



Full wwPDB EM Validation Report ⓘ

Mar 9, 2026 – 01:26 AM UTC

PDB ID : 8HPO / pdb_00008hpo
EMDB ID : EMD-34935
Title : Cryo-EM structure of a SIN3/HDAC complex from budding yeast
Authors : Guo, Z.; Zhan, X.; Wang, C.
Deposited on : 2022-12-12
Resolution : 2.60 Å(reported)

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

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/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.dev132
Mogul : 2022.3.0, CSD as543be (2022)
MolProbity : 4-5-2 with Phenix2.0
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) : 2.49

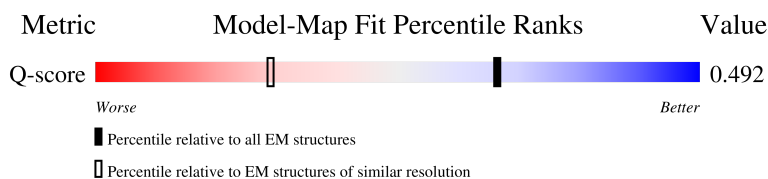
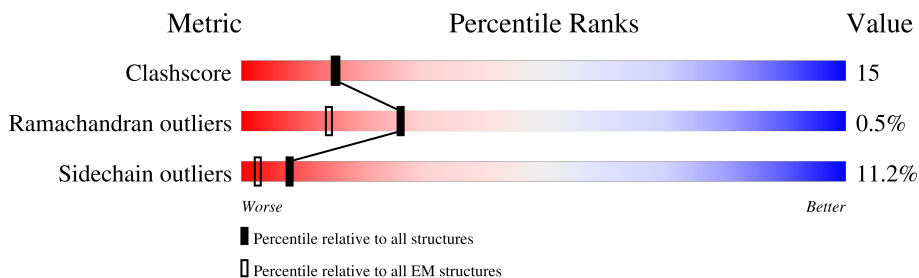
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 2.60 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.



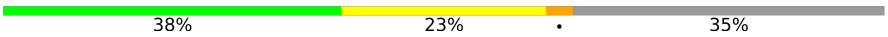
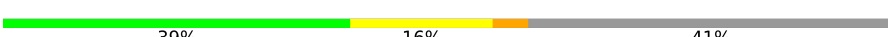
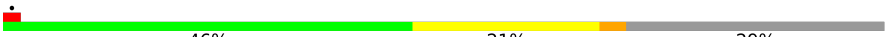
Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
Q-score	-	25397	8728 (2.10 - 3.10)

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	K	460	89% 86% 10%
2	D	327	7% 28% 17% 6% 50%
3	F	433	65% 21% 9%
4	G	433	62% 22% 5% 11%

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Mol	Chain	Length	Quality of chain
5	I	201	
6	A	1536	
6	B	1536	
7	H	405	
8	C	330	
9	E	430	
10	J	294	

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
3	SEP	F	265	-	-	X	-
3	TPO	F	365	-	-	X	-
9	TPO	E	167	-	-	X	-

2 Entry composition

There are 12 unique types of molecules in this entry. The entry contains 27950 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 Transcriptional regulatory protein UME1.

Mol	Chain	Residues	Atoms				AltConf	Trace
1	K	413	Total	C	N	O	0	0
			2038	1212	413	413		

- Molecule 2 is a protein called Transcriptional regulatory protein SDS3.

Mol	Chain	Residues	Atoms						AltConf	Trace
2	D	165	Total	C	N	O	P	S	0	0
			1385	863	248	271	1	2		

- Molecule 3 is a protein called Histone deacetylase RPD3.

Mol	Chain	Residues	Atoms						AltConf	Trace
3	F	393	Total	C	N	O	P	S	0	0
			3143	1986	525	601	6	25		

- Molecule 4 is a protein called Histone deacetylase RPD3.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	G	385	Total	C	N	O	S	0	0
			3057	1948	513	571	25		

- Molecule 5 is a protein called Transcriptional regulatory protein SAP30.

Mol	Chain	Residues	Atoms						AltConf	Trace
5	I	130	Total	C	N	O	P	S	0	0
			1104	696	203	201	1	3		

- Molecule 6 is a protein called Transcriptional regulatory protein SIN3.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	A	637	Total	C	N	O	S	0	0
			5283	3392	887	987	17		

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Mol	Chain	Residues	Atoms					AltConf	Trace
6	B	613	Total	C	N	O	S	0	0
			5129	3295	862	955	17		

- Molecule 7 is a protein called Transcriptional regulatory protein DEP1.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	H	233	Total	C	N	O	S	0	0
			1936	1218	340	368	10		

- Molecule 8 is a protein called Transcriptional regulatory protein PHO23.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	C	138	Total	C	N	O	S	0	0
			1116	703	195	211	7		

- Molecule 9 is a protein called Transcriptional regulatory protein RXT2.

Mol	Chain	Residues	Atoms						AltConf	Trace
9	E	255	Total	C	N	O	P	S	0	0
			2077	1306	375	391	2	3		

- Molecule 10 is a protein called Transcriptional regulatory protein RXT3.

Mol	Chain	Residues	Atoms					AltConf	Trace
10	J	209	Total	C	N	O	S	0	0
			1676	1069	284	321	2		

- Molecule 11 is ZINC ION (CCD ID: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		AltConf
11	F	1	Total	Zn	0
			1	1	
11	G	1	Total	Zn	0
			1	1	

- Molecule 12 is POTASSIUM ION (CCD ID: K) (formula: K).

Mol	Chain	Residues	Atoms		AltConf
12	F	2	Total	K	0
			2	2	

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Mol	Chain	Residues	Atoms		AltConf
12	G	2	Total	K	0
			2	2	

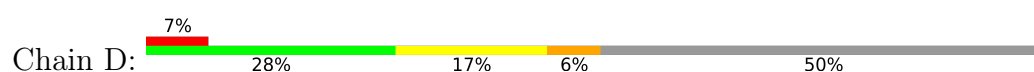
3 Residue-property plots

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.

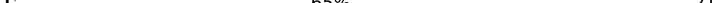
- Molecule 1: Transcriptional regulatory protein UME1

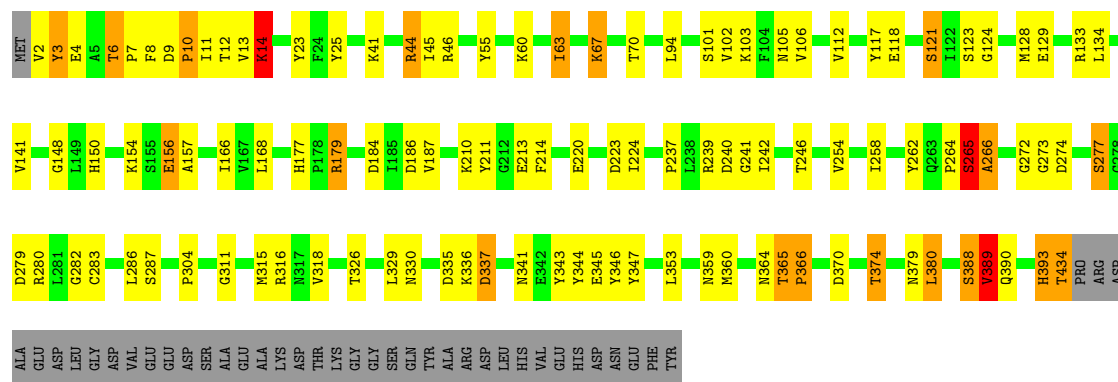


- Molecule 2: Transcriptional regulatory protein SDS3



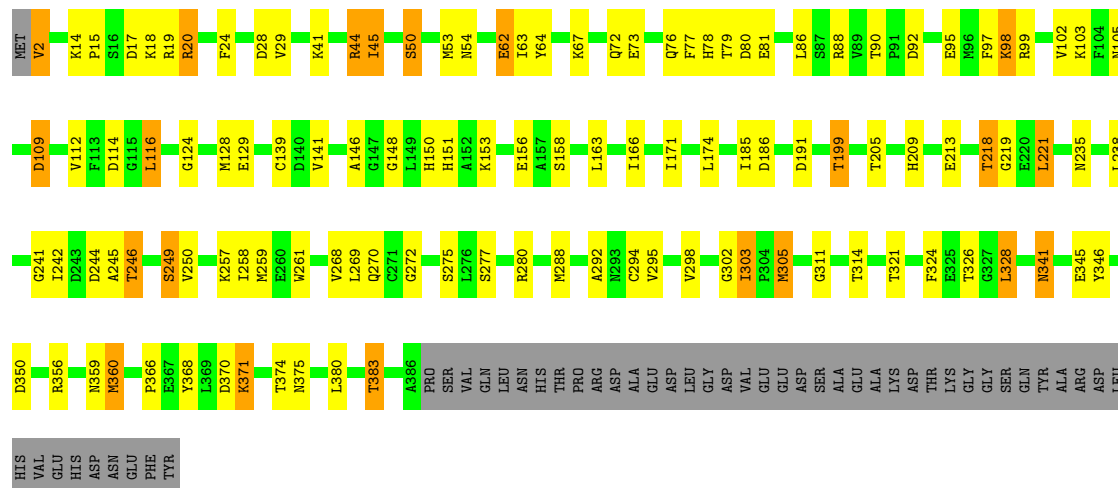
- Molecule 3: Histone deacetylase RPD3

Chain F:  65% 21% . . 9%



- Molecule 4: Histone deacetylase RPD3

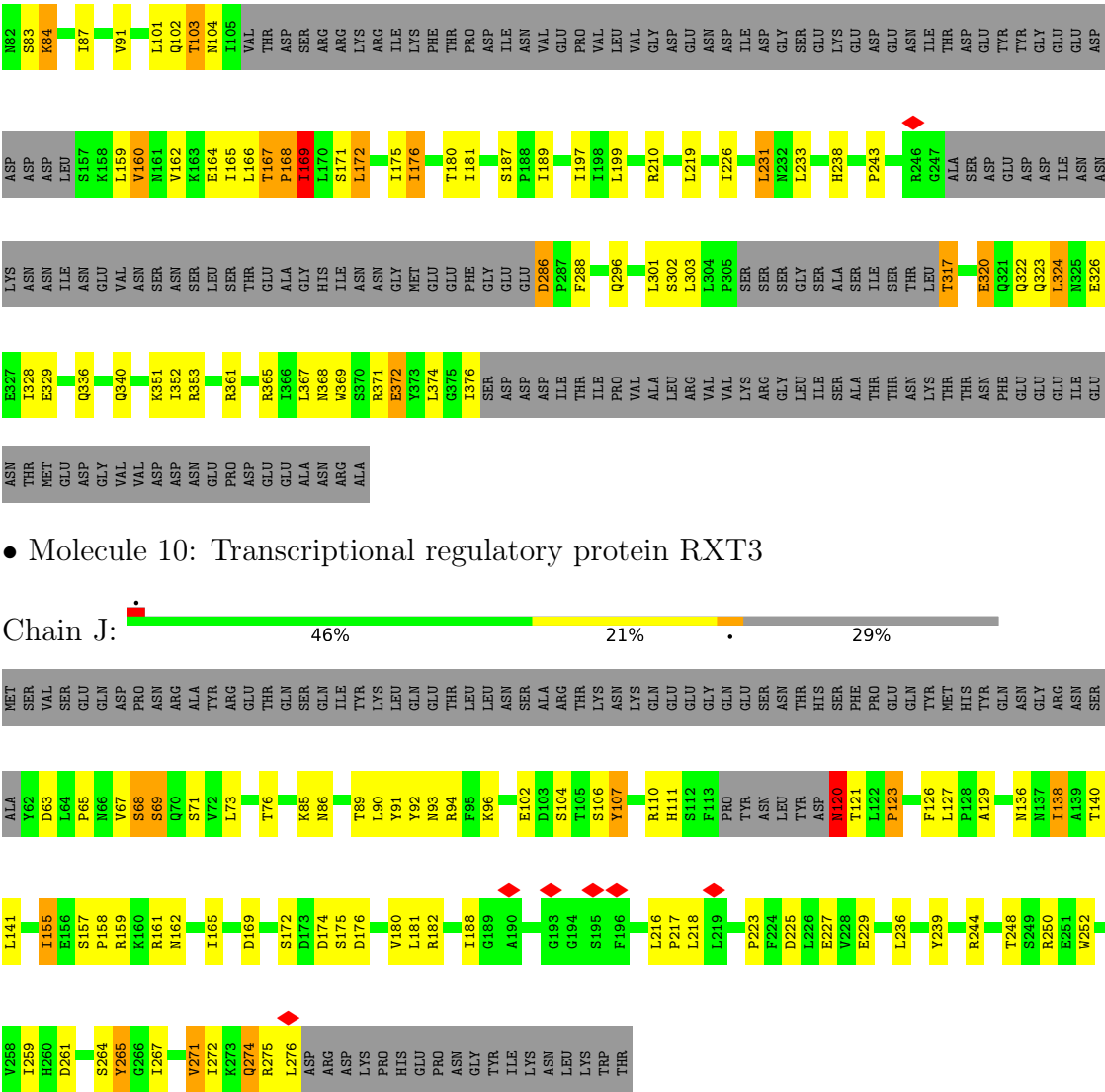
Chain G: 62% 22% 5% 11%





Chain H:





• Molecule 10: Transcriptional regulatory protein RXT3

4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	665105	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 ($e^-/\text{\AA}^2$)	50	Depositor
Minimum defocus (nm)	1800	Depositor
Maximum defocus (nm)	2300	Depositor
Magnification	Not provided	
Image detector	GATAN K3 (6k x 4k)	Depositor
Maximum map value	4.442	Depositor
Minimum map value	-2.664	Depositor
Average map value	0.001	Depositor
Map value standard deviation	0.066	Depositor
Recommended contour level	0.3	Depositor
Map size ($\text{\AA}$)	434.80002, 434.80002, 434.80002	wwPDB
Map dimensions	400, 400, 400	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing ($\text{\AA}$)	1.087, 1.087, 1.087	Depositor

5 Model quality [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: TPO, K, SEP, ZN

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	K	0.12	0/2033	0.37	0/2822
2	D	0.60	1/1393 (0.1%)	0.93	7/1866 (0.4%)
3	F	0.65	3/3156 (0.1%)	0.81	14/4262 (0.3%)
4	G	0.24	0/3137	0.45	0/4246
5	I	0.34	0/1119	0.66	1/1500 (0.1%)
6	A	0.24	0/5400	0.48	0/7289
6	B	0.21	0/5245	0.53	1/7077 (0.0%)
7	H	0.26	0/1976	0.52	0/2674
8	C	0.23	0/1134	0.50	0/1529
9	E	0.42	1/2082 (0.0%)	0.67	5/2799 (0.2%)
10	J	0.44	2/1718 (0.1%)	0.69	5/2335 (0.2%)
All	All	0.36	7/28393 (0.0%)	0.59	33/38399 (0.1%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
3	F	0	1
5	I	0	1
6	A	0	1
6	B	0	2
7	H	0	4
9	E	0	2
All	All	0	11

All (7) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	F	10	PRO	N-CA	19.07	1.69	1.47

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	F	14	LYS	C-N	18.50	1.50	1.33
10	J	123	PRO	C-N	13.41	1.49	1.33
2	D	294	PRO	C-N	12.91	1.50	1.33
3	F	9	ASP	C-N	10.66	1.46	1.33
10	J	123	PRO	C-O	-5.85	1.18	1.24
9	E	169	ILE	C-O	-5.08	1.18	1.24

All (33) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	F	9	ASP	CA-C-N	17.51	138.67	119.93
3	F	9	ASP	C-N-CA	17.51	138.67	119.93
2	D	307	ASP	CB-CA-C	-13.79	87.91	110.79
10	J	123	PRO	CA-C-N	13.09	133.87	120.38
10	J	123	PRO	C-N-CA	13.09	133.87	120.38
2	D	294	PRO	CA-C-N	11.12	130.88	119.76
2	D	294	PRO	C-N-CA	11.12	130.88	119.76
3	F	14	LYS	CA-C-N	9.53	132.43	120.89
3	F	14	LYS	C-N-CA	9.53	132.43	120.89
3	F	9	ASP	CB-CA-C	-8.92	95.42	109.42
10	J	123	PRO	CB-CA-C	-7.92	101.26	110.92
3	F	14	LYS	CB-CA-C	-7.71	99.83	109.31
3	F	10	PRO	N-CA-C	-7.60	98.88	111.26
3	F	10	PRO	CA-N-CD	-6.99	102.21	112.00
3	F	266	ALA	N-CA-CB	6.67	120.40	110.40
10	J	120	ASN	CA-C-N	6.35	133.67	121.54
10	J	120	ASN	C-N-CA	6.35	133.67	121.54
9	E	168	PRO	N-CA-CB	-6.27	96.10	103.00
2	D	294	PRO	O-C-N	-6.11	114.25	121.46
2	D	305	THR	CA-CB-OG1	-5.75	100.98	109.60
9	E	168	PRO	CA-C-N	5.73	128.18	120.50
9	E	168	PRO	C-N-CA	5.73	128.18	120.50
6	B	732	CYS	N-CA-C	-5.65	107.03	114.04
3	F	3	TYR	CA-C-N	-5.61	115.25	123.00
3	F	3	TYR	C-N-CA	-5.61	115.25	123.00
9	E	40	ASN	CA-C-N	5.59	132.22	121.54
9	E	40	ASN	C-N-CA	5.59	132.22	121.54
3	F	393	HIS	CB-CA-C	5.58	120.71	110.10
5	I	177	GLU	O-C-N	5.53	129.95	122.59
2	D	290	THR	CB-CA-C	5.36	119.34	111.73
2	D	306	GLU	CA-C-O	-5.35	115.20	120.82
3	F	344	TYR	N-CA-C	-5.28	107.37	112.97

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	F	10	PRO	CB-CA-C	5.05	118.05	111.64

There are no chirality outliers.

All (11) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
6	A	891	ALA	Peptide
6	B	741	HIS	Peptide
6	B	891	ALA	Peptide
9	E	41	TYR	Peptide
9	E	42	GLN	Peptide
3	F	265	SEP	Mainchain
7	H	314	LYS	Peptide
7	H	342	GLU	Peptide
7	H	343	SER	Peptide
7	H	344	ILE	Peptide
5	I	174	SEP	Mainchain

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	K	2038	0	890	9	0
2	D	1385	0	1388	87	0
3	F	3143	0	2983	91	0
4	G	3057	0	2932	74	0
5	I	1104	0	1087	47	0
6	A	5283	0	5216	167	0
6	B	5129	0	5096	204	0
7	H	1936	0	1896	66	0
8	C	1116	0	1133	43	0
9	E	2077	0	2136	76	0
10	J	1676	0	1637	45	0
11	F	1	0	0	0	0
11	G	1	0	0	0	0
12	F	2	0	0	0	0
12	G	2	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
All	All	27950	0	26394	794	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 15.

All (794) 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)
3:F:10:PRO:N	3:F:10:PRO:CA	1.69	1.36
3:F:6:TPO:CG2	3:F:7:PRO:HD2	1.68	1.23
9:E:176:ILE:CD1	9:E:374:LEU:HD12	1.77	1.15
9:E:167:TPO:CG2	9:E:168:PRO:HD2	1.81	1.10
5:I:177:GLU:O	5:I:179:ASP:N	1.82	1.09
2:D:304:VAL:CG1	6:A:875:ARG:HH21	1.66	1.07
3:F:6:TPO:HG23	3:F:7:PRO:CD	1.84	1.06
2:D:312:ARG:HD2	2:D:317:GLN:OE1	1.55	1.05
3:F:365:TPO:HG23	3:F:366:PRO:HD2	1.39	1.01
9:E:167:TPO:HG23	9:E:168:PRO:HD2	1.03	1.01
9:E:167:TPO:HG23	9:E:168:PRO:CD	1.90	1.00
6:B:987:ASP:O	6:B:990:CYS:HB2	1.60	1.00
9:E:176:ILE:HD11	9:E:374:LEU:HD12	1.40	0.99
6:A:923:VAL:O	6:A:927:SER:HB2	1.63	0.96
9:E:176:ILE:HD11	9:E:374:LEU:CD1	1.96	0.96
2:D:291:LYS:HE3	2:D:291:LYS:HA	1.48	0.95
2:D:304:VAL:HG12	6:A:875:ARG:HH21	1.29	0.95
3:F:6:TPO:HG23	3:F:7:PRO:HD2	0.94	0.93
2:D:311:ILE:CD1	6:A:890:THR:HG23	2.00	0.91
9:E:176:ILE:CD1	9:E:374:LEU:CD1	2.49	0.90
6:A:837:LYS:NZ	6:A:841:MET:SD	2.46	0.88
3:F:265:SEP:O1P	3:F:265:SEP:N	2.06	0.88
9:E:176:ILE:HD12	9:E:374:LEU:HD12	1.56	0.88
4:G:90:THR:HG22	4:G:92:ASP:H	1.38	0.87
3:F:365:TPO:HG23	3:F:366:PRO:CD	2.07	0.83
2:D:132:ARG:HH12	7:H:198:GLN:HA	1.42	0.83
3:F:156:GLU:OE2	6:A:742:ARG:NH2	2.12	0.83
6:B:972:LYS:O	6:B:1315:GLN:NE2	2.12	0.82
6:B:1287:ARG:NH2	6:B:1321:ASP:O	2.12	0.81
2:D:291:LYS:HA	2:D:291:LYS:CE	2.06	0.81
5:I:177:GLU:C	5:I:179:ASP:H	1.88	0.81
6:B:1013:LEU:HD11	6:B:1257:MET:HG3	1.63	0.81
6:A:1330:ASP:HA	6:A:1333:LYS:HE2	1.62	0.81

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:J:227:GLU:HB2	10:J:271:VAL:HG22	1.64	0.80
2:D:304:VAL:HG12	6:A:875:ARG:NH2	1.96	0.79
6:A:770:ARG:HG2	6:A:774:CYS:HB3	1.64	0.79
6:B:1169:THR:O	6:B:1173:ASN:ND2	2.16	0.78
6:A:939:ASP:OD2	6:A:1157:ARG:NH2	2.15	0.77
2:D:302:ASP:HA	2:D:305:THR:HG22	1.67	0.77
5:I:177:GLU:O	5:I:180:CYS:N	2.15	0.76
2:D:312:ARG:HH12	2:D:320:ALA:HB2	1.51	0.76
3:F:4:GLU:N	3:F:4:GLU:OE1	2.18	0.76
10:J:162:ASN:O	10:J:250:ARG:NH1	2.19	0.76
6:B:1004:ASN:HA	6:B:1007:LYS:HD3	1.68	0.75
2:D:311:ILE:HD13	6:A:890:THR:HG23	1.68	0.75
4:G:50:SER:O	4:G:54:ASN:ND2	2.20	0.75
4:G:350:ASP:OD2	4:G:356:ARG:NH2	2.19	0.74
2:D:313:GLU:HA	2:D:313:GLU:OE2	1.85	0.74
9:E:103:THR:HG23	9:E:104:ASN:H	1.53	0.74
3:F:10:PRO:N	3:F:10:PRO:C	2.45	0.74
3:F:337:ASP:HB3	6:A:1178:VAL:HG22	1.69	0.74
9:E:164:GLU:HA	9:E:167:TPO:O2P	1.88	0.74
6:B:1327:PRO:HB3	6:B:1333:LYS:HD3	1.69	0.73
3:F:365:TPO:CG2	3:F:366:PRO:HD2	2.15	0.73
4:G:148:GLY:HA2	4:G:166:ILE:HD11	1.70	0.73
5:I:79:TYR:OH	6:A:878:GLU:OE1	2.07	0.73
7:H:220:HIS:NE2	7:H:222:GLU:HB3	2.05	0.72
3:F:179:ARG:O	3:F:265:SEP:O1P	2.07	0.72
7:H:242:TYR:OH	9:E:243:PRO:O	2.07	0.72
4:G:2:VAL:N	4:G:370:ASP:OD1	2.23	0.72
6:B:1067:ASP:HA	6:B:1070:HIS:HB2	1.71	0.71
2:D:310:LEU:C	2:D:310:LEU:HD23	2.15	0.71
6:A:956:LYS:HE2	6:A:959:GLN:HE21	1.56	0.71
7:H:317:SER:OG	7:H:354:ASP:OD1	2.09	0.70
2:D:18:ARG:HG2	6:A:666:VAL:HG21	1.73	0.69
7:H:218:GLY:O	7:H:224:GLN:NE2	2.25	0.69
2:D:64:ARG:HD3	5:I:113:ARG:HD3	1.74	0.69
9:E:25:ILE:HD13	6:B:690:ASN:HB2	1.75	0.69
9:E:67:LYS:NZ	10:J:174:ASP:OD2	2.26	0.69
6:B:902:ASP:OD1	6:B:906:ARG:NH2	2.26	0.69
6:B:1287:ARG:NH2	6:B:1319:LEU:O	2.25	0.69
7:H:342:GLU:HG3	8:C:122:ARG:HH21	1.57	0.68
6:A:1140:ALA:HB1	6:A:1144:ILE:HB	1.75	0.68
3:F:154:LYS:NZ	6:A:780:ASP:OD1	2.27	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:I:177:GLU:C	5:I:179:ASP:N	2.49	0.68
9:E:30:THR:HB	6:B:662:LEU:HD11	1.74	0.68
3:F:265:SEP:HB2	3:F:434:TPO:HB	1.76	0.68
6:B:1291:ARG:HG3	6:B:1319:LEU:HD21	1.75	0.68
2:D:43:ARG:NH2	5:I:196:LYS:O	2.27	0.68
6:B:981:ASP:OD2	6:B:1162:LYS:NZ	2.24	0.68
2:D:95:PHE:HB2	7:H:245:GLN:HG3	1.75	0.67
2:D:15:ASP:OD2	2:D:18:ARG:NH1	2.22	0.67
4:G:19:ARG:HH22	4:G:302:GLY:HA2	1.59	0.67
8:C:128:HIS:O	8:C:130:ALA:N	2.27	0.67
6:A:1006:ASP:OD1	6:A:1006:ASP:N	2.22	0.67
4:G:280:ARG:NH1	6:B:812:GLU:OE2	2.25	0.67
10:J:239:TYR:OH	10:J:264:SER:OG	2.10	0.67
4:G:15:PRO:O	4:G:18:LYS:NZ	2.28	0.66
5:I:186:TYR:O	5:I:190:ASN:ND2	2.28	0.66
6:B:1191:LEU:HD12	6:B:1191:LEU:H	1.60	0.66
6:A:1295:SER:OG	6:A:1296:ASN:N	2.28	0.66
8:C:135:HIS:O	8:C:139:GLU:HB2	1.96	0.66
2:D:291:LYS:HE3	2:D:291:LYS:CA	2.24	0.66
7:H:204:GLN:HE22	7:H:205:LEU:HD13	1.61	0.66
6:A:1265:ILE:HG12	6:A:1290:VAL:HG23	1.78	0.65
8:C:8:PHE:O	8:C:12:ASN:ND2	2.24	0.65
9:E:70:GLN:C	9:E:72:SER:H	2.04	0.65
6:B:1175:ARG:NH1	6:B:1231:ALA:O	2.29	0.65
6:B:1009:ARG:NH2	6:B:1069:LEU:O	2.28	0.65
6:B:1213:ARG:HE	6:B:1218:ASP:HB3	1.62	0.65
6:B:860:MET:SD	6:B:860:MET:N	2.65	0.65
2:D:80:LEU:HD11	7:H:259:THR:HG23	1.77	0.65
4:G:95:GLU:HA	4:G:98:LYS:HD2	1.78	0.65
2:D:304:VAL:HG22	6:A:871:TYR:HD1	1.62	0.65
6:A:1268:LEU:HD23	6:A:1286:TYR:HD2	1.61	0.65
10:J:85:LYS:HZ3	10:J:86:ASN:H	1.45	0.65
6:A:951:GLU:HG2	6:A:969:PRO:HG2	1.79	0.64
6:A:1042:GLU:OE1	6:A:1209:ARG:NH1	2.30	0.64
9:E:70:GLN:O	9:E:72:SER:N	2.30	0.64
7:H:348:TYR:O	8:C:113:LYS:NZ	2.30	0.64
6:A:976:ASP:OD1	6:A:1311:HIS:NE2	2.20	0.64
6:B:1063:MET:HE2	6:B:1068:ILE:HG13	1.80	0.64
2:D:90:ARG:NH1	6:A:902:ASP:OD2	2.30	0.64
3:F:4:GLU:O	3:F:4:GLU:HG2	1.95	0.64
6:A:1233:ASN:OD1	6:A:1233:ASN:N	2.28	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:C:94:LEU:HD23	9:E:352:ILE:HG13	1.79	0.64
6:A:1343:LEU:HD12	6:A:1344:PRO:HD2	1.78	0.64
9:E:169:ILE:HG13	9:E:181:ILE:HD13	1.80	0.64
6:B:790:SER:HA	10:J:129:ALA:HB3	1.80	0.64
6:B:996:ILE:HD13	6:B:1010:LEU:HD21	1.78	0.64
4:G:80:ASP:HB2	6:B:765:MET:HE1	1.78	0.64
9:E:41:TYR:O	9:E:42:GLN:HB2	1.96	0.64
6:B:990:CYS:O	6:B:994:THR:OG1	2.15	0.63
2:D:311:ILE:HD11	6:A:890:THR:HG23	1.79	0.63
3:F:129:GLU:OE1	7:H:269:LYS:NZ	2.31	0.63
6:B:1037:LYS:O	6:B:1041:SER:OG	2.14	0.63
4:G:258:ILE:HG22	4:G:380:LEU:HD21	1.80	0.63
6:A:767:CYS:SG	6:A:770:ARG:NH1	2.71	0.63
6:A:1181:ALA:HA	6:A:1186:LEU:HD12	1.80	0.63
6:A:1019:SER:HA	6:A:1024:ILE:HB	1.80	0.63
2:D:58:ASP:N	2:D:58:ASP:OD1	2.31	0.63
6:A:1161:ILE:HG12	6:A:1239:LEU:HD11	1.81	0.63
7:H:398:ASP:OD2	6:B:871:TYR:OH	2.17	0.63
7:H:324:SER:OG	7:H:325:ALA:N	2.31	0.63
6:A:1325:LYS:H	6:A:1325:LYS:HD2	1.64	0.62
6:B:1233:ASN:HD22	6:B:1235:LYS:HG3	1.64	0.62
4:G:81:GLU:HG3	6:B:765:MET:HE3	1.81	0.62
6:B:1166:GLU:O	6:B:1169:THR:OG1	2.16	0.62
9:E:176:ILE:HG13	9:E:374:LEU:HD11	1.81	0.62
6:B:959:GLN:OE1	6:B:974:GLN:NE2	2.28	0.62
6:B:652:PRO:O	6:B:653:THR:OG1	2.17	0.62
9:E:197:ILE:HG21	9:E:353:ARG:HB2	1.79	0.62
2:D:18:ARG:NH2	2:D:22:GLU:OE2	2.32	0.61
10:J:180:VAL:HG22	10:J:267:ILE:HD11	1.82	0.61
3:F:359:ASN:HB3	6:A:1234:ASN:HB2	1.82	0.61
2:D:304:VAL:HG11	6:A:875:ARG:HH21	1.62	0.61
4:G:368:TYR:HD2	4:G:371:LYS:HZ3	1.47	0.61
5:I:121:LEU:HD21	5:I:169:HIS:CD2	2.35	0.61
6:A:1262:THR:HA	6:A:1265:ILE:HD12	1.83	0.61
9:E:84:LYS:O	9:E:87:ILE:HG13	2.01	0.61
5:I:105:GLU:O	5:I:159:LYS:NZ	2.26	0.61
5:I:100:HIS:HD2	5:I:102:MET:H	1.48	0.61
5:I:169:HIS:O	5:I:169:HIS:ND1	2.33	0.61
1:K:216:LEU:O	1:K:227:LEU:N	2.32	0.60
3:F:2:VAL:HG13	3:F:2:VAL:O	2.01	0.60
6:A:678:ASN:OD1	6:A:679:LYS:N	2.33	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:C:16:ASP:OD1	6:B:910:ARG:NH1	2.34	0.60
6:B:1189:SER:O	6:B:1192:SER:HB2	2.02	0.60
8:C:45:ASN:OD1	8:C:45:ASN:N	2.35	0.60
6:B:1065:LEU:HA	6:B:1068:ILE:HB	1.82	0.60
6:A:639:ILE:HG22	7:H:368:GLU:HA	1.83	0.60
6:A:945:THR:HG23	6:A:1146:ILE:HG13	1.84	0.60
7:H:175:MET:O	7:H:179:ARG:HG2	2.02	0.60
2:D:48:GLN:O	2:D:48:GLN:NE2	2.35	0.60
2:D:312:ARG:HB2	2:D:312:ARG:HH11	1.66	0.60
9:E:81:ASN:OD1	9:E:83:SER:OG	2.18	0.60
10:J:93:ASN:OD1	10:J:94:ARG:N	2.35	0.59
4:G:141:VAL:HG22	4:G:305:MET:HG2	1.83	0.59
6:B:993:ASP:HA	6:B:996:ILE:HG13	1.83	0.59
10:J:120:ASN:HD22	10:J:121:THR:H	1.49	0.59
2:D:125:ILE:HD12	7:H:208:LEU:HD11	1.85	0.59
4:G:99:ARG:HH21	4:G:103:LYS:HB2	1.68	0.59
6:A:1133:ARG:NH1	6:A:1272:ASP:O	2.34	0.59
6:A:1303:ILE:HG12	6:A:1314:ILE:HG12	1.83	0.59
9:E:372:GLU:HG3	9:E:372:GLU:O	2.03	0.59
6:A:986:TYR:HB3	6:A:1033:LEU:HD23	1.84	0.59
9:E:167:TPO:O1P	9:E:167:TPO:HG21	2.01	0.59
6:B:1167:ARG:HA	6:B:1170:LYS:HG2	1.84	0.59
6:B:1305:PHE:HE2	6:B:1310:LEU:HA	1.68	0.59
6:A:1288:LEU:HD22	6:A:1345:HIS:HD2	1.68	0.59
4:G:62:GLU:OE1	4:G:64:TYR:OH	2.16	0.59
5:I:74:ALA:O	5:I:78:GLN:NE2	2.33	0.59
6:A:978:ASP:OD1	6:A:979:PHE:N	2.36	0.59
6:B:732:CYS:HA	10:J:65:PRO:HB3	1.83	0.59
6:B:929:ASP:OD1	6:B:929:ASP:N	2.35	0.58
10:J:104:SER:HB2	10:J:107:TYR:CE1	2.37	0.58
2:D:87:ARG:HB3	7:H:252:ILE:HD13	1.84	0.58
6:A:838:ILE:HD13	6:A:888:ALA:HA	1.86	0.58
4:G:371:LYS:HA	4:G:374:THR:HG22	1.85	0.58
6:A:1288:LEU:O	6:A:1292:SER:OG	2.21	0.58
7:H:311:LEU:HB2	7:H:314:LYS:HB2	1.84	0.58
6:B:1069:LEU:HD13	6:B:1266:MET:HE2	1.86	0.58
6:B:1140:ALA:HB1	6:B:1144:ILE:HB	1.84	0.58
3:F:6:TPO:CG2	3:F:7:PRO:CD	2.61	0.58
7:H:265:GLN:NE2	9:E:226:ILE:O	2.33	0.58
8:C:122:ARG:HG3	9:E:369:TRP:CZ2	2.39	0.58
6:B:1033:LEU:HD22	6:B:1037:LYS:HZ1	1.67	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:F:343:TYR:OH	6:A:822:GLU:OE1	2.11	0.58
6:B:1203:ALA:O	6:B:1207:VAL:HG23	2.04	0.58
2:D:87:ARG:NH2	7:H:255:GLU:OE1	2.34	0.58
2:D:306:GLU:OE2	2:D:306:GLU:HA	2.02	0.58
3:F:365:TPO:N	3:F:365:TPO:O1P	2.36	0.58
4:G:246:THR:O	4:G:250:VAL:HG23	2.04	0.58
9:E:361:ARG:O	9:E:365:ARG:HG2	2.04	0.58
2:D:288:TYR:N	2:D:288:TYR:CD2	2.72	0.57
5:I:173:HIS:C	5:I:173:HIS:CD2	2.82	0.57
6:A:1331:GLU:O	6:A:1335:LYS:HG3	2.04	0.57
6:B:890:THR:O	6:B:890:THR:OG1	2.20	0.57
6:B:985:PHE:HD1	6:B:1151:TRP:HZ2	1.50	0.57
7:H:341:CYS:O	9:E:361:ARG:NH1	2.37	0.57
6:A:1134:SER:OG	6:A:1308:ARG:NE	2.38	0.57
4:G:20:ARG:HG3	4:G:139:CYS:HA	1.87	0.57
6:B:1261:LYS:O	6:B:1265:ILE:HG12	2.04	0.57
4:G:238:LEU:HD13	4:G:242:ILE:HD13	1.87	0.57
4:G:294:CYS:O	4:G:298:VAL:HG23	2.04	0.57
2:D:291:LYS:HE3	2:D:292:THR:H	1.69	0.57
5:I:148:ASN:O	5:I:148:ASN:ND2	2.38	0.57
3:F:14:LYS:HG3	3:F:14:LYS:O	2.05	0.57
9:E:323:GLN:O	9:E:326:GLU:HG2	2.04	0.57
6:A:1009:ARG:HA	6:A:1068:ILE:HD11	1.86	0.56
7:H:208:LEU:O	7:H:211:GLU:HG3	2.05	0.56
9:E:160:VAL:HG21	6:B:919:LEU:HD12	1.86	0.56
6:A:929:ASP:HB3	6:A:933:LEU:HD13	1.85	0.56
6:A:932:GLY:HA2	6:A:935:PHE:HB3	1.86	0.56
7:H:215:CYS:HB2	7:H:220:HIS:ND1	2.19	0.56
6:B:951:GLU:O	6:B:954:SER:OG	2.22	0.56
7:H:342:GLU:OE1	9:E:365:ARG:NH2	2.39	0.56
7:H:343:SER:OG	7:H:344:ILE:N	2.39	0.56
4:G:53:MET:HE1	4:G:63:ILE:HD11	1.88	0.56
6:B:691:LEU:HD12	6:B:697:LEU:HD22	1.88	0.56
4:G:44:ARG:NH1	4:G:311:GLY:O	2.39	0.56
4:G:280:ARG:HH21	9:E:83:SER:HB2	1.71	0.56
6:A:1331:GLU:HA	6:A:1334:TRP:HB3	1.88	0.55
6:B:738:HIS:ND1	6:B:739:GLU:O	2.36	0.55
6:B:1162:LYS:HE2	6:B:1204:TYR:CZ	2.41	0.55
1:K:78:GLU:HA	1:K:124:GLU:HA	1.88	0.55
6:A:678:ASN:HD21	6:A:680:HIS:HB3	1.71	0.55
6:A:1268:LEU:HD21	6:A:1289:GLN:HB3	1.88	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:C:53:PHE:HB2	8:C:68:LEU:HD22	1.88	0.55
3:F:390:GLN:O	9:E:199:LEU:HD13	2.06	0.55
9:E:24:ASN:O	9:E:28:THR:HG23	2.06	0.55
2:D:37:ASP:O	2:D:41:LYS:NZ	2.38	0.55
4:G:245:ALA:O	4:G:249:SER:OG	2.25	0.55
8:C:13:ASP:OD2	8:C:103:ARG:NH2	2.38	0.55
6:A:1063:MET:HE1	6:A:1067:ASP:HB2	1.88	0.55
7:H:369:ILE:HD11	9:E:166:LEU:O	2.06	0.55
3:F:258:ILE:HG12	3:F:380:LEU:HD11	1.88	0.55
4:G:368:TYR:O	4:G:371:LYS:HD3	2.07	0.55
6:B:1214:LEU:HD13	6:B:1224:PHE:HD2	1.70	0.55
1:K:292:THR:O	1:K:308:ILE:N	2.36	0.55
6:A:1173:ASN:HD21	6:A:1200:GLY:HA2	1.72	0.54
7:H:363:MET:HG2	6:B:648:VAL:HG11	1.88	0.54
2:D:122:GLU:O	2:D:125:ILE:HG22	2.06	0.54
3:F:6:TPO:O1P	3:F:6:TPO:HG21	2.07	0.54
3:F:211:TYR:HB2	3:F:237:PRO:HB3	1.88	0.54
6:A:738:HIS:ND1	6:A:764:PHE:HB2	2.23	0.54
10:J:175:SER:O	10:J:265:TYR:OH	2.21	0.54
6:A:732:CYS:SG	6:A:733:ILE:N	2.81	0.54
1:K:70:PRO:HA	1:K:83:ASP:HA	1.89	0.54
6:B:700:ASP:N	6:B:700:ASP:OD1	2.39	0.54
7:H:195:GLN:HA	7:H:198:GLN:HG2	1.88	0.54
7:H:200:LEU:O	7:H:204:GLN:HG3	2.08	0.54
2:D:304:VAL:CG1	6:A:875:ARG:NH2	2.50	0.54
3:F:211:TYR:OH	3:F:220:GLU:OE2	2.23	0.54
6:B:1167:ARG:O	6:B:1171:GLU:HG2	2.07	0.54
3:F:434:TPO:O2P	3:F:434:TPO:HG22	2.08	0.54
6:B:1152:THR:HG22	6:B:1156:GLU:OE1	2.08	0.54
2:D:312:ARG:CD	2:D:317:GLN:OE1	2.43	0.54
3:F:365:TPO:N	3:F:365:TPO:P	2.80	0.54
6:A:841:MET:HE3	6:A:846:LYS:HA	1.90	0.54
8:C:73:ASN:O	8:C:77:GLU:HG3	2.08	0.54
6:B:788:TRP:CD1	6:B:788:TRP:H	2.24	0.54
6:B:1168:VAL:HG21	6:B:1232:TYR:CZ	2.43	0.54
2:D:312:ARG:HG3	2:D:317:GLN:HB2	1.89	0.53
2:D:71:GLU:HG2	5:I:131:GLY:HA3	1.90	0.53
9:E:226:ILE:HD12	9:E:231:LEU:HD21	1.90	0.53
2:D:290:THR:HG23	2:D:290:THR:O	2.07	0.53
8:C:101:THR:O	8:C:105:GLU:HG3	2.08	0.53
3:F:134:LEU:HD22	3:F:304:PRO:HB3	1.90	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:G:24:PHE:CE1	4:G:129:GLU:HG2	2.43	0.53
3:F:389:VAL:HG12	3:F:389:VAL:O	2.08	0.53
4:G:209:HIS:HE1	4:G:235:ASN:HB3	1.73	0.53
6:A:760:LYS:O	6:A:763:THR:OG1	2.27	0.53
6:B:1012:ASP:HA	6:B:1015:LYS:HE2	1.90	0.53
3:F:223:ASP:OD2	6:A:754:SER:OG	2.22	0.53
6:A:1268:LEU:HD23	6:A:1286:TYR:CD2	2.43	0.53
6:B:838:ILE:HD11	6:B:849:PHE:CE1	2.44	0.53
2:D:126:LYS:O	2:D:130:GLU:HG2	2.09	0.52
2:D:135:MET:HA	2:D:138:ALA:HB3	1.91	0.52
4:G:292:ALA:HB1	4:G:328:LEU:HD21	1.90	0.52
6:B:987:ASP:OD1	6:B:1204:TYR:OH	2.23	0.52
3:F:346:TYR:OH	6:A:818:ASP:OD1	2.17	0.52
5:I:127:LEU:N	5:I:157:ILE:O	2.40	0.52
6:A:692:TYR:CG	6:A:702:LEU:HD22	2.44	0.52
6:A:1165:ASN:O	6:A:1169:THR:HG22	2.10	0.52
8:C:47:ASN:HD22	9:E:210:ARG:HD2	1.73	0.52
5:I:157:ILE:HD12	5:I:161:ASP:HB2	1.91	0.52
7:H:193:PHE:O	7:H:197:ARG:HG3	2.10	0.52
6:B:678:ASN:OD1	6:B:680:HIS:N	2.42	0.52
6:B:993:ASP:O	6:B:997:THR:HG23	2.09	0.52
2:D:138:ALA:HA	2:D:141:HIS:CD2	2.45	0.52
3:F:277:SER:OG	3:F:286:LEU:O	2.27	0.52
6:B:1156:GLU:HA	6:B:1159:LEU:HD23	1.91	0.52
6:A:864:LYS:O	6:A:868:ARG:HG2	2.10	0.52
6:B:1065:LEU:HA	6:B:1068:ILE:HD12	1.92	0.52
2:D:136:ASP:HA	2:D:139:ASN:ND2	2.25	0.52
6:A:944:THR:HB	6:A:946:LYS:HD2	1.92	0.52
2:D:84:GLU:OE1	9:E:238:HIS:ND1	2.39	0.51
9:E:167:TPO:CB	9:E:168:PRO:HD2	2.33	0.51
6:B:1213:ARG:O	6:B:1218:ASP:N	2.43	0.51
6:B:1263:ALA:O	6:B:1266:MET:HG3	2.10	0.51
6:B:721:LYS:HG2	6:B:726:TYR:HD2	1.76	0.51
5:I:128:THR:OG1	5:I:129:LEU:N	2.39	0.51
6:B:987:ASP:HA	6:B:990:CYS:SG	2.50	0.51
3:F:177:HIS:ND1	3:F:265:SEP:O2P	2.40	0.51
4:G:366:PRO:O	4:G:370:ASP:HB2	2.11	0.51
6:A:727:GLN:O	6:A:727:GLN:NE2	2.44	0.51
10:J:69:SER:O	10:J:69:SER:OG	2.25	0.51
7:H:266:ASP:O	7:H:270:LYS:HG3	2.11	0.51
4:G:191:ASP:OD1	4:G:191:ASP:N	2.36	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:A:1280:ALA:O	6:A:1284:ILE:HG12	2.10	0.51
2:D:18:ARG:HB3	2:D:18:ARG:CZ	2.41	0.51
3:F:370:ASP:O	3:F:374:THR:OG1	2.26	0.51
6:A:948:LEU:HA	6:A:951:GLU:OE1	2.11	0.51
6:B:1338:VAL:O	6:B:1342:ALA:HB2	2.11	0.51
9:E:167:TPO:CG2	9:E:168:PRO:CD	2.70	0.51
4:G:261:TRP:HB3	4:G:383:THR:O	2.11	0.51
6:B:1223:TRP:O	6:B:1227:SER:OG	2.17	0.51
3:F:55:TYR:OH	3:F:335:ASP:O	2.22	0.50
3:F:210:LYS:HD2	3:F:283:CYS:SG	2.51	0.50
6:A:1012:ASP:O	6:A:1016:TYR:HD2	1.93	0.50
6:A:1322:LEU:HA	6:A:1348:GLU:HG3	1.92	0.50
6:B:1148:PHE:O	6:B:1152:THR:OG1	2.29	0.50
2:D:91:SER:OG	7:H:248:GLU:HG2	2.11	0.50
2:D:132:ARG:HH21	2:D:135:MET:HE3	1.76	0.50
4:G:109:ASP:OD1	4:G:109:ASP:N	2.43	0.50
6:A:1321:ASP:OD2	6:A:1321:ASP:N	2.39	0.50
10:J:169:ASP:OD1	10:J:244:ARG:NH2	2.44	0.50
2:D:307:ASP:OD2	6:A:871:TYR:HE1	1.95	0.50
3:F:128:MET:HE3	3:F:168:LEU:HB3	1.94	0.50
4:G:346:TYR:OH	6:B:818:ASP:OD2	2.16	0.50
6:A:1295:SER:HB3	6:A:1298:GLU:HG3	1.94	0.50
9:E:286:ASP:OD1	9:E:286:ASP:N	2.44	0.50
2:D:110:ILE:HG13	2:D:111:LYS:N	2.27	0.50
4:G:105:ASN:HB2	4:G:156:GLU:HG2	1.93	0.50
6:B:1004:ASN:OD1	6:B:1004:ASN:N	2.43	0.50
6:B:1162:LYS:HG3	6:B:1204:TYR:CG	2.46	0.50
7:H:300:ILE:HD13	6:B:895:LEU:HD23	1.94	0.50
6:B:924:PHE:O	6:B:927:SER:OG	2.29	0.50
4:G:77:PHE:HA	6:B:770:ARG:HH21	1.77	0.50
2:D:300:LYS:HB2	2:D:303:GLU:HG3	1.93	0.50
8:C:93:MET:HE2	9:E:352:ILE:HG21	1.94	0.50
6:A:1214:LEU:HD11	6:A:1221:HIS:ND1	2.27	0.50
7:H:330:TYR:HD1	7:H:331:PRO:HD2	1.76	0.50
10:J:85:LYS:NZ	10:J:86:ASN:H	2.10	0.50
2:D:106:HIS:HE1	7:H:230:ILE:HG23	1.76	0.49
3:F:118:GLU:OE2	3:F:118:GLU:N	2.41	0.49
3:F:336:LYS:O	3:F:353:LEU:N	2.39	0.49
8:C:76:TYR:O	8:C:80:MET:HG2	2.12	0.49
6:B:942:LEU:HG	6:B:947:GLN:HG2	1.94	0.49
6:B:1158:LEU:O	6:B:1161:ILE:HG22	2.13	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:124:LYS:O	2:D:127:LYS:HB3	2.12	0.49
7:H:310:LYS:HG2	7:H:354:ASP:HB2	1.95	0.49
9:E:172:LEU:HD12	9:E:175:ILE:HD12	1.93	0.49
6:B:986:TYR:HE1	6:B:1029:ILE:HG22	1.76	0.49
6:B:1207:VAL:O	6:B:1211:SER:OG	2.29	0.49
2:D:64:ARG:HH11	5:I:113:ARG:HB3	1.77	0.49
3:F:210:LYS:HE3	3:F:240:ASP:OD1	2.12	0.49
4:G:209:HIS:CE1	4:G:235:ASN:HB3	2.47	0.49
6:B:1199:VAL:C	6:B:1201:GLU:H	2.19	0.49
4:G:244:ASP:OD1	4:G:244:ASP:N	2.45	0.49
6:B:954:SER:HA	6:B:957:VAL:HG12	1.95	0.49
9:E:73:GLU:HB3	10:J:257:THR:HG22	1.94	0.49
6:B:857:HIS:HB3	6:B:860:MET:HA	1.94	0.49
2:D:307:ASP:OD2	6:A:871:TYR:CE1	2.66	0.49
2:D:312:ARG:HH11	2:D:312:ARG:CB	2.25	0.49
6:A:672:ALA:O	6:A:676:ILE:HG13	2.11	0.49
6:A:1288:LEU:HD22	6:A:1345:HIS:CD2	2.46	0.49
6:A:1286:TYR:O	6:A:1290:VAL:HG12	2.13	0.49
7:H:275:ARG:NH1	9:E:219:LEU:HB3	2.27	0.49
6:B:1065:LEU:HD11	6:B:1270:VAL:HG11	1.95	0.49
3:F:148:GLY:HA2	3:F:166:ILE:HD11	1.93	0.49
8:C:77:GLU:HA	8:C:80:MET:HG2	1.95	0.49
6:B:1285:ILE:O	6:B:1289:GLN:NE2	2.46	0.49
1:K:132:LYS:O	1:K:148:LEU:N	2.34	0.49
2:D:138:ALA:O	2:D:141:HIS:HB2	2.13	0.49
6:B:739:GLU:HG3	6:B:740:LYS:N	2.27	0.49
6:B:830:CYS:SG	6:B:831:LEU:N	2.85	0.49
4:G:86:LEU:HD22	4:G:116:LEU:HD11	1.95	0.48
6:A:1030:GLU:O	6:A:1034:TYR:HB2	2.13	0.48
6:B:1138:LEU:HD22	6:B:1140:ALA:HB2	1.95	0.48
3:F:102:VAL:HG21	8:C:141:ILE:HD11	1.94	0.48
6:A:667:THR:O	6:A:671:LYS:HG2	2.13	0.48
6:A:1322:LEU:HD23	6:A:1322:LEU:H	1.78	0.48
6:B:960:THR:HA	6:B:963:LYS:HE3	1.95	0.48
3:F:105:ASN:ND2	3:F:157:ALA:O	2.46	0.48
10:J:89:THR:HA	10:J:140:THR:HB	1.96	0.48
6:A:1229:ARG:O	6:A:1233:ASN:HA	2.13	0.48
6:B:1014:LEU:O	6:B:1018:ILE:HG22	2.14	0.48
2:D:80:LEU:HD21	7:H:259:THR:HG21	1.96	0.48
6:B:1129:ILE:HG12	6:B:1131:GLN:HG3	1.96	0.48
4:G:359:ASN:HB3	6:B:1234:ASN:HD22	1.78	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:B:963:LYS:HE2	6:B:971:PRO:HD3	1.95	0.48
8:C:16:ASP:OD2	8:C:103:ARG:NH1	2.39	0.48
6:B:951:GLU:O	6:B:955:ILE:HG13	2.14	0.48
2:D:312:ARG:NH1	2:D:312:ARG:CG	2.72	0.48
6:A:1335:LYS:O	6:A:1339:THR:HG22	2.13	0.48
10:J:120:ASN:N	10:J:120:ASN:ND2	2.60	0.48
10:J:223:PRO:O	10:J:275:ARG:HB2	2.14	0.48
3:F:117:TYR:O	3:F:121:SER:OG	2.28	0.48
8:C:17:VAL:HG22	8:C:103:ARG:HG2	1.96	0.48
6:B:1164:MET:O	6:B:1168:VAL:HG23	2.14	0.48
4:G:368:TYR:HA	4:G:371:LYS:NZ	2.29	0.47
6:A:663:ASN:O	6:A:667:THR:OG1	2.22	0.47
6:B:1295:SER:OG	6:B:1296:ASN:N	2.46	0.47
7:H:342:GLU:OE2	9:E:365:ARG:NH1	2.48	0.47
6:B:729:LYS:O	6:B:731:LYS:N	2.46	0.47
2:D:291:LYS:HE3	2:D:292:THR:N	2.28	0.47
6:A:1261:LYS:NZ	6:A:1261:LYS:H	2.11	0.47
10:J:123:PRO:HG3	10:J:158:PRO:HG2	1.96	0.47
4:G:99:ARG:O	4:G:102:VAL:HG22	2.15	0.47
7:H:346:TYR:CZ	8:C:113:LYS:HE2	2.49	0.47
9:E:176:ILE:CG1	9:E:374:LEU:HD11	2.43	0.47
6:B:851:LEU:HD12	6:B:851:LEU:HA	1.79	0.47
3:F:103:LYS:HD2	6:A:740:LYS:O	2.14	0.47
5:I:126:ASN:HD22	5:I:159:LYS:HG2	1.80	0.47
6:A:699:LEU:O	6:A:703:VAL:HG23	2.13	0.47
6:A:1004:ASN:O	6:A:1008:GLU:HG2	2.15	0.47
6:A:1283:GLN:HB2	6:A:1324:LEU:HD21	1.95	0.47
6:B:1282:ASP:HA	6:B:1285:ILE:HB	1.97	0.47
2:D:94:GLU:HG2	6:A:910:ARG:NH1	2.30	0.47
2:D:312:ARG:HH22	2:D:320:ALA:HA	1.79	0.47
3:F:326:THR:O	3:F:330:ASN:ND2	2.47	0.47
6:A:965:HIS:CE1	6:A:967:LEU:HD12	2.49	0.47
2:D:122:GLU:HA	2:D:125:ILE:HG22	1.95	0.47
2:D:312:ARG:HD2	2:D:317:GLN:HB2	1.97	0.47
2:D:312:ARG:HH11	2:D:312:ARG:CG	2.26	0.47
3:F:213:GLU:HG2	6:A:789:ALA:O	2.15	0.47
5:I:113:ARG:NH2	5:I:126:ASN:OD1	2.41	0.47
6:A:807:LEU:O	6:A:811:GLU:HG3	2.14	0.47
9:E:70:GLN:C	9:E:72:SER:N	2.69	0.47
6:B:820:TYR:CE2	6:B:869:LYS:HD2	2.50	0.47
6:B:1004:ASN:O	6:B:1008:GLU:HG2	2.14	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:B:1222:GLN:OE1	6:B:1222:GLN:N	2.47	0.47
10:J:216:LEU:HD23	10:J:217:PRO:HD2	1.97	0.47
6:B:851:LEU:HD23	6:B:855:LEU:HD22	1.96	0.47
3:F:265:SEP:P	3:F:265:SEP:O	2.73	0.47
4:G:199:THR:O	4:G:199:THR:OG1	2.27	0.47
7:H:356:LEU:O	7:H:360:VAL:HG23	2.14	0.47
6:B:739:GLU:HG3	6:B:741:HIS:H	1.80	0.47
10:J:217:PRO:HG3	10:J:274:GLN:CD	2.40	0.47
2:D:18:ARG:CD	6:A:663:ASN:ND2	2.78	0.47
7:H:233:ILE:HD12	7:H:233:ILE:HA	1.69	0.47
2:D:81:ARG:HB2	9:E:288:PHE:CE1	2.50	0.46
6:B:803:TYR:CD1	6:B:923:VAL:HG13	2.50	0.46
6:B:1026:PHE:O	6:B:1029:ILE:HG12	2.15	0.46
6:B:1035:SER:O	6:B:1039:ASN:ND2	2.48	0.46
10:J:90:LEU:N	10:J:140:THR:O	2.43	0.46
3:F:186:ASP:OD2	3:F:272:GLY:HA3	2.14	0.46
5:I:92:HIS:CD2	5:I:93:PRO:HD2	2.50	0.46
7:H:185:GLU:O	7:H:189:ILE:HG13	2.14	0.46
9:E:56:GLU:HG3	9:E:70:GLN:HG3	1.97	0.46
9:E:64:ARG:NH1	10:J:127:LEU:O	2.41	0.46
10:J:123:PRO:O	10:J:123:PRO:HG2	2.15	0.46
3:F:94:LEU:HD13	3:F:112:VAL:HG21	1.97	0.46
8:C:46:LEU:HB2	8:C:75:ILE:HG21	1.97	0.46
9:E:167:TPO:CB	9:E:168:PRO:CD	2.90	0.46
4:G:73:GLU:O	4:G:76:GLN:HG3	2.15	0.46
5:I:173:HIS:CD2	5:I:173:HIS:O	2.69	0.46
6:B:1033:LEU:HD22	6:B:1037:LYS:NZ	2.31	0.46
8:C:43:MET:N	8:C:44:PRO:HD2	2.31	0.46
6:B:1036:HIS:O	6:B:1040:VAL:HG23	2.14	0.46
6:B:1147:PHE:CE2	6:B:1253:ALA:HB2	2.51	0.46
2:D:94:GLU:HG2	6:A:910:ARG:HH11	1.80	0.46
6:A:792:ASP:OD1	6:A:792:ASP:N	2.48	0.46
6:A:1197:ASP:OD1	6:A:1198:PHE:N	2.49	0.46
7:H:307:VAL:HG12	7:H:353:VAL:HG23	1.98	0.46
9:E:71:ARG:O	9:E:74:VAL:HG22	2.15	0.46
6:B:868:ARG:HD2	6:B:873:LYS:HG2	1.97	0.46
10:J:136:ASN:ND2	10:J:136:ASN:O	2.49	0.46
7:H:305:TYR:O	8:C:103:ARG:HD2	2.15	0.46
6:B:958:ASP:HA	6:B:961:ASN:ND2	2.31	0.46
6:B:1006:ASP:HA	6:B:1009:ARG:HD3	1.96	0.46
6:B:1033:LEU:O	6:B:1037:LYS:NZ	2.49	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:126:LYS:HA	2:D:129:GLN:HB2	1.98	0.46
5:I:194:LYS:HB3	7:H:289:ILE:HD13	1.97	0.46
6:A:1237:PHE:H	6:A:1237:PHE:HD1	1.64	0.46
5:I:108:THR:C	5:I:110:ALA:H	2.24	0.46
6:B:894:VAL:O	6:B:898:LEU:HG	2.16	0.46
6:B:901:LYS:HA	6:B:901:LYS:HD2	1.58	0.46
6:B:1168:VAL:HA	6:B:1171:GLU:HG2	1.96	0.46
10:J:92:TYR:HB2	10:J:141:LEU:HD11	1.98	0.46
3:F:3:TYR:O	3:F:3:TYR:CD1	2.68	0.46
4:G:151:HIS:ND1	4:G:191:ASP:OD1	2.42	0.46
5:I:180:CYS:SG	6:A:686:LEU:HD22	2.56	0.46
6:B:702:LEU:O	6:B:706:VAL:HG23	2.16	0.46
3:F:273:GLY:H	3:F:311:GLY:C	2.23	0.45
4:G:78:HIS:CD2	4:G:163:LEU:HD12	2.51	0.45
5:I:90:ASP:OD1	5:I:90:ASP:N	2.40	0.45
6:A:802:GLN:H	6:A:802:GLN:HG3	1.46	0.45
7:H:346:TYR:CE2	8:C:113:LYS:HE2	2.51	0.45
9:E:56:GLU:HA	9:E:70:GLN:HB2	1.97	0.45
9:E:87:ILE:HG22	9:E:87:ILE:O	2.16	0.45
8:C:25:THR:HG23	8:C:93:MET:HE3	1.98	0.45
8:C:65:GLN:HB3	9:E:303:LEU:HD23	1.97	0.45
6:B:773:MET:HE3	6:B:773:MET:HB3	1.88	0.45
6:B:1201:GLU:HB3	6:B:1206:GLN:CD	2.41	0.45
3:F:241:GLY:HA2	3:F:360:MET:HE2	1.98	0.45
5:I:100:HIS:CD2	5:I:102:MET:H	2.31	0.45
5:I:181:ILE:HB	5:I:182:PRO:HD3	1.97	0.45
6:A:1139:PHE:HD2	6:A:1286:TYR:CE1	2.34	0.45
6:A:1256:LEU:HD13	6:A:1266:MET:SD	2.56	0.45
8:C:121:LEU:HD21	9:E:372:GLU:HG2	1.99	0.45
6:B:651:GLU:CD	6:B:651:GLU:H	2.24	0.45
6:B:1020:LEU:HD12	6:B:1021:PHE:N	2.31	0.45
3:F:179:ARG:HG2	3:F:262:TYR:CZ	2.51	0.45
3:F:341:ASN:ND2	3:F:343:TYR:H	2.14	0.45
5:I:92:HIS:HD2	5:I:93:PRO:HD2	1.82	0.45
7:H:343:SER:O	7:H:344:ILE:HB	2.15	0.45
6:B:842:THR:OG1	6:B:845:GLU:HG2	2.17	0.45
6:B:1289:GLN:O	6:B:1293:HIS:NE2	2.48	0.45
4:G:171:ILE:HA	4:G:174:LEU:HD12	1.98	0.45
8:C:47:ASN:ND2	9:E:210:ARG:HD2	2.32	0.45
6:B:849:PHE:O	6:B:850:LYS:HD2	2.16	0.45
4:G:24:PHE:HE1	4:G:129:GLU:HG2	1.81	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:I:193:LYS:HA	5:I:193:LYS:HD3	1.74	0.45
6:A:802:GLN:O	6:A:806:THR:HG23	2.16	0.45
6:A:940:LYS:HE3	6:A:940:LYS:HB3	1.74	0.45
6:A:1164:MET:SD	6:A:1235:LYS:HD2	2.57	0.45
7:H:351:ASN:H	8:C:113:LYS:HZ2	1.65	0.45
7:H:396:ILE:HG13	6:B:875:ARG:HH22	1.81	0.45
6:B:863:TYR:O	6:B:867:ILE:HD12	2.16	0.45
6:B:1143:ASN:N	6:B:1143:ASN:OD1	2.47	0.45
10:J:86:ASN:HA	10:J:138:ILE:HD12	1.99	0.45
1:K:77:SER:O	1:K:125:PHE:N	2.40	0.45
2:D:67:ARG:HH11	5:I:156:ARG:HD2	1.81	0.45
2:D:304:VAL:HG22	6:A:871:TYR:CD1	2.48	0.45
5:I:136:SER:HB3	6:A:837:LYS:HA	1.98	0.45
10:J:188:ILE:HA	10:J:216:LEU:HD11	1.99	0.45
2:D:79:ARG:NH2	6:A:830:CYS:SG	2.85	0.45
6:A:1022:PHE:HA	6:A:1305:PHE:CZ	2.51	0.45
6:B:770:ARG:HB2	6:B:775:TRP:NE1	2.32	0.45
6:B:1201:GLU:HB3	6:B:1206:GLN:NE2	2.32	0.45
2:D:73:ARG:O	2:D:76:GLU:HB2	2.17	0.45
3:F:46:ARG:HD3	3:F:343:TYR:OH	2.16	0.44
4:G:218:THR:HG22	4:G:219:GLY:H	1.82	0.44
5:I:98:LYS:HB2	5:I:98:LYS:HE2	1.73	0.44
5:I:109:ASP:OD1	5:I:109:ASP:C	2.60	0.44
6:B:1260:ALA:O	6:B:1264:GLU:HG3	2.18	0.44
6:B:1286:TYR:HA	6:B:1289:GLN:NE2	2.32	0.44
3:F:365:TPO:CB	3:F:366:PRO:HD2	2.47	0.44
6:B:946:LYS:O	6:B:950:SER:OG	2.29	0.44
4:G:45:ILE:HD13	4:G:146:ALA:HA	1.99	0.44
7:H:370:SER:HA	7:H:373:GLU:HG2	1.98	0.44
8:C:8:PHE:HD1	8:C:11:LEU:HD12	1.83	0.44
2:D:18:ARG:O	2:D:22:GLU:HG3	2.16	0.44
4:G:241:GLY:HA2	4:G:360:MET:SD	2.58	0.44
8:C:131:MET:HE3	8:C:131:MET:HB2	1.82	0.44
9:E:70:GLN:HB3	9:E:71:ARG:H	1.61	0.44
6:B:653:THR:HG22	6:B:654:GLU:N	2.32	0.44
6:B:790:SER:C	6:B:792:ASP:H	2.25	0.44
6:B:1010:LEU:O	6:B:1013:LEU:HB2	2.17	0.44
3:F:141:VAL:HG11	3:F:329:LEU:HD22	1.98	0.44
3:F:150:HIS:ND1	3:F:184:ASP:OD2	2.47	0.44
8:C:30:THR:O	8:C:34:GLU:HG3	2.17	0.44
10:J:181:LEU:HD23	10:J:181:LEU:HA	1.86	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:14:LYS:HD2	2:D:16:LYS:HZ3	1.82	0.44
6:A:844:ASN:O	6:A:848:ASN:HB2	2.17	0.44
6:A:1327:PRO:HD2	6:A:1333:LYS:HG2	2.00	0.44
6:B:691:LEU:HD13	6:B:696:ILE:HB	1.99	0.44
3:F:274:ASP:O	3:F:282:GLY:HA3	2.16	0.44
6:A:864:LYS:HE3	6:A:864:LYS:HB3	1.83	0.44
6:A:1276:SER:OG	6:A:1277:THR:N	2.50	0.44
6:A:1343:LEU:HG	6:A:1345:HIS:H	1.83	0.44
9:E:166:LEU:HD23	9:E:166:LEU:HA	1.81	0.44
6:B:1020:LEU:O	6:B:1273:ARG:NH2	2.47	0.44
6:B:1333:LYS:HA	6:B:1336:TYR:HB3	2.00	0.44
5:I:72:LEU:HD12	5:I:73:THR:HG23	2.00	0.44
6:A:982:LYS:HB2	6:A:982:LYS:HE2	1.78	0.44
9:E:66:ASN:HB3	9:E:69:LEU:HD12	2.00	0.44
6:B:957:VAL:HA	6:B:960:THR:HG22	2.00	0.44
10:J:223:PRO:HB2	10:J:275:ARG:HD2	1.99	0.44
4:G:257:LYS:HG3	4:G:380:LEU:HD23	2.00	0.43
5:I:107:TYR:O	5:I:109:ASP:N	2.50	0.43
6:A:1173:ASN:ND2	6:A:1200:GLY:HA2	2.33	0.43
9:E:176:ILE:CG1	9:E:374:LEU:CD1	2.96	0.43
6:B:684:GLU:O	6:B:687:LYS:HB3	2.18	0.43
6:B:984:ILE:O	6:B:988:ILE:HG13	2.18	0.43
6:B:1202:ASP:C	6:B:1206:GLN:HE21	2.26	0.43
6:B:1305:PHE:CE2	6:B:1310:LEU:HA	2.50	0.43
10:J:126:PHE:HB2	10:J:159:ARG:NH2	2.33	0.43
10:J:155:ILE:HD12	10:J:155:ILE:O	2.18	0.43
4:G:86:LEU:HD23	4:G:86:LEU:HA	1.90	0.43
4:G:186:ASP:OD2	4:G:272:GLY:HA3	2.17	0.43
9:E:317:THR:N	9:E:320:GLU:OE1	2.51	0.43
10:J:274:GLN:HE21	10:J:274:GLN:HB3	1.59	0.43
6:A:851:LEU:HD12	6:A:887:PRO:HB3	2.00	0.43
6:A:1003:SER:OG	6:A:1004:ASN:N	2.50	0.43
6:A:1199:VAL:O	6:A:1201:GLU:N	2.50	0.43
6:A:1334:TRP:O	6:A:1338:VAL:HG23	2.18	0.43
7:H:372:LEU:HD22	7:H:383:PRO:HB3	2.00	0.43
6:B:889:VAL:HG13	6:B:890:THR:HG22	1.99	0.43
6:B:1013:LEU:HD13	6:B:1256:LEU:HD23	2.01	0.43
6:B:1242:ILE:O	6:B:1245:VAL:HG12	2.18	0.43
10:J:73:LEU:HA	10:J:76:THR:HG22	1.99	0.43
3:F:345:GLU:O	3:F:346:TYR:HB2	2.16	0.43
7:H:278:LEU:O	7:H:282:THR:HG23	2.18	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:C:63:GLN:HG2	8:C:64:THR:HG23	2.01	0.43
6:B:1327:PRO:CB	6:B:1333:LYS:HD3	2.43	0.43
2:D:131:GLU:O	2:D:135:MET:HG3	2.18	0.43
3:F:390:GLN:H	3:F:390:GLN:HG2	1.45	0.43
4:G:114:ASP:HB3	6:B:859:SER:HB3	2.00	0.43
6:A:1157:ARG:O	6:A:1160:GLU:HG2	2.19	0.43
6:A:1168:VAL:HG21	6:A:1232:TYR:CE1	2.54	0.43
6:B:936:LYS:HB2	6:B:936:LYS:HE2	1.62	0.43
6:B:1145:TYR:CE2	6:B:1149:ARG:HD2	2.53	0.43
6:B:1253:ALA:O	6:B:1256:LEU:HB3	2.18	0.43
6:B:1268:LEU:HB3	6:B:1286:TYR:HE2	1.84	0.43
2:D:64:ARG:NH1	5:I:113:ARG:HB3	2.34	0.43
4:G:150:HIS:CD2	4:G:150:HIS:H	2.35	0.43
6:A:983:ASN:HA	6:A:986:TYR:CE2	2.54	0.43
6:A:1214:LEU:HD11	6:A:1221:HIS:CE1	2.54	0.43
7:H:309:ILE:HG23	7:H:352:PRO:HB2	2.00	0.43
8:C:13:ASP:O	8:C:17:VAL:HG23	2.19	0.43
6:B:979:PHE:HB2	6:B:1310:LEU:HD23	2.01	0.43
6:B:1235:LYS:HB2	6:B:1235:LYS:HE2	1.74	0.43
6:B:1069:LEU:HG	6:B:1257:MET:HG2	2.00	0.43
6:B:1136:PHE:CE2	6:B:1307:LYS:HD2	2.54	0.43
10:J:85:LYS:HZ2	10:J:85:LYS:HG3	1.71	0.43
6:A:943:LEU:HD12	6:A:943:LEU:HA	1.82	0.43
6:A:1268:LEU:HD21	6:A:1289:GLN:CB	2.48	0.43
7:H:205:LEU:HA	7:H:208:LEU:HD22	2.00	0.43
8:C:80:MET:N	8:C:81:PRO:HD2	2.33	0.43
6:B:986:TYR:CE1	6:B:1029:ILE:HG22	2.53	0.43
6:B:1287:ARG:HE	6:B:1300:MET:HE1	1.83	0.43
6:A:1013:LEU:HD13	6:A:1257:MET:HE3	1.99	0.43
6:A:1237:PHE:HA	6:A:1240:TYR:CE1	2.53	0.43
6:A:1258:THR:HG22	6:A:1258:THR:O	2.19	0.43
6:A:1331:GLU:HG3	6:A:1334:TRP:HD1	1.84	0.43
6:B:993:ASP:OD1	6:B:993:ASP:N	2.46	0.43
3:F:343:TYR:C	3:F:345:GLU:H	2.27	0.43
4:G:79:THR:HB	6:B:765:MET:SD	2.59	0.43
5:I:118:HIS:NE2	6:A:694:GLN:OE1	2.52	0.43
7:H:222:GLU:O	7:H:225:VAL:HG12	2.18	0.43
9:E:226:ILE:O	9:E:226:ILE:HG13	2.18	0.43
2:D:51:LEU:HD21	9:E:336:GLN:NE2	2.34	0.42
3:F:211:TYR:CB	3:F:237:PRO:HB3	2.49	0.42
3:F:341:ASN:HD22	3:F:343:TYR:H	1.67	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:F:360:MET:HB3	6:A:930:HIS:CD2	2.54	0.42
5:I:121:LEU:HD21	5:I:169:HIS:HD2	1.81	0.42
6:A:986:TYR:O	6:A:989:LEU:HB2	2.19	0.42
6:A:1327:PRO:HG2	6:A:1333:LYS:HG2	2.00	0.42
6:B:736:ILE:HB	10:J:236:LEU:HD13	2.01	0.42
6:B:943:LEU:HD12	6:B:943:LEU:HA	1.76	0.42
6:B:1031:GLU:O	6:B:1035:SER:OG	2.31	0.42
6:B:1205:LYS:HE2	6:B:1205:LYS:HB2	1.68	0.42
2:D:312:ARG:NH1	2:D:312:ARG:HG2	2.33	0.42
4:G:88:ARG:HH21	4:G:97:PHE:HE1	1.67	0.42
5:I:133:LEU:HD23	6:A:837:LYS:HD2	2.01	0.42
5:I:133:LEU:HA	6:A:837:LYS:HG3	2.01	0.42
6:A:983:ASN:HA	6:A:986:TYR:CD2	2.54	0.42
6:B:787:VAL:O	6:B:787:VAL:HG13	2.19	0.42
6:B:1007:LYS:O	6:B:1010:LEU:HD23	2.19	0.42
6:B:1159:LEU:O	6:B:1163:GLN:HG3	2.19	0.42
2:D:49:THR:HA	2:D:52:THR:HG22	2.01	0.42
4:G:269:LEU:HD21	4:G:295:VAL:HG22	2.01	0.42
6:B:685:PHE:HE2	6:B:706:VAL:HG13	1.84	0.42
6:B:734:GLU:CD	10:J:67:VAL:HG12	2.44	0.42
6:B:787:VAL:O	6:B:789:ALA:N	2.52	0.42
2:D:16:LYS:HD2	2:D:16:LYS:H	1.85	0.42
6:A:714:LYS:HE3	6:A:714:LYS:HB3	1.64	0.42
7:H:391:LEU:HD11	6:B:897:ARG:HD3	2.01	0.42
9:E:296:GLN:HB3	9:E:301:LEU:HD23	2.02	0.42
2:D:111:LYS:HB3	2:D:111:LYS:HE3	1.66	0.42
4:G:185:ILE:HG12	4:G:270:GLN:O	2.19	0.42
5:I:113:ARG:NH2	5:I:156:ARG:HH21	2.17	0.42
6:A:673:LYS:HG3	6:A:682:TYR:CE1	2.54	0.42
6:A:1162:LYS:HE2	6:A:1162:LYS:HB3	1.88	0.42
10:J:91:TYR:CD2	10:J:102:GLU:HG2	2.54	0.42
6:B:1016:TYR:O	6:B:1020:LEU:HG	2.20	0.42
6:B:1242:ILE:O	6:B:1246:THR:HG23	2.19	0.42
6:B:1300:MET:HE2	6:B:1319:LEU:HD23	2.01	0.42
3:F:23:TYR:CE1	3:F:25:TYR:HB2	2.55	0.42
3:F:345:GLU:C	3:F:347:TYR:H	2.28	0.42
6:A:690:ASN:HA	6:A:693:SER:OG	2.19	0.42
6:A:745:LEU:O	6:A:756:LYS:HD2	2.19	0.42
6:B:1302:ARG:O	6:B:1302:ARG:HG3	2.20	0.42
4:G:259:MET:HE1	4:G:303:ILE:HD11	2.01	0.42
4:G:341:ASN:H	4:G:341:ASN:ND2	2.18	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:E:48:LEU:HA	9:E:48:LEU:HD23	1.74	0.42
6:B:684:GLU:HB3	6:B:709:TYR:OH	2.20	0.42
10:J:140:THR:HG23	10:J:229:GLU:OE2	2.20	0.42
3:F:41:LYS:HD3	3:F:315:MET:HE2	2.01	0.42
3:F:44:ARG:HG2	3:F:45:ILE:N	2.35	0.42
3:F:63:ILE:HD12	7:H:262:PHE:CZ	2.55	0.42
7:H:362:ARG:CZ	9:E:168:PRO:HG3	2.50	0.42
8:C:128:HIS:O	8:C:129:PRO:C	2.63	0.42
9:E:165:ILE:HG23	9:E:180:THR:HG21	2.02	0.42
6:B:995:PHE:CD1	6:B:1250:VAL:HG21	2.54	0.42
6:A:714:LYS:O	6:A:718:THR:HG22	2.19	0.41
6:A:1333:LYS:H	6:A:1333:LYS:HG3	1.69	0.41
9:E:26:ILE:HD13	6:B:669:PHE:CG	2.55	0.41
9:E:73:GLU:HA	10:J:252:TRP:CH2	2.55	0.41
3:F:239:ARG:HB2	3:F:364:ASN:OD1	2.20	0.41
3:F:365:TPO:CB	3:F:366:PRO:CD	2.97	0.41
4:G:288:MET:HE3	4:G:324:PHE:CG	2.54	0.41
9:E:231:LEU:O	9:E:233:LEU:N	2.45	0.41
6:B:1141:ASN:HB2	6:B:1298:GLU:OE2	2.21	0.41
2:D:310:LEU:HD23	2:D:310:LEU:O	2.20	0.41
3:F:3:TYR:O	3:F:3:TYR:CG	2.70	0.41
3:F:274:ASP:HA	3:F:279:ASP:OD1	2.20	0.41
7:H:344:ILE:HD12	7:H:344:ILE:HA	1.83	0.41
6:B:735:ASN:ND2	10:J:68:SER:O	2.54	0.41
6:B:1267:ALA:O	6:B:1271:LYS:HG3	2.20	0.41
4:G:257:LYS:HD2	4:G:261:TRP:CE3	2.56	0.41
5:I:118:HIS:HD2	5:I:119:PHE:CD2	2.37	0.41
6:A:1228:LEU:HD23	6:A:1228:LEU:HA	1.93	0.41
7:H:315:THR:HB	7:H:357:GLU:OE2	2.20	0.41
6:B:701:ASP:O	6:B:705:LYS:HG2	2.20	0.41
6:B:1226:GLU:O	6:B:1230:GLN:HG2	2.20	0.41
6:B:1289:GLN:O	6:B:1292:SER:OG	2.38	0.41
10:J:261:ASP:OD1	10:J:261:ASP:N	2.54	0.41
1:K:113:LYS:O	1:K:117:THR:N	2.53	0.41
6:A:831:LEU:HD22	6:A:891:ALA:HB1	2.01	0.41
6:A:960:THR:HG22	6:A:962:LYS:HG2	2.03	0.41
6:A:1203:ALA:O	6:A:1207:VAL:HG12	2.21	0.41
6:A:1304:GLU:OE2	6:A:1325:LYS:HE2	2.19	0.41
7:H:353:VAL:HB	8:C:110:VAL:HG21	2.03	0.41
6:B:938:ALA:O	6:B:942:LEU:HB2	2.20	0.41
6:B:1165:ASN:OD1	6:B:1204:TYR:N	2.47	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:B:1287:ARG:HD2	6:B:1323:THR:HB	2.01	0.41
2:D:86:TYR:OH	6:A:902:ASP:OD1	2.26	0.41
3:F:14:LYS:HB2	3:F:14:LYS:HE2	1.75	0.41
3:F:265:SEP:O1P	3:F:265:SEP:CA	2.67	0.41
3:F:434:TPO:O2P	3:F:434:TPO:CG2	2.69	0.41
6:A:679:LYS:O	6:A:683:THR:OG1	2.24	0.41
3:F:254:VAL:O	3:F:258:ILE:HG13	2.21	0.41
3:F:365:TPO:CG2	3:F:366:PRO:CD	2.85	0.41
6:A:1004:ASN:N	6:A:1004:ASN:OD1	2.53	0.41
8:C:143:SER:OG	8:C:144:LYS:N	2.54	0.41
6:B:729:LYS:O	6:B:729:LYS:HD2	2.20	0.41
6:B:765:MET:HE2	6:B:766:PRO:HD2	2.03	0.41
6:B:1330:ASP:O	6:B:1334:TRP:HD1	2.04	0.41
3:F:124:GLY:O	3:F:128:MET:HG3	2.20	0.41
4:G:19:ARG:NH2	4:G:302:GLY:HA2	2.32	0.41
6:A:744:ASP:HB2	8:C:133:LEU:HB2	2.02	0.41
6:A:993:ASP:HA	6:A:996:ILE:HD12	2.03	0.41
7:H:361:ASP:OD1	7:H:364:ARG:NH1	2.54	0.41
8:C:47:ASN:ND2	9:E:210:ARG:HH11	2.18	0.41
6:B:864:LYS:HG2	6:B:880:ILE:HD13	2.02	0.41
6:B:885:GLU:O	6:B:886:HIS:ND1	2.54	0.41
6:B:1322:LEU:HD21	6:B:1326:GLU:OE1	2.20	0.41
2:D:310:LEU:C	2:D:310:LEU:CD2	2.85	0.41
3:F:8:PHE:O	3:F:8:PHE:CD1	2.74	0.41
3:F:239:ARG:N	3:F:364:ASN:OD1	2.41	0.41
4:G:124:GLY:O	4:G:128:MET:HG3	2.21	0.41
5:I:90:ASP:O	5:I:92:HIS:N	2.46	0.41
6:A:1162:LYS:HD2	6:A:1204:TYR:CE1	2.56	0.41
6:A:1168:VAL:O	6:A:1172:ILE:HG13	2.21	0.41
7:H:202:ASP:O	7:H:206:VAL:HG23	2.21	0.41
7:H:362:ARG:NH2	8:C:7:LEU:HD12	2.36	0.41
6:B:1004:ASN:N	6:B:1005:PRO:HD2	2.36	0.41
1:K:149:SER:N	1:K:153:SER:O	2.35	0.41
3:F:242:ILE:HG13	3:F:246:THR:HB	2.02	0.41
6:A:770:ARG:HH21	6:A:778:LEU:HD13	1.86	0.41
9:E:103:THR:HG23	9:E:104:ASN:N	2.30	0.41
9:E:324:LEU:O	9:E:328:ILE:HG13	2.20	0.41
6:B:684:GLU:OE2	6:B:709:TYR:OH	2.16	0.41
6:B:1220:GLU:HG3	6:B:1223:TRP:HD1	1.86	0.41
6:B:1251:LYS:HB3	6:B:1251:LYS:HE3	1.72	0.41
4:G:128:MET:HE2	4:G:128:MET:HB3	2.00	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:I:113:ARG:O	5:I:117:ASP:HB2	2.21	0.40
10:J:182:ARG:HE	10:J:182:ARG:HB3	1.77	0.40
4:G:14:LYS:HE3	4:G:14:LYS:HB3	1.94	0.40
4:G:257:LYS:HD2	4:G:261:TRP:CD2	2.56	0.40
6:A:1281:LYS:HD3	6:A:1281:LYS:H	1.86	0.40
6:B:913:ASN:HA	6:B:916:TRP:HB2	2.03	0.40
10:J:176:ASP:O	10:J:180:VAL:HG12	2.22	0.40
3:F:67:LYS:HE2	3:F:67:LYS:HB2	1.71	0.40
3:F:224:ILE:HD13	3:F:379:ASN:OD1	2.21	0.40
4:G:153:LYS:HE2	4:G:158:SER:OG	2.21	0.40
6:A:809:LYS:HB3	6:A:809:LYS:HE2	1.94	0.40
6:A:1161:ILE:HD12	6:A:1164:MET:HE2	2.04	0.40
8:C:125:VAL:HG12	8:C:126:ASP:N	2.36	0.40
1:K:368:HIS:O	1:K:399:ALA:N	2.50	0.40
3:F:388:SEP:O3P	4:G:54:ASN:O	2.40	0.40
3:F:389:VAL:O	3:F:389:VAL:CG1	2.69	0.40
4:G:221:LEU:O	4:G:221:LEU:HD13	2.22	0.40
4:G:359:ASN:HD22	6:B:1234:ASN:HD22	1.69	0.40
6:A:906:ARG:O	6:A:910:ARG:HG2	2.21	0.40
2:D:44:LEU:HG	7:H:286:TRP:HE1	1.86	0.40
4:G:341:ASN:H	4:G:341:ASN:HD22	1.68	0.40
6:A:636:ARG:HA	6:A:636:ARG:HD2	1.76	0.40
6:B:1287:ARG:O	6:B:1290:VAL:HG12	2.22	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all 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	K	403/460 (88%)	396 (98%)	7 (2%)	0	100	100
2	D	160/327 (49%)	157 (98%)	3 (2%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
3	F	386/433 (89%)	357 (92%)	26 (7%)	3 (1%)	16	34
4	G	383/433 (88%)	360 (94%)	23 (6%)	0	100	100
5	I	127/201 (63%)	110 (87%)	14 (11%)	3 (2%)	4	9
6	A	627/1536 (41%)	593 (95%)	32 (5%)	2 (0%)	36	58
6	B	605/1536 (39%)	551 (91%)	54 (9%)	0	100	100
7	H	231/405 (57%)	208 (90%)	20 (9%)	3 (1%)	9	21
8	C	134/330 (41%)	128 (96%)	3 (2%)	3 (2%)	5	10
9	E	245/430 (57%)	217 (89%)	24 (10%)	4 (2%)	7	16
10	J	205/294 (70%)	188 (92%)	17 (8%)	0	100	100
All	All	3506/6385 (55%)	3265 (93%)	223 (6%)	18 (0%)	26	46

All (18) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
5	I	177	GLU
5	I	178	THR
7	H	344	ILE
9	E	42	GLN
9	E	71	ARG
3	F	266	ALA
3	F	389	VAL
7	H	343	SER
5	I	128	THR
8	C	129	PRO
9	E	72	SER
9	E	103	THR
3	F	366	PRO
6	A	1233	ASN
7	H	315	THR
8	C	128	HIS
8	C	130	ALA
6	A	1200	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	
2	D	153/289 (53%)	125 (82%)	28 (18%)	2	3
3	F	328/361 (91%)	300 (92%)	28 (8%)	10	22
4	G	326/367 (89%)	288 (88%)	38 (12%)	5	11
5	I	119/178 (67%)	107 (90%)	12 (10%)	7	15
6	A	585/1391 (42%)	524 (90%)	61 (10%)	7	14
6	B	574/1391 (41%)	515 (90%)	59 (10%)	7	15
7	H	213/371 (57%)	186 (87%)	27 (13%)	4	9
8	C	129/290 (44%)	120 (93%)	9 (7%)	14	31
9	E	234/391 (60%)	201 (86%)	33 (14%)	3	6
10	J	190/269 (71%)	165 (87%)	25 (13%)	4	8
All	All	2851/5298 (54%)	2531 (89%)	320 (11%)	8	12

All (320) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	D	34	SER
2	D	36	ARG
2	D	47	LEU
2	D	51	LEU
2	D	53	SER
2	D	54	LEU
2	D	58	ASP
2	D	71	GLU
2	D	80	LEU
2	D	89	SER
2	D	94	GLU
2	D	98	ASP
2	D	99	ILE
2	D	106	HIS
2	D	110	ILE
2	D	127	LYS
2	D	128	LEU
2	D	129	GLN
2	D	133	LEU
2	D	141	HIS
2	D	288	TYR
2	D	290	THR

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Mol	Chain	Res	Type
2	D	291	LYS
2	D	304	VAL
2	D	308	ILE
2	D	311	ILE
2	D	312	ARG
2	D	313	GLU
3	F	11	ILE
3	F	13	VAL
3	F	14	LYS
3	F	44	ARG
3	F	60	LYS
3	F	63	ILE
3	F	67	LYS
3	F	70	THR
3	F	101	SER
3	F	106	VAL
3	F	121	SER
3	F	123	SER
3	F	133	ARG
3	F	156	GLU
3	F	179	ARG
3	F	187	VAL
3	F	214	PHE
3	F	264	PRO
3	F	277	SER
3	F	280	ARG
3	F	287	SER
3	F	316	ARG
3	F	318	VAL
3	F	337	ASP
3	F	374	THR
3	F	380	LEU
3	F	389	VAL
3	F	393	HIS
4	G	2	VAL
4	G	17	ASP
4	G	20	ARG
4	G	28	ASP
4	G	29	VAL
4	G	41	LYS
4	G	44	ARG
4	G	45	ILE

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Mol	Chain	Res	Type
4	G	50	SER
4	G	62	GLU
4	G	67	LYS
4	G	72	GLN
4	G	98	LYS
4	G	109	ASP
4	G	112	VAL
4	G	116	LEU
4	G	199	THR
4	G	205	THR
4	G	213	GLU
4	G	218	THR
4	G	221	LEU
4	G	246	THR
4	G	249	SER
4	G	268	VAL
4	G	275	SER
4	G	277	SER
4	G	303	ILE
4	G	305	MET
4	G	314	THR
4	G	321	THR
4	G	326	THR
4	G	328	LEU
4	G	341	ASN
4	G	345	GLU
4	G	360	MET
4	G	371	LYS
4	G	375	ASN
4	G	383	THR
5	I	72	LEU
5	I	80	ILE
5	I	109	ASP
5	I	117	ASP
5	I	123	VAL
5	I	138	LEU
5	I	149	THR
5	I	172	GLU
5	I	173	HIS
5	I	175	ILE
5	I	177	GLU
5	I	180	CYS

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Mol	Chain	Res	Type
6	A	639	ILE
6	A	641	LEU
6	A	645	ILE
6	A	646	VAL
6	A	691	LEU
6	A	700	ASP
6	A	736	ILE
6	A	747	LEU
6	A	761	SER
6	A	801	ASN
6	A	802	GLN
6	A	823	SER
6	A	825	LEU
6	A	826	ARG
6	A	827	THR
6	A	833	THR
6	A	848	ASN
6	A	859	SER
6	A	860	MET
6	A	861	THR
6	A	864	LYS
6	A	868	ARG
6	A	872	ASP
6	A	889	VAL
6	A	893	VAL
6	A	896	LYS
6	A	920	GLU
6	A	981	ASP
6	A	999	THR
6	A	1006	ASP
6	A	1013	LEU
6	A	1020	LEU
6	A	1029	ILE
6	A	1033	LEU
6	A	1036	HIS
6	A	1040	VAL
6	A	1062	GLU
6	A	1064	SER
6	A	1067	ASP
6	A	1069	LEU
6	A	1144	ILE
6	A	1153	THR

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Mol	Chain	Res	Type
6	A	1156	GLU
6	A	1161	ILE
6	A	1170	LYS
6	A	1199	VAL
6	A	1233	ASN
6	A	1248	SER
6	A	1249	LEU
6	A	1256	LEU
6	A	1261	LYS
6	A	1262	THR
6	A	1274	ASN
6	A	1277	THR
6	A	1288	LEU
6	A	1319	LEU
6	A	1321	ASP
6	A	1328	LYS
6	A	1331	GLU
6	A	1337	TYR
6	A	1345	HIS
7	H	192	LYS
7	H	195	GLN
7	H	200	LEU
7	H	205	LEU
7	H	208	LEU
7	H	210	THR
7	H	222	GLU
7	H	233	ILE
7	H	244	ARG
7	H	245	GLN
7	H	248	GLU
7	H	250	SER
7	H	251	CYS
7	H	274	LEU
7	H	299	VAL
7	H	313	ASN
7	H	324	SER
7	H	333	GLU
7	H	338	ASP
7	H	344	ILE
7	H	349	ARG
7	H	351	ASN
7	H	363	MET

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Mol	Chain	Res	Type
7	H	370	SER
7	H	371	ASP
7	H	395	GLU
7	H	396	ILE
8	C	21	PHE
8	C	45	ASN
8	C	54	LEU
8	C	64	THR
8	C	66	VAL
8	C	76	TYR
8	C	92	ILE
8	C	137	LEU
8	C	142	GLU
9	E	32	ARG
9	E	42	GLN
9	E	49	ASP
9	E	60	ILE
9	E	61	SER
9	E	76	THR
9	E	84	LYS
9	E	91	VAL
9	E	101	LEU
9	E	102	GLN
9	E	159	LEU
9	E	160	VAL
9	E	162	VAL
9	E	169	ILE
9	E	172	LEU
9	E	176	ILE
9	E	187	SER
9	E	189	ILE
9	E	231	LEU
9	E	286	ASP
9	E	302	SER
9	E	317	THR
9	E	320	GLU
9	E	322	GLN
9	E	324	LEU
9	E	329	GLU
9	E	340	GLN
9	E	351	LYS
9	E	367	LEU

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Mol	Chain	Res	Type
9	E	368	ASN
9	E	371	ARG
9	E	372	GLU
9	E	376	ILE
6	B	648	VAL
6	B	656	ILE
6	B	657	GLU
6	B	660	ILE
6	B	664	GLU
6	B	689	LEU
6	B	697	LEU
6	B	718	THR
6	B	732	CYS
6	B	733	ILE
6	B	734	GLU
6	B	742	ARG
6	B	760	LYS
6	B	768	SER
6	B	821	ILE
6	B	822	GLU
6	B	828	ILE
6	B	830	CYS
6	B	831	LEU
6	B	833	THR
6	B	838	ILE
6	B	844	ASN
6	B	858	THR
6	B	861	THR
6	B	881	ASP
6	B	883	LEU
6	B	884	HIS
6	B	890	THR
6	B	901	LYS
6	B	917	ARG
6	B	918	GLU
6	B	929	ASP
6	B	933	LEU
6	B	948	LEU
6	B	953	SER
6	B	991	LEU
6	B	999	THR
6	B	1004	ASN

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Mol	Chain	Res	Type
6	B	1010	LEU
6	B	1016	TYR
6	B	1019	SER
6	B	1025	SER
6	B	1029	ILE
6	B	1137	ASN
6	B	1143	ASN
6	B	1152	THR
6	B	1159	LEU
6	B	1164	MET
6	B	1211	SER
6	B	1220	GLU
6	B	1226	GLU
6	B	1261	LYS
6	B	1285	ILE
6	B	1288	LEU
6	B	1298	GLU
6	B	1309	THR
6	B	1321	ASP
6	B	1333	LYS
6	B	1339	THR
10	J	63	ASP
10	J	68	SER
10	J	69	SER
10	J	71	SER
10	J	96	LYS
10	J	106	SER
10	J	107	TYR
10	J	110	ARG
10	J	111	HIS
10	J	120	ASN
10	J	138	ILE
10	J	155	ILE
10	J	157	SER
10	J	161	ARG
10	J	165	ILE
10	J	172	SER
10	J	218	LEU
10	J	225	ASP
10	J	248	THR
10	J	259	ILE
10	J	265	TYR

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Mol	Chain	Res	Type
10	J	271	VAL
10	J	272	ILE
10	J	274	GLN
10	J	276	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (74) such sidechains are listed below:

Mol	Chain	Res	Type
2	D	20	ASN
2	D	59	ASN
2	D	106	HIS
2	D	141	HIS
3	F	188	HIS
3	F	231	ASN
3	F	235	ASN
3	F	341	ASN
4	G	38	HIS
4	G	188	HIS
4	G	231	ASN
4	G	330	ASN
4	G	341	ASN
5	I	82	ASN
5	I	92	HIS
5	I	100	HIS
5	I	173	HIS
6	A	663	ASN
6	A	690	ASN
6	A	741	HIS
6	A	779	ASN
6	A	798	HIS
6	A	802	GLN
6	A	829	GLN
6	A	836	ASN
6	A	840	ASN
6	A	848	ASN
6	A	857	HIS
6	A	884	HIS
6	A	947	GLN
6	A	959	GLN
6	A	965	HIS
6	A	983	ASN
6	A	1132	ASN

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Mol	Chain	Res	Type
6	A	1150	HIS
6	A	1173	ASN
6	A	1252	HIS
6	A	1293	HIS
6	A	1299	ASN
6	A	1345	HIS
7	H	204	GLN
7	H	253	ASN
7	H	264	HIS
7	H	280	ASN
7	H	327	GLN
7	H	351	ASN
8	C	6	ASN
8	C	47	ASN
8	C	128	HIS
8	C	135	HIS
9	E	24	ASN
9	E	102	GLN
9	E	213	GLN
9	E	322	GLN
9	E	336	GLN
9	E	340	GLN
9	E	360	ASN
6	B	694	GLN
6	B	779	ASN
6	B	801	ASN
6	B	815	HIS
6	B	900	GLN
6	B	965	HIS
6	B	1070	HIS
6	B	1163	GLN
6	B	1206	GLN
6	B	1216	ASN
6	B	1230	GLN
6	B	1233	ASN
6	B	1234	ASN
6	B	1296	ASN
10	J	120	ASN
10	J	260	HIS
10	J	274	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

10 non-standard protein/DNA/RNA residues 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
3	TPO	F	365	3	8,10,11	0.91	0	10,14,16	1.28	2 (20%)
3	TPO	F	12	3	8,10,11	0.84	0	10,14,16	1.17	1 (10%)
3	TPO	F	6	3	8,10,11	1.06	1 (12%)	10,14,16	1.37	1 (10%)
2	SEP	D	309	2	8,9,10	0.97	0	7,12,14	0.83	0
9	SEP	E	171	9	8,9,10	0.71	0	7,12,14	1.52	2 (28%)
3	SEP	F	265	3	8,9,10	2.07	1 (12%)	7,12,14	2.39	3 (42%)
3	TPO	F	434	3	8,10,11	0.65	0	10,14,16	1.46	2 (20%)
5	SEP	I	174	5	8,9,10	1.00	0	7,12,14	0.82	0
9	TPO	E	167	9	8,10,11	3.24	1 (12%)	10,14,16	1.70	2 (20%)
3	SEP	F	388	3	8,9,10	0.75	0	7,12,14	1.11	1 (14%)

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
3	TPO	F	365	3	-	7/9/11/13	-
3	TPO	F	12	3	-	1/9/11/13	-
3	TPO	F	6	3	-	1/9/11/13	-
2	SEP	D	309	2	-	3/6/8/10	-
9	SEP	E	171	9	-	3/6/8/10	-
3	SEP	F	265	3	-	5/6/8/10	-
3	TPO	F	434	3	-	3/9/11/13	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	SEP	I	174	5	-	2/6/8/10	-
9	TPO	E	167	9	-	5/9/11/13	-
3	SEP	F	388	3	-	4/6/8/10	-

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
9	E	167	TPO	P-OG1	-8.69	1.44	1.59
3	F	265	SEP	O-C	-4.82	1.01	1.20
3	F	6	TPO	P-O3P	-2.03	1.47	1.54

All (14) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	F	265	SEP	O2P-P-OG	-4.57	94.74	106.67
9	E	167	TPO	P-OG1-CB	-3.99	112.48	123.33
3	F	434	TPO	O-C-CA	-3.01	117.03	124.77
3	F	265	SEP	OG-P-O1P	2.84	114.11	106.44
3	F	365	TPO	P-OG1-CB	-2.82	115.66	123.33
9	E	171	SEP	O3P-P-OG	-2.78	99.41	106.67
3	F	388	SEP	OG-CB-CA	2.70	110.78	108.14
3	F	6	TPO	O-C-CA	-2.58	118.13	124.77
9	E	167	TPO	O2P-P-OG1	-2.55	95.91	105.85
3	F	12	TPO	O-C-CA	-2.45	118.47	124.77
3	F	265	SEP	O3P-P-O2P	2.45	116.97	107.80
3	F	365	TPO	O-C-CA	-2.28	118.91	124.77
3	F	434	TPO	P-OG1-CB	2.13	129.12	123.33
9	E	171	SEP	O2P-P-OG	2.03	111.97	106.67

There are no chirality outliers.

All (34) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	D	309	SEP	C-CA-CB-OG
3	F	12	TPO	O-C-CA-CB
3	F	265	SEP	N-CA-CB-OG
3	F	265	SEP	C-CA-CB-OG
3	F	265	SEP	CB-OG-P-O2P
3	F	265	SEP	CB-OG-P-O3P
3	F	365	TPO	N-CA-CB-CG2

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Mol	Chain	Res	Type	Atoms
3	F	365	TPO	N-CA-CB-OG1
3	F	365	TPO	C-CA-CB-CG2
3	F	365	TPO	CA-CB-OG1-P
3	F	388	SEP	N-CA-CB-OG
3	F	388	SEP	C-CA-CB-OG
3	F	434	TPO	N-CA-CB-OG1
3	F	434	TPO	CG2-CB-OG1-P
9	E	167	TPO	N-CA-CB-CG2
9	E	167	TPO	N-CA-CB-OG1
9	E	167	TPO	C-CA-CB-CG2
9	E	167	TPO	O-C-CA-CB
9	E	171	SEP	N-CA-CB-OG
9	E	171	SEP	C-CA-CB-OG
9	E	167	TPO	CG2-CB-OG1-P
3	F	265	SEP	CA-CB-OG-P
3	F	388	SEP	CA-CB-OG-P
9	E	171	SEP	CA-CB-OG-P
2	D	309	SEP	CB-OG-P-O1P
5	I	174	SEP	N-CA-CB-OG
2	D	309	SEP	CB-OG-P-O2P
3	F	388	SEP	CB-OG-P-O2P
3	F	365	TPO	O-C-CA-CB
5	I	174	SEP	C-CA-CB-OG
3	F	365	TPO	CB-OG1-P-O1P
3	F	6	TPO	N-CA-CB-CG2
3	F	434	TPO	N-CA-CB-CG2
3	F	365	TPO	CG2-CB-OG1-P

There are no ring outliers.

6 monomers are involved in 30 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	F	365	TPO	8	0
3	F	6	TPO	5	0
3	F	265	SEP	6	0
3	F	434	TPO	3	0
9	E	167	TPO	8	0
3	F	388	SEP	1	0

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 6 ligands modelled in this entry, 6 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

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.

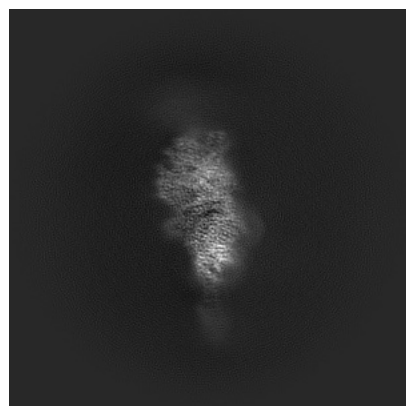
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-34935. These allow visual inspection of the internal detail of the map and identification of artifacts.

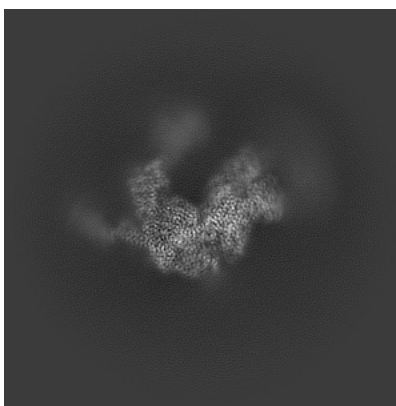
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

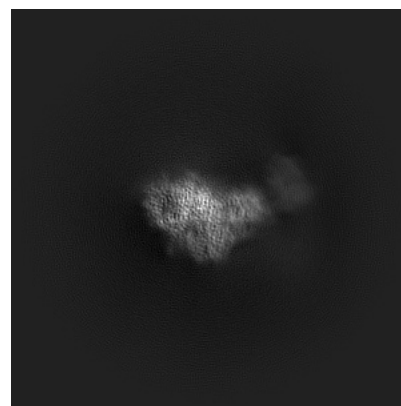
6.1.1 Primary map



X

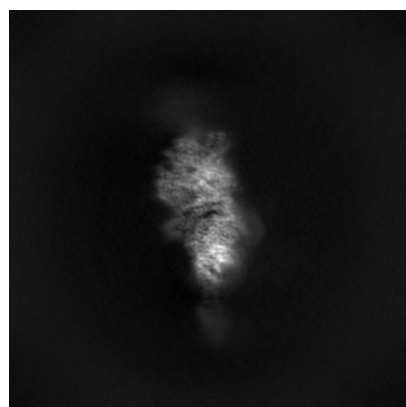


Y

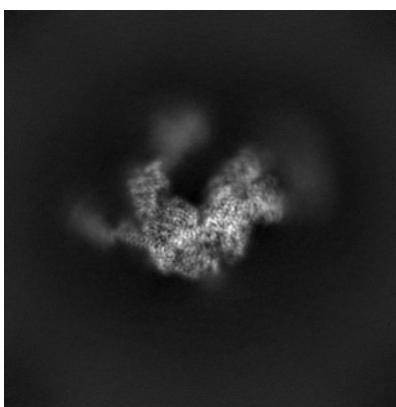


Z

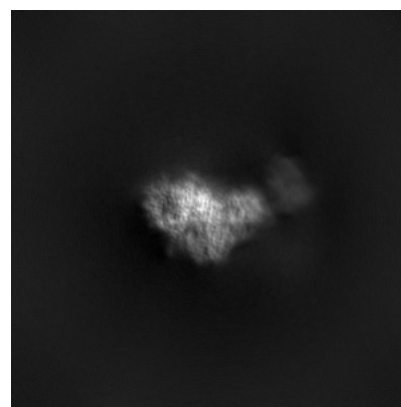
6.1.2 Raw map



X



Y

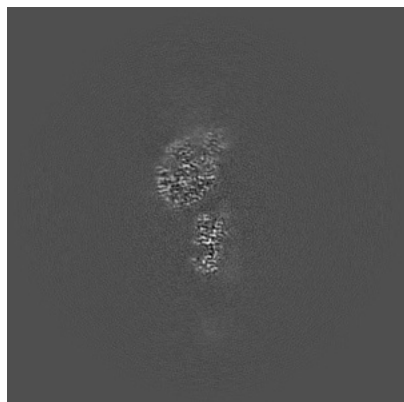


Z

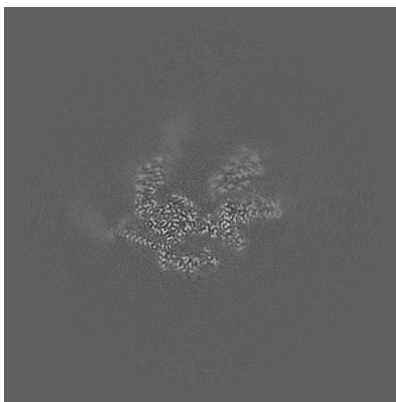
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

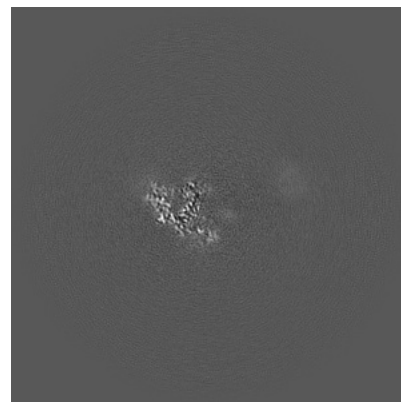
6.2.1 Primary map



X Index: 200

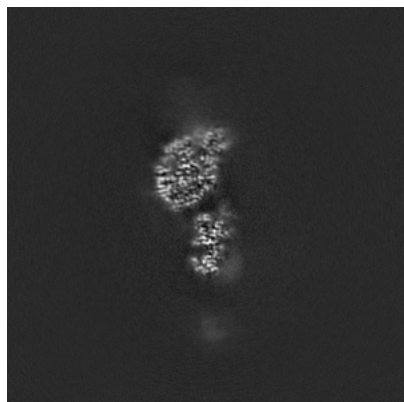


Y Index: 200

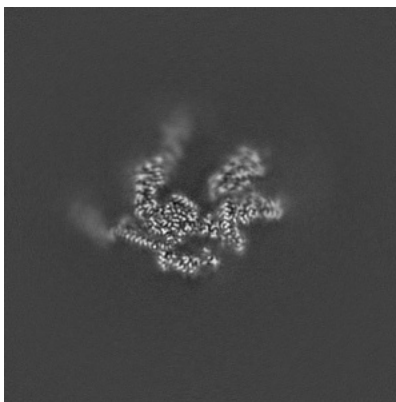


Z Index: 200

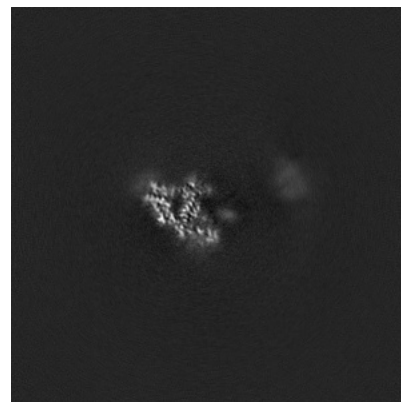
6.2.2 Raw map



X Index: 200



Y Index: 200

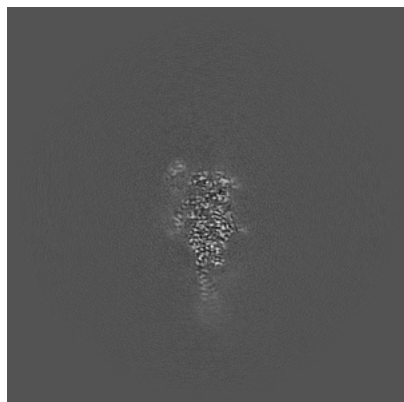


Z Index: 200

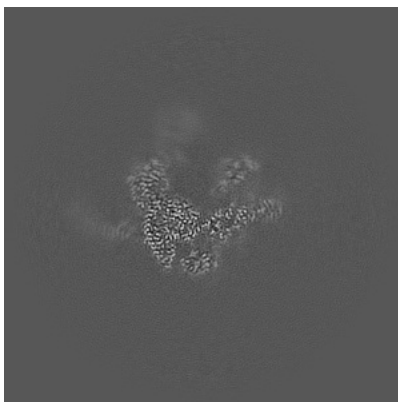
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

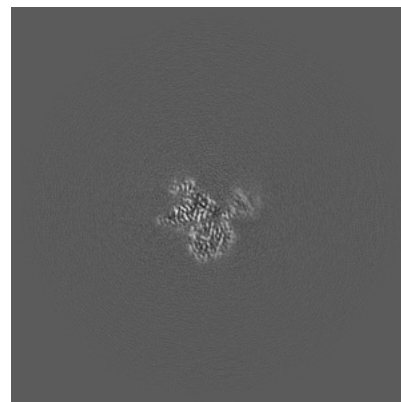
6.3.1 Primary map



X Index: 176

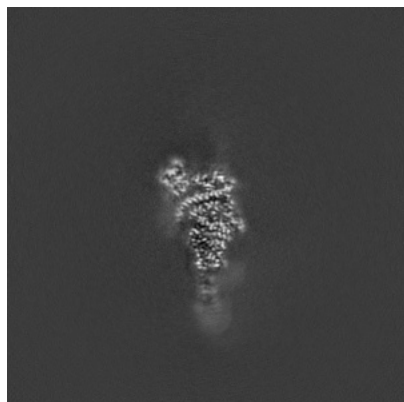


Y Index: 208

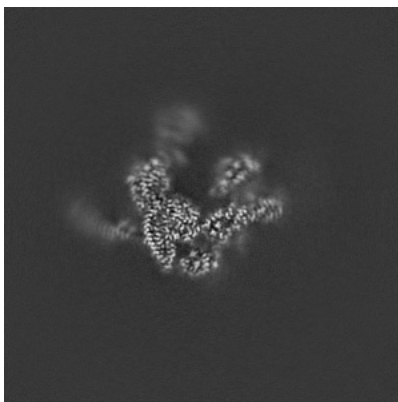


Z Index: 225

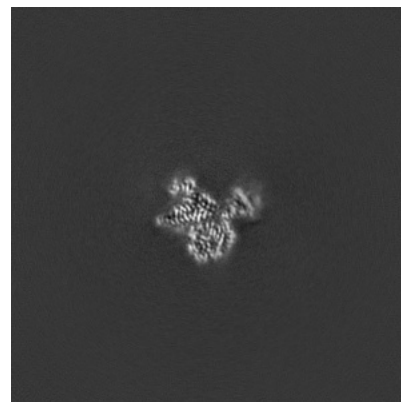
6.3.2 Raw map



X Index: 180



Y Index: 208

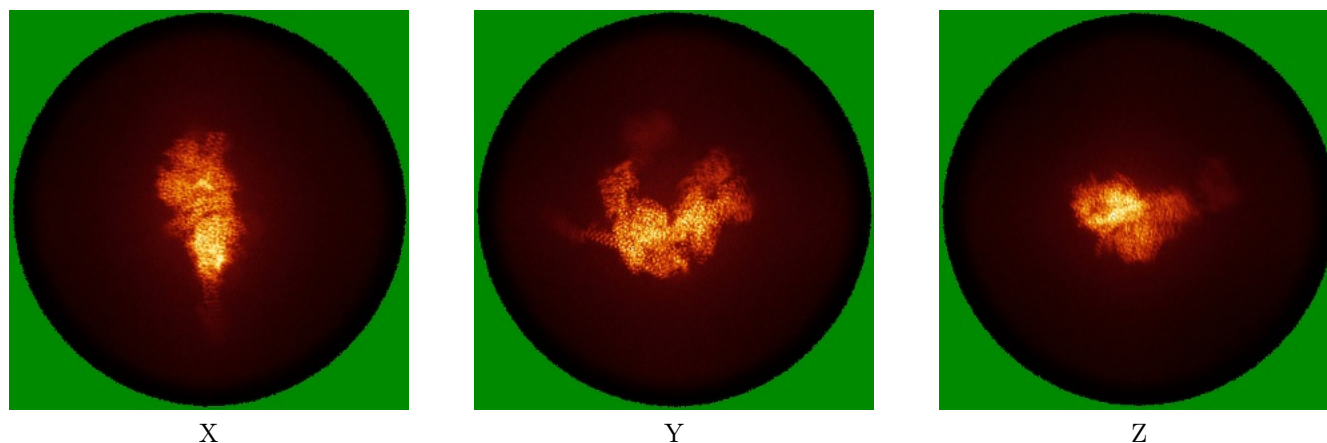


Z Index: 225

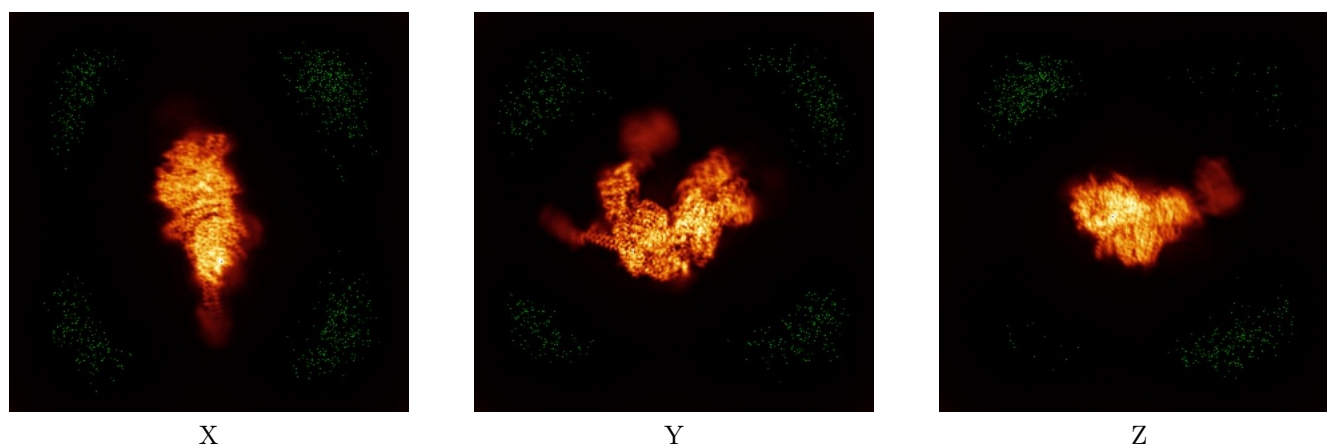
The images above show the largest variance slices of the map in three orthogonal directions.

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

6.4.1 Primary map



6.4.2 Raw map



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](#)

This section was not generated.

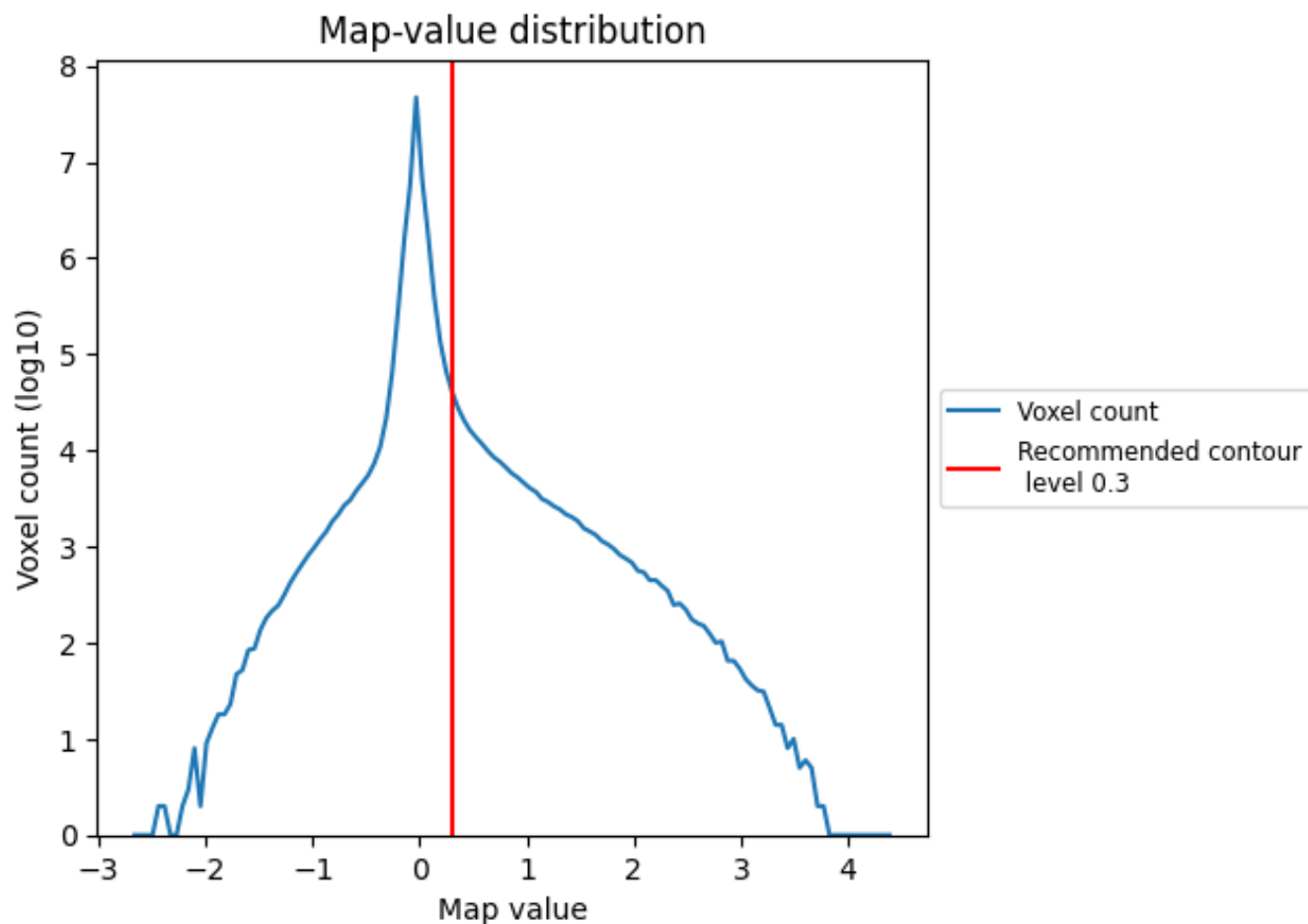
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

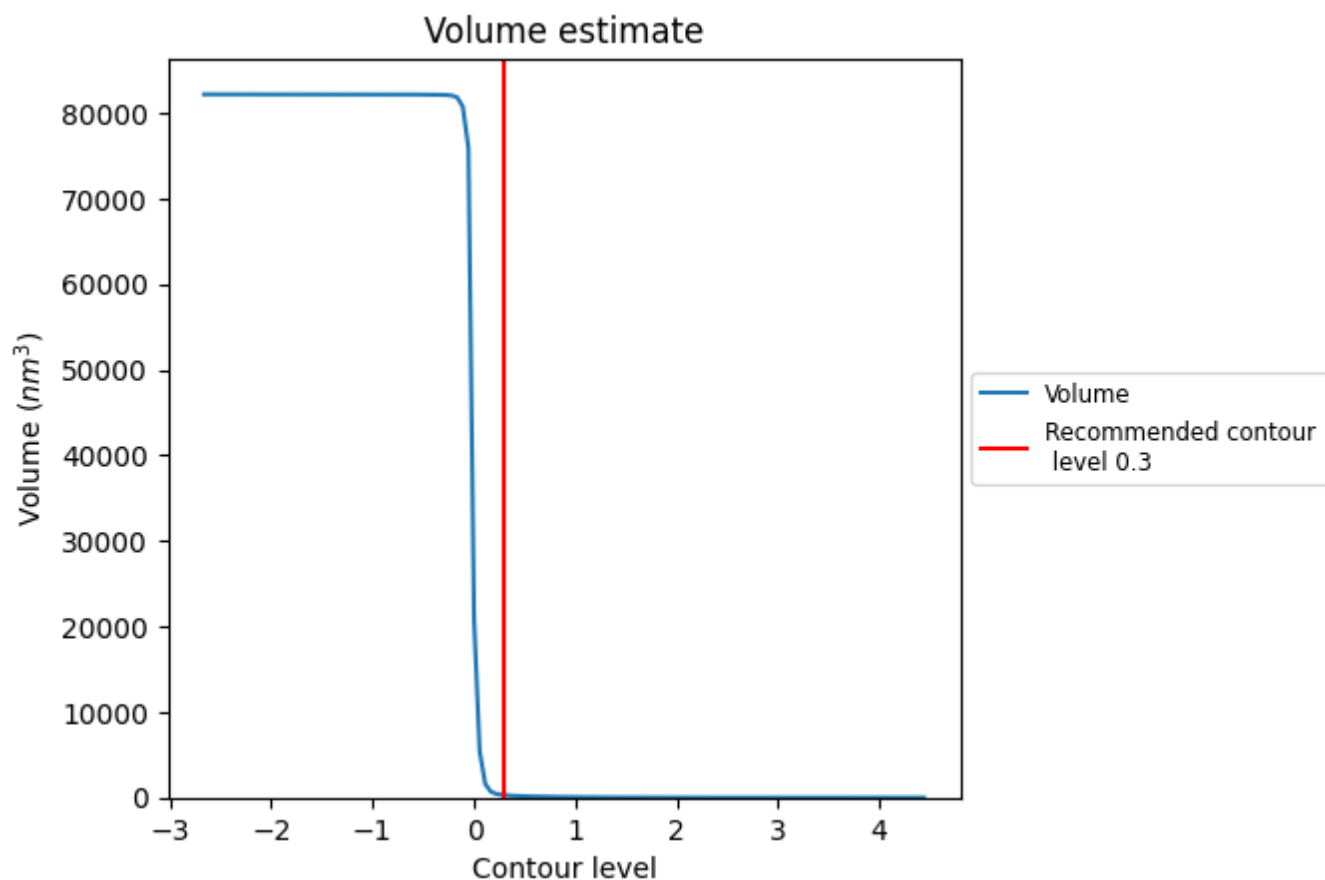
This section contains the results of statistical analysis of the map.

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.

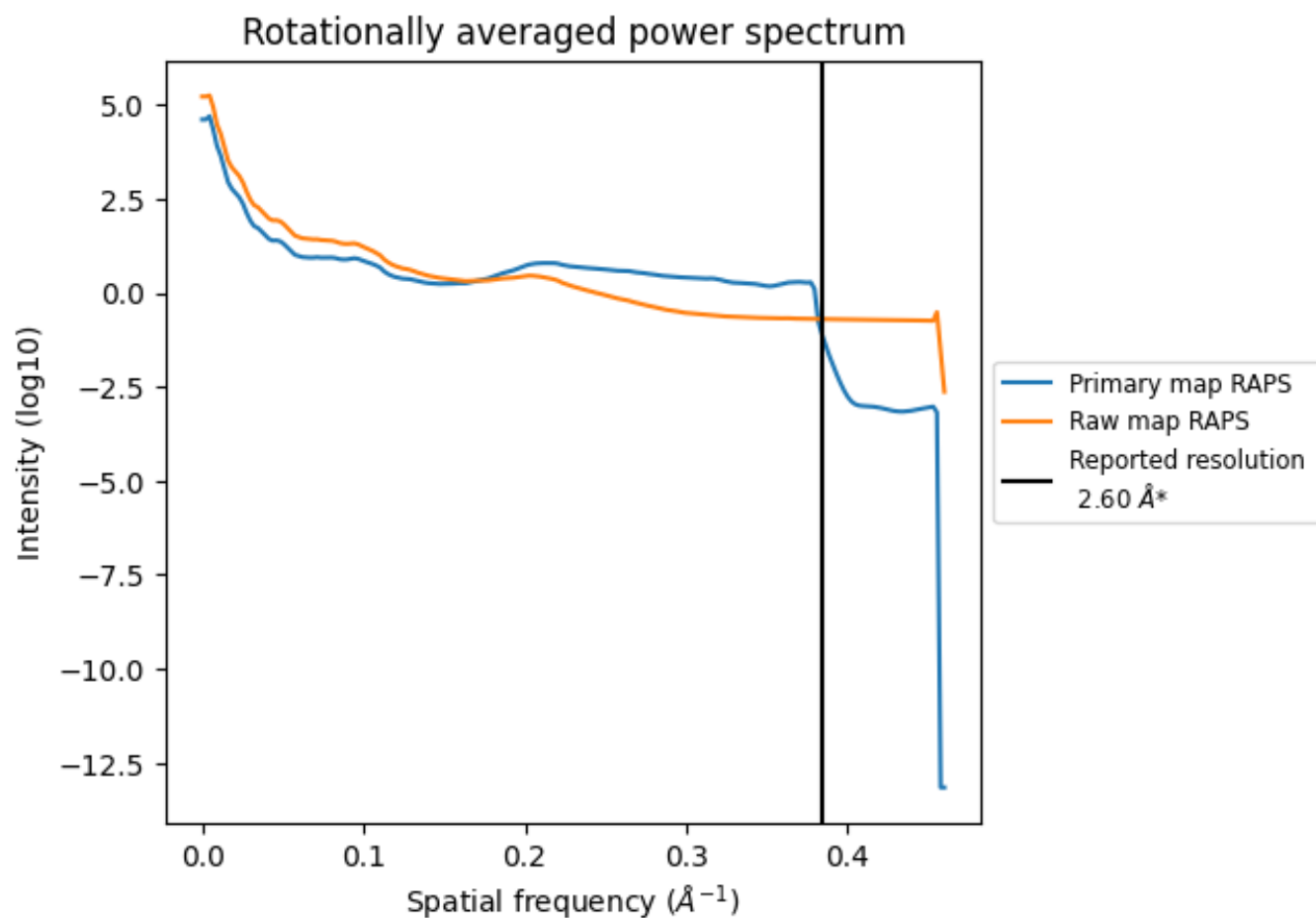
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 285 nm^3 ; this corresponds to an approximate mass of 257 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 ⓘ

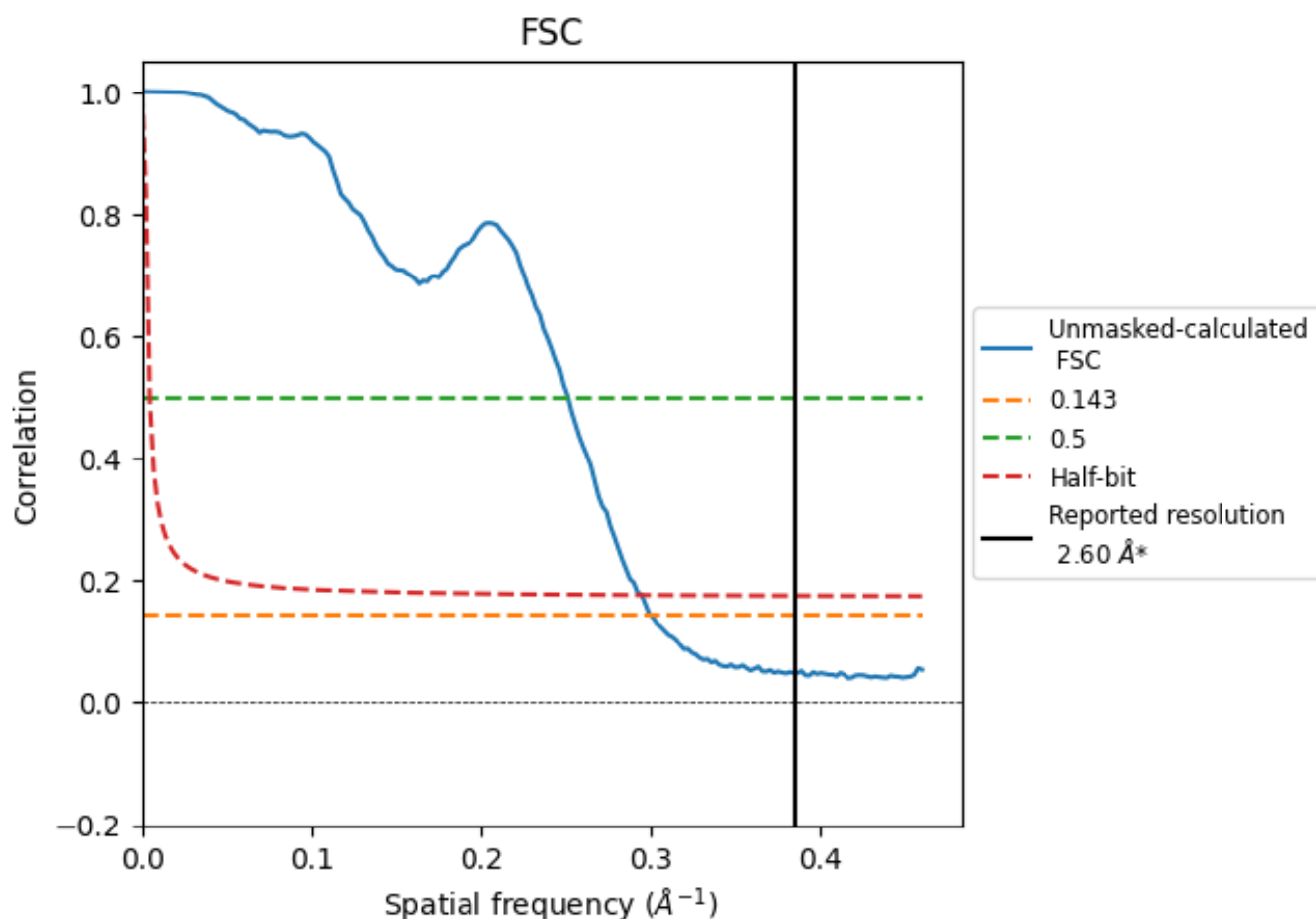


*Reported resolution corresponds to spatial frequency of 0.385 Å⁻¹

8 Fourier-Shell correlation [i](#)

Fourier-Shell Correlation (FSC) is the most commonly used method to estimate the resolution of single-particle and subtomogram-averaged maps. The shape of the curve depends on the imposed symmetry, mask and whether or not the two 3D reconstructions used were processed from a common reference. The reported resolution is shown as a black line. A curve is displayed for the half-bit criterion in addition to lines showing the 0.143 gold standard cut-off and 0.5 cut-off.

8.1 FSC [i](#)



*Reported resolution corresponds to spatial frequency of 0.385 $\text{\AA}^{-1}$

8.2 Resolution estimates [i](#)

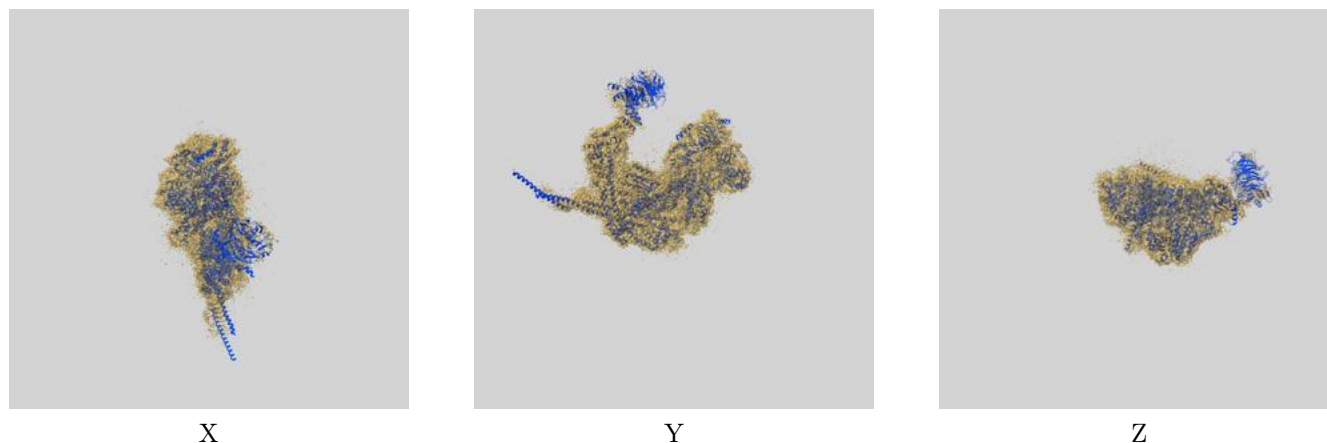
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	2.60	-	-
Author-provided FSC curve	-	-	-
Unmasked-calculated*	3.34	3.99	3.40

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 3.34 differs from the reported value 2.6 by more than 10 %

9 Map-model fit [i](#)

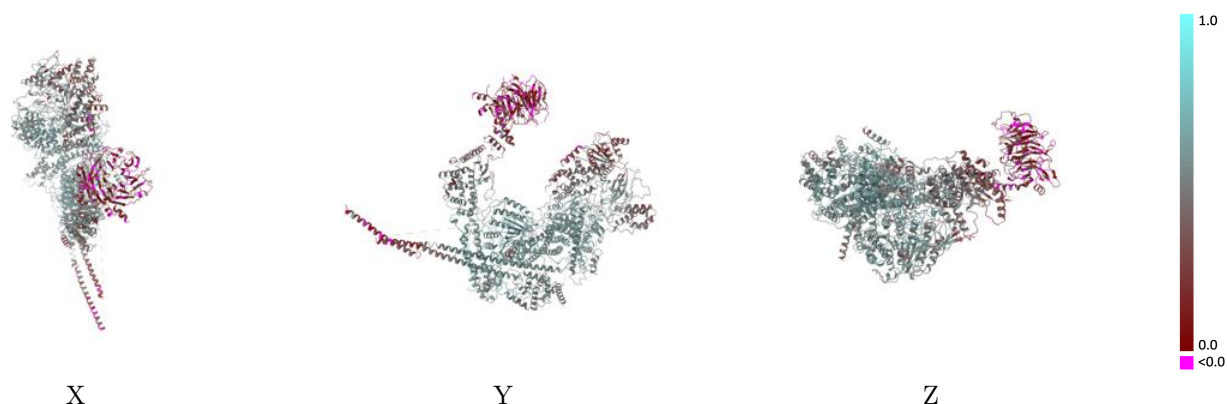
This section contains information regarding the fit between EMDB map EMD-34935 and PDB model 8HPO. Per-residue inclusion information can be found in [section 3](#) on [page 7](#).

9.1 Map-model overlay [i](#)



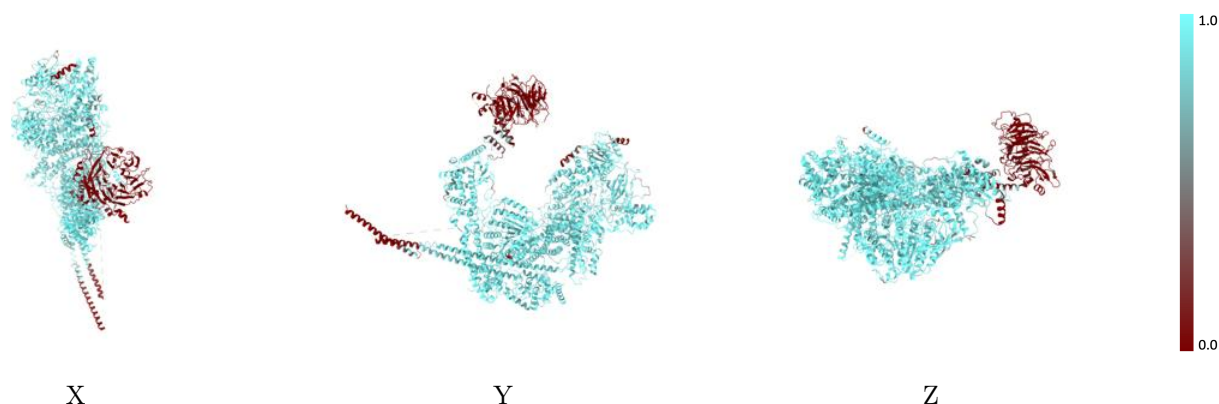
The images above show the 3D surface view of the map at the recommended contour level 0.3 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



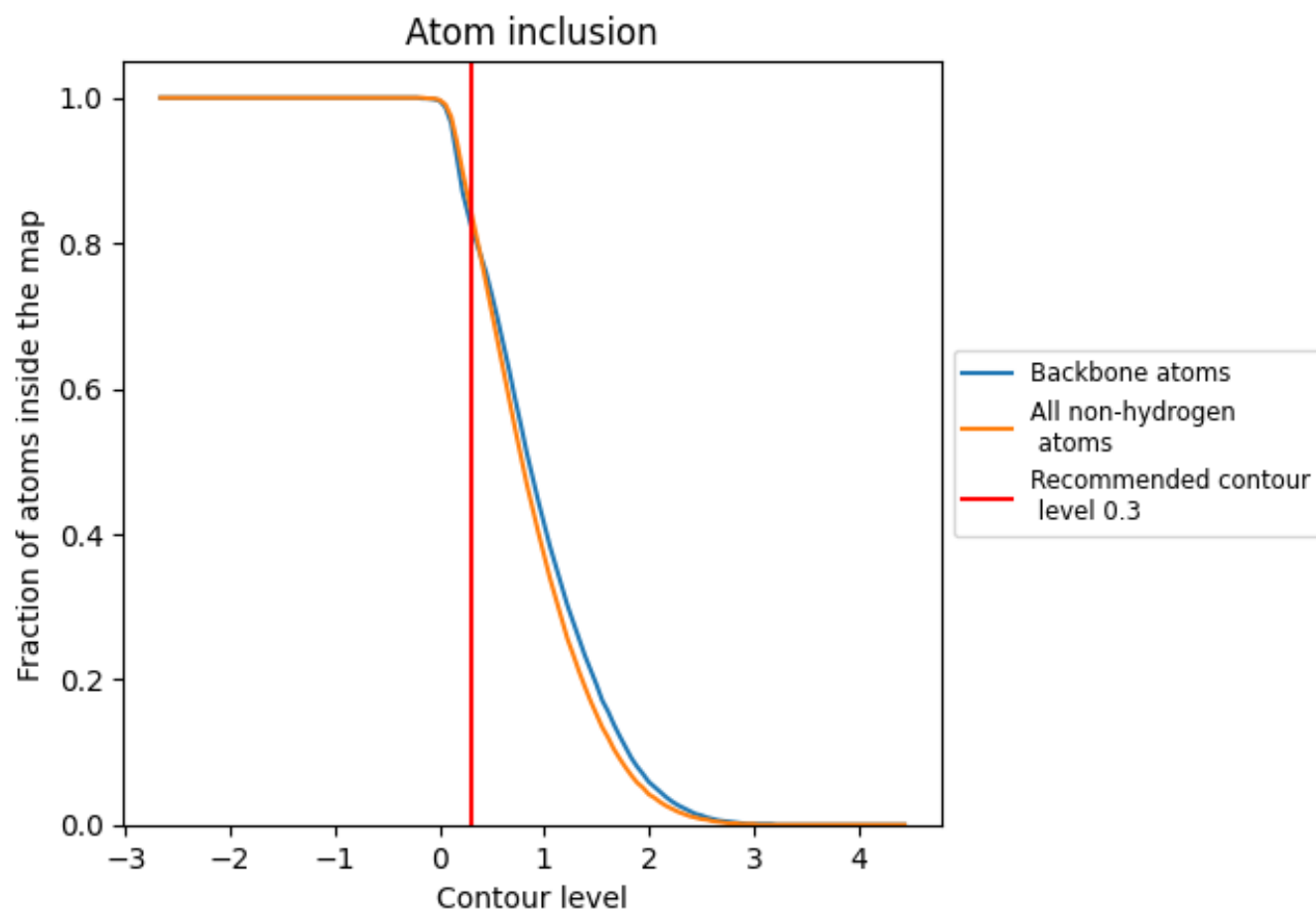
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.3).

9.4 Atom inclusion [i](#)



At the recommended contour level, 82% of all backbone atoms, 84% 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 (0.3) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.8450	0.4920
A	0.9060	0.5100
B	0.8730	0.4350
C	0.9450	0.5490
D	0.8150	0.4870
E	0.9620	0.5630
F	0.9820	0.6110
G	0.9760	0.5680
H	0.7740	0.4960
I	0.9440	0.5560
J	0.9110	0.4930
K	0.0340	0.1540

1.0

0.0

<0.0