3	12:M:359:ASN:HB3	1.92	0.51
12:M:89:VAL:HB	12:M:94:MET:HG3	1.91	0.51
12:M:188:GLU:O	12:M:419:ARG:NE	2.40	0.51
12:M:573:GLY:HA3	13:N:137:TRP:NE1	2.25	0.51
13:N:30:THR:HG21	13:N:63:VAL:HG22	1.91	0.51
16:Q:99:MET:HE2	16:Q:109:CYS:SG	2.49	0.51
16:Q:404:LYS:HZ3	16:Q:457:VAL:HB	1.74	0.51
11:L:84:ARG:HG3	11:L:90:GLY:O	2.10	0.51
11:L:169:ARG:NH1	12:M:426:ASP:HA	2.25	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
1:A:113:LEU:HD23	1:A:113:LEU:C	2.35	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
1:A:126:LYS:HZ3	1:A:246:GLU:HG3	1.75	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
9:J:62:THR:HB	22:J:401:NDP:HO3A	1.76	0.51
13:N:137:TRP:HH2	13:N:140:PRO:HD3	1.75	0.51
2:B:201:ALA:HB1	13:N:88:ARG:NH1	2.26	0.51
3:C:137:VAL:HA	3:C:140:GLN:CD	2.36	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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:81:GLU:CD	12:M:108:LYS:HB3	2.36	0.51
12:M:151:SER:OG	16:Q:374:SER:HB2	2.11	0.51
12:M:302:LEU:HB3	12:M:585:PRO:HB3	1.93	0.51
12:M:430:ALA:HA	12:M:442:TYR:HB2	1.93	0.51
13:N:18:GLY:O	13:N:20:LEU:N	2.44	0.51
14:O:63:ILE:HA	14:O:66:ILE:HD12	1.92	0.51
14:O:130:TYR:HA	14:O:189:ASN:HD21	1.76	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:76:ARG:HE	12:M:79:LEU:HD21	1.74	0.50
12:M:307:VAL:HB	12:M:317:THR:HG21	1.93	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: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
14:O:135:CYS:O	14:O:145:SER:OG	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
1:A:152:ARG:HH12	10:K:99:PRO:HB3	1.76	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:281:HIS:NE2	14:O:142:LEU:O	2.38	0.50
2:B:109:GLU:OE2	2:B:139:ARG:HD2	2.11	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
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
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
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: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
12:M:506:VAL:HG12	12:M:508:GLY:N	2.25	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:CG	9:J:85:ARG:NH1	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:37:LYS:HE2	8:I:110:GLN:O	2.11	0.50
2:B:108:GLU:OE1	17:T:68:ALA:HB1	2.12	0.50
8:I:9:GLN:O	8:I:13:ASN:ND2	2.40	0.50
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
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
16:Q:374:SER:HG	16:Q:377:SER:HG	1.57	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:32:ILE:HG23	12:M:98:LYS:HB2	1.93	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: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
7:H:115:PRO:O	15:P:247:GLN:NE2	2.45	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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: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:OE1	10:K:104:GLU:N	2.46	0.49
11:L:92:ASN:HB2	15:P:239:TRP:H	1.77	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
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
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
12:M:381:LEU:C	12:M:383:SER:H	2.16	0.49
1:A:71:LYS:HA	1:A:147:ARG:HH21	1.77	0.49
1:A:208:GLU:OE1	1:A:211:ALA:N	2.39	0.49
2:B:36:TYR:CD2	8:I:104:TRP:HB2	2.48	0.49
7:H:107:PRO:HD3	15:P:74:GLN:HE22	1.76	0.49
9:J:64:PHE:HE2	9:J:242:VAL:HG21	1.77	0.49
9:J:209:ARG:HD2	15:P:217:LYS:HE2	1.93	0.49
12:M:300:GLN:HA	13:N:135:GLN:O	2.12	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:160:GLY:HA2	1:A:199:ARG:NH1	2.27	0.49
7:H:111:GLN:HE22	15:P:122:ARG:HB3	1.77	0.49
9:J:179:ARG:NH1	9:J:179:ARG:HB3	2.27	0.49
12:M:64:CYS:O	12:M:184:ARG:NH2	2.46	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
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:171:THR:HB	12:M:173:MET:HE3	1.94	0.49
12:M:372:PHE:CE1	12:M:481:LEU:HD13	2.48	0.49
16:Q:438:MET:HE1	16:Q:454:GLN:HE22	1.78	0.49
1:A:274:LYS:HZ2	1:A:352:ALA:HB3	1.76	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: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
16:Q:179:ARG:HG2	16:Q:183:HIS:CD2	2.48	0.48
1:A:36:LYS:HB2	1:A:39:ASP:CG	2.38	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
13:N:129:THR:HA	17:T:44:GLN:NE2	2.28	0.48
16:Q:140:ASP:HB3	16:Q:147:ASN:ND2	2.28	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
1:A:118:ASP:O	1:A:119:GLU:C	2.55	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
11:L:95:LYS:NZ	15:P:240:GLU:OE2	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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
2:B:142:ARG:NH2	11:L:112:MET:O	2.47	0.48
5:F:68:ARG:HA	5:F:74:GLU:HG2	1.95	0.48
12:M:266:ARG:NE	12:M:271:MET:HE3	2.29	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
9:J:212:ARG:NH1	9:J:212:ARG:CG	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
1:A:256:ARG:O	14:O:246:GLN:HB3	2.13	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: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:OE1	6:G:77:GLU:N	2.38	0.47
8:I:11:LEU:O	8:I:14:TRP:HB3	2.13	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:I:44:GLY:HA2	16:Q:355:GLU:HG3	1.95	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
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
2:B:138:ARG:HG2	12:M:238:PHE:CG	2.48	0.47
7:H:32:LEU:HG	7:H:52:THR:HG21	1.96	0.47
9:J:91:ILE:HA	9:J:93:HIS:CE1	2.49	0.47
9:J:141:PHE:HE2	9:J:183:ASN:HD22	1.62	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
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
17:T:109:THR:HB	17:T:118:GLN:HB3	1.95	0.47
3:C:95:HIS:HE1	16:Q:211:PHE:CE2	2.32	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
10:K:96:MET:HE3	10:K:97:PRO:HD2	1.96	0.47
16:Q:99:MET:HE1	16:Q:447:VAL:HG21	1.97	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:84:TYR:CE2	2:B:85:PRO:HB3	2.49	0.47
2:B:198:GLU:OE2	2:B:202:ASN:ND2	2.46	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
9:J:221:HIS:ND1	9:J:221:HIS:C	2.73	0.47
11:L:121:LEU:HA	15:P:203:PRO:HB3	1.97	0.47
1:A:276:PHE:CE2	1:A:290:GLU:HB3	2.50	0.47
2:B:40:ASN:C	2:B:42:GLN:H	2.21	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
6:G:104:PHE:CD1	6:G:108:LEU:HD22	2.50	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:H:28:TYR:HD1	7:H:52:THR:HG23	1.80	0.47
9:J:41:MET:HE3	9:J:42:PRO:HD2	1.96	0.47
9:J:141:PHE:CE2	9:J:183:ASN:ND2	2.83	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
16:Q:281:GLU:N	16:Q:281:GLU:CD	2.73	0.47
1:A:69:LEU:HD11	1:A:143:LEU:HD21	1.96	0.47
2:B:91:LEU:HG	16:Q:215:GLU:OE2	2.15	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
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:311:TRP:CD1	1:A:314:LEU:HD12	2.50	0.47
9:J:41:MET:HB3	9:J:42:PRO:HD2	1.97	0.47
9:J:229:GLY:HA2	9:J:293:LEU:O	2.15	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
3:C:100:ARG:NH2	16:Q:208:GLU:HB3	2.18	0.46
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
16:Q:241:MET:HE3	18:W:16:TYR:OH	2.15	0.46
1:A:177:TYR:CE2	10:K:91:LEU:HD13	2.50	0.46
3:C:106:PHE:CE2	3:C:191:LEU:HD11	2.51	0.46
3:C:147:VAL:CG2	3:C:176:VAL:HA	2.46	0.46
14:O:138:THR:OG1	14:O:139:PRO:HD3	2.15	0.46
2:B:94:ARG:NH2	16:Q:237:PRO:HG3	2.30	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
16:Q:315:GLU:HB2	16:Q:346:GLN:HE22	1.80	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
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
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:64:TYR:CE2	15:P:68:ILE:HD11	2.50	0.46
15:P:201:ASP:OD1	15:P:202:PHE:N	2.48	0.46
2:B:138:ARG:HD3	12:M:130:ILE:HG22	1.98	0.46
4:E:62:LYS:HE3	4:E:66:MET:HE2	1.98	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
12:M:323:LEU:HG	12:M:629:ILE:HD12	1.98	0.46
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
9:J:319:VAL:C	9:J:323:HIS:HD1	2.22	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:69:GLU:HB2	11:L:73:LYS:NZ	2.30	0.46
11:L:69:GLU:HB2	11:L:73:LYS:HZ2	1.80	0.46
11:L:109:ASN:OD1	11:L:110:PRO:HD2	2.16	0.46
14:O:78:ALA:O	14:O:82:VAL:HG23	2.15	0.46
16:Q:97:LEU:HD12	16:Q:97:LEU:O	2.15	0.46
4:E:40:TYR:CE1	4:E:60:ARG:HD3	2.51	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
14:O:236:GLU:C	14:O:238:PRO:HD2	2.41	0.46
15:P:83:GLU:HB3	15:P:142:ARG:NH1	2.29	0.46
15:P:97:LEU:HA	15:P:100:LEU:HD12	1.97	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:64:CYS:SG	12:M:75:CYS:HB3	2.56	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
1:A:89:GLY:HA2	1:A:244:ASN:ND2	2.28	0.45
1:A:203:ALA:HB2	14:O:119:TYR:CE1	2.50	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
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: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
14:O:218:PRO:HG2	14:O:222:ARG:O	2.16	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:99:ASP:H	9:J:102:GLN:HB2	1.82	0.45
9:J:299:ARG:HE	9:J:316:ARG:HH11	1.62	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
1:A:201:ALA:O	14:O:119:TYR:HB3	2.17	0.45
2:B:94:ARG:HE	16:Q:234:GLN:NE2	2.15	0.45
2:B:160:CYS:O	16:Q:368:ARG:NH1	2.41	0.45
3:C:153:CYS:SG	19:C:301:SF4:S2	3.07	0.45
3:C:161:HIS:CE1	3:C:168:ARG:HD2	2.51	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:158:ARG:HH21	12:M:178:GLN:HE22	1.64	0.45
12:M:164:ASN:OD1	12:M:165:ILE:N	2.49	0.45
2:B:127:THR:HA	15:P:231:ARG:HH12	1.81	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
15:P:167:GLU:HG2	15:P:181:HIS:CD2	2.52	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
2:B:90:PRO:HG2	13:N:56:PHE:CE2	2.52	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:OD1	11:L:102:ASP:N	2.50	0.45
13:N:48:TYR:HB3	13:N:89:TRP:HZ3	1.81	0.45
14:O:84:ASP:O	14:O:88:ARG:N	2.47	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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:M:471:LYS:HB3	12:M:510:TRP:CH2	2.52	0.45
12:M:498:GLN:HE22	12:M:501:ARG:HD2	1.82	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: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:63:GLU:O	15:P:67:GLU:HG3	2.17	0.44
15:P:214:ASP:O	15:P:217:LYS:HD2	2.16	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:157:LYS:HB2	17:T:100:TYR:CD2	2.52	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
1:A:99:TRP:HA	1:A:149:MET:HE1	1.99	0.44
1:A:369:ARG:NH2	14:O:175:GLU:OE2	2.33	0.44
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
4:E:53:ASP:OD2	9:J:351:GLU:HB3	2.17	0.44
6:G:99:SER:OG	6:G:102:SER:OG	2.29	0.44
12:M:546:PHE:CZ	12:M:566:ILE:HD12	2.52	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
13:N:29:ARG:HH22	13:N:65:THR:C	2.17	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:116:ASN:HD21	20:A:502:FMN:C8	2.22	0.44
1:A:173:ILE:HG22	1:A:177:TYR:CE2	2.52	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
22:J:401:NDP:O2X	22:J:401:NDP:O3B	2.33	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:371:VAL:HG12	12:M:533:GLY:O	2.17	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: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
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
8:I:97:PRO:HG3	15:P:61:PHE:CD1	2.52	0.44
12:M:255:ASP:HB3	12:M:257:VAL:HG23	1.98	0.44
16:Q:307:PRO:HB2	16:Q:312:ASP:HB3	2.00	0.44
1:A:123:GLY:CA	1:A:355:ILE:HD11	2.48	0.44
1:A:167:SER:O	1:A:171:VAL:HG23	2.18	0.44
5:F:39:LYS:HG3	5:F:40:ARG:N	2.29	0.44
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
1:A:152:ARG:NH1	10:K:99:PRO:HB3	2.33	0.44
9:J:71:ASN:ND2	15:P:214:ASP:HB3	2.33	0.44
9:J:168:SER:O	9:J:203:PRO:HD2	2.18	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
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
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:72:ILE:HA	11:L:143:TRP:CD1	2.53	0.43
11:L:133:ASP:O	11:L:136:SER:OG	2.21	0.43
12:M:136:GLU:HB3	12:M:242:PRO:HG2	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
2:B:61:TRP:HB2	2:B:65:PHE:HE2	1.82	0.43
2:B:128:ILE:HG12	2:B:143:TYR:HD1	1.83	0.43
4:E:39:TRP:O	4:E:43:VAL:HG23	2.18	0.43
4:E:50:PHE:CD2	4:E:103:VAL:HG21	2.52	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
3:C:88:CYS:HB3	16:Q:141:TYR:CG	2.54	0.43
3:C:163:SER:HB3	16:Q:123:LEU:HD11	2.00	0.43
4:E:53:ASP:HA	9:J:366:ILE:HD11	2.00	0.43
9:J:168:SER:CA	9:J:184:LYS:HE3	2.47	0.43
1:A:37:ASP:OD2	14:O:235:THR:N	2.49	0.43
2:B:35:THR:N	8:I:105:GLU:O	2.51	0.43
2:B:169:PRO:HG3	2:B:198:GLU:HG2	2.00	0.43
4:E:126:HIS:HD2	12:M:612:PRO:HD2	1.84	0.43
7:H:50:GLN:NE2	8:I:93:LYS:HD2	2.32	0.43
9:J:81:ILE:HG22	9:J:83:PRO:HD3	2.00	0.43
9:J:125:VAL:HG12	9:J:163:LYS:HB2	2.00	0.43
9:J:204:SER:OG	9:J:240:VAL:HG23	2.18	0.43
9:J:220:MET:HA	9:J:223:PHE:CD2	2.53	0.43
12:M:200:ARG:HB3	14:O:118:PHE:CD1	2.54	0.43
12:M:501:ARG:HH12	12:M:666:GLN:HB2	1.82	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:65:LEU:O	5:F:76:ASN:HA	2.18	0.43
5:F:67:ALA:HB3	5:F:75:THR:OG1	2.18	0.43
6:G:115:GLN:NE2	6:G:135:ALA:HB1	2.34	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
3:C:211:TYR:CD1	3:C:211:TYR:C	2.96	0.43
4:E:43:VAL:O	4:E:47:VAL:HG23	2.19	0.43
4:E:118:PHE:HZ	12:M:621:LYS:HG3	1.83	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
14:O:163:THR:HG22	14:O:170:THR:HG22	2.01	0.43
17:T:96:HIS:NE2	17:T:115:CYS:SG	2.90	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
4:E:48:HIS:HE1	9:J:363:SER:O	2.02	0.43
5:F:87:VAL:O	5:F:91:LEU:HG	2.18	0.43
10:K:78:ASP:HA	14:O:215:LYS:HD3	2.00	0.43
12:M:221:ASN:HB3	12:M:285:TRP:CZ3	2.53	0.43
12:M:243:TRP:CD1	12:M:244:GLU:HG3	2.54	0.43
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:90:PRO:O	15:P:93:VAL:HG23	2.18	0.43
15:P:129:VAL:HG22	15:P:144:LYS:HB3	2.01	0.43
16:Q:144:MET:HA	16:Q:147:ASN:HD22	1.84	0.43
16:Q:372:LYS:HD2	17:T:93:ALA:HA	2.00	0.43
16:Q:410:TYR:O	16:Q:422:CYS:HA	2.19	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:153:PHE:C	12:M:154:LEU:HD12	2.44	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
3:C:150:MET:HE3	3:C:185:PRO:HG2	1.99	0.43
8:I:42:PRO:HG3	16:Q:354:GLY:O	2.19	0.43
9:J:293:LEU:HD23	9:J:298:TYR:HD1	1.84	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:K:82:TYR:HB3	14:O:62:ARG:HH22	1.84	0.43
12:M:323:LEU:HA	12:M:326:VAL:HG22	1.99	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
17:T:79:GLU:OE1	17:T:122:HIS:HB3	2.19	0.43
1:A:88:ARG:C	1:A:244:ASN:HD22	2.26	0.42
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:99:HIS:ND1	2:B:147:MET:HE1	2.34	0.42
2:B:104:TYR:N	2:B:108:GLU:O	2.32	0.42
3:C:175:PRO:HB3	9:J:96:PRO:HD3	2.01	0.42
7:H:7:LYS:O	7:H:8:THR:OG1	2.29	0.42
7:H:21:HIS:NE2	7:H:63:PRO:O	2.52	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
11:L:131:LYS:HD2	11:L:147:ILE:CG2	2.49	0.42
11:L:154:LYS:HG2	12:M:279:GLU:HG3	2.02	0.42
12:M:153:PHE:O	12:M:154:LEU:HD12	2.19	0.42
13:N:66:THR:HG23	13:N:74:PHE:H	1.85	0.42
16:Q:167:ALA:O	16:Q:171:ARG:HG3	2.18	0.42
1:A:270:ASN:CG	1:A:338:ASP:HB2	2.44	0.42
1:A:418:GLN:CD	12:M:115:GLY:HA2	2.44	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: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
14:O:46:GLU:C	14:O:49:PRO:HD3	2.44	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
12:M:381:LEU:C	12:M:383:SER:N	2.77	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:N:106:ARG:O	13:N:109:ILE:HG12	2.18	0.42
16:Q:119:GLY:H	16:Q:463:ARG:C	2.27	0.42
1:A:47:GLY:HA2	1:A:133:HIS:HB3	2.00	0.42
2:B:176:GLU:OE1	3:C:200:LYS:HD2	2.20	0.42
9:J:336:GLU:C	9:J:339:GLY:H	2.28	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
7:H:47:TYR:OH	8:I:92:LYS:HG3	2.20	0.42
8:I:5:THR:HB	8:I:8:ILE:HD12	2.00	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:49:VAL:HG23	12:M:94:MET:O	2.20	0.42
12:M:319:TRP:HH2	12:M:617:ARG:NE	2.18	0.42
12:M:543:LYS:HD2	12:M:543:LYS:N	2.35	0.42
12:M:559:ASP:OD1	12:M:560:LEU:N	2.51	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
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:44:TYR:CD2	7:H:94:MET:HE2	2.54	0.42
8:I:40:LYS:HG2	18:W:8:GLN:HA	2.00	0.42
9:J:240:VAL:HG22	9:J:266:VAL:C	2.45	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
17:T:40:THR:OG1	17:T:44:GLN:HG2	2.20	0.42
1:A:184:LYS:C	1:A:186:ALA:H	2.27	0.42
1:A:257:ARG:HH12	14:O:239:LYS:NZ	2.17	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
7:H:18:ASN:O	7:H:19:THR:OG1	2.31	0.42
9:J:152:ILE:HG22	9:J:164:PHE:CE1	2.55	0.42
12:M:66:HIS:CE1	12:M:68:ARG:HG2	2.53	0.42
12:M:307:VAL:HA	12:M:582:VAL:HA	2.01	0.42
12:M:314:LEU:HD22	12:M:583:ILE:HD12	2.02	0.42
14:O:213:ILE:HG22	14:O:214:PRO:O	2.20	0.42
16:Q:116:LEU:HD11	16:Q:141:TYR:OH	2.20	0.42
16:Q:371:MET:HE1	16:Q:381:HIS:CE1	2.55	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
9:J:209:ARG:HD2	15:P:217:LYS:CE	2.50	0.42
11:L:86:ASN:ND2	12:M:224:ASP:OD2	2.53	0.42
12:M:342:ALA:HA	12:M:547:LEU:HB2	2.00	0.42
12:M:541:PRO:HA	12:M:542:PRO:HD2	1.77	0.42
14:O:53:PHE:HE2	14:O:55:PHE:CE1	2.38	0.42
14:O:176:CYS:HA	23:O:301:FES:S1	2.60	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
2:B:184:ASN:ND2	13:N:126:PRO:HA	2.35	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:33:GLU:O	12:M:98:LYS:HA	2.20	0.41
12:M:83:GLU:HB2	12:M:101:ASN:HB3	2.02	0.41
13:N:117:VAL:HG11	13:N:122:GLU:HB2	2.02	0.41
14:O:100:LYS:O	14:O:104:VAL:HG23	2.20	0.41
16:Q:290:GLY:C	16:Q:294:ARG:HE	2.28	0.41
1:A:220:GLN:NE2	14:O:114:GLU:HB3	2.34	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
15:P:96:VAL:O	15:P:100:LEU:HG	2.20	0.41
16:Q:84:PHE:HE2	16:Q:99:MET:HE3	1.85	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
8:I:60:ARG:HD2	16:Q:390:GLN:O	2.19	0.41
9:J:50:SER:O	9:J:77:GLY:HA3	2.20	0.41
9:J:157:LYS:HA	9:J:195:PHE:HE1	1.85	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
1:A:244:ASN:ND2	20:A:502:FMN:HM82	2.35	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
4:E:84:ILE:HD13	15:P:177:PHE:CE1	2.56	0.41
7:H:81:ILE:HG13	7:H:82:LEU:N	2.34	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
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
2:B:133:ARG:C	2:B:136:GLY:H	2.29	0.41
3:C:118:ASP:CG	3:C:119:VAL:H	2.28	0.41
12:M:236:TYR:CE1	12:M:272:ARG:HB3	2.55	0.41
12:M:433:GLY:HA3	12:M:684:LEU:HD23	2.01	0.41
12:M:492:ALA:O	12:M:496:ILE:HG13	2.19	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
16:Q:333:ARG:HE	16:Q:455:ASP:CG	2.29	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
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
9:J:98:GLY:HA3	9:J:103:LEU:HG	2.01	0.41
22:J:401:NDP:O3B	22:J:401:NDP:P2B	2.79	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:L:117:THR:OG1	15:P:229:GLU:OE1	2.39	0.41
1:A:122:PRO:HA	14:O:176:CYS:SG	2.61	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
16:Q:358:VAL:O	16:Q:364:SER:OG	2.24	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
3:C:98:ALA:HB1	3:C:99:PRO:HD2	2.03	0.41
3:C:213:ARG:HG2	3:C:213:ARG:O	2.19	0.41
7:H:19:THR:N	7:H:20:PRO:HD3	2.35	0.41
8:I:23:LYS:NZ	16:Q:252:SER:HG	2.18	0.41
9:J:179:ARG:HB3	9:J:179:ARG:HH11	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
14:O:148:ILE:O	14:O:152:ILE:HG13	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
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
1:A:284:HIS:CE1	14:O:229:GLY:HA3	2.56	0.41
2:B:62:THR:OG1	2:B:63:GLU:N	2.53	0.41
2:B:101:LEU:O	2:B:192:GLY:HA3	2.21	0.41
3:C:81:PRO:HA	3:C:119:VAL:HG13	2.03	0.41
3:C:137:VAL:HA	3:C:140:GLN:OE1	2.20	0.41
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:O	12:M:483:ARG:HG3	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:86:ARG:C	1:A:95:THR:HG23	2.46	0.40
2:B:90:PRO:O	2:B:91:LEU:HD12	2.22	0.40
2:B:102:ARG:HB2	2:B:196:GLU:OE2	2.21	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
15:P:190:ASP:CG	15:P:191:TYR:N	2.77	0.40
16:Q:316:PHE:HB2	16:Q:339:GLN:CG	2.51	0.40
2:B:120:ILE:O	2:B:121:CYS:C	2.64	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
12:M:198:THR:CG2	14:O:39:PHE:HB3	2.47	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
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:169:TRP:C	16:Q:351:MET:HE2	2.46	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:84:TYR:CD1	2:B:85:PRO:HA	2.56	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
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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:H:12:VAL:CG1	16:Q:280:ALA:N	2.81	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
14:O:144:ASN:O	14:O:147:SER:OG	2.35	0.40
15:P:100:LEU:O	15:P:108:PHE:HD2	2.05	0.40
1:A:73:PRO:O	1:A:75:TRP:N	2.55	0.40
1:A:222:LYS:HB2	11:L:175:LYS:O	2.22	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
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
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 ⓘ

5.3.1 Protein backbone ⓘ

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%)	5	24
2	B	174/176 (99%)	163 (94%)	10 (6%)	1 (1%)	21	50
3	C	154/156 (99%)	137 (89%)	12 (8%)	5 (3%)	3	17
4	E	111/113 (98%)	101 (91%)	8 (7%)	2 (2%)	6	26
5	F	81/83 (98%)	74 (91%)	7 (9%)	0	100	100
6	G	83/85 (98%)	78 (94%)	3 (4%)	2 (2%)	4	22
7	H	110/112 (98%)	100 (91%)	5 (4%)	5 (4%)	2	12

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

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
8	I	93	LYS

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Mol	Chain	Res	Type
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
8	I	108	SER

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Mol	Chain	Res	Type
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%)	106 (100%)	0	100	100
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%)	99 (99%)	1 (1%)	68	75
8	I	87/96 (91%)	87 (100%)	0	100	100
9	J	292/292 (100%)	288 (99%)	4 (1%)	59	70
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%)	86	84
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%)	328 (99%)	3 (1%)	70	76
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%)	2996 (100%)	10 (0%)	84	84

All (10) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
7	H	81	ILE
9	J	85	ARG
9	J	91	ILE
9	J	206	ILE
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
16	Q	275	ILE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (67) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	44	ASN
1	A	49	HIS
1	A	116	ASN
1	A	164	ASN
1	A	170	GLN
1	A	220	GLN
1	A	270	ASN
1	A	284	HIS
1	A	313	ASN
1	A	376	HIS
1	A	441	HIS
2	B	184	ASN
3	C	72	ASN
3	C	95	HIS
4	E	48	HIS
4	E	49	GLN
4	E	51	GLN
4	E	70	ASN
4	E	108	HIS
5	F	62	GLN
5	F	81	ASN
6	G	80	GLN
6	G	142	GLN
7	H	50	GLN
7	H	76	GLN
7	H	83	GLN
7	H	111	GLN
9	J	71	ASN
9	J	93	HIS
9	J	102	GLN
9	J	183	ASN
10	K	77	HIS
11	L	86	ASN
12	M	415	ASN

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Mol	Chain	Res	Type
12	M	460	HIS
12	M	464	GLN
12	M	498	GLN
12	M	514	ASN
12	M	663	ASN
12	M	666	GLN
12	M	669	ASN
13	N	72	ASN
13	N	91	HIS
13	N	113	HIS
13	N	135	GLN
14	O	69	ASN
14	O	187	GLN
14	O	189	ASN
14	O	191	ASN
15	P	74	GLN
15	P	82	ASN
15	P	105	ASN
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 [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

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	$\# Z > 2$
21	8Q1	E	201	-	31,34,34	1.65	6 (19%)	40,43,43	1.38	7 (17%)
23	FES	O	301	14	0,4,4	-	-	-		
19	SF4	M	801	12	0,12,12	-	-	-		
20	FMN	A	502	-	33,33,33	1.40	6 (18%)	48,50,50	1.34	8 (16%)
19	SF4	A	501	1	0,12,12	-	-	-		
19	SF4	B	302	2	0,12,12	-	-	-		
19	SF4	C	301	3	0,12,12	-	-	-		
23	FES	M	803	-	0,4,4	-	-	-		
22	NDP	J	401	-	49,52,52	1.20	5 (10%)	66,80,80	1.75	11 (16%)
19	SF4	M	802	12	0,12,12	-	-	-		
19	SF4	B	301	2	0,12,12	-	-	-		

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
21	8Q1	E	201	-	-	18/41/41/41	-
23	FES	O	301	14	-	-	0/1/1/1
19	SF4	M	801	12	-	-	0/6/5/5
20	FMN	A	502	-	-	7/18/18/18	0/3/3/3
19	SF4	A	501	1	-	-	0/6/5/5
19	SF4	B	302	2	-	-	0/6/5/5
19	SF4	C	301	3	-	-	0/6/5/5
23	FES	M	803	-	-	-	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
22	NDP	J	401	-	-	15/34/77/77	0/5/5/5
19	SF4	M	802	12	-	-	0/6/5/5
19	SF4	B	301	2	-	-	0/6/5/5

All (17) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
21	E	201	8Q1	C34-N36	5.24	1.45	1.33
21	E	201	8Q1	C39-N41	4.94	1.44	1.33
20	A	502	FMN	C9A-C5A	4.43	1.48	1.41
22	J	401	NDP	C5A-C4A	3.92	1.46	1.39
22	J	401	NDP	C6N-C5N	3.08	1.38	1.33
20	A	502	FMN	C8-C7	3.07	1.48	1.40
20	A	502	FMN	C4-N3	-3.05	1.33	1.38
22	J	401	NDP	C5A-N7A	-2.82	1.33	1.39
21	E	201	8Q1	O35-C34	-2.46	1.18	1.23
21	E	201	8Q1	C1-S44	2.34	1.81	1.76
21	E	201	8Q1	O40-C39	-2.33	1.18	1.23
21	E	201	8Q1	C6-C1	2.28	1.53	1.50
20	A	502	FMN	C5A-N5	-2.27	1.35	1.39
22	J	401	NDP	C5A-C6A	2.18	1.47	1.41
22	J	401	NDP	C8A-N7A	2.11	1.35	1.31
20	A	502	FMN	C4A-N5	2.11	1.34	1.30
20	A	502	FMN	C2-N3	-2.02	1.34	1.39

All (26) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	J	401	NDP	C5A-C4A-N3A	-6.20	118.66	126.75
22	J	401	NDP	PN-O3-PA	-5.21	114.95	132.83
22	J	401	NDP	N3A-C4A-N9A	4.95	135.24	127.08
21	E	201	8Q1	C6-C1-S44	4.52	118.72	113.46
22	J	401	NDP	C2A-N3A-C4A	4.04	121.30	111.75
22	J	401	NDP	N3A-C2A-N1A	-3.73	122.77	128.60
22	J	401	NDP	C4A-C5A-N7A	-3.10	106.84	110.62
20	A	502	FMN	C4-C4A-N5	2.84	122.27	118.23
22	J	401	NDP	C5A-N7A-C8A	2.82	107.52	103.51
21	E	201	8Q1	C43-S44-C1	2.79	110.57	101.87
20	A	502	FMN	C4A-C10-N1	-2.76	118.32	124.73
21	E	201	8Q1	C32-C34-N36	2.73	122.02	116.58
22	J	401	NDP	C4A-N9A-C8A	2.67	108.63	105.73
21	E	201	8Q1	O4-C1-C6	-2.54	120.99	123.99

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
21	E	201	8Q1	C42-N41-C39	-2.43	118.33	122.84
20	A	502	FMN	C4A-C10-N10	2.42	120.01	116.48
21	E	201	8Q1	C37-N36-C34	-2.40	118.30	122.59
20	A	502	FMN	O2-C2-N1	-2.32	117.98	121.83
20	A	502	FMN	C4-N3-C2	-2.23	121.52	125.64
22	J	401	NDP	C3D-C2D-C1D	2.22	105.64	101.43
22	J	401	NDP	N9A-C8A-N7A	-2.19	110.91	113.91
20	A	502	FMN	C4A-C4-N3	2.16	118.67	113.19
20	A	502	FMN	C10-N1-C2	2.16	121.22	116.90
22	J	401	NDP	C6A-C5A-N7A	2.15	136.03	132.02
20	A	502	FMN	N3-C2-N1	2.11	123.53	119.38
21	E	201	8Q1	O35-C34-N36	-2.11	118.46	122.99

There are no chirality outliers.

All (40) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
20	A	502	FMN	C1'-C2'-C3'-O3'
20	A	502	FMN	C1'-C2'-C3'-C4'
20	A	502	FMN	C3'-C4'-C5'-O5'
20	A	502	FMN	O4'-C4'-C5'-O5'
21	E	201	8Q1	C1-C6-C7-C8
21	E	201	8Q1	O4-C1-S44-C43
21	E	201	8Q1	C6-C1-S44-C43
21	E	201	8Q1	C29-C32-C34-N36
21	E	201	8Q1	C29-C32-C34-O35
21	E	201	8Q1	C42-C43-S44-C1
21	E	201	8Q1	C28-O27-P24-O3
21	E	201	8Q1	C28-O27-P24-O2
21	E	201	8Q1	C28-O27-P24-O1
22	J	401	NDP	C5B-O5B-PA-O1A
22	J	401	NDP	C5D-O5D-PN-O1N
21	E	201	8Q1	C38-C39-N41-C42
22	J	401	NDP	O4B-C4B-C5B-O5B
22	J	401	NDP	C3B-C4B-C5B-O5B
22	J	401	NDP	C1B-C2B-O2B-P2B
21	E	201	8Q1	O40-C39-N41-C42
22	J	401	NDP	C3B-C2B-O2B-P2B
21	E	201	8Q1	C12-C13-C14-C15
21	E	201	8Q1	N41-C42-C43-S44
20	A	502	FMN	O2'-C2'-C3'-O3'
20	A	502	FMN	O2'-C2'-C3'-C4'

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Mol	Chain	Res	Type	Atoms
21	E	201	8Q1	C7-C8-C9-C10
22	J	401	NDP	C5B-O5B-PA-O3
22	J	401	NDP	C5D-O5D-PN-O3
21	E	201	8Q1	C6-C7-C8-C9
22	J	401	NDP	C5B-O5B-PA-O2A
22	J	401	NDP	C5D-O5D-PN-O2N
21	E	201	8Q1	O33-C32-C34-O35
22	J	401	NDP	O4D-C1D-N1N-C6N
22	J	401	NDP	C2D-C1D-N1N-C6N
21	E	201	8Q1	O27-C28-C29-C30
21	E	201	8Q1	O33-C32-C34-N36
22	J	401	NDP	O4D-C4D-C5D-O5D
22	J	401	NDP	O4D-C1D-N1N-C2N
22	J	401	NDP	C2D-C1D-N1N-C2N
20	A	502	FMN	N10-C1'-C2'-O2'

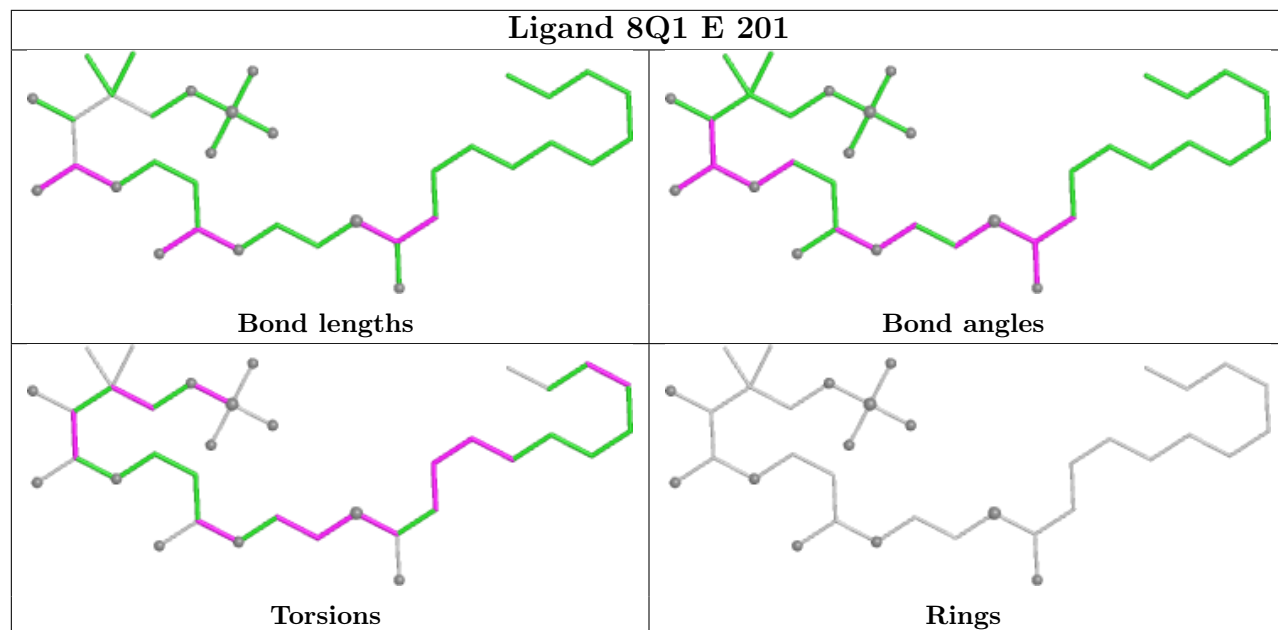
There are no ring outliers.

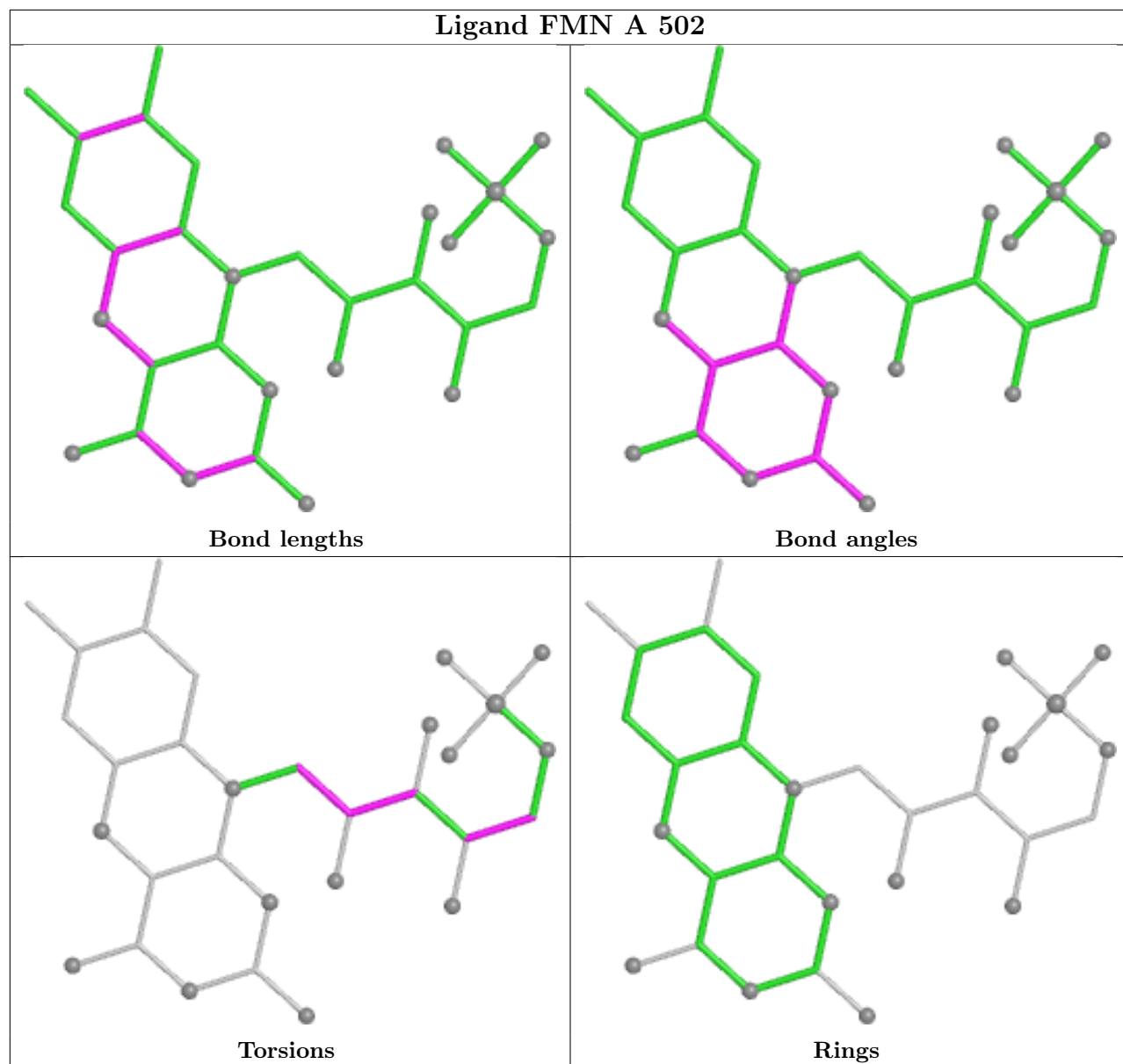
10 monomers are involved in 64 short contacts:

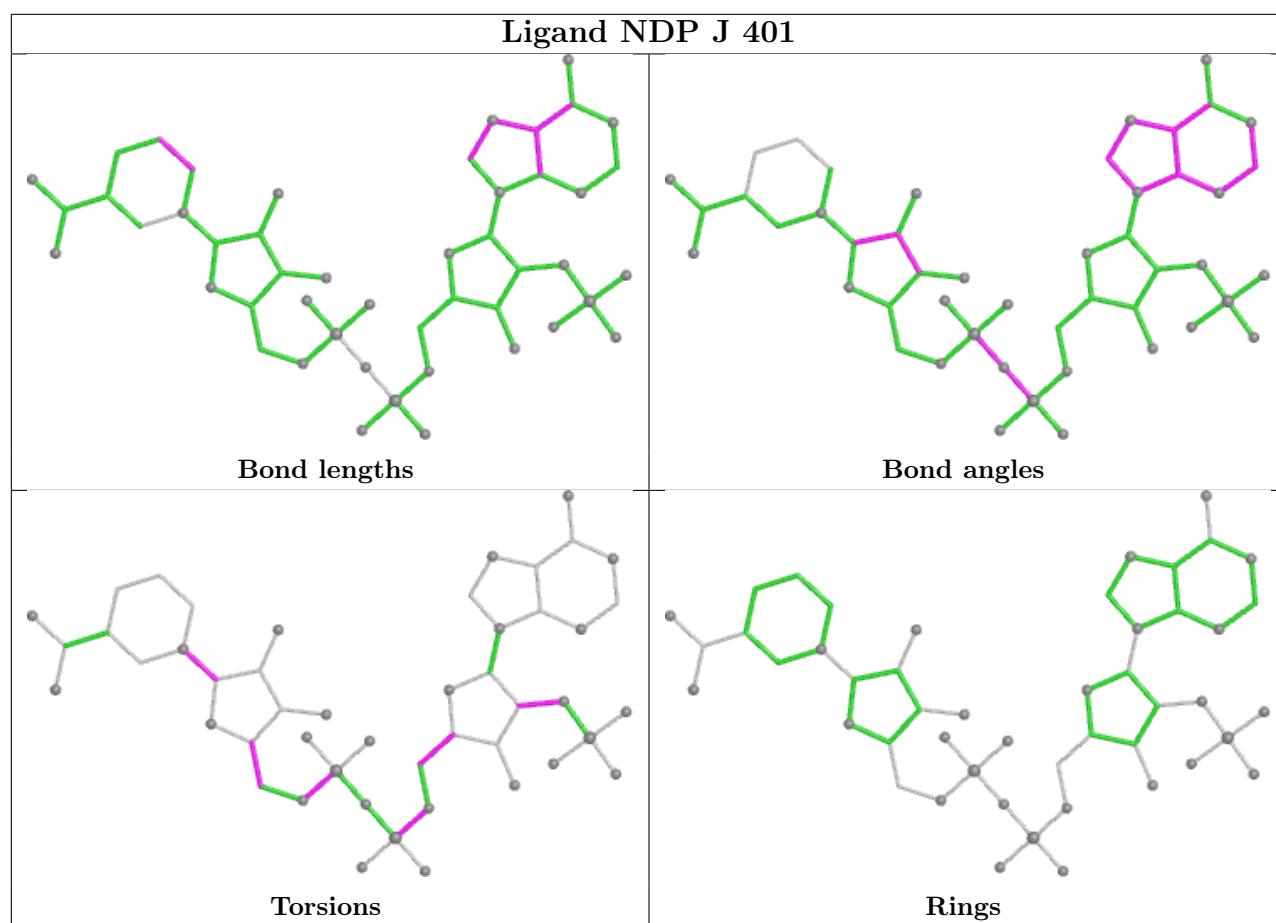
Mol	Chain	Res	Type	Clashes	Symm-Clashes
21	E	201	8Q1	4	0
23	O	301	FES	2	0
19	M	801	SF4	4	0
20	A	502	FMN	16	0
19	A	501	SF4	6	0
19	B	302	SF4	2	0
19	C	301	SF4	1	0
23	M	803	FES	1	0
22	J	401	NDP	27	0
19	B	301	SF4	1	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient

equivalents in the CSD to analyse the geometry.







5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

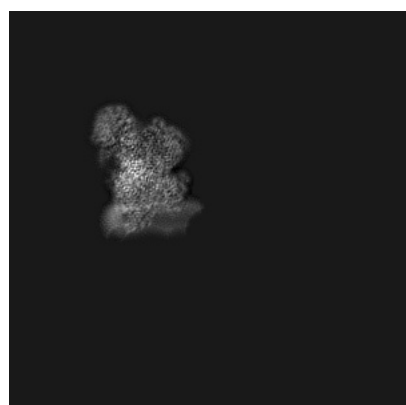
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-6771. These allow visual inspection of the internal detail of the map and identification of artifacts.

No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

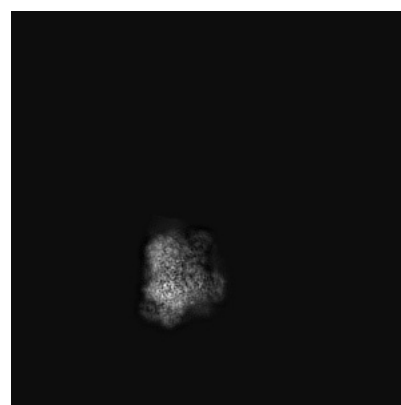
6.1.1 Primary map



X



Y



Z

The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

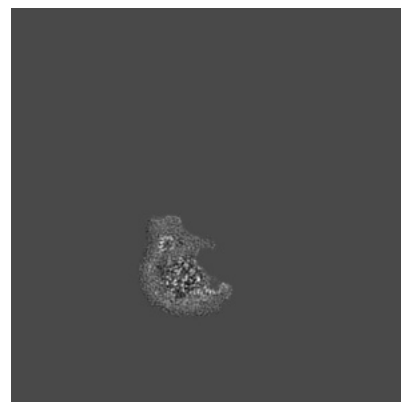
6.2.1 Primary map



X Index: 240



Y Index: 240

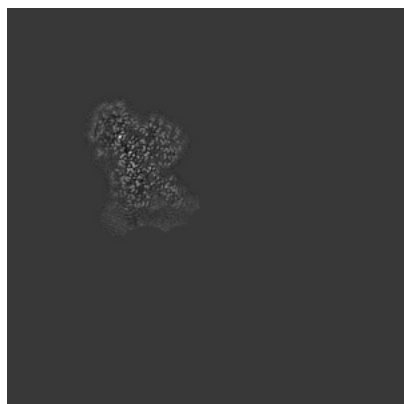


Z Index: 240

The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

6.3.1 Primary map



X Index: 189



Y Index: 147

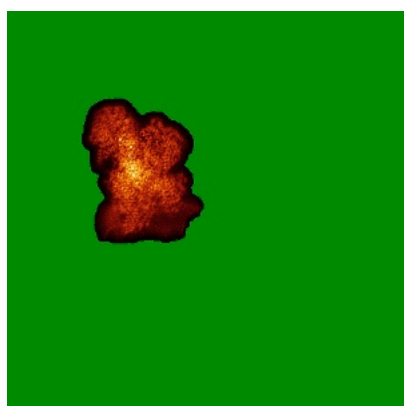


Z Index: 281

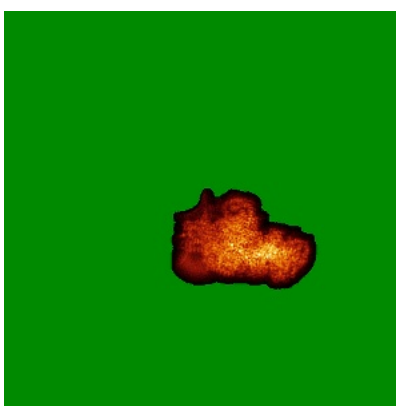
The images above show the largest variance slices of the map in three orthogonal directions.

6.4 Orthogonal standard-deviation projections (False-color) [i](#)

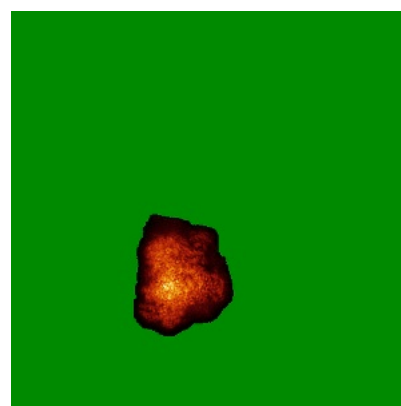
6.4.1 Primary map



X



Y

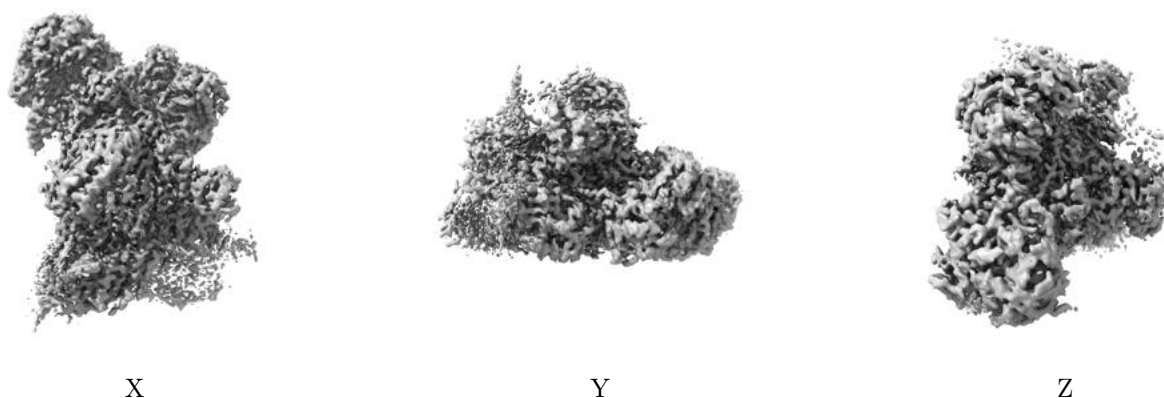


Z

The images above show the map standard deviation projections with false color in three orthogonal directions. Minimum values are shown in green, max in blue, and dark to light orange shades represent small to large values respectively.

6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.0516. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

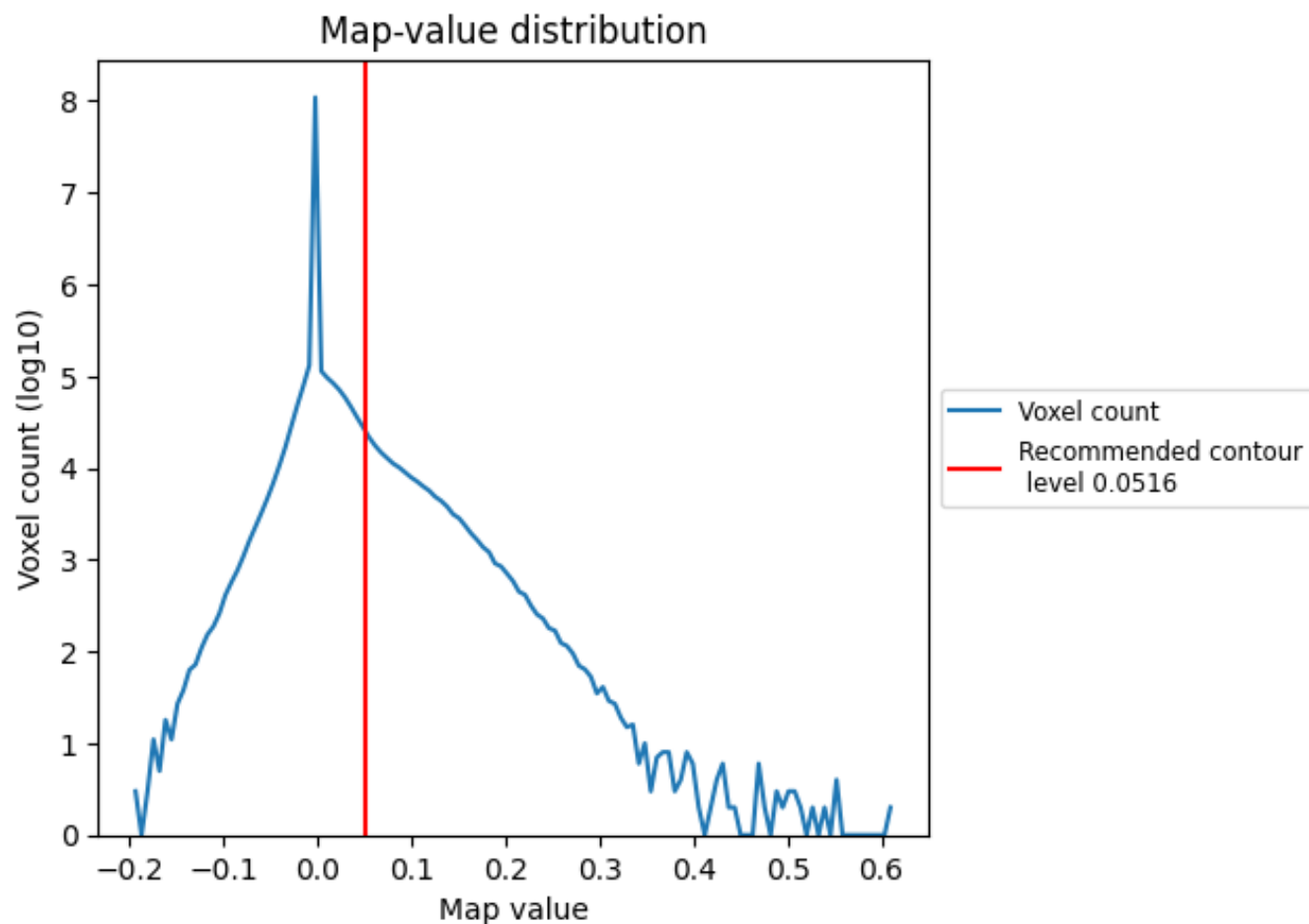
6.6 Mask visualisation [i](#)

This section was not generated. No masks/segmentation were deposited.

7 Map analysis [i](#)

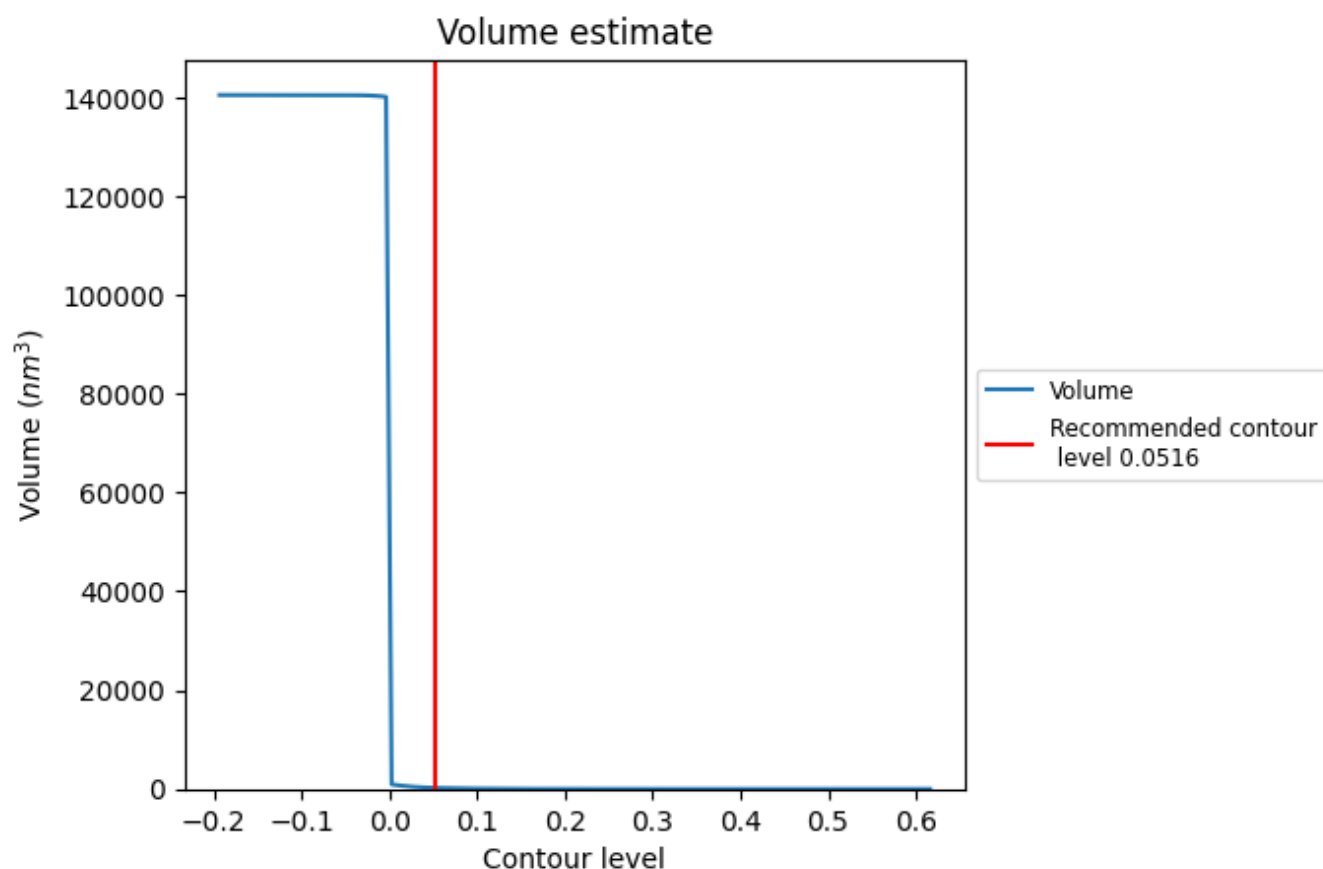
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution [i](#)



The map-value distribution is plotted in 128 intervals along the x-axis. The y-axis is logarithmic. A spike in this graph at zero usually indicates that the volume has been masked.

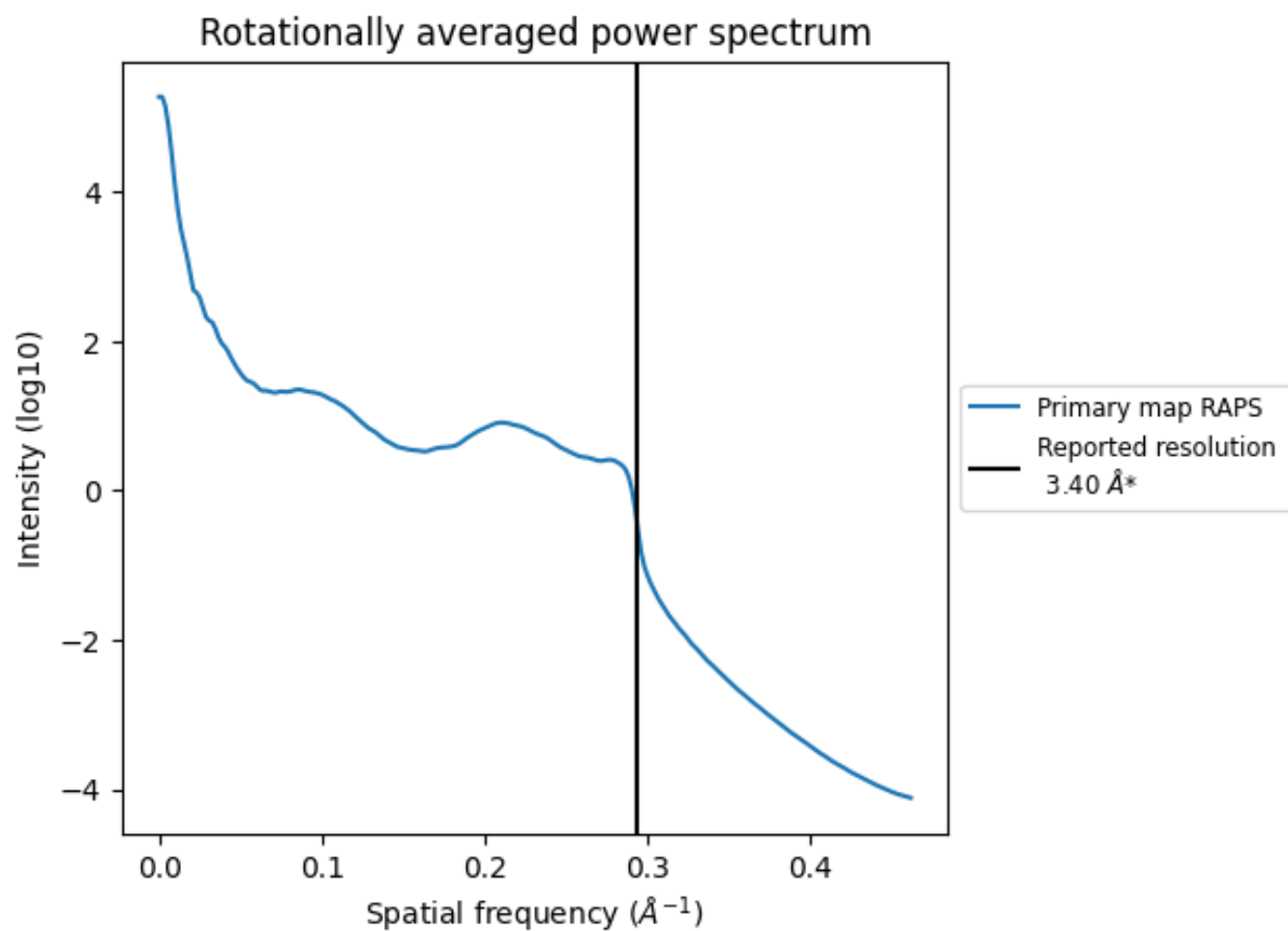
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 219 nm^3 ; this corresponds to an approximate mass of 198 kDa.

The volume estimate graph shows how the enclosed volume varies with the contour level. The recommended contour level is shown as a vertical line and the intersection between the line and the curve gives the volume of the enclosed surface at the given level.

7.3 Rotationally averaged power spectrum ⓘ



*Reported resolution corresponds to spatial frequency of 0.294 Å⁻¹

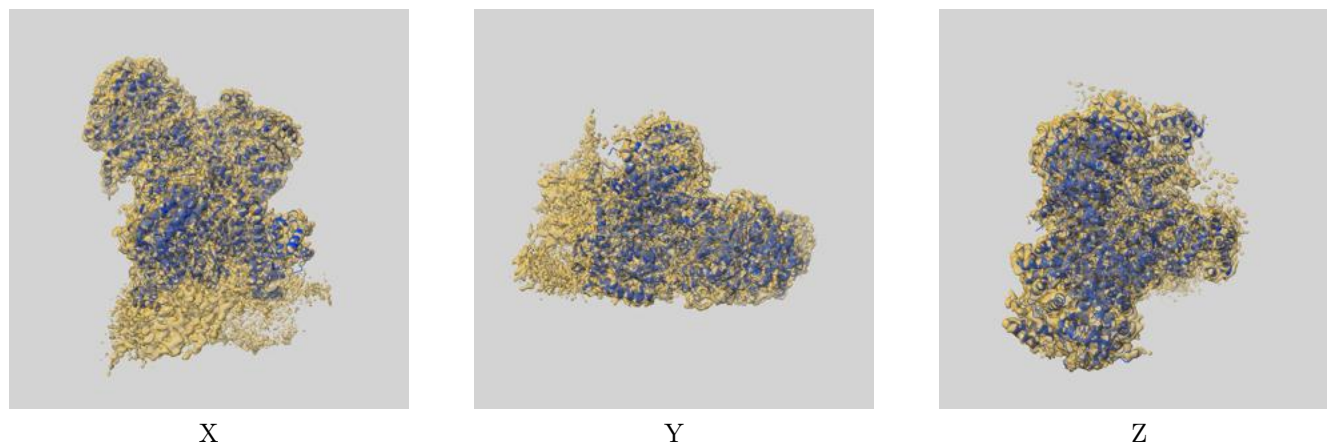
8 Fourier-Shell correlation

This section was not generated. No FSC curve or half-maps provided.

9 Map-model fit [i](#)

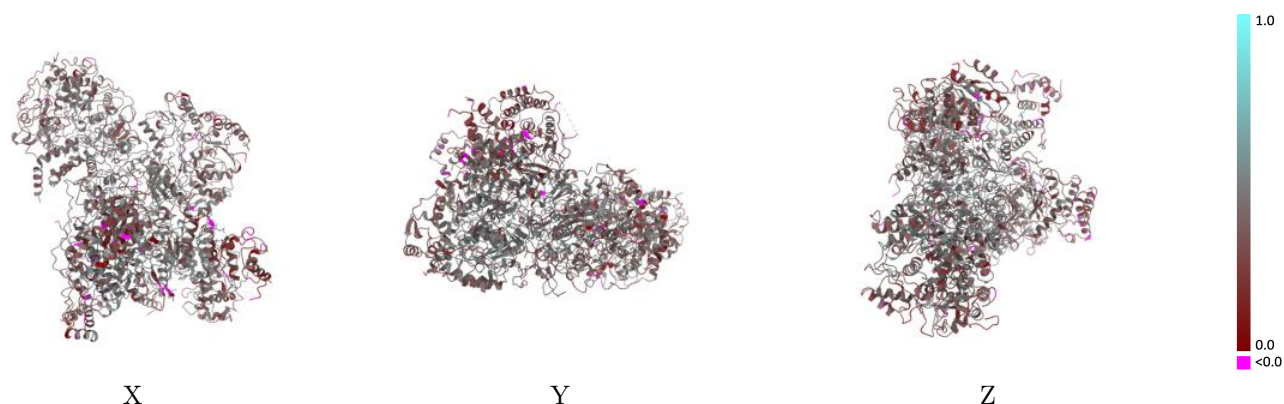
This section contains information regarding the fit between EMDB map EMD-6771 and PDB model 5XTB. Per-residue inclusion information can be found in section 3 on page 10.

9.1 Map-model overlay [i](#)



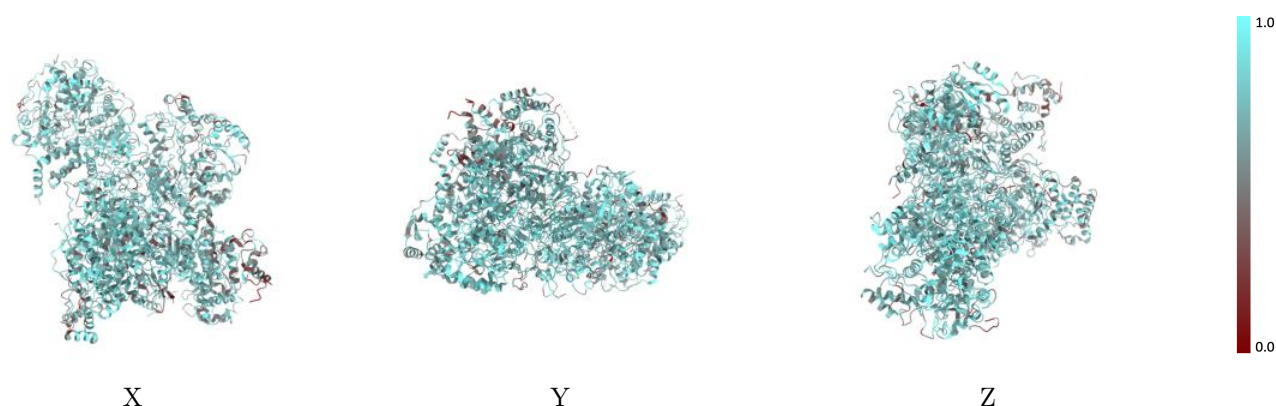
The images above show the 3D surface view of the map at the recommended contour level 0.0516 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

9.2 Q-score mapped to coordinate model [i](#)



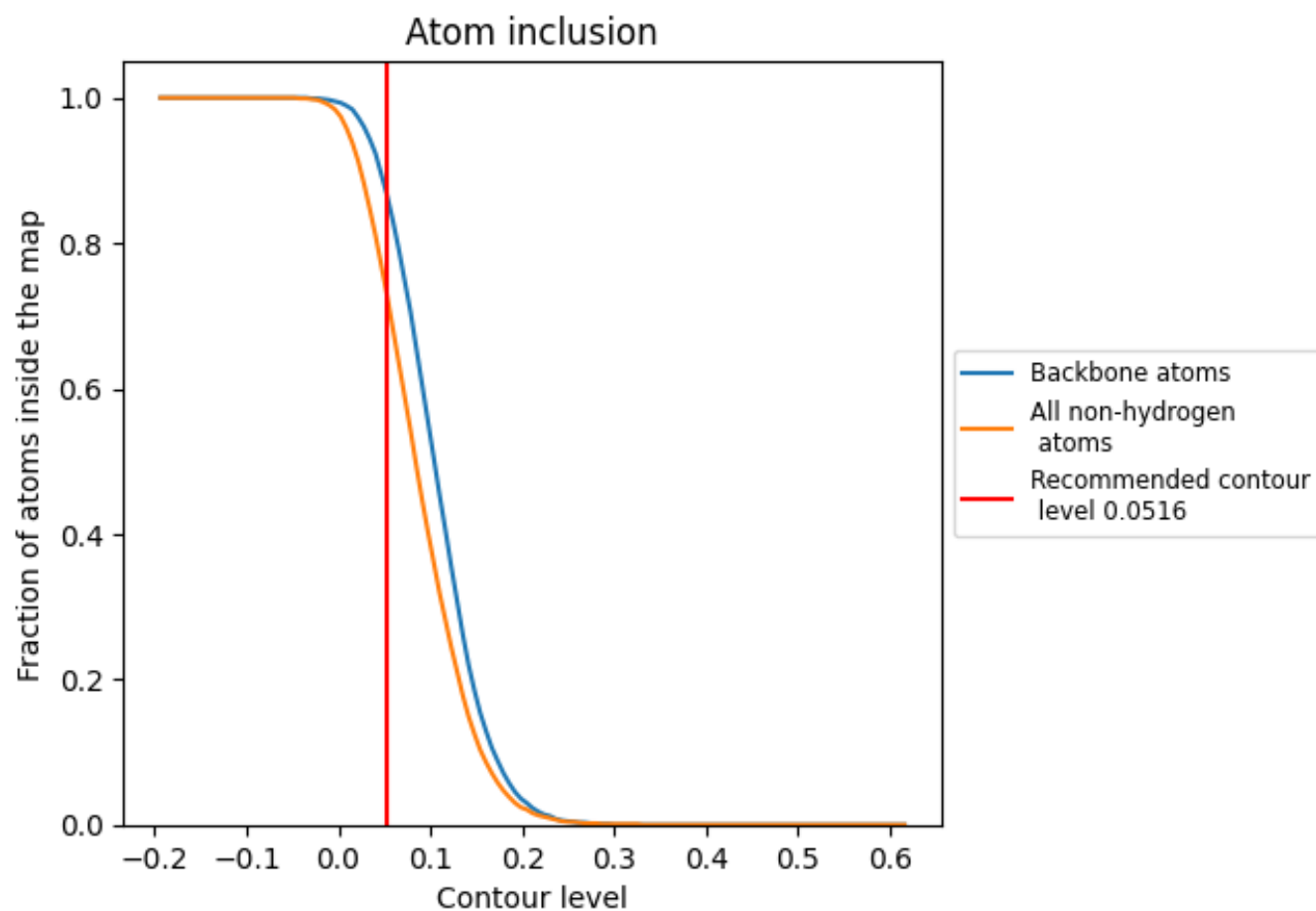
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions at which atoms can be resolved. Low Q-score values may therefore be expected for many entries.

9.3 Atom inclusion mapped to coordinate model [i](#)



The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.0516).

9.4 Atom inclusion ⓘ



At the recommended contour level, 87% of all backbone atoms, 74% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary

The table lists the average atom inclusion at the recommended contour level (0.0516) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.7370	 0.3890
A	 0.7470	 0.3790
B	 0.8260	 0.4490
C	 0.8320	 0.4710
E	 0.7080	 0.3800
F	 0.7390	 0.3330
G	 0.5150	 0.2360
H	 0.6730	 0.2830
I	 0.6250	 0.3560
J	 0.7500	 0.4070
K	 0.6790	 0.3400
L	 0.7430	 0.4100
M	 0.7460	 0.3910
N	 0.6790	 0.3760
O	 0.7260	 0.3710
P	 0.7330	 0.3860
Q	 0.7640	 0.4220
T	 0.7060	 0.3980
W	 0.7370	 0.3580

