



Full wwPDB EM Validation Report ⓘ

Mar 9, 2026 – 05:46 AM UTC

PDB ID : 9QO0 / pdb_00009qo0
EMDB ID : EMD-53252
Title : Pre-activated 9-subunit COP9 signalosome and neddylated SCF (Skp1-Skp2-Cks1) complex structure
Authors : Ding, S.; Clapperton, J.A.; Maeots, M.E.; Shaaban, M.; Enchev, R.I.
Deposited on : 2025-03-25
Resolution : 3.26 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:

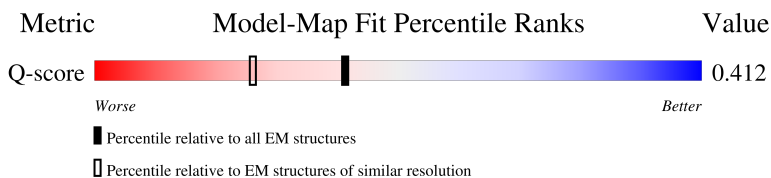
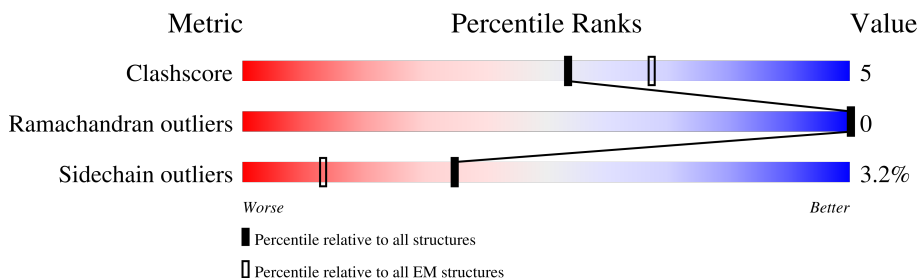
EMDB validation analysis : 0.0.1.dev132
Mogul : 2022.3.0, CSD as543be (2022)
MolProbity : 4-5-2 with Phenix2.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data 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) : 2.49

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 3.26 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	14557 (2.76 - 3.76)

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	D	406	
2	G	264	
3	K	76	
4	N	79	

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Mol	Chain	Length	Quality of chain
5	P	57	
6	A	491	
7	B	443	
8	C	423	
9	E	334	
10	F	327	
11	H	209	
12	I	776	
13	J	108	
14	L	163	
15	M	424	

2 Entry composition

There are 17 unique types of molecules in this entry. The entry contains 29373 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 COP9 signalosome complex subunit 4.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	D	394	Total	C	N	O	S	0	0
			3168	2000	550	604	14		

- Molecule 2 is a protein called COP9 signalosome complex subunit 7b.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	G	214	Total	C	N	O	S	0	0
			1694	1074	288	326	6		

- Molecule 3 is a protein called NEDD8.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	K	76	Total	C	N	O	S	0	0
			526	338	93	93	2		

- Molecule 4 is a protein called Cyclin-dependent kinases regulatory subunit 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	N	67	Total	C	N	O	S	0	0
			581	376	99	103	3		

- Molecule 5 is a protein called COP9 signalosome complex subunit 9.

Mol	Chain	Residues	Atoms				AltConf	Trace
5	P	21	Total	C	N	O	0	0
			179	113	26	40		

- Molecule 6 is a protein called COP9 signalosome complex subunit 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	A	406	Total	C	N	O	S	0	0
			3099	1969	529	579	22		

- Molecule 7 is a protein called COP9 signalosome complex subunit 2.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	B	404	Total	C	N	O	S	0	0
			3301	2099	567	620	15		

- Molecule 8 is a protein called COP9 signalosome complex subunit 3.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	C	354	Total	C	N	O	S	0	0
			2843	1816	475	528	24		

- Molecule 9 is a protein called COP9 signalosome complex subunit 5.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	E	288	Total	C	N	O	S	0	0
			2276	1458	377	428	13		

- Molecule 10 is a protein called COP9 signalosome complex subunit 6.

Mol	Chain	Residues	Atoms					AltConf	Trace
10	F	282	Total	C	N	O	S	0	0
			2238	1430	369	424	15		

- Molecule 11 is a protein called COP9 signalosome complex subunit 8.

Mol	Chain	Residues	Atoms					AltConf	Trace
11	H	173	Total	C	N	O	S	0	0
			1384	884	241	255	4		

- Molecule 12 is a protein called Cullin-1.

Mol	Chain	Residues	Atoms					AltConf	Trace
12	I	644	Total	C	N	O	S	0	0
			4699	2994	809	876	20		

- Molecule 13 is a protein called E3 ubiquitin-protein ligase RBX1.

Mol	Chain	Residues	Atoms					AltConf	Trace
13	J	80	Total	C	N	O	S	0	0
			665	425	119	112	9		

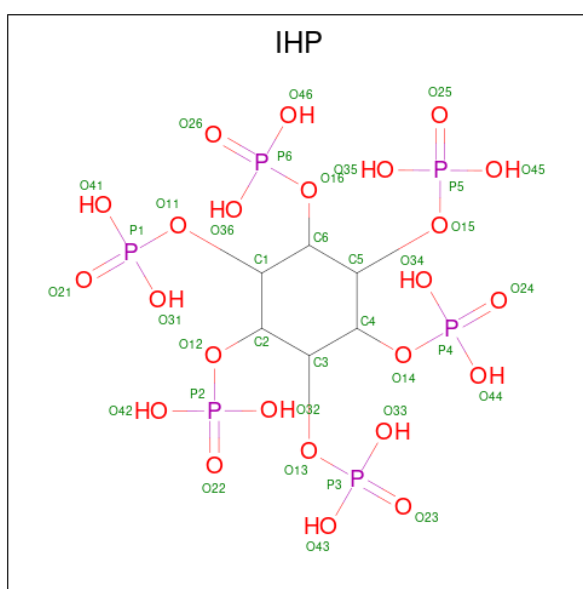
- Molecule 14 is a protein called S-phase kinase-associated protein 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
14	L	104	Total	C	N	O	S	0	0
			830	531	135	160	4		

- Molecule 15 is a protein called S-phase kinase-associated protein 2.

Mol	Chain	Residues	Atoms					AltConf	Trace
15	M	237	Total	C	N	O	S	0	0
			1851	1165	328	344	14		

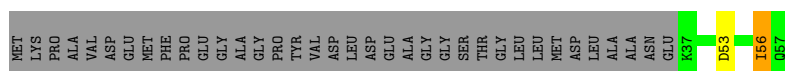
- Molecule 16 is INOSITOL HEXAKISPHOSPHATE (CCD ID: IHP) (formula: $C_6H_{18}O_{24}P_6$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms				AltConf
16	B	1	Total	C	O	P	0
			36	6	24	6	

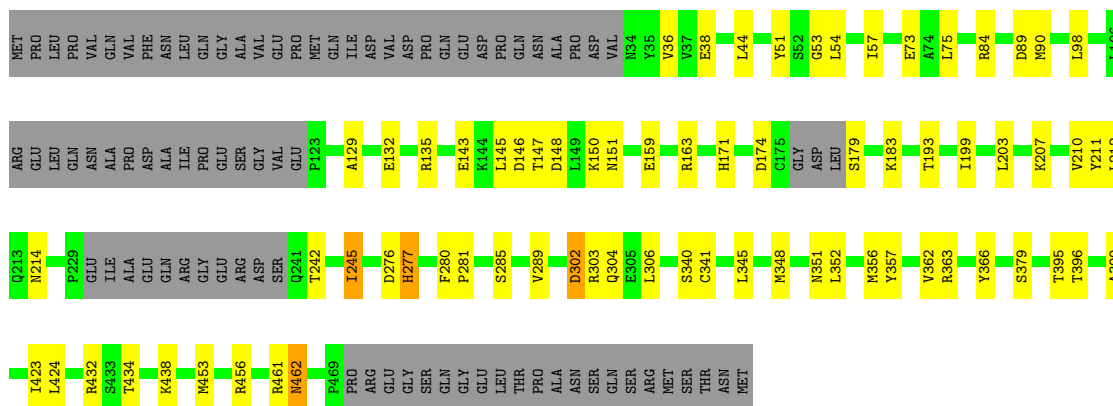
- Molecule 17 is ZINC ION (CCD ID: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		AltConf
17	J	3	Total	Zn	0
			3	3	



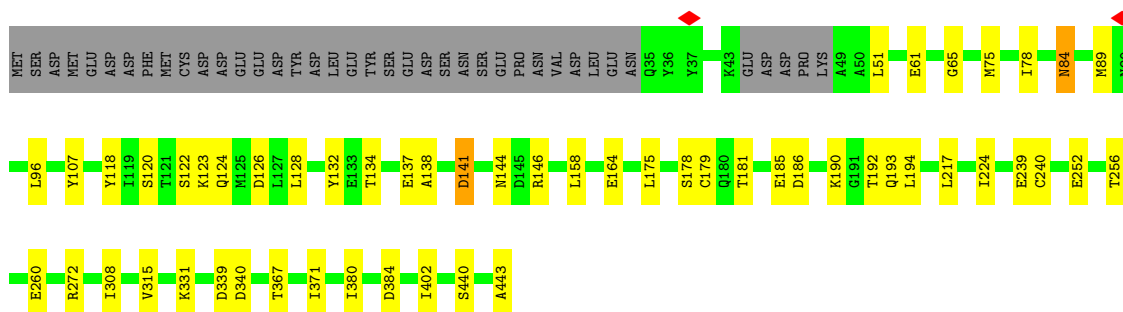
• Molecule 6: COP9 signalosome complex subunit 1

Chain A: 68% 14% 17%



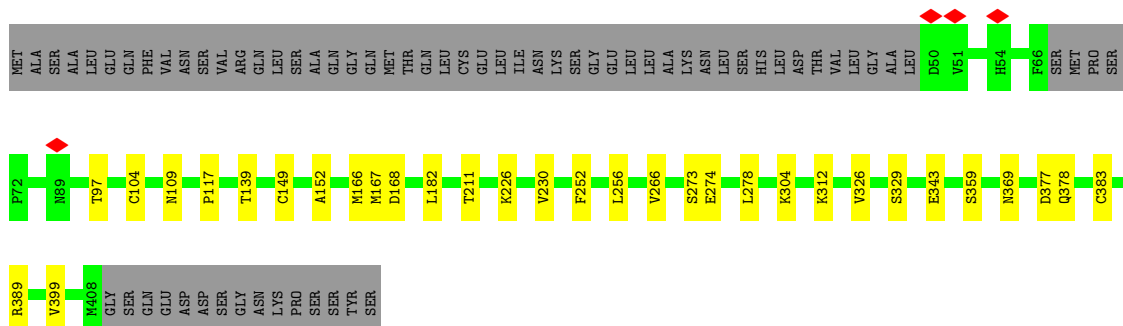
• Molecule 7: COP9 signalosome complex subunit 2

Chain B: 79% 12% 9%




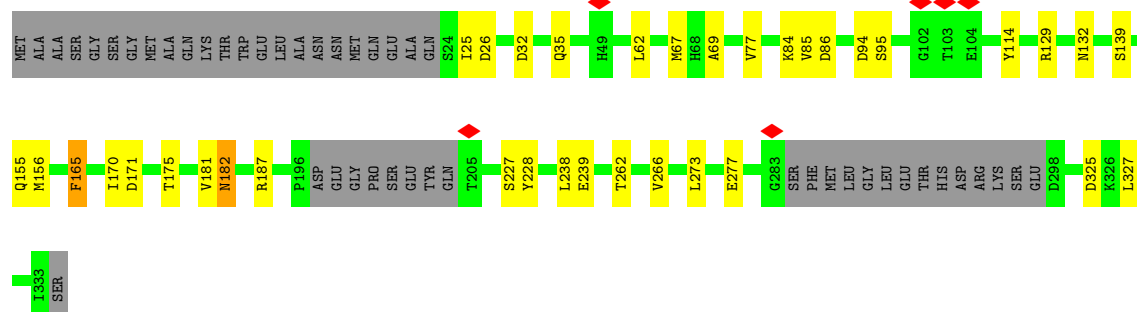
• Molecule 8: COP9 signalosome complex subunit 3

Chain C: 76% 8% 16%



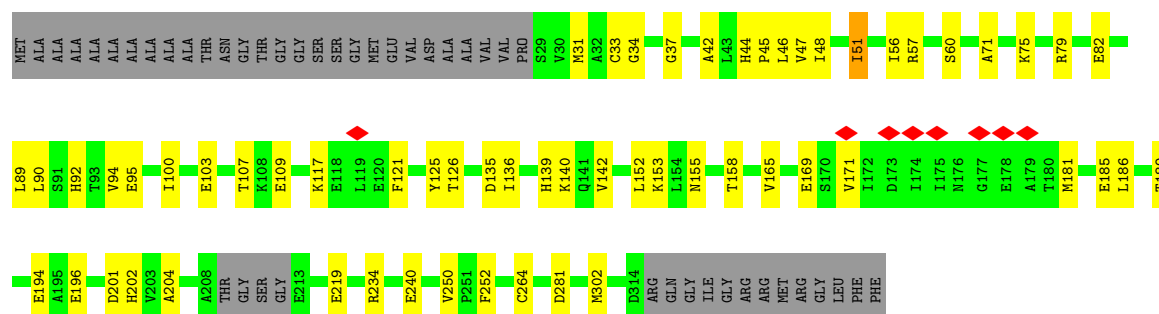
• Molecule 9: COP9 signalosome complex subunit 5

Chain E:  75% 10% 14%



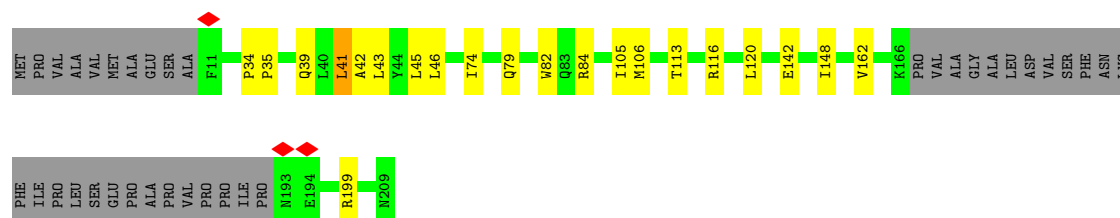
- Molecule 10: COP9 signalosome complex subunit 6

Chain F:  68% 18% 14%



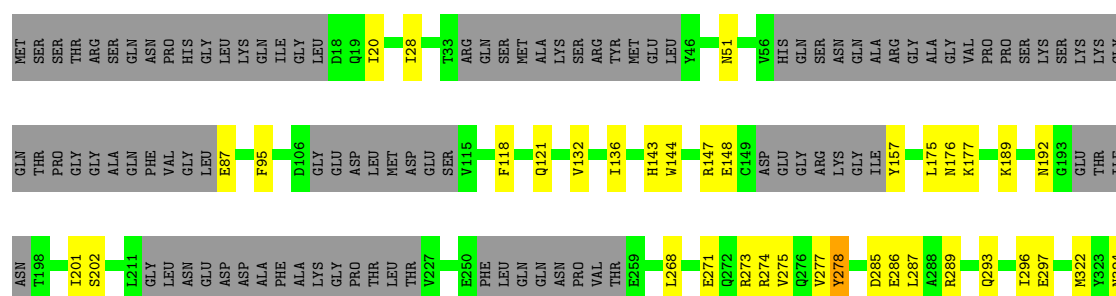
- Molecule 11: COP9 signalosome complex subunit 8

Chain H:  73% 10% 17%



- Molecule 12: Cullin-1

Chain I:  71% 12% 17%



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	400018	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	TFS KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	47	Depositor
Minimum defocus (nm)	500	Depositor
Maximum defocus (nm)	5000	Depositor
Magnification	Not provided	
Image detector	FEI FALCON III (4k x 4k)	Depositor
Maximum map value	2.033	Depositor
Minimum map value	-0.002	Depositor
Average map value	0.002	Depositor
Map value standard deviation	0.028	Depositor
Recommended contour level	0.0108	Depositor
Map size (Å)	345.6, 345.6, 345.6	wwPDB
Map dimensions	320, 320, 320	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.08, 1.08, 1.08	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: ZN, IHP

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	D	0.12	0/3217	0.29	1/4345 (0.0%)
2	G	0.13	0/1714	0.29	0/2319
3	K	0.15	0/531	0.34	0/722
4	N	0.10	0/601	0.26	0/814
5	P	0.34	0/183	0.61	0/245
6	A	0.17	0/3151	0.37	0/4270
7	B	0.15	0/3357	0.33	0/4514
8	C	0.14	0/2898	0.30	0/3910
9	E	0.16	0/2323	0.35	0/3138
10	F	0.15	0/2284	0.33	0/3096
11	H	0.13	0/1416	0.30	0/1923
12	I	0.15	0/4764	0.34	0/6480
13	J	0.14	0/685	0.35	0/929
14	L	0.10	0/841	0.28	0/1133
15	M	0.10	0/1873	0.28	0/2524
All	All	0.14	0/29838	0.33	1/40362 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	103	VAL	N-CA-C	-5.26	107.70	112.96

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	D	3168	0	3169	24	0
2	G	1694	0	1737	11	0
3	K	526	0	523	12	0
4	N	581	0	555	0	0
5	P	179	0	144	5	0
6	A	3099	0	3018	44	0
7	B	3301	0	3349	30	0
8	C	2843	0	2850	18	0
9	E	2276	0	2264	23	0
10	F	2238	0	2223	45	0
11	H	1384	0	1365	17	0
12	I	4699	0	4291	59	0
13	J	665	0	613	7	0
14	L	830	0	834	16	0
15	M	1851	0	1897	12	0
16	B	36	0	6	2	0
17	J	3	0	0	0	0
All	All	29373	0	28838	301	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 5.

All (301) 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)
5:P:56:ILE:HG13	11:H:79:GLN:HG2	1.55	0.89
12:I:621:THR:HG22	12:I:668:LEU:HD22	1.59	0.82
12:I:621:THR:OG1	12:I:624:GLN:HG3	1.79	0.79
12:I:466:TYR:OH	12:I:488:MET:SD	2.41	0.77
3:K:14:GLU:O	3:K:33:LYS:NZ	2.20	0.74
6:A:57:ILE:HD12	6:A:90:MET:HE2	1.69	0.73
7:B:252:GLU:OE2	13:J:98:ASN:ND2	2.22	0.73
6:A:199:ILE:O	6:A:203:LEU:HD12	1.88	0.72
10:F:201:ASP:OD1	10:F:202:HIS:N	2.23	0.72
14:L:106:ALA:O	14:L:110:LEU:HD12	1.90	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:A:159:GLU:OE2	6:A:163:ARG:NH1	2.22	0.71
6:A:276:ASP:OD1	6:A:277:HIS:N	2.24	0.69
9:E:69:ALA:CB	9:E:170:ILE:HD11	2.22	0.69
2:G:78:TYR:CE1	2:G:88:LEU:HD13	2.28	0.69
3:K:39:GLN:N	3:K:39:GLN:OE1	2.25	0.69
13:J:50:MET:HE2	13:J:50:MET:HA	1.74	0.68
12:I:520:GLN:OE1	12:I:573:ARG:NH1	2.26	0.68
6:A:73:GLU:N	6:A:73:GLU:OE1	2.25	0.68
10:F:103:GLU:O	10:F:107:THR:HG23	1.95	0.66
12:I:285:ASP:O	12:I:289:ARG:N	2.28	0.66
12:I:274:ARG:O	12:I:278:TYR:N	2.29	0.66
2:G:45:GLU:N	2:G:45:GLU:OE1	2.29	0.66
1:D:345:GLU:OE1	1:D:347:ARG:NH1	2.29	0.65
10:F:194:GLU:N	10:F:194:GLU:OE1	2.28	0.65
12:I:420:GLU:OE2	12:I:424:ARG:NE	2.30	0.65
12:I:189:LYS:O	12:I:192:ASN:ND2	2.29	0.65
12:I:87:GLU:OE1	12:I:87:GLU:N	2.31	0.64
16:B:501:IHP:O21	16:B:501:IHP:O32	2.15	0.64
12:I:510:ASP:OD2	12:I:541:SER:N	2.30	0.64
1:D:203:GLU:N	1:D:203:GLU:OE1	2.31	0.64
12:I:51:ASN:OD1	14:L:49:ASN:ND2	2.31	0.64
12:I:277:VAL:O	12:I:277:VAL:HG22	1.99	0.63
10:F:71:ALA:HB1	10:F:121:PHE:CE1	2.33	0.62
10:F:71:ALA:HB1	10:F:121:PHE:HE1	1.65	0.62
14:L:21:ALA:HB1	14:L:27:ILE:HG21	1.82	0.62
6:A:36:VAL:HG23	6:A:36:VAL:O	1.99	0.61
10:F:185:GLU:OE2	10:F:185:GLU:N	2.32	0.61
7:B:124:GLN:OE1	7:B:126:ASP:N	2.32	0.61
12:I:296:ILE:HD12	12:I:297:GLU:N	2.16	0.61
6:A:54:LEU:CD1	6:A:57:ILE:HD11	2.30	0.61
6:A:54:LEU:HD12	6:A:57:ILE:HD11	1.82	0.61
9:E:165:PHE:O	9:E:187:ARG:NH1	2.33	0.61
12:I:705:GLU:O	12:I:709:LEU:HD22	2.01	0.60
7:B:146:ARG:NH1	12:I:483:ASP:OD1	2.33	0.60
9:E:155:GLN:O	9:E:155:GLN:NE2	2.34	0.60
6:A:51:TYR:OH	6:A:84:ARG:NE	2.32	0.60
5:P:56:ILE:HD11	11:H:79:GLN:HA	1.84	0.60
1:D:257:GLN:OE1	1:D:257:GLN:N	2.31	0.60
9:E:25:ILE:HG23	9:E:26:ASP:OD1	2.02	0.59
9:E:156:MET:HE3	9:E:156:MET:O	2.01	0.59
7:B:194:LEU:HD23	7:B:224:ILE:HD11	1.85	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
15:M:131:ALA:O	15:M:137:TRP:NE1	2.34	0.59
6:A:146:ASP:OD1	6:A:147:THR:N	2.35	0.59
6:A:432:ARG:NH2	10:F:281:ASP:OD1	2.36	0.59
9:E:77:VAL:HG22	9:E:139:SER:OG	2.02	0.58
9:E:238:LEU:HD13	10:F:204:ALA:HA	1.85	0.58
7:B:239:GLU:OE1	7:B:272:ARG:NH1	2.37	0.58
8:C:167:MET:SD	8:C:389:ARG:NH1	2.76	0.58
12:I:176:ASN:OD1	12:I:177:LYS:N	2.37	0.58
1:D:270:ASP:OD2	1:D:314:LYS:NZ	2.31	0.58
12:I:621:THR:OG1	12:I:624:GLN:CG	2.52	0.57
12:I:621:THR:HG1	12:I:624:GLN:HG3	1.70	0.57
12:I:326:VAL:HG11	12:I:336:LEU:HD11	1.86	0.56
7:B:190:LYS:NZ	7:B:193:GLN:OE1	2.38	0.56
9:E:94:ASP:OD2	9:E:129:ARG:NH2	2.39	0.56
13:J:48:HIS:NE2	13:J:50:MET:O	2.38	0.56
3:K:15:ILE:CD1	3:K:30:VAL:HG12	2.36	0.56
9:E:262:THR:O	9:E:266:VAL:HG23	2.05	0.55
14:L:30:MET:O	14:L:34:LEU:N	2.34	0.55
6:A:453:MET:HE1	10:F:302:MET:HG3	1.89	0.54
15:M:114:LEU:H	15:M:114:LEU:HD12	1.73	0.54
1:D:234:ILE:O	1:D:242:ARG:NH2	2.41	0.54
10:F:94:VAL:HG13	10:F:95:GLU:H	1.72	0.54
6:A:132:GLU:O	6:A:135:ARG:NH2	2.41	0.54
7:B:61:GLU:OE2	7:B:65:GLY:N	2.41	0.54
11:H:74:ILE:HD13	11:H:106:MET:HE1	1.89	0.54
1:D:68:ASP:OD1	1:D:72:HIS:NE2	2.41	0.54
1:D:206:GLN:NE2	1:D:241:GLN:OE1	2.38	0.54
10:F:42:ALA:HB3	10:F:82:GLU:OE2	2.08	0.53
1:D:385:LEU:HD13	10:F:234:ARG:HD2	1.89	0.53
2:G:75:TYR:CE2	2:G:93:GLN:NE2	2.76	0.53
2:G:75:TYR:HE2	2:G:93:GLN:NE2	2.05	0.53
16:B:501:IHP:O46	16:B:501:IHP:O11	2.25	0.53
14:L:17:ASP:OD1	14:L:19:GLU:N	2.39	0.53
2:G:184:VAL:HG11	9:E:327:LEU:HD13	1.91	0.53
12:I:28:ILE:HD11	12:I:95:PHE:CD1	2.44	0.53
12:I:613:GLN:OE1	12:I:613:GLN:N	2.42	0.53
10:F:75:LYS:NZ	10:F:117:LYS:O	2.42	0.53
10:F:57:ARG:O	10:F:60:SER:OG	2.27	0.52
6:A:462:ASN:OD1	6:A:462:ASN:N	2.41	0.52
7:B:51:LEU:HD13	7:B:78:ILE:HG21	1.91	0.52
1:D:252:ASP:OD1	1:D:253:GLU:N	2.42	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:H:74:ILE:HD13	11:H:106:MET:CE	2.39	0.52
12:I:549:GLN:OE1	12:I:550:SER:N	2.43	0.52
12:I:722:ARG:NH1	12:I:733:GLU:OE2	2.43	0.52
13:J:69:THR:HG21	13:J:107:GLY:HA2	1.91	0.52
6:A:89:ASP:OD1	6:A:90:MET:N	2.43	0.52
15:M:168:SER:O	15:M:191:SER:OG	2.25	0.51
7:B:308:ILE:HG22	7:B:308:ILE:O	2.09	0.51
12:I:286:GLU:OE1	12:I:286:GLU:N	2.42	0.51
14:L:4:ILE:N	14:L:15:GLU:OE2	2.44	0.51
10:F:165:VAL:HG23	10:F:165:VAL:O	2.10	0.51
3:K:49:GLN:OE1	3:K:50:MET:N	2.43	0.51
10:F:136:ILE:HD12	10:F:181:MET:HE3	1.92	0.50
1:D:214:LYS:NZ	1:D:217:VAL:HG13	2.27	0.50
15:M:201:ILE:O	15:M:201:ILE:HG13	2.11	0.50
1:D:142:ASP:OD1	1:D:143:TYR:N	2.45	0.50
14:L:119:THR:O	14:L:122:THR:OG1	2.29	0.50
1:D:214:LYS:HZ3	1:D:217:VAL:HG13	1.76	0.50
3:K:15:ILE:HD12	3:K:30:VAL:HG12	1.94	0.50
3:K:70:VAL:HG21	9:E:114:TYR:CG	2.47	0.49
6:A:456:ARG:NH2	7:B:443:ALA:OXT	2.41	0.49
15:M:192:VAL:HG13	15:M:192:VAL:O	2.13	0.49
9:E:32:ASP:OD2	9:E:35:GLN:N	2.43	0.49
8:C:182:LEU:HD21	8:C:211:THR:HG21	1.93	0.49
12:I:20:ILE:O	12:I:20:ILE:HG22	2.13	0.49
6:A:434:THR:O	6:A:438:LYS:HG3	2.13	0.48
15:M:201:ILE:O	15:M:201:ILE:CG1	2.61	0.48
14:L:104:ILE:HG22	14:L:119:THR:HG23	1.94	0.48
7:B:84:ASN:OD1	7:B:84:ASN:N	2.46	0.48
8:C:266:VAL:HG21	8:C:278:LEU:HD12	1.95	0.48
12:I:638:GLN:OE1	12:I:638:GLN:N	2.33	0.48
14:L:123:VAL:HG11	15:M:108:ILE:HG23	1.95	0.48
6:A:302:ASP:OD1	6:A:303:ARG:N	2.47	0.48
10:F:126:THR:HG23	10:F:153:LYS:HD2	1.94	0.48
12:I:775:LEU:O	12:I:775:LEU:HD12	2.13	0.48
9:E:238:LEU:HD12	9:E:239:GLU:N	2.29	0.48
8:C:326:VAL:HG12	8:C:326:VAL:O	2.14	0.47
12:I:118:PHE:O	12:I:121:GLN:NE2	2.47	0.47
6:A:395:THR:HG22	6:A:396:THR:N	2.29	0.47
10:F:71:ALA:HB2	10:F:89:LEU:HD11	1.95	0.47
6:A:280:PHE:N	6:A:281:PRO:HD2	2.30	0.47
12:I:296:ILE:HD12	12:I:296:ILE:C	2.38	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:F:51:ILE:HD12	10:F:125:TYR:CZ	2.50	0.47
10:F:90:LEU:O	10:F:100:ILE:HD12	2.15	0.47
2:G:150:GLN:O	2:G:151:LEU:HD12	2.14	0.47
2:G:181:CYS:O	2:G:184:VAL:HG12	2.15	0.47
12:I:753:ILE:HG21	12:I:772:TYR:HE2	1.80	0.47
15:M:367:VAL:O	15:M:389:ASN:ND2	2.48	0.47
11:H:41:LEU:HD23	11:H:45:LEU:HD13	1.97	0.47
10:F:42:ALA:HB2	10:F:189:THR:OG1	2.14	0.46
10:F:169:GLU:CD	10:F:186:LEU:HD12	2.40	0.46
12:I:275:VAL:HG11	12:I:287:LEU:HD22	1.97	0.46
12:I:427:ASP:OD2	12:I:431:LYS:HD2	2.15	0.46
1:D:69:PHE:CE2	1:D:73:LEU:HD11	2.49	0.46
1:D:306:GLU:OE2	1:D:347:ARG:NH2	2.48	0.46
6:A:302:ASP:OD1	6:A:304:GLN:N	2.46	0.46
11:H:42:ALA:HB3	11:H:105:ILE:HD12	1.98	0.46
12:I:201:ILE:HG13	12:I:202:SER:N	2.30	0.46
6:A:53:GLY:O	6:A:211:TYR:OH	2.28	0.46
9:E:26:ASP:OD2	10:F:56:ILE:HD11	2.16	0.46
12:I:144:TRP:O	12:I:148:GLU:N	2.49	0.46
12:I:402:PHE:C	12:I:402:PHE:CD1	2.94	0.46
1:D:130:ILE:O	1:D:132:LEU:N	2.47	0.46
8:C:377:ASP:OD2	11:H:199:ARG:NH1	2.48	0.46
9:E:273:LEU:O	9:E:277:GLU:HG3	2.16	0.46
6:A:203:LEU:HD21	6:A:245:ILE:HG13	1.97	0.46
5:P:56:ILE:HD13	11:H:82:TRP:CG	2.51	0.46
3:K:31:GLU:O	3:K:35:GLY:N	2.45	0.45
12:I:132:VAL:HG12	12:I:136:ILE:HD11	1.97	0.45
12:I:753:ILE:HG21	12:I:772:TYR:CE2	2.51	0.45
12:I:589:GLU:HG2	12:I:600:THR:HG23	1.98	0.45
7:B:128:LEU:HD22	7:B:132:TYR:OH	2.17	0.45
12:I:621:THR:HG22	12:I:668:LEU:CD2	2.38	0.45
5:P:53:ASP:OD1	5:P:53:ASP:N	2.49	0.45
8:C:97:THR:CG2	8:C:97:THR:O	2.64	0.45
15:M:113:CYS:SG	15:M:114:LEU:HD12	2.57	0.45
15:M:187:ASP:OD1	15:M:187:ASP:N	2.49	0.45
14:L:104:ILE:HG22	14:L:119:THR:CG2	2.46	0.45
6:A:150:LYS:N	6:A:150:LYS:HD2	2.32	0.45
7:B:158:LEU:C	7:B:158:LEU:HD23	2.42	0.45
8:C:226:LYS:O	8:C:230:VAL:HG22	2.16	0.45
8:C:399:VAL:O	8:C:399:VAL:HG13	2.16	0.45
12:I:143:HIS:O	12:I:147:ARG:N	2.46	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:I:273:ARG:O	12:I:277:VAL:HG12	2.16	0.45
7:B:120:SER:HA	7:B:128:LEU:HD21	1.99	0.45
7:B:175:LEU:O	7:B:179:CYS:N	2.45	0.45
8:C:343:GLU:OE1	11:H:84:ARG:NH1	2.49	0.45
13:J:75:CYS:O	13:J:77:HIS:N	2.49	0.45
12:I:405:ASN:OD1	12:I:405:ASN:N	2.50	0.44
12:I:601:LEU:HD21	12:I:680:LEU:HD23	1.97	0.44
12:I:427:ASP:OD2	12:I:427:ASP:C	2.60	0.44
7:B:141:ASP:OD2	7:B:141:ASP:N	2.50	0.44
3:K:36:ILE:O	3:K:41:GLN:NE2	2.51	0.44
10:F:201:ASP:OD1	10:F:201:ASP:C	2.60	0.44
6:A:362:VAL:HG13	6:A:363:ARG:N	2.32	0.44
7:B:380:ILE:HD11	7:B:384:ASP:CB	2.47	0.44
10:F:140:LYS:HD2	10:F:181:MET:HE2	1.99	0.44
10:F:152:LEU:HD12	10:F:153:LYS:N	2.32	0.44
10:F:250:VAL:HG23	10:F:252:PHE:H	1.82	0.44
14:L:6:LEU:HD23	14:L:45:VAL:HG23	2.00	0.44
14:L:47:LEU:HB3	14:L:50:VAL:HG22	2.00	0.44
1:D:73:LEU:HD13	1:D:84:ILE:HD11	2.00	0.44
7:B:51:LEU:HD11	7:B:75:MET:HG3	1.99	0.44
12:I:706:ASP:O	12:I:710:LEU:HG	2.17	0.44
13:J:39:VAL:HG13	13:J:40:ASP:N	2.33	0.44
1:D:185:ILE:HD12	1:D:188:LYS:HD2	1.99	0.44
10:F:48:ILE:HG12	10:F:165:VAL:HG11	1.99	0.44
6:A:207:LYS:O	6:A:211:TYR:HD2	2.01	0.43
12:I:528:SER:OG	12:I:529:GLU:N	2.50	0.43
1:D:385:LEU:HD13	10:F:234:ARG:CD	2.48	0.43
6:A:179:SER:O	6:A:183:LYS:N	2.48	0.43
15:M:394:THR:O	15:M:398:ARG:NE	2.46	0.43
6:A:212:LEU:O	6:A:212:LEU:HD12	2.18	0.43
6:A:289:VAL:HG12	6:A:289:VAL:O	2.19	0.43
8:C:273:SER:OG	8:C:274:GLU:N	2.51	0.43
10:F:31:MET:SD	10:F:31:MET:N	2.91	0.43
6:A:171:HIS:O	6:A:174:ASP:HB2	2.19	0.43
12:I:712:GLN:HG2	12:I:756:LEU:HD21	2.00	0.43
9:E:94:ASP:OD1	9:E:95:SER:N	2.47	0.43
3:K:51:ASN:N	3:K:59:TYR:OH	2.47	0.43
6:A:453:MET:HE1	10:F:302:MET:CG	2.49	0.43
10:F:33:CYS:SG	10:F:34:GLY:N	2.92	0.43
10:F:152:LEU:HD12	10:F:153:LYS:H	1.84	0.43
12:I:275:VAL:CG1	12:I:287:LEU:HD22	2.48	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:I:468:LYS:O	12:I:468:LYS:HD3	2.19	0.43
6:A:145:LEU:O	6:A:148:ASP:OD1	2.37	0.43
8:C:343:GLU:HG3	11:H:120:LEU:HD13	2.00	0.43
9:E:175:THR:HG23	9:E:181:VAL:HA	2.00	0.43
10:F:155:ASN:ND2	10:F:158:THR:OG1	2.52	0.43
11:H:46:LEU:O	11:H:46:LEU:HD23	2.18	0.43
12:I:277:VAL:O	12:I:277:VAL:CG2	2.66	0.43
8:C:109:ASN:OD1	8:C:109:ASN:C	2.62	0.42
10:F:44:HIS:O	10:F:47:VAL:HG22	2.18	0.42
2:G:138:THR:O	2:G:138:THR:HG22	2.20	0.42
9:E:85:VAL:HG12	9:E:86:ASP:N	2.34	0.42
6:A:461:ARG:NH2	8:C:168:ASP:OD1	2.52	0.42
7:B:89:MET:HE1	7:B:134:THR:HG21	2.00	0.42
14:L:120:CYS:O	14:L:123:VAL:HG12	2.20	0.42
6:A:38:GLU:N	6:A:38:GLU:OE1	2.53	0.42
10:F:135:ASP:N	10:F:135:ASP:OD2	2.48	0.42
7:B:371:ILE:HD11	7:B:402:ILE:CD1	2.50	0.42
11:H:39:GLN:O	11:H:43:LEU:HD23	2.20	0.42
6:A:345:LEU:HD12	6:A:366:TYR:CZ	2.53	0.42
12:I:332:GLY:O	12:I:336:LEU:HG	2.20	0.42
12:I:551:CYS:SG	12:I:552:THR:N	2.93	0.42
6:A:423:ILE:HG22	6:A:424:LEU:N	2.35	0.42
8:C:278:LEU:O	8:C:278:LEU:HD23	2.20	0.42
2:G:37:ALA:HB3	2:G:40:VAL:HG22	2.02	0.42
9:E:175:THR:OG1	9:E:182:ASN:OD1	2.37	0.42
12:I:709:LEU:HD22	12:I:709:LEU:H	1.84	0.42
2:G:78:TYR:CZ	2:G:88:LEU:HD13	2.54	0.42
3:K:42:ARG:HB2	3:K:70:VAL:HG22	2.02	0.42
8:C:252:PHE:O	8:C:256:LEU:HD12	2.20	0.42
11:H:45:LEU:HD22	11:H:74:ILE:HD11	2.01	0.42
12:I:369:THR:O	12:I:372:ASP:OD2	2.38	0.42
1:D:101:GLU:OE2	1:D:101:GLU:C	2.63	0.41
1:D:125:GLN:OE1	1:D:125:GLN:HA	2.21	0.41
11:H:34:PRO:N	11:H:35:PRO:HD2	2.35	0.41
12:I:175:LEU:HD12	12:I:175:LEU:O	2.20	0.41
8:C:369:ASN:N	8:C:369:ASN:OD1	2.52	0.41
9:E:171:ASP:OD1	9:E:171:ASP:N	2.54	0.41
10:F:109:GLU:C	10:F:109:GLU:OE1	2.63	0.41
11:H:42:ALA:CB	11:H:105:ILE:HD12	2.50	0.41
1:D:92:ILE:O	1:D:92:ILE:HG22	2.20	0.41
6:A:129:ALA:HA	6:A:132:GLU:OE1	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:H:142:GLU:CD	11:H:142:GLU:H	2.29	0.41
7:B:181:THR:OG1	7:B:185:GLU:N	2.53	0.41
7:B:380:ILE:HD11	7:B:384:ASP:HB3	2.02	0.41
9:E:62:LEU:HD22	9:E:228:TYR:CE1	2.56	0.41
10:F:140:LYS:CD	10:F:181:MET:HE2	2.51	0.41
6:A:214:ASN:OD1	6:A:214:ASN:C	2.64	0.41
6:A:351:ASN:OD1	6:A:351:ASN:C	2.63	0.41
7:B:123:LYS:HE3	7:B:123:LYS:HB3	1.95	0.41
7:B:178:SER:HA	7:B:181:THR:HG22	2.02	0.41
7:B:186:ASP:OD1	7:B:186:ASP:N	2.53	0.41
9:E:67:MET:HE3	10:F:46:LEU:HD22	2.01	0.41
1:D:289:GLN:O	1:D:299:ILE:HD11	2.21	0.41
10:F:90:LEU:HD23	10:F:90:LEU:H	1.86	0.41
1:D:234:ILE:HG21	1:D:281:PHE:CZ	2.56	0.41
7:B:137:GLU:OE1	7:B:138:ALA:N	2.53	0.41
8:C:97:THR:O	8:C:97:THR:HG22	2.21	0.41
8:C:117:PRO:HB2	8:C:152:ALA:HB2	2.02	0.41
10:F:37:GLY:O	10:F:79:ARG:NH2	2.47	0.41
10:F:45:PRO:HG2	10:F:196:GLU:OE1	2.21	0.41
14:L:8:SER:OG	14:L:50:VAL:HG23	2.21	0.41
15:M:259:ASP:OD1	15:M:259:ASP:C	2.64	0.41
1:D:367:LEU:HB2	1:D:368:PRO:HD3	2.03	0.41
3:K:40:GLN:O	3:K:42:ARG:NH1	2.54	0.41
6:A:356:MET:HE2	6:A:357:TYR:CE2	2.56	0.41
7:B:340:ASP:OD2	7:B:340:ASP:C	2.64	0.41
7:B:96:LEU:C	7:B:96:LEU:HD12	2.46	0.40
10:F:240:GLU:HA	10:F:240:GLU:OE1	2.20	0.40
12:I:330:GLN:N	12:I:330:GLN:OE1	2.55	0.40
13:J:37:ILE:HD13	13:J:37:ILE:N	2.36	0.40
3:K:44:ILE:CD1	3:K:68:HIS:HB2	2.51	0.40
12:I:268:LEU:HA	12:I:271:GLU:HG3	2.04	0.40
6:A:36:VAL:O	6:A:36:VAL:CG2	2.69	0.40
6:A:395:THR:CG2	6:A:399:ALA:HB3	2.51	0.40
7:B:339:ASP:OD1	7:B:339:ASP:N	2.53	0.40
9:E:85:VAL:HG12	9:E:86:ASP:H	1.86	0.40
14:L:58:VAL:HG23	14:L:59:ILE:N	2.37	0.40
2:G:174:LEU:HD13	10:F:264:CYS:SG	2.60	0.40
5:P:56:ILE:HD13	11:H:82:TRP:CD1	2.56	0.40
6:A:75:LEU:HB3	6:A:98:LEU:CD2	2.51	0.40
12:I:532:ASP:OD1	12:I:533:LEU:N	2.55	0.40
6:A:193:THR:O	6:A:193:THR:HG23	2.22	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:B:146:ARG:HD3	7:B:192:THR:HG22	2.04	0.40
10:F:139:HIS:O	10:F:142:VAL:HG12	2.22	0.40
12:I:322:MET:O	12:I:326:VAL:HG12	2.21	0.40
14:L:6:LEU:HD23	14:L:45:VAL:CG2	2.52	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	D	388/406 (96%)	379 (98%)	9 (2%)	0	100	100
2	G	212/264 (80%)	206 (97%)	6 (3%)	0	100	100
3	K	74/76 (97%)	70 (95%)	4 (5%)	0	100	100
4	N	65/79 (82%)	60 (92%)	5 (8%)	0	100	100
5	P	19/57 (33%)	18 (95%)	1 (5%)	0	100	100
6	A	398/491 (81%)	380 (96%)	18 (4%)	0	100	100
7	B	400/443 (90%)	377 (94%)	23 (6%)	0	100	100
8	C	350/423 (83%)	340 (97%)	10 (3%)	0	100	100
9	E	282/334 (84%)	269 (95%)	13 (5%)	0	100	100
10	F	278/327 (85%)	266 (96%)	12 (4%)	0	100	100
11	H	169/209 (81%)	160 (95%)	9 (5%)	0	100	100
12	I	618/776 (80%)	590 (96%)	28 (4%)	0	100	100
13	J	76/108 (70%)	70 (92%)	6 (8%)	0	100	100
14	L	94/163 (58%)	92 (98%)	2 (2%)	0	100	100
15	M	221/424 (52%)	208 (94%)	13 (6%)	0	100	100
All	All	3644/4580 (80%)	3485 (96%)	159 (4%)	0	100	100

There are no Ramachandran outliers to report.

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	D	339/347 (98%)	330 (97%)	9 (3%)	39	61
2	G	186/229 (81%)	174 (94%)	12 (6%)	15	42
3	K	48/66 (73%)	47 (98%)	1 (2%)	47	66
4	N	64/76 (84%)	61 (95%)	3 (5%)	23	51
5	P	19/45 (42%)	18 (95%)	1 (5%)	20	48
6	A	320/429 (75%)	304 (95%)	16 (5%)	22	49
7	B	365/405 (90%)	350 (96%)	15 (4%)	27	53
8	C	318/377 (84%)	308 (97%)	10 (3%)	35	59
9	E	244/283 (86%)	238 (98%)	6 (2%)	42	63
10	F	251/276 (91%)	247 (98%)	4 (2%)	55	70
11	H	144/173 (83%)	139 (96%)	5 (4%)	32	56
12	I	440/698 (63%)	430 (98%)	10 (2%)	44	65
13	J	70/90 (78%)	68 (97%)	2 (3%)	37	60
14	L	95/150 (63%)	89 (94%)	6 (6%)	16	43
15	M	220/392 (56%)	219 (100%)	1 (0%)	81	82
All	All	3123/4036 (77%)	3022 (97%)	101 (3%)	35	58

All (101) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	D	13	MET
1	D	45	LEU
1	D	69	PHE
1	D	89	LEU
1	D	177	GLU
1	D	179	THR
1	D	185	ILE

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Mol	Chain	Res	Type
1	D	221	GLU
1	D	237	SER
2	G	11	LEU
2	G	18	LEU
2	G	28	THR
2	G	48	GLU
2	G	64	LEU
2	G	67	LEU
2	G	93	GLN
2	G	103	SER
2	G	134	GLU
2	G	157	CYS
2	G	197	GLN
2	G	205	THR
3	K	27	LYS
4	N	24	LEU
4	N	39	SER
4	N	68	LEU
5	P	56	ILE
6	A	44	LEU
6	A	143	GLU
6	A	151	ASN
6	A	210	VAL
6	A	242	THR
6	A	245	ILE
6	A	277	HIS
6	A	285	SER
6	A	302	ASP
6	A	306	LEU
6	A	340	SER
6	A	341	CYS
6	A	348	MET
6	A	352	LEU
6	A	379	SER
6	A	462	ASN
7	B	84	ASN
7	B	107	TYR
7	B	118	TYR
7	B	122	SER
7	B	141	ASP
7	B	144	ASN
7	B	164	GLU

Continued on next page...

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Mol	Chain	Res	Type
7	B	217	LEU
7	B	240	CYS
7	B	256	THR
7	B	260	GLU
7	B	315	VAL
7	B	331	LYS
7	B	367	THR
7	B	440	SER
8	C	104	CYS
8	C	139	THR
8	C	149	CYS
8	C	166	MET
8	C	304	LYS
8	C	312	LYS
8	C	329	SER
8	C	359	SER
8	C	378	GLN
8	C	383	CYS
9	E	84	LYS
9	E	132	ASN
9	E	165	PHE
9	E	182	ASN
9	E	227	SER
9	E	325	ASP
10	F	51	ILE
10	F	92	HIS
10	F	171	VAL
10	F	219	GLU
11	H	41	LEU
11	H	113	THR
11	H	116	ARG
11	H	148	ILE
11	H	162	VAL
12	I	157	TYR
12	I	278	TYR
12	I	293	GLN
12	I	324	ASN
12	I	469	MET
12	I	502	SER
12	I	511	ILE
12	I	587	LYS
12	I	597	ASN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
12	I	666	ASP
13	J	68	CYS
13	J	84	ILE
14	L	17	ASP
14	L	24	SER
14	L	31	LEU
14	L	34	LEU
14	L	88	TRP
14	L	103	LEU
15	M	241	SER

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (18) such sidechains are listed below:

Mol	Chain	Res	Type
1	D	136	GLN
1	D	390	GLN
2	G	168	ASN
7	B	321	ASN
8	C	106	GLN
8	C	180	HIS
8	C	378	GLN
9	E	74	ASN
10	F	111	GLN
10	F	224	GLN
10	F	284	ASN
11	H	68	ASN
11	H	96	HIS
12	I	374	HIS
12	I	378	ASN
14	L	60	GLN
14	L	108	ASN
15	M	185	HIS

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 4 ligands modelled in this entry, 3 are monoatomic - leaving 1 for Mogul analysis.

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	$\# Z > 2$
16	IHP	B	501	-	36,36,36	0.67	1 (2%)	60,60,60	0.68	0

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
16	IHP	B	501	-	-	5/30/54/54	0/1/1/1

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
16	B	501	IHP	P3-O13	2.76	1.64	1.59

There are no bond angle outliers.

There are no chirality outliers.

All (5) torsion outliers are listed below:

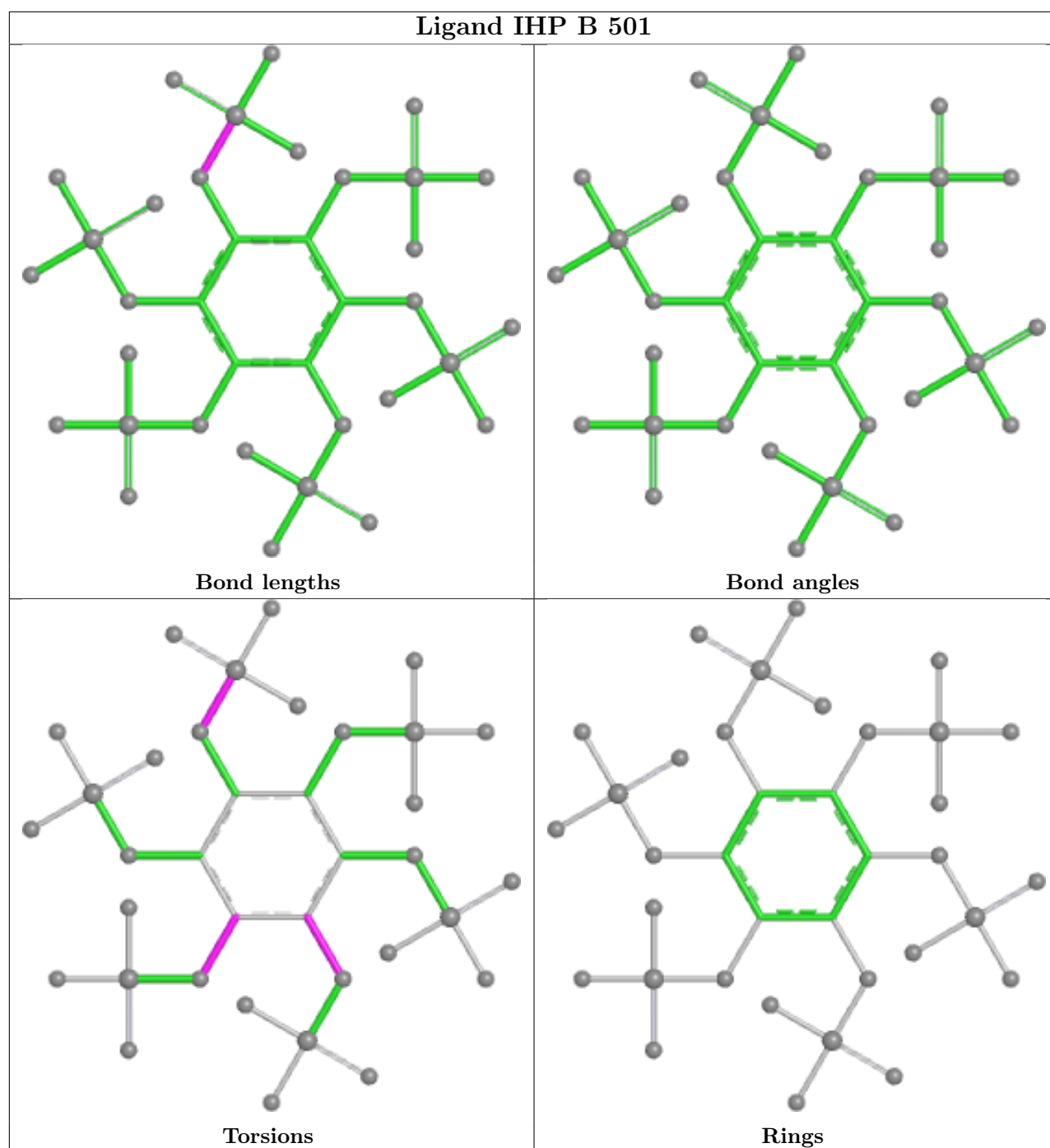
Mol	Chain	Res	Type	Atoms
16	B	501	IHP	C2-C1-O11-P1
16	B	501	IHP	C6-C1-O11-P1
16	B	501	IHP	C3-O13-P3-O23
16	B	501	IHP	C1-C6-O16-P6
16	B	501	IHP	C3-O13-P3-O43

There are no ring outliers.

1 monomer is involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
16	B	501	IHP	2	0

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

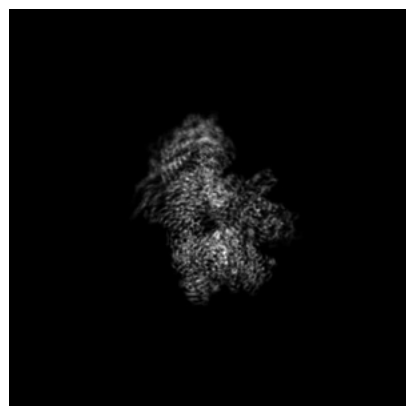
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-53252. These allow visual inspection of the internal detail of the map and identification of artifacts.

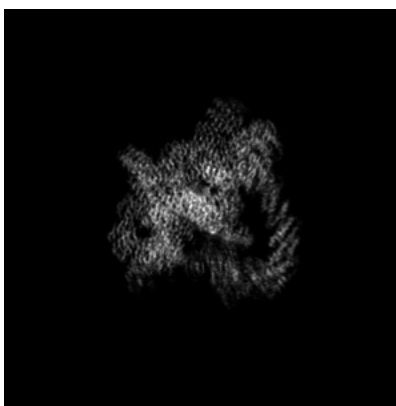
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

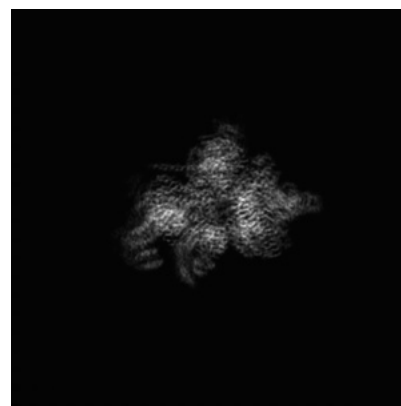
6.1.1 Primary map



X

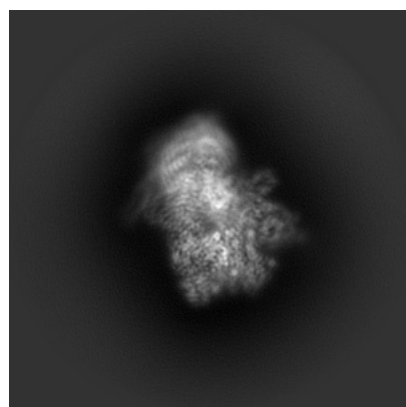


Y

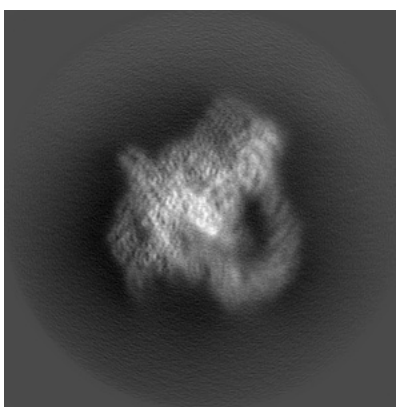


Z

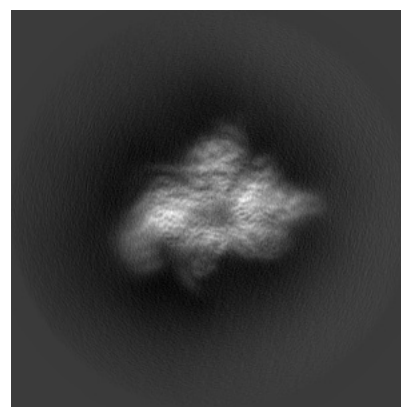
6.1.2 Raw map



X



Y



Z

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

6.2 Central slices [i](#)

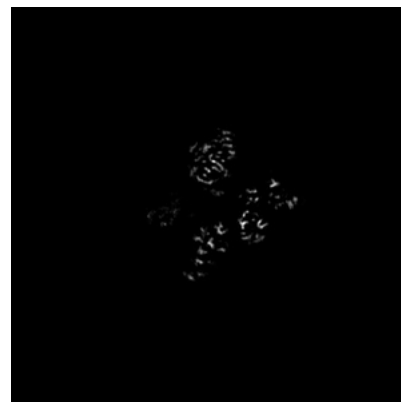
6.2.1 Primary map



X Index: 160

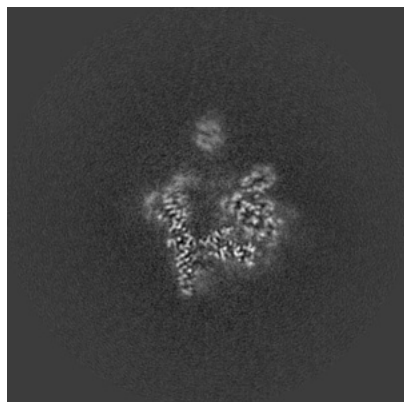


Y Index: 160

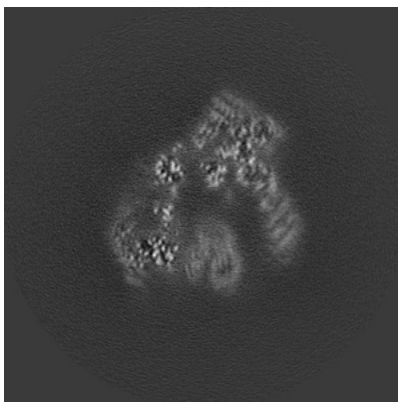


Z Index: 160

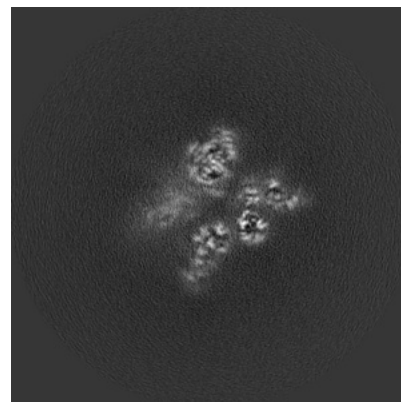
6.2.2 Raw map



X Index: 160



Y Index: 160



Z Index: 160

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: 184

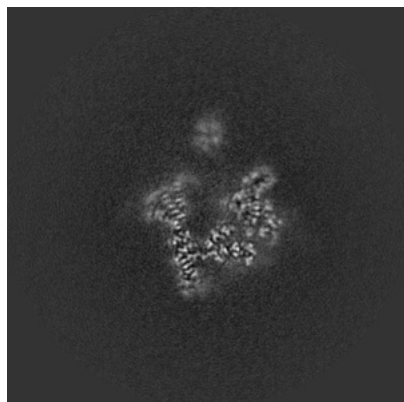


Y Index: 167

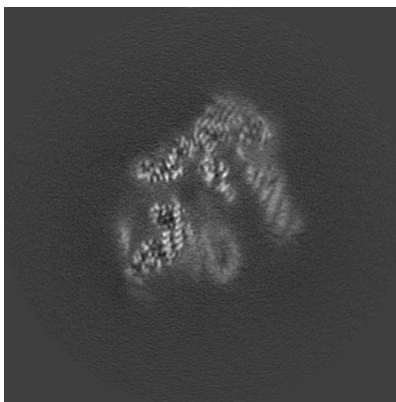


Z Index: 124

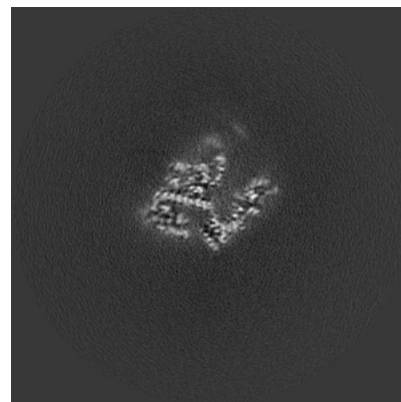
6.3.2 Raw map



X Index: 158



Y Index: 167

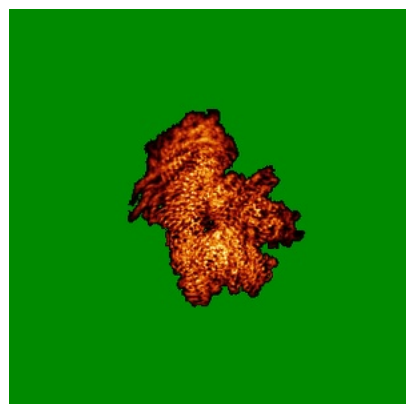


Z Index: 131

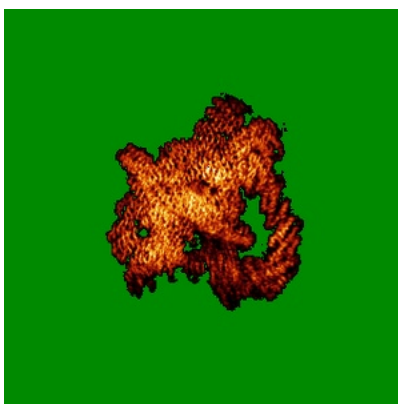
The images above show the largest variance slices of the map in three orthogonal directions.

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

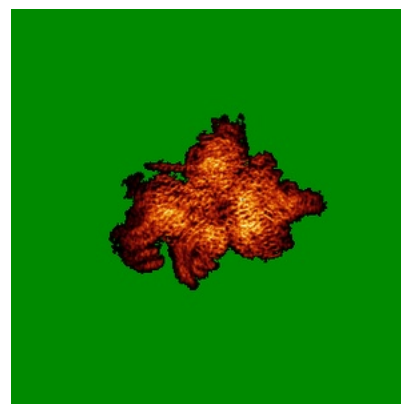
6.4.1 Primary map



X

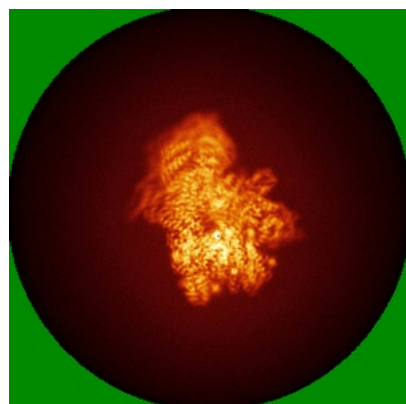


Y

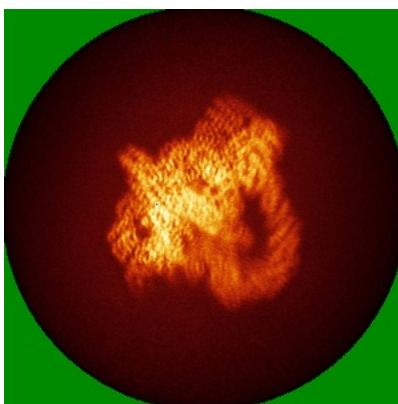


Z

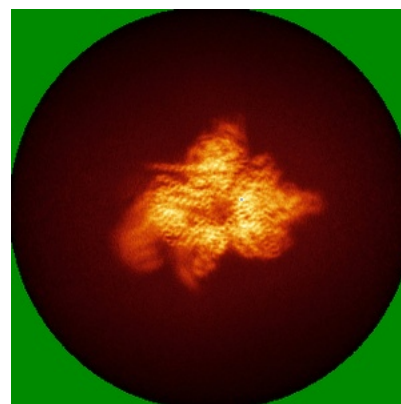
6.4.2 Raw map



X



Y

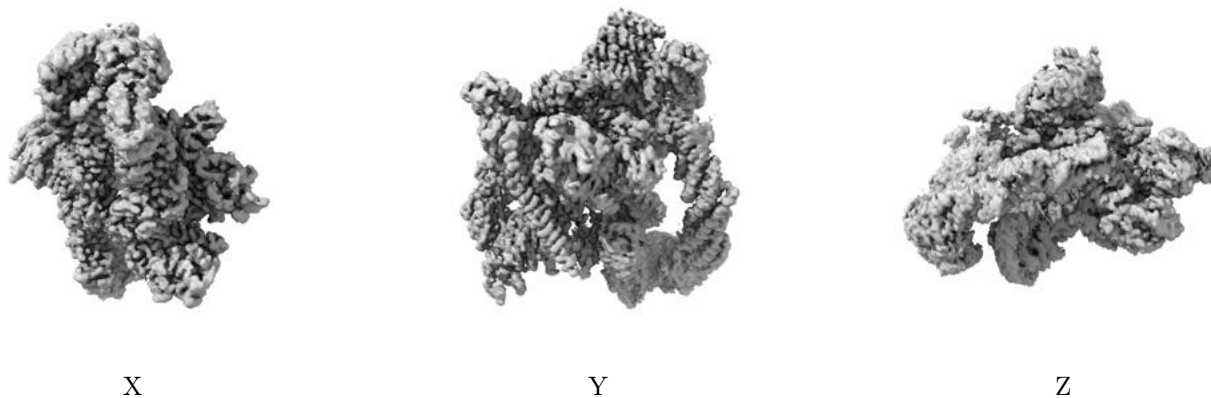


Z

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.

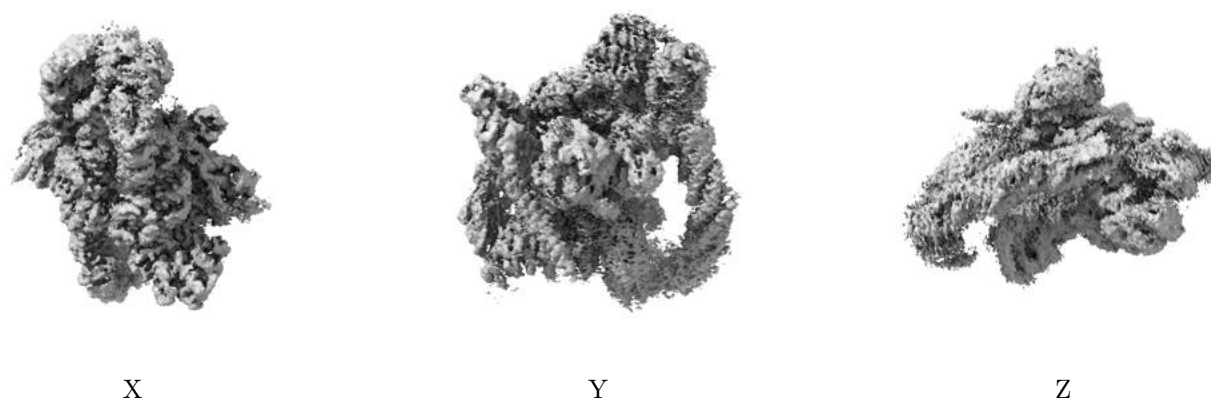
6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.0108. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

6.5.2 Raw map



These images show the 3D surface of the raw map. The raw map's contour level was selected so that its surface encloses the same volume as the primary map does at its recommended contour level.

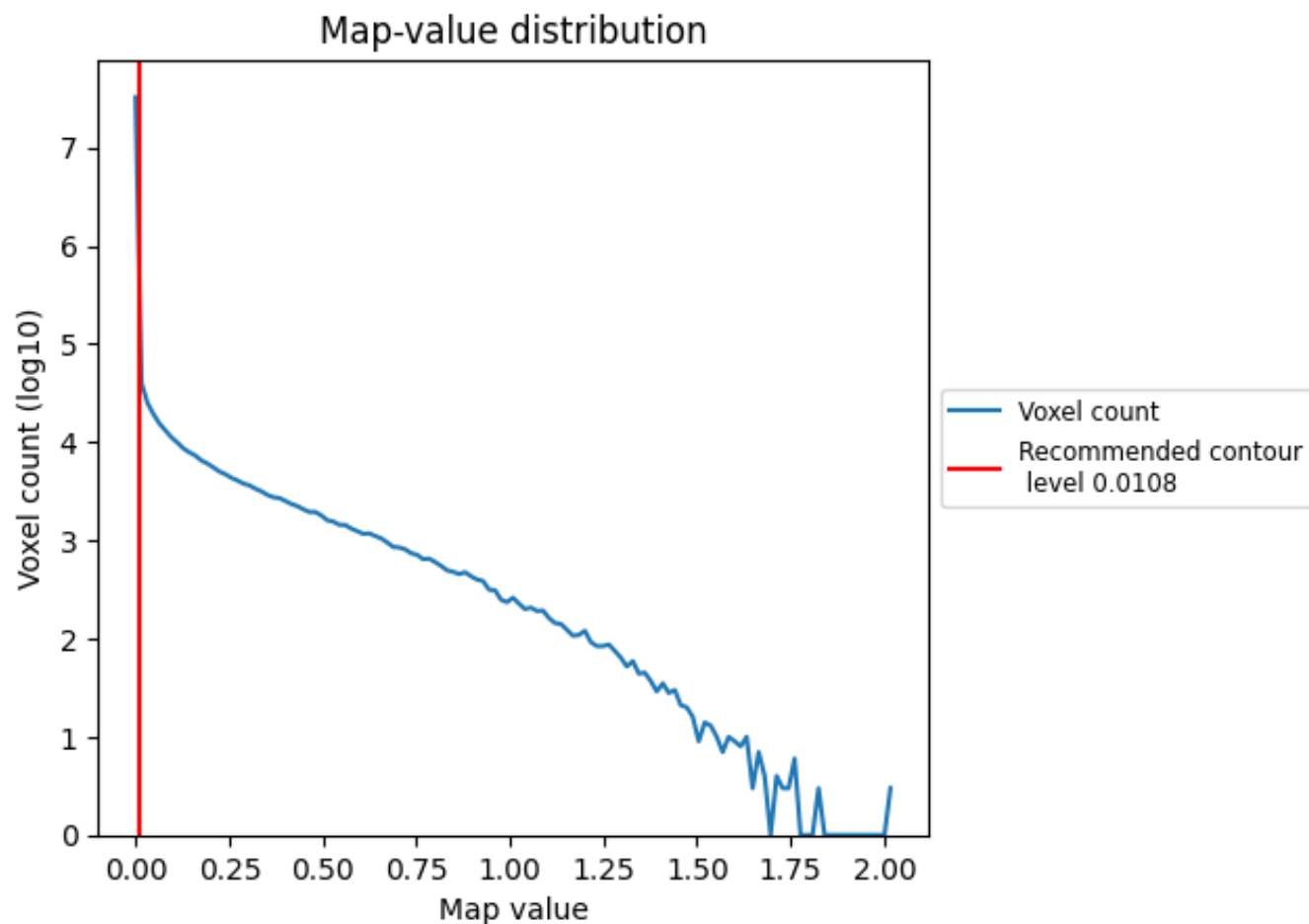
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

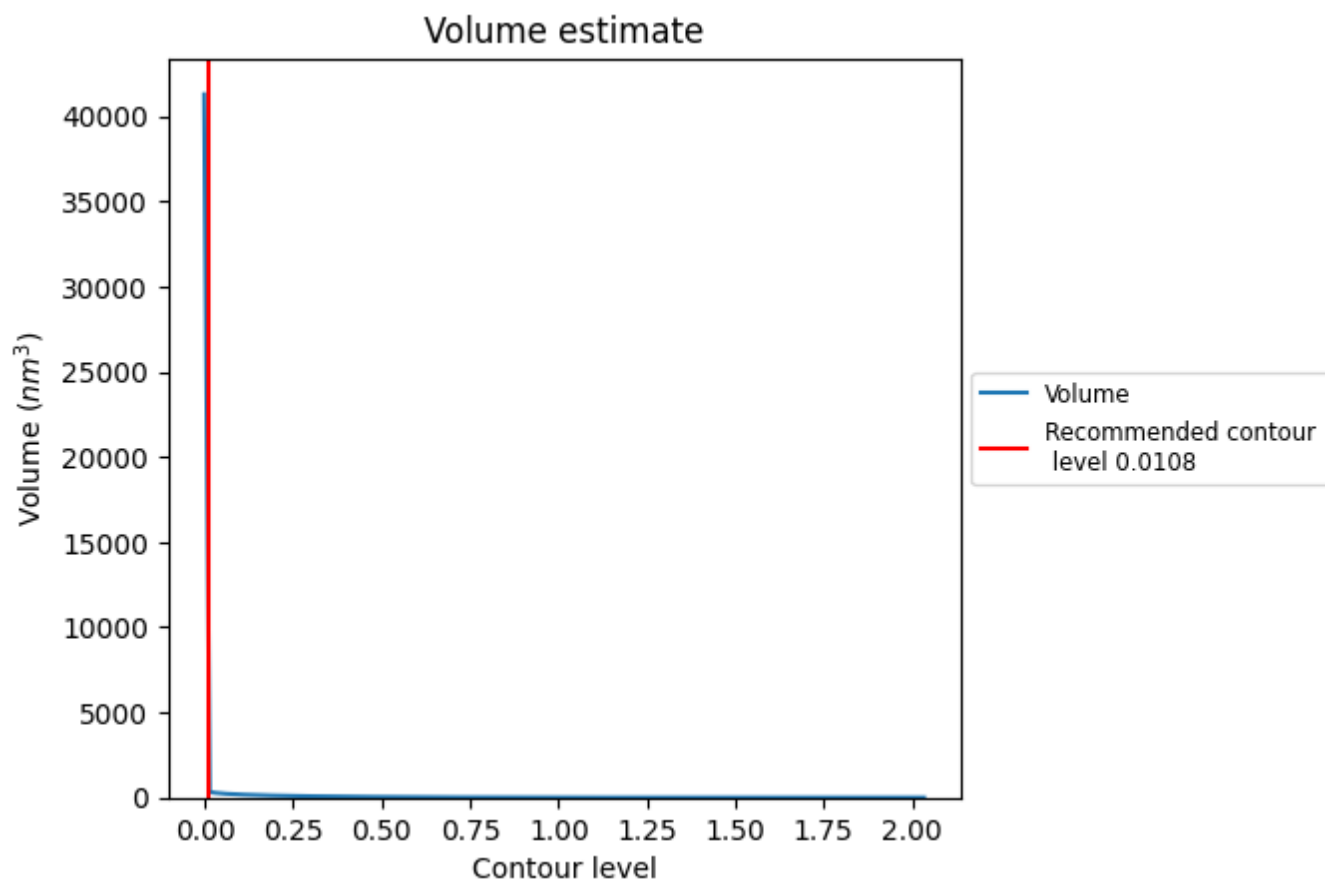
This section contains the results of statistical analysis of the map.

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.

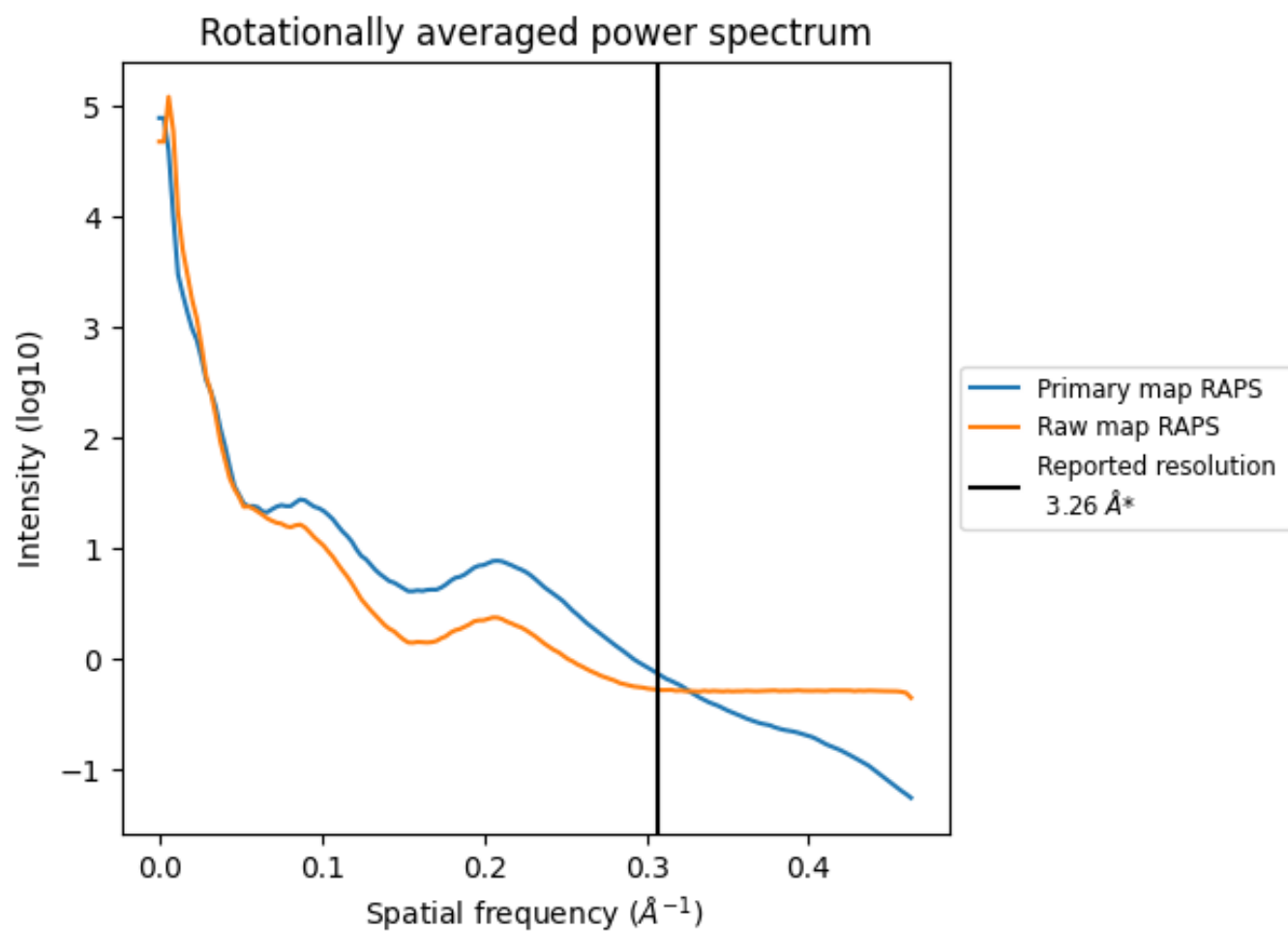
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 9063 nm³; this corresponds to an approximate mass of 8186 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 ⓘ

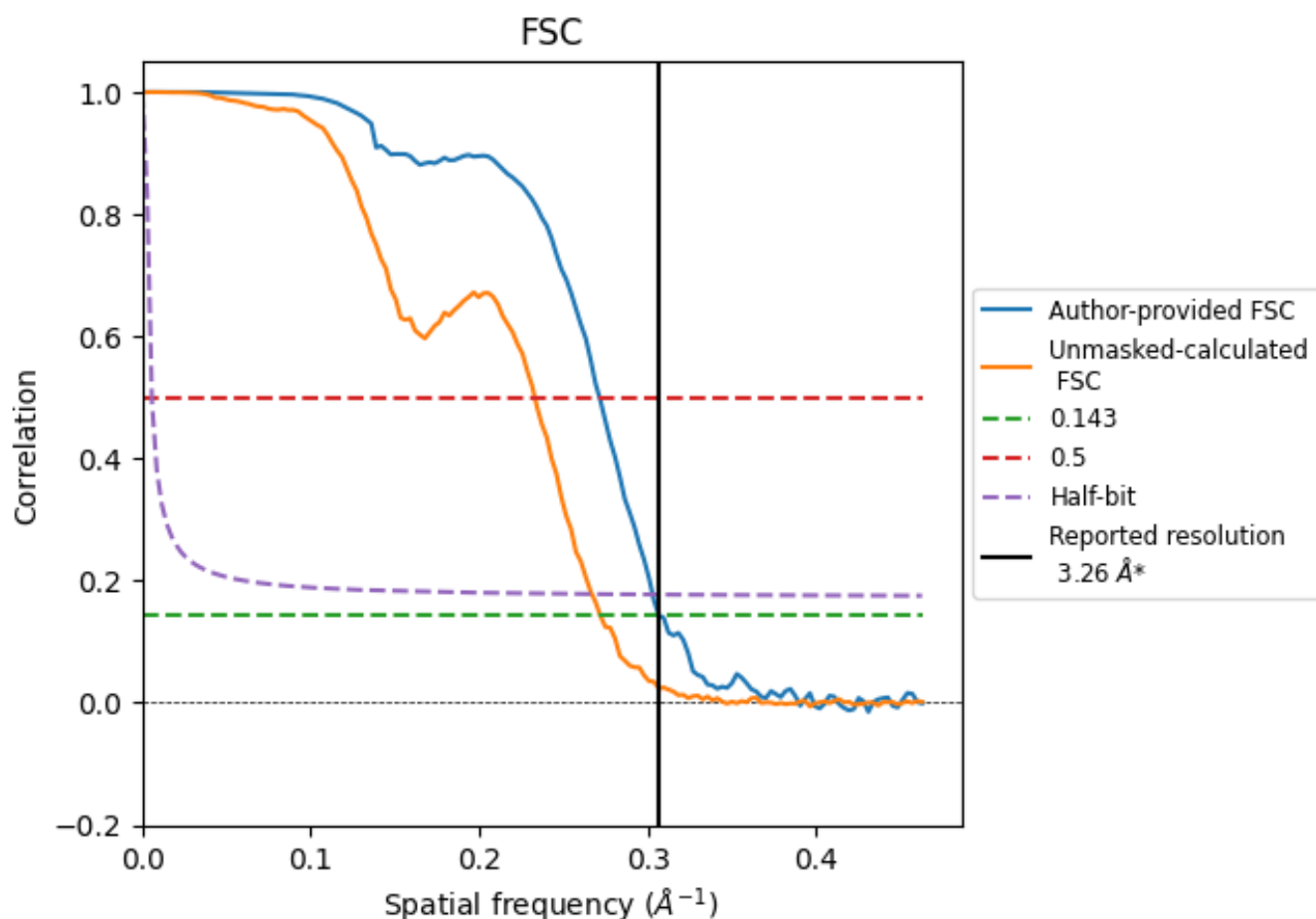


*Reported resolution corresponds to spatial frequency of 0.307 \AA^{-1}

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 0.307 Å⁻¹

8.2 Resolution estimates [i](#)

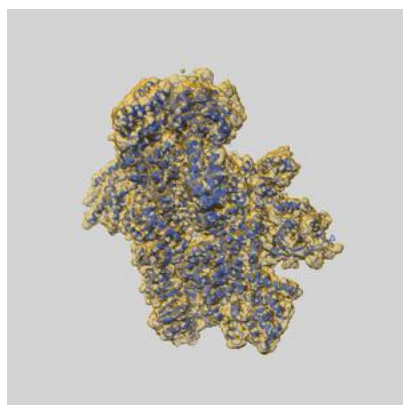
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.26	-	-
Author-provided FSC curve	3.26	3.68	3.30
Unmasked-calculated*	3.68	4.29	3.75

*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 3.68 differs from the reported value 3.26 by more than 10 %

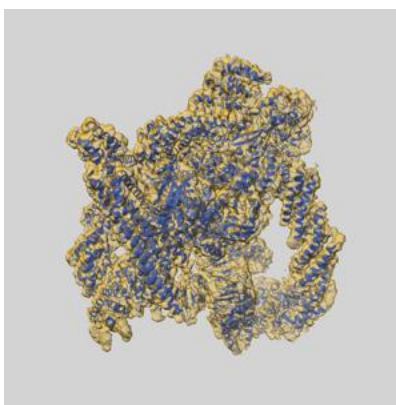
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-53252 and PDB model 9QO0. Per-residue inclusion information can be found in section 3 on page 7.

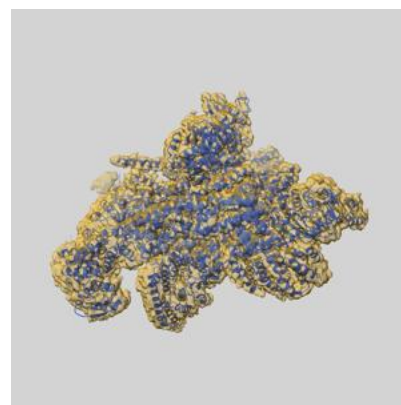
9.1 Map-model overlay [i](#)



X



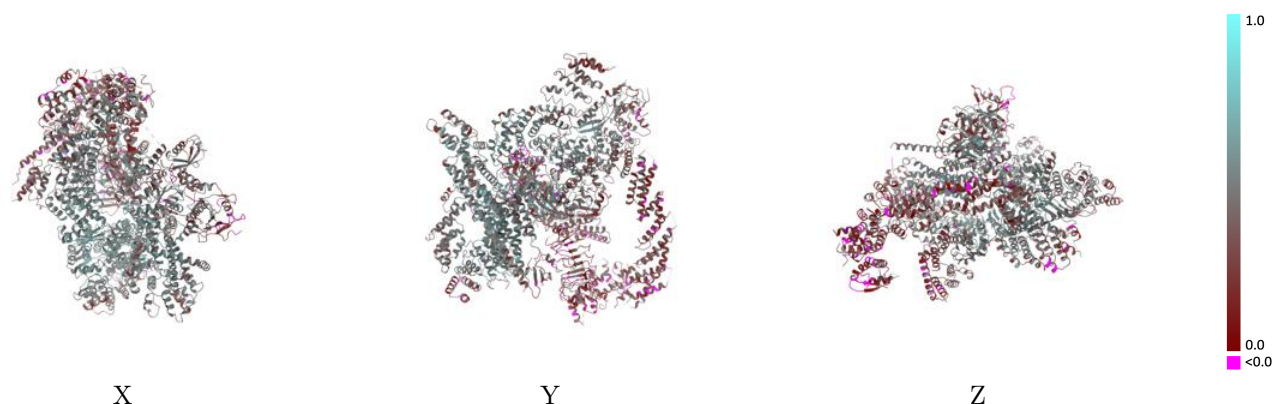
Y



Z

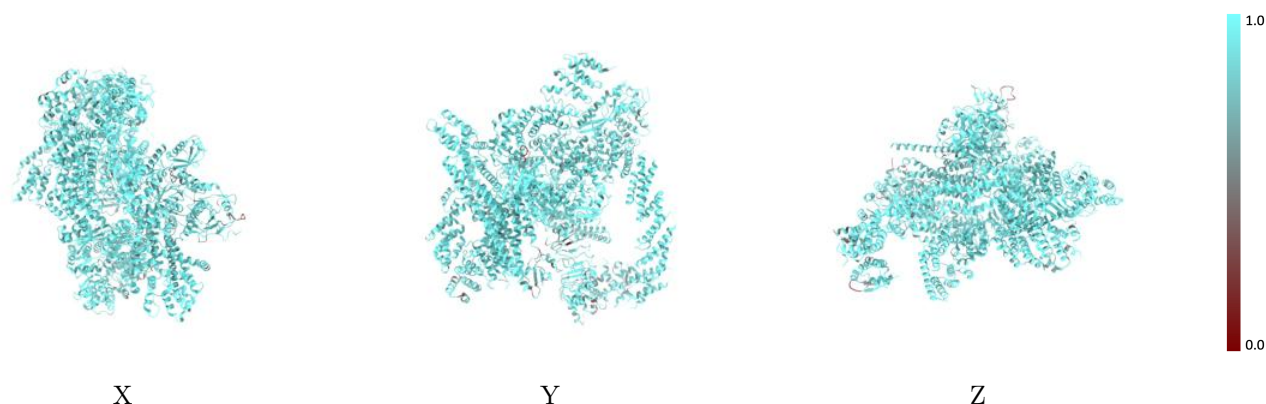
The images above show the 3D surface view of the map at the recommended contour level 0.0108 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



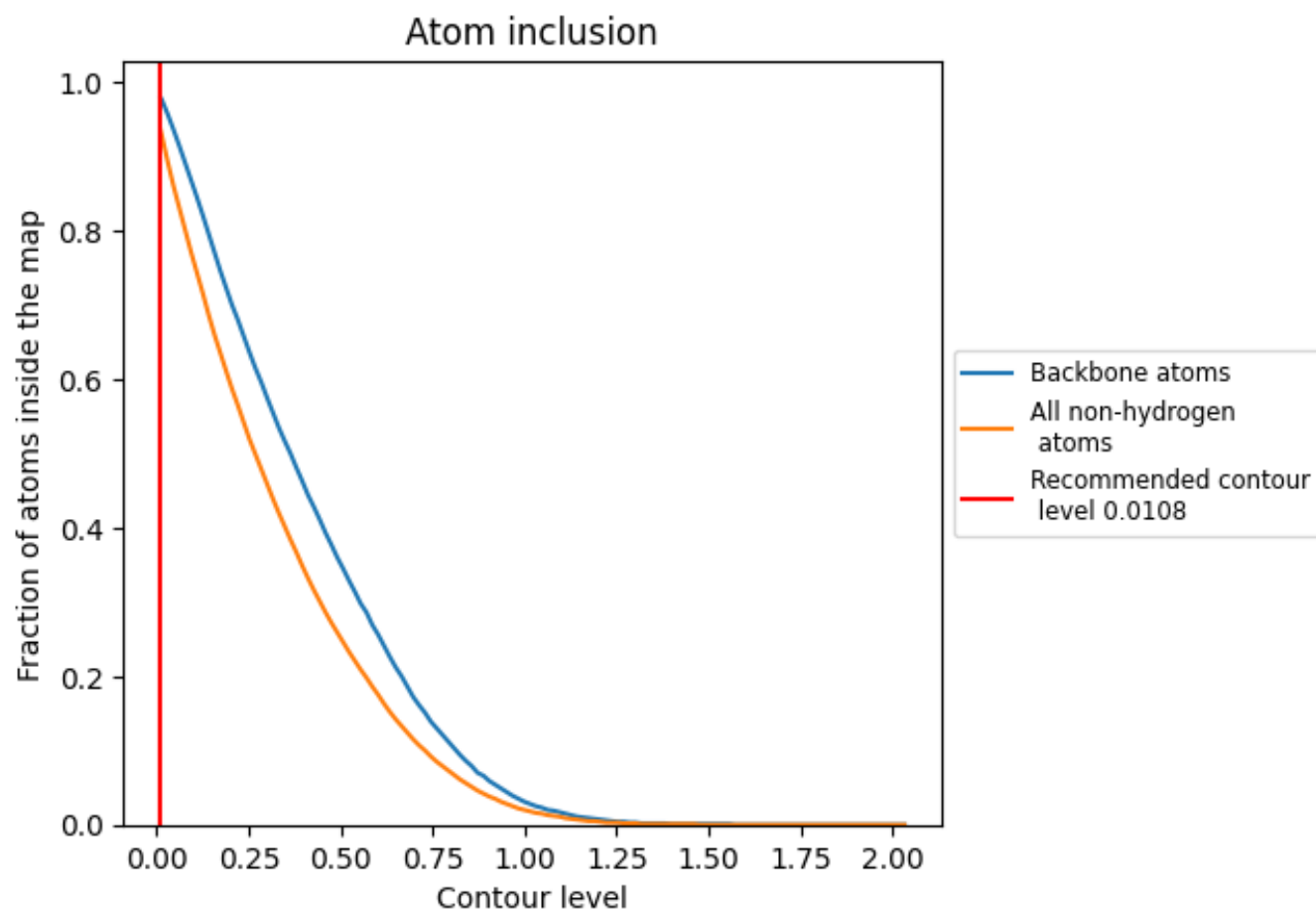
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.0108).

































9.4 Atom inclusion [i](#)



At the recommended contour level, 98% of all backbone atoms, 94% 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 (0.0108) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.9350	 0.4120
A	 0.9640	 0.4260
B	 0.9450	 0.4610
C	 0.9530	 0.4950
D	 0.9510	 0.4610
E	 0.9210	 0.4310
F	 0.9100	 0.4060
G	 0.9490	 0.4890
H	 0.9400	 0.4560
I	 0.9670	 0.3660
J	 0.9560	 0.4880
K	 0.9650	 0.4210
L	 0.8190	 0.1560
M	 0.8420	 0.2110
N	 0.8090	 0.2800
P	 0.9220	 0.4700

