



Full wwPDB EM Validation Report ⓘ

Mar 5, 2026 – 05:36 PM UTC

PDB ID : 9QO4 / pdb_00009qo4
EMDB ID : EMD-53256
Title : Dissociation-state-3 of 9-subunit CSN and SCF (SKP1-SKP2-CKS1) complex
Authors : Ding, S.; Clapperton, J.A.; Maeots, M.E.; Enchev, R.I.
Deposited on : 2025-03-25
Resolution : 2.95 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:

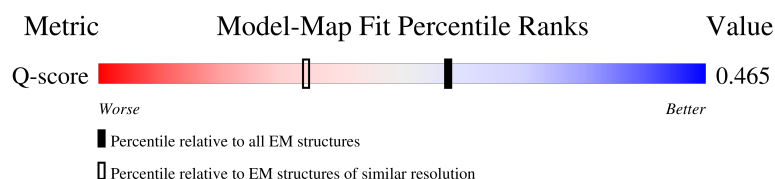
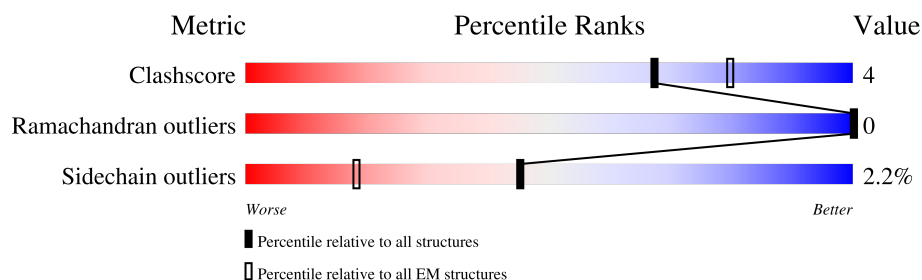
EMDB validation analysis : 0.0.1.dev132
Mogul : 2022.3.0, CSD as543be (2022)
MolProbity : 4-5-2 with Phenix2.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data 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 2.95 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.



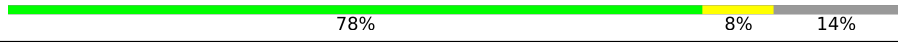
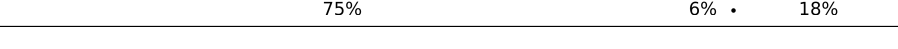
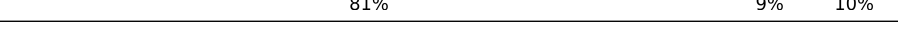
Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
Q-score	-	25397	13114 (2.45 - 3.45)

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

Mol	Chain	Length	Quality of chain
1	A	491	 76% 8% 16%
2	B	443	 79% 11% 10%
3	C	423	 87% 7% • 5%
4	D	406	 87% 6% 7%

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Mol	Chain	Length	Quality of chain
5	E	334	
6	F	327	
7	G	264	
8	H	209	
9	I	776	
10	J	108	
11	L	163	
12	M	424	
13	N	79	
14	P	57	

2 Entry composition [i](#)

There are 17 unique types of molecules in this entry. The entry contains 30681 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 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	414	Total	C	N	O	S	0	0
			3308	2090	576	620	22		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
2	B	398	Total	C	N	O	S	0	0
			3267	2082	559	611	15		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
3	C	400	Total	C	N	O	S	0	0
			3191	2032	536	596	27		

- Molecule 4 is a protein called COP9 signalosome complex subunit 4.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	D	379	Total	C	N	O	S	0	0
			3050	1929	528	579	14		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
5	E	300	Total	C	N	O	S	0	0
			2381	1522	395	450	14		

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
E	104	ALA	GLU	conflict	UNP Q92905

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

Mol	Chain	Residues	Atoms					AltConf	Trace
6	F	282	Total	C	N	O	S	0	0
			2244	1434	373	422	15		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
7	G	216	Total	C	N	O	S	0	0
			1705	1080	290	329	6		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
8	H	172	Total	C	N	O	S	0	0
			1374	880	239	251	4		

- Molecule 9 is a protein called Cullin-1.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	I	619	Total	C	N	O	S	0	0
			5049	3203	860	961	25		

- Molecule 10 is a protein called E3 ubiquitin-protein ligase RBX1.

Mol	Chain	Residues	Atoms					AltConf	Trace
10	J	85	Total	C	N	O	S	0	0
			701	443	128	121	9		

- Molecule 11 is a protein called S-phase kinase-associated protein 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
11	L	127	Total	C	N	O	S	0	0
			1021	651	167	198	5		

- Molecule 12 is a protein called S-phase kinase-associated protein 2.

Mol	Chain	Residues	Atoms					AltConf	Trace
12	M	324	Total	C	N	O	S	0	0
			2565	1630	442	477	16		

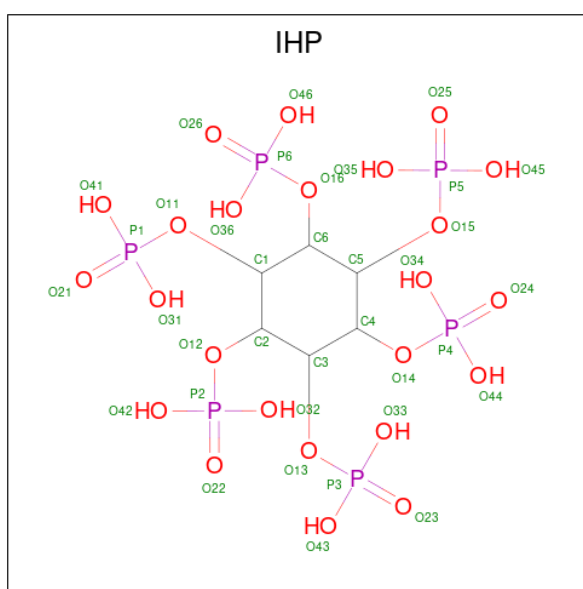
- Molecule 13 is a protein called Cyclin-dependent kinases regulatory subunit 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
13	N	71	Total	C	N	O	S	0	0
			614	398	105	108	3		

- Molecule 14 is a protein called COP9 signalosome complex subunit 9.

Mol	Chain	Residues	Atoms				AltConf	Trace
14	P	20	Total	C	N	O	0	0
			170	107	24	39		

- Molecule 15 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
15	B	1	Total	C	O	P	0
			36	6	24	6	

- Molecule 16 is ZINC ION (CCD ID: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		AltConf
16	E	1	Total	Zn	0
			1	1	
16	J	3	Total	Zn	0
			3	3	

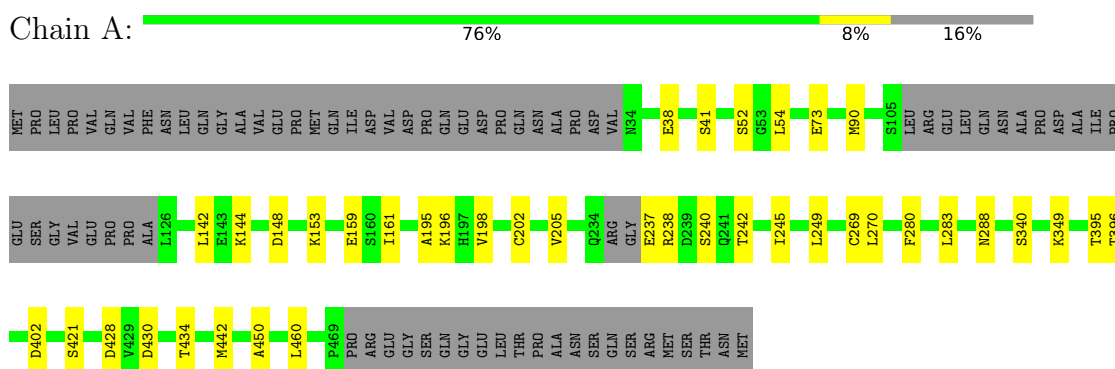
- Molecule 17 is water.

Mol	Chain	Residues	Atoms		AltConf
17	E	1	Total 1	O 1	0

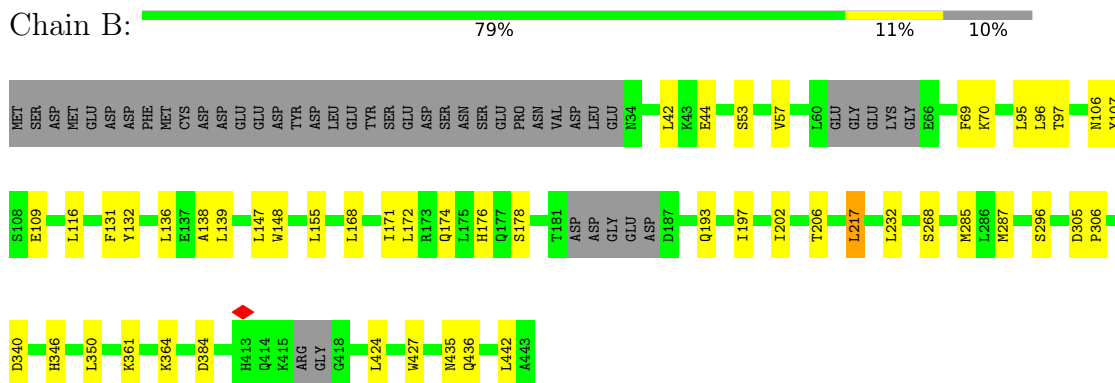
3 Residue-property plots

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion in map density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red diamond above a residue indicates a poor fit to the EM map for this residue (all-atom inclusion < 40%). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

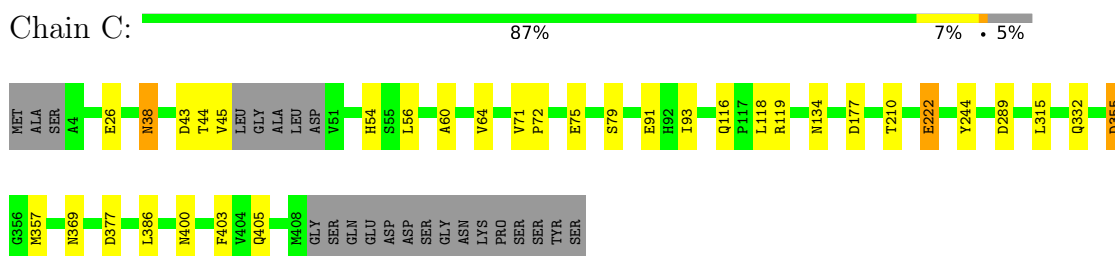
• Molecule 1: COP9 signalosome complex subunit 1



• Molecule 2: COP9 signalosome complex subunit 2

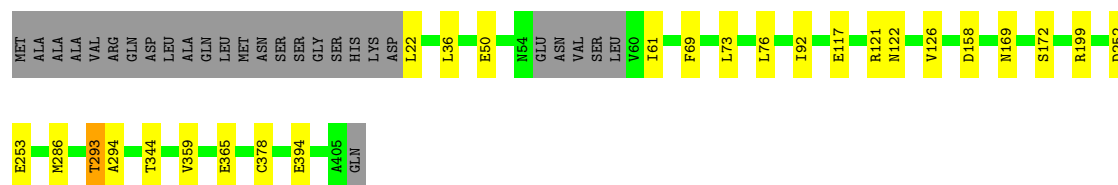


• Molecule 3: COP9 signalosome complex subunit 3



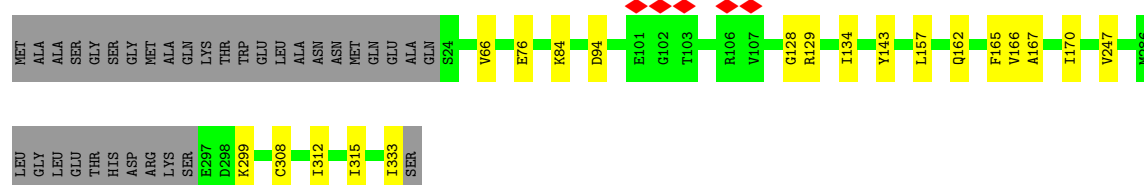
- Molecule 4: COP9 signalosome complex subunit 4

Chain D:  87% 6% 7%



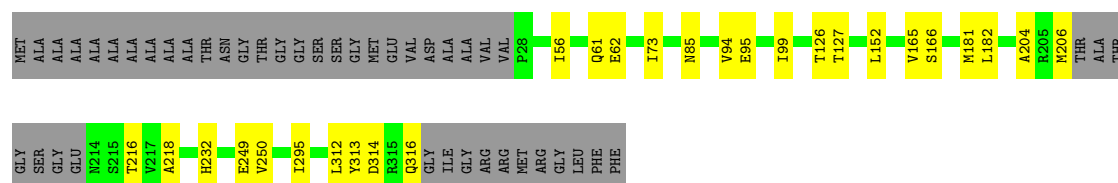
- Molecule 5: COP9 signalosome complex subunit 5

Chain E:  84% 6% 10%



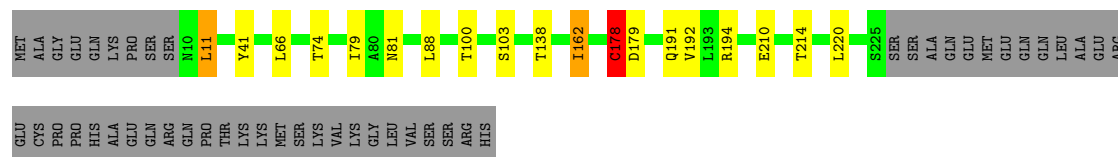
- Molecule 6: COP9 signalosome complex subunit 6

Chain F:  78% 8% 14%



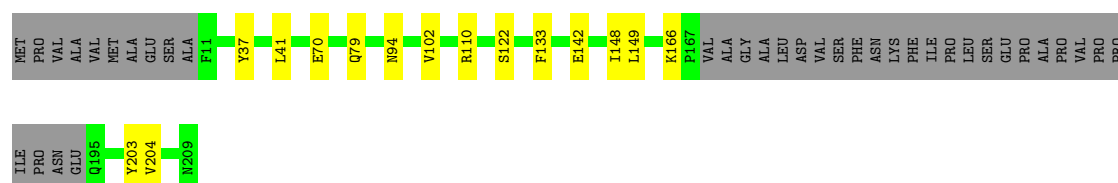
- Molecule 7: COP9 signalosome complex subunit 7b

Chain G:  75% 6% 18%

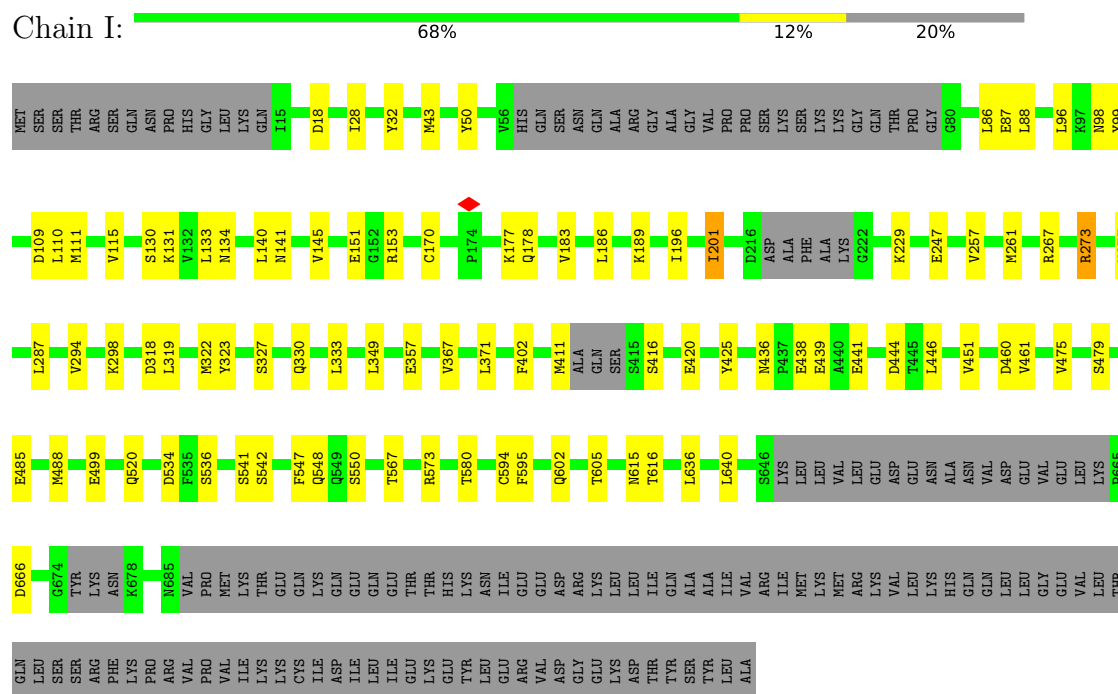


- Molecule 8: COP9 signalosome complex subunit 8

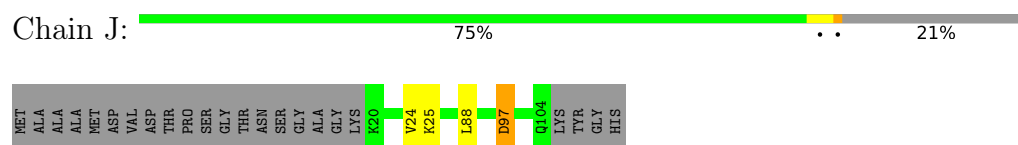
Chain H:  75% 7% 18%



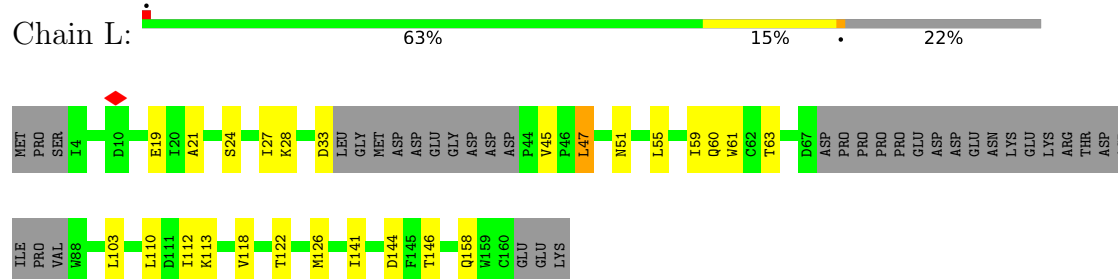
- Molecule 9: Cullin-1



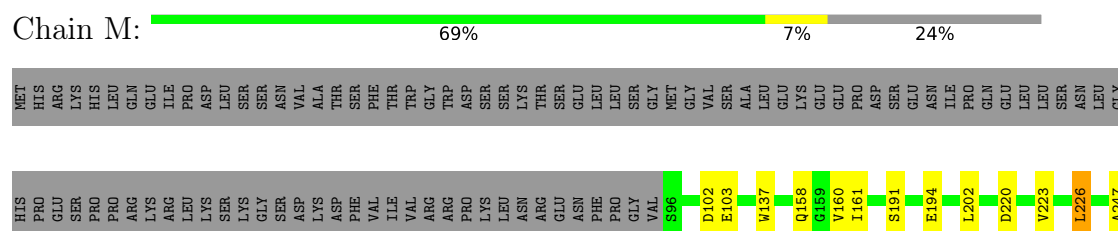
- Molecule 10: E3 ubiquitin-protein ligase RBX1



- Molecule 11: S-phase kinase-associated protein 1

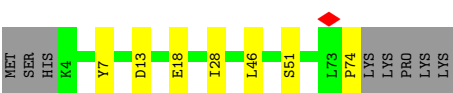
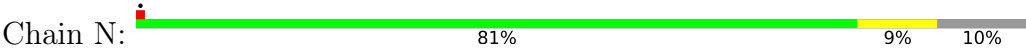


- Molecule 12: S-phase kinase-associated protein 2

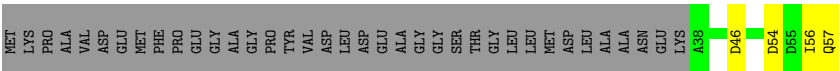




- Molecule 13: Cyclin-dependent kinases regulatory subunit 1



- Molecule 14: COP9 signalosome complex subunit 9



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	409455	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	1.775	Depositor
Minimum map value	-0.002	Depositor
Average map value	0.002	Depositor
Map value standard deviation	0.028	Depositor
Recommended contour level	0.00796	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

5.1 Standard geometry

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	A	0.18	0/3362	0.37	0/4531
2	B	0.16	0/3322	0.35	0/4467
3	C	0.16	0/3249	0.32	0/4385
4	D	0.15	0/3100	0.30	0/4187
5	E	0.17	0/2433	0.34	0/3287
6	F	0.33	0/2291	0.47	1/3104 (0.0%)
7	G	0.37	0/1725	0.58	2/2334 (0.1%)
8	H	0.16	0/1407	0.31	0/1912
9	I	0.19	0/5134	0.44	1/6911 (0.0%)
10	J	0.18	0/721	0.41	0/980
11	L	0.19	0/1036	0.49	0/1398
12	M	0.15	0/2615	0.31	0/3548
13	N	0.15	0/635	0.32	0/860
14	P	0.48	0/174	0.71	0/234
All	All	0.20	0/31204	0.39	4/42138 (0.0%)

There are no bond length outliers.

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	G	179	ASP	N-CA-C	-7.49	103.12	111.28
9	I	201	ILE	N-CA-C	-6.89	106.32	111.90
6	F	204	ALA	CA-C-O	-5.43	114.67	120.42
7	G	178	CYS	CB-CA-C	5.34	120.39	109.55

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts ⓘ

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3308	0	3335	23	0
2	B	3267	0	3323	29	0
3	C	3191	0	3212	25	0
4	D	3050	0	3054	16	0
5	E	2381	0	2357	14	0
6	F	2244	0	2234	18	0
7	G	1705	0	1745	9	0
8	H	1374	0	1360	9	0
9	I	5049	0	5028	63	0
10	J	701	0	654	3	0
11	L	1021	0	1023	20	0
12	M	2565	0	2596	14	0
13	N	614	0	594	6	0
14	P	170	0	131	4	0
15	B	36	0	6	2	0
16	E	1	0	0	0	0
16	J	3	0	0	0	0
17	E	1	0	0	0	0
All	All	30681	0	30652	235	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 4.

All (235) 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)
2:B:109:GLU:HG2	2:B:147:LEU:HD21	1.50	0.93
5:E:299:LYS:NZ	13:N:7:TYR:HE1	1.69	0.89
5:E:299:LYS:HZ2	13:N:7:TYR:HE1	0.90	0.89
9:I:602:GLN:OE1	9:I:602:GLN:N	2.13	0.81
6:F:249:GLU:N	6:F:249:GLU:OE2	2.16	0.79
5:E:299:LYS:NZ	13:N:7:TYR:CE1	2.45	0.79
9:I:499:GLU:OE1	9:I:499:GLU:N	2.16	0.77
11:L:158:GLN:NE2	11:L:158:GLN:O	2.20	0.73
1:A:159:GLU:N	1:A:159:GLU:OE2	2.23	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
15:B:501:IHP:O36	15:B:501:IHP:O31	2.07	0.71
9:I:441:GLU:N	9:I:441:GLU:OE1	2.23	0.70
14:P:56:ILE:O	14:P:57:GLN:OXT	2.09	0.70
1:A:38:GLU:N	1:A:38:GLU:OE2	2.25	0.70
12:M:298:GLN:N	12:M:298:GLN:OE1	2.26	0.68
9:I:322:MET:N	9:I:322:MET:HE2	2.09	0.68
6:F:62:GLU:N	6:F:62:GLU:OE2	2.27	0.67
9:I:460:ASP:OD1	9:I:461:VAL:N	2.27	0.67
9:I:261:MET:HE2	9:I:261:MET:H	1.59	0.67
1:A:144:LYS:NZ	1:A:148:ASP:OD2	2.28	0.67
4:D:199:ARG:NH2	10:J:88:LEU:O	2.26	0.67
2:B:109:GLU:HG2	2:B:147:LEU:CD2	2.23	0.66
9:I:420:GLU:N	9:I:420:GLU:OE1	2.28	0.66
2:B:44:GLU:N	2:B:44:GLU:OE1	2.29	0.66
9:I:141:ASN:O	9:I:145:VAL:HG22	1.96	0.65
2:B:96:LEU:HD13	2:B:138:ALA:HB1	1.79	0.65
12:M:194:GLU:N	12:M:194:GLU:OE2	2.26	0.65
9:I:446:LEU:HD22	9:I:488:MET:HE3	1.77	0.65
3:C:222:GLU:N	3:C:222:GLU:OE2	2.30	0.65
6:F:95:GLU:OE2	6:F:95:GLU:N	2.29	0.65
3:C:403:PHE:HB2	6:F:312:LEU:HD12	1.78	0.65
3:C:400:ASN:HD22	6:F:312:LEU:HD11	1.63	0.64
9:I:438:GLU:N	9:I:438:GLU:OE1	2.30	0.64
3:C:60:ALA:O	3:C:64:VAL:HG23	1.96	0.64
12:M:220:ASP:OD1	12:M:247:ALA:HB2	1.98	0.64
2:B:364:LYS:NZ	4:D:344:THR:OG1	2.32	0.63
11:L:27:ILE:HD12	11:L:28:LYS:N	2.14	0.63
2:B:139:LEU:HD13	2:B:139:LEU:O	2.00	0.62
10:J:97:ASP:N	10:J:97:ASP:OD1	2.30	0.62
9:I:541:SER:OG	9:I:542:SER:N	2.33	0.62
9:I:475:VAL:HG21	9:I:547:PHE:HE2	1.65	0.61
14:P:56:ILE:O	14:P:57:GLN:C	2.43	0.61
4:D:252:ASP:OD2	4:D:253:GLU:N	2.34	0.60
9:I:87:GLU:OE1	9:I:87:GLU:N	2.33	0.60
9:I:98:ASN:OD1	9:I:99:TYR:N	2.34	0.60
9:I:439:GLU:N	9:I:439:GLU:OE1	2.35	0.60
1:A:442:MET:HE1	6:F:295:ILE:HG21	1.84	0.60
3:C:91:GLU:OE2	3:C:91:GLU:N	2.35	0.60
9:I:189:LYS:HE2	9:I:196:ILE:HG13	1.84	0.60
9:I:318:ASP:OD1	9:I:319:LEU:N	2.35	0.60
5:E:162:GLN:N	5:E:162:GLN:OE1	2.36	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:69:PHE:CD1	2:B:95:LEU:HD11	2.37	0.58
2:B:116:LEU:HD21	2:B:132:TYR:CE1	2.39	0.58
6:F:94:VAL:HG21	6:F:99:ILE:HD12	1.86	0.58
12:M:354:LEU:HD12	12:M:383:LEU:HD21	1.84	0.58
6:F:152:LEU:HD11	6:F:165:VAL:HG13	1.86	0.58
9:I:520:GLN:OE1	9:I:573:ARG:NH1	2.36	0.58
8:H:70:GLU:OE2	8:H:102:VAL:HG21	2.03	0.58
9:I:327:SER:HA	9:I:333:LEU:HD21	1.86	0.58
11:L:33:ASP:OD1	11:L:33:ASP:N	2.34	0.58
8:H:94:ASN:OD1	8:H:110:ARG:NH2	2.38	0.57
5:E:94:ASP:OD2	5:E:129:ARG:NH2	2.37	0.57
9:I:294:VAL:HG23	9:I:298:LYS:NZ	2.21	0.56
1:A:283:LEU:HD22	1:A:288:ASN:CG	2.31	0.56
3:C:116:GLN:OE1	3:C:119:ARG:NH1	2.39	0.56
4:D:121:ARG:NH2	4:D:158:ASP:OD2	2.39	0.56
1:A:196:LYS:HE2	1:A:196:LYS:H	1.71	0.56
3:C:44:THR:O	3:C:45:VAL:HG22	2.04	0.56
9:I:479:SER:OG	9:I:485:GLU:OE2	2.23	0.56
11:L:59:ILE:HD12	11:L:60:GLN:N	2.21	0.55
2:B:171:ILE:HG23	2:B:172:LEU:HD22	1.87	0.55
9:I:548:GLN:OE1	9:I:550:SER:HB3	2.06	0.55
5:E:66:VAL:HG22	5:E:170:ILE:HD11	1.89	0.55
11:L:45:VAL:HG13	11:L:47:LEU:HD13	1.88	0.55
4:D:50:GLU:OE2	4:D:50:GLU:N	2.40	0.55
2:B:435:ASN:OD1	2:B:436:GLN:N	2.41	0.54
11:L:51:ASN:O	11:L:55:LEU:N	2.39	0.54
9:I:229:LYS:HE3	9:I:229:LYS:HA	1.90	0.54
3:C:405:GLN:OE1	7:G:220:LEU:HD11	2.07	0.54
3:C:45:VAL:HB	3:C:54:HIS:CE1	2.43	0.53
11:L:118:VAL:O	11:L:122:THR:HG23	2.08	0.53
9:I:189:LYS:HG2	9:I:196:ILE:HG13	1.90	0.53
2:B:116:LEU:HD21	2:B:132:TYR:CZ	2.43	0.53
1:A:195:ALA:HA	1:A:198:VAL:HG22	1.90	0.53
12:M:370:ILE:HD12	12:M:371:VAL:HG13	1.89	0.53
2:B:232:LEU:HD13	2:B:268:SER:OG	2.08	0.53
12:M:313:VAL:HG13	12:M:314:HIS:ND1	2.23	0.53
9:I:111:MET:HE3	9:I:111:MET:HA	1.91	0.53
9:I:151:GLU:OE2	9:I:153:ARG:NH2	2.42	0.52
9:I:460:ASP:OD1	9:I:461:VAL:HG13	2.10	0.52
6:F:232:HIS:ND1	7:G:178:CYS:SG	2.72	0.52
7:G:162:ILE:HD12	7:G:162:ILE:O	2.10	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:96:LEU:HD12	2:B:97:THR:N	2.25	0.52
12:M:286:THR:O	12:M:313:VAL:HG12	2.10	0.51
9:I:488:MET:HE2	9:I:488:MET:HA	1.91	0.51
3:C:210:THR:HG21	3:C:244:TYR:HE1	1.75	0.51
3:C:38:ASN:OD1	3:C:38:ASN:N	2.43	0.51
9:I:330:GLN:N	9:I:330:GLN:OE1	2.44	0.51
2:B:193:GLN:O	2:B:197:ILE:HG23	2.10	0.51
7:G:41:TYR:OH	7:G:138:THR:HG21	2.11	0.51
13:N:18:GLU:HG3	13:N:74:PRO:HG2	1.93	0.50
9:I:186:LEU:HD11	9:I:196:ILE:HG12	1.92	0.50
9:I:273:ARG:O	9:I:277:VAL:HG23	2.12	0.50
2:B:176:HIS:CE1	2:B:197:ILE:HD12	2.47	0.50
11:L:59:ILE:O	11:L:63:THR:HG23	2.12	0.50
1:A:430:ASP:OD1	1:A:430:ASP:N	2.40	0.50
5:E:84:LYS:HA	5:E:134:ILE:HD12	1.94	0.49
13:N:18:GLU:CG	13:N:74:PRO:HG2	2.42	0.49
4:D:378:CYS:HB3	5:E:247:VAL:HG22	1.95	0.49
3:C:210:THR:HG21	3:C:244:TYR:CE1	2.47	0.49
4:D:293:THR:HG22	4:D:294:ALA:H	1.76	0.49
9:I:43:MET:HE2	9:I:43:MET:O	2.13	0.49
3:C:45:VAL:HB	3:C:54:HIS:HE1	1.77	0.49
4:D:122:ASN:O	4:D:126:VAL:HG23	2.12	0.49
3:C:355:ASP:OD1	3:C:355:ASP:N	2.43	0.49
13:N:28:ILE:HG23	13:N:46:LEU:HD22	1.94	0.48
9:I:580:THR:O	9:I:580:THR:OG1	2.30	0.48
9:I:130:SER:O	9:I:134:ASN:ND2	2.46	0.48
3:C:43:ASP:OD2	3:C:43:ASP:N	2.46	0.48
8:H:142:GLU:OE1	8:H:142:GLU:N	2.47	0.48
2:B:285:MET:HE1	2:B:350:LEU:HD11	1.96	0.47
2:B:168:LEU:HA	2:B:172:LEU:HD23	1.95	0.47
4:D:365:GLU:OE1	4:D:365:GLU:N	2.46	0.47
6:F:181:MET:C	6:F:182:LEU:HD12	2.40	0.47
11:L:144:ASP:HB3	11:L:146:THR:HG23	1.97	0.47
12:M:223:VAL:HB	12:M:247:ALA:HB1	1.97	0.47
1:A:460:LEU:HD13	6:F:316:GLN:HB3	1.96	0.47
4:D:69:PHE:CZ	4:D:73:LEU:HD21	2.49	0.47
3:C:26:GLU:OE2	3:C:26:GLU:N	2.42	0.47
9:I:323:TYR:CE1	9:I:333:LEU:HD22	2.49	0.47
11:L:126:MET:SD	11:L:126:MET:N	2.87	0.47
6:F:126:THR:OG1	6:F:127:THR:N	2.48	0.47
11:L:126:MET:HA	11:L:126:MET:HE3	1.96	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:L:141:ILE:HG22	11:L:141:ILE:O	2.14	0.47
5:E:128:GLY:O	6:F:61:GLN:NE2	2.48	0.46
8:H:79:GLN:HG3	14:P:56:ILE:HG13	1.98	0.46
9:I:436:ASN:OD1	9:I:436:ASN:N	2.47	0.46
11:L:27:ILE:HD12	11:L:28:LYS:H	1.80	0.46
4:D:394:GLU:OE2	4:D:394:GLU:N	2.38	0.46
2:B:53:SER:O	2:B:57:VAL:HG23	2.15	0.46
2:B:106:ASN:OD1	2:B:107:TYR:N	2.49	0.46
5:E:76:GLU:OE1	5:E:143:TYR:OH	2.34	0.46
9:I:186:LEU:CD1	9:I:196:ILE:HG12	2.46	0.46
1:A:450:ALA:HB1	3:C:386:LEU:HD21	1.98	0.46
2:B:340:ASP:OD1	2:B:340:ASP:N	2.47	0.46
6:F:152:LEU:HD12	6:F:166:SER:O	2.16	0.46
9:I:444:ASP:OD1	9:I:444:ASP:N	2.49	0.45
3:C:75:GLU:OE2	3:C:79:SER:OG	2.33	0.45
4:D:92:ILE:N	4:D:92:ILE:HD12	2.31	0.45
9:I:261:MET:HE2	9:I:261:MET:N	2.29	0.45
2:B:70:LYS:HZ1	15:B:501:IHP:P6	2.39	0.45
9:I:367:VAL:HG11	9:I:425:TYR:CD2	2.51	0.45
3:C:93:ILE:C	3:C:93:ILE:HD12	2.41	0.45
5:E:66:VAL:HG22	5:E:170:ILE:CD1	2.46	0.45
9:I:18:ASP:N	9:I:18:ASP:OD1	2.49	0.45
5:E:315:ILE:HG21	8:H:204:VAL:HG23	1.98	0.45
9:I:131:LYS:HD3	9:I:131:LYS:C	2.42	0.45
1:A:196:LYS:HE2	1:A:196:LYS:N	2.32	0.45
3:C:377:ASP:OD1	8:H:203:TYR:OH	2.35	0.45
9:I:186:LEU:HD13	9:I:186:LEU:O	2.16	0.45
9:I:287:LEU:HD13	9:I:287:LEU:C	2.42	0.44
11:L:110:LEU:HD13	11:L:112:ILE:HD11	1.98	0.44
1:A:395:THR:HG22	1:A:396:THR:O	2.18	0.44
9:I:666:ASP:OD1	9:I:666:ASP:N	2.50	0.44
11:L:19:GLU:OE2	11:L:19:GLU:HA	2.17	0.44
11:L:24:SER:HB2	11:L:27:ILE:HD11	2.00	0.44
4:D:169:ASN:O	4:D:172:SER:OG	2.22	0.44
7:G:11:LEU:HD13	7:G:11:LEU:O	2.18	0.44
9:I:294:VAL:HG23	9:I:298:LYS:HZ1	1.83	0.43
12:M:202:LEU:HD23	12:M:226:LEU:CD1	2.48	0.43
1:A:402:ASP:OD2	1:A:402:ASP:N	2.50	0.43
2:B:139:LEU:HD12	2:B:148:TRP:HB2	1.99	0.43
9:I:111:MET:O	9:I:115:VAL:HG23	2.18	0.43
1:A:202:CYS:HA	1:A:205:VAL:HG12	1.99	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:H:122:SER:OG	8:H:166:LYS:O	2.35	0.43
9:I:615:ASN:OD1	9:I:616:THR:N	2.51	0.43
12:M:102:ASP:OD1	12:M:103:GLU:N	2.52	0.43
1:A:142:LEU:HD12	1:A:142:LEU:O	2.18	0.43
1:A:153:LYS:HA	1:A:161:ILE:HD11	2.01	0.43
9:I:416:SER:O	9:I:416:SER:OG	2.34	0.43
12:M:367:VAL:HG23	12:M:367:VAL:O	2.19	0.43
6:F:218:ALA:HB2	7:G:192:VAL:HG13	2.00	0.43
9:I:109:ASP:OD1	9:I:109:ASP:N	2.52	0.43
9:I:247:GLU:OE2	9:I:267:ARG:NH2	2.51	0.43
9:I:257:VAL:HG23	9:I:261:MET:HE1	2.01	0.43
2:B:384:ASP:OD2	2:B:384:ASP:N	2.51	0.43
7:G:74:THR:CG2	7:G:100:THR:HG23	2.49	0.43
3:C:369:ASN:OD1	3:C:369:ASN:N	2.52	0.42
9:I:88:LEU:HD23	9:I:140:LEU:HD12	2.01	0.42
12:M:271:GLU:O	12:M:275:GLN:HG3	2.19	0.42
1:A:238:ARG:O	1:A:240:SER:N	2.52	0.42
9:I:594:CYS:SG	9:I:595:PHE:N	2.88	0.42
4:D:22:LEU:HD11	4:D:61:ILE:HG21	2.00	0.42
9:I:110:LEU:O	9:I:178:GLN:NE2	2.53	0.42
11:L:21:ALA:HA	11:L:27:ILE:HD13	2.00	0.42
12:M:160:VAL:C	12:M:161:ILE:HD12	2.44	0.42
2:B:305:ASP:OD1	2:B:306:PRO:HD2	2.19	0.42
3:C:210:THR:HG22	3:C:210:THR:O	2.20	0.42
7:G:191:GLN:OE1	7:G:194:ARG:NH1	2.53	0.42
11:L:60:GLN:OE1	11:L:61:TRP:N	2.53	0.42
3:C:71:VAL:N	3:C:72:PRO:CD	2.83	0.42
5:E:166:VAL:HG12	5:E:167:ALA:N	2.34	0.42
9:I:534:ASP:N	10:J:25:LYS:O	2.47	0.42
9:I:183:VAL:HG12	9:I:201:ILE:CD1	2.50	0.41
9:I:50:TYR:C	9:I:50:TYR:CD2	2.98	0.41
11:L:103:LEU:HD13	11:L:103:LEU:C	2.45	0.41
4:D:36:LEU:O	4:D:36:LEU:HD12	2.20	0.41
9:I:86:LEU:HD13	9:I:86:LEU:C	2.44	0.41
14:P:46:ASP:OD1	14:P:46:ASP:N	2.49	0.41
3:C:134:ASN:N	3:C:134:ASN:OD1	2.52	0.41
1:A:52:SER:OG	1:A:280:PHE:O	2.33	0.41
2:B:424:LEU:HD23	2:B:427:TRP:HE1	1.86	0.41
2:B:132:TYR:CD1	2:B:155:LEU:HD13	2.55	0.41
9:I:636:LEU:HD13	9:I:640:LEU:HD22	2.03	0.41
8:H:148:ILE:HD12	8:H:149:LEU:N	2.36	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:I:357:GLU:OE1	9:I:357:GLU:HA	2.20	0.41
1:A:41:SER:O	1:A:41:SER:OG	2.33	0.41
1:A:73:GLU:C	1:A:73:GLU:OE2	2.64	0.41
2:B:42:LEU:HD22	2:B:53:SER:HB2	2.02	0.41
5:E:308:CYS:O	5:E:312:ILE:HG13	2.20	0.41
6:F:313:TYR:O	6:F:314:ASP:C	2.63	0.41
7:G:66:LEU:HD11	7:G:88:LEU:HD21	2.02	0.41
8:H:133:PHE:CE2	8:H:148:ILE:HG21	2.56	0.41
4:D:359:VAL:O	4:D:359:VAL:HG13	2.20	0.41
6:F:73:ILE:HD11	6:F:85:ASN:HB3	2.01	0.41
9:I:32:TYR:OH	9:I:96:LEU:HD21	2.21	0.41
11:L:112:ILE:HG22	11:L:113:LYS:N	2.36	0.41
12:M:137:TRP:NE1	12:M:158:GLN:OE1	2.54	0.41
1:A:269:CYS:SG	1:A:270:LEU:N	2.93	0.41
1:A:245:ILE:O	1:A:249:LEU:HG	2.21	0.40
3:C:177:ASP:OD1	3:C:177:ASP:C	2.64	0.40
9:I:189:LYS:CE	9:I:196:ILE:HG13	2.50	0.40
1:A:237:GLU:HA	1:A:242:THR:HG21	2.03	0.40
2:B:174:GLN:O	2:B:178:SER:OG	2.39	0.40
6:F:312:LEU:HD23	6:F:312:LEU:O	2.21	0.40
2:B:202:ILE:HD11	2:B:217:LEU:HD11	2.02	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all PDB entries followed by that with respect to all EM entries.

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	408/491 (83%)	380 (93%)	28 (7%)	0	100	100
2	B	390/443 (88%)	374 (96%)	16 (4%)	0	100	100
3	C	396/423 (94%)	378 (96%)	18 (4%)	0	100	100
4	D	375/406 (92%)	368 (98%)	7 (2%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
5	E	296/334 (89%)	279 (94%)	17 (6%)	0	100	100
6	F	278/327 (85%)	266 (96%)	12 (4%)	0	100	100
7	G	214/264 (81%)	205 (96%)	9 (4%)	0	100	100
8	H	168/209 (80%)	164 (98%)	4 (2%)	0	100	100
9	I	607/776 (78%)	576 (95%)	31 (5%)	0	100	100
10	J	83/108 (77%)	73 (88%)	10 (12%)	0	100	100
11	L	121/163 (74%)	108 (89%)	13 (11%)	0	100	100
12	M	322/424 (76%)	304 (94%)	18 (6%)	0	100	100
13	N	69/79 (87%)	68 (99%)	1 (1%)	0	100	100
14	P	18/57 (32%)	17 (94%)	1 (6%)	0	100	100
All	All	3745/4504 (83%)	3560 (95%)	185 (5%)	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	A	362/429 (84%)	355 (98%)	7 (2%)	50	71
2	B	364/405 (90%)	355 (98%)	9 (2%)	42	66
3	C	359/377 (95%)	350 (98%)	9 (2%)	42	66
4	D	325/347 (94%)	321 (99%)	4 (1%)	63	79
5	E	256/282 (91%)	253 (99%)	3 (1%)	63	79
6	F	252/276 (91%)	248 (98%)	4 (2%)	55	75
7	G	187/229 (82%)	179 (96%)	8 (4%)	26	52
8	H	143/173 (83%)	141 (99%)	2 (1%)	59	77
9	I	557/698 (80%)	544 (98%)	13 (2%)	44	67
10	J	75/90 (83%)	73 (97%)	2 (3%)	39	64
11	L	115/150 (77%)	114 (99%)	1 (1%)	70	83

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
12	M	300/392 (76%)	292 (97%)	8 (3%)	39	64
13	N	68/76 (90%)	66 (97%)	2 (3%)	37	61
14	P	18/45 (40%)	17 (94%)	1 (6%)	19	43
All	All	3381/3969 (85%)	3308 (98%)	73 (2%)	45	69

All (73) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	54	LEU
1	A	90	MET
1	A	340	SER
1	A	349	LYS
1	A	421	SER
1	A	428	ASP
1	A	434	THR
2	B	131	PHE
2	B	136	LEU
2	B	206	THR
2	B	217	LEU
2	B	287	MET
2	B	296	SER
2	B	346	HIS
2	B	361	LYS
2	B	442	LEU
3	C	38	ASN
3	C	56	LEU
3	C	118	LEU
3	C	222	GLU
3	C	289	ASP
3	C	315	LEU
3	C	332	GLN
3	C	355	ASP
3	C	357	MET
4	D	76	LEU
4	D	117	GLU
4	D	286	MET
4	D	293	THR
5	E	157	LEU
5	E	165	PHE
5	E	333	ILE
6	F	56	ILE

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Mol	Chain	Res	Type
6	F	206	MET
6	F	216	THR
6	F	250	VAL
7	G	11	LEU
7	G	79	ILE
7	G	81	ASN
7	G	103	SER
7	G	162	ILE
7	G	178	CYS
7	G	210	GLU
7	G	214	THR
8	H	37	TYR
8	H	41	LEU
9	I	28	ILE
9	I	133	LEU
9	I	170	CYS
9	I	177	LYS
9	I	273	ARG
9	I	349	LEU
9	I	371	LEU
9	I	402	PHE
9	I	411	MET
9	I	451	VAL
9	I	536	SER
9	I	567	THR
9	I	605	THR
10	J	24	VAL
10	J	97	ASP
11	L	47	LEU
12	M	191	SER
12	M	226	LEU
12	M	290	LEU
12	M	294	ARG
12	M	325	ASN
12	M	361	THR
12	M	394	THR
12	M	400	THR
13	N	13	ASP
13	N	51	SER
14	P	54	ASP

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (32) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	265	GLN
2	B	84	ASN
2	B	176	HIS
2	B	203	GLN
2	B	353	ASN
3	C	7	GLN
3	C	92	HIS
3	C	180	HIS
3	C	271	ASN
3	C	378	GLN
3	C	400	ASN
4	D	308	ASN
4	D	403	GLN
5	E	275	GLN
5	E	321	GLN
6	F	137	HIS
6	F	220	HIS
7	G	68	ASN
7	G	93	GLN
7	G	98	HIS
8	H	51	ASN
9	I	29	GLN
9	I	276	GLN
9	I	324	ASN
9	I	343	HIS
9	I	477	GLN
9	I	524	HIS
9	I	549	GLN
10	J	41	ASN
10	J	48	HIS
12	M	273	HIS
12	M	389	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates

There are no oligosaccharides in this entry.

5.6 Ligand geometry

Of 5 ligands modelled in this entry, 4 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
15	IHP	B	501	-	36,36,36	0.66	1 (2%)	60,60,60	0.67	3 (5%)

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
15	IHP	B	501	-	-	9/30/54/54	0/1/1/1

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
15	B	501	IHP	P3-O13	3.02	1.64	1.59

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
15	B	501	IHP	P2-O12-C2	2.54	130.21	123.43
15	B	501	IHP	P4-O14-C4	2.48	130.06	123.43
15	B	501	IHP	P6-O16-C6	2.13	129.12	123.43

There are no chirality outliers.

All (9) torsion outliers are listed below:

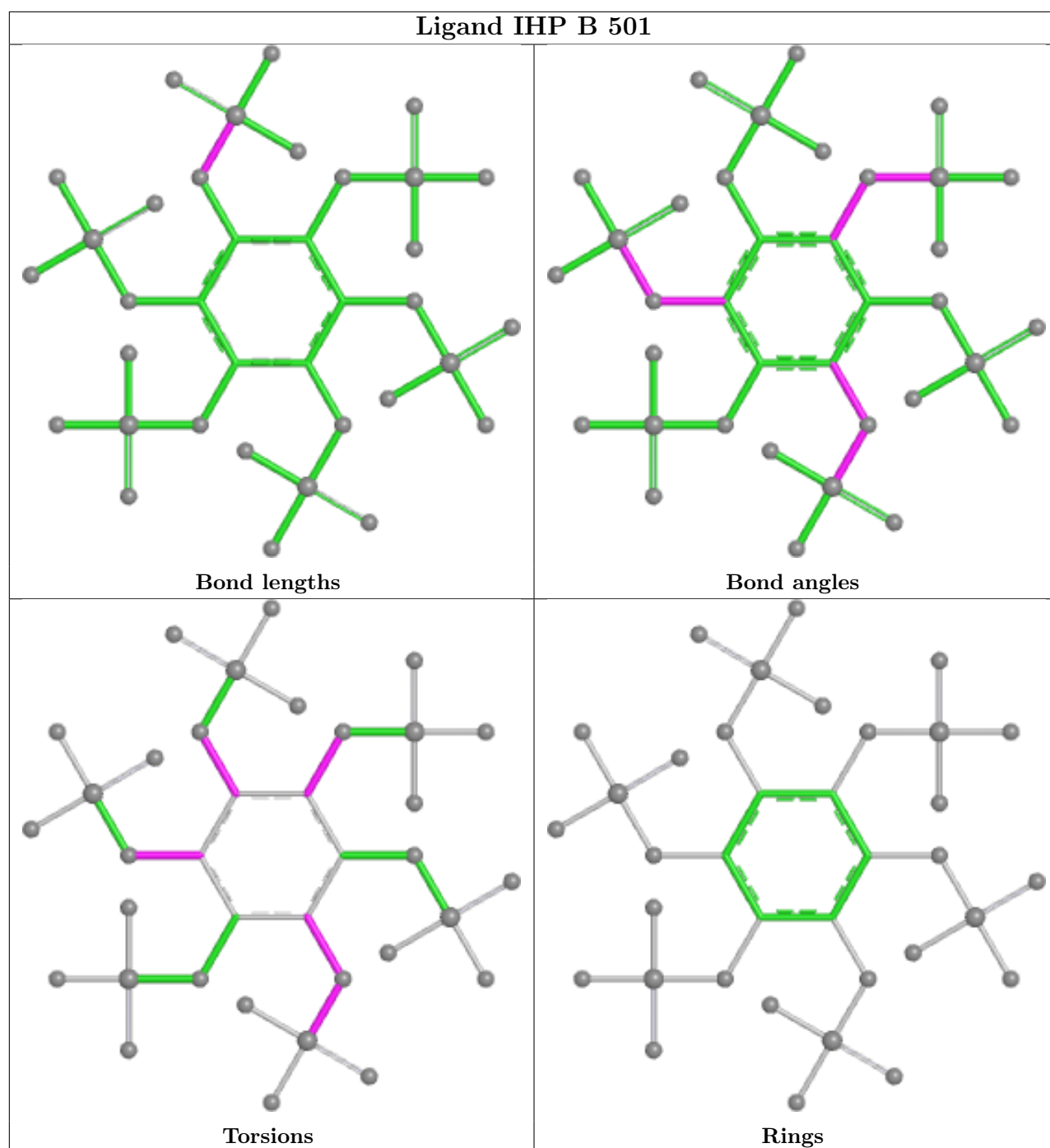
Mol	Chain	Res	Type	Atoms
15	B	501	IHP	C3-C2-O12-P2
15	B	501	IHP	C3-C4-O14-P4
15	B	501	IHP	C5-C4-O14-P4
15	B	501	IHP	C1-C2-O12-P2
15	B	501	IHP	C1-C6-O16-P6
15	B	501	IHP	C6-O16-P6-O36
15	B	501	IHP	C6-O16-P6-O26
15	B	501	IHP	C5-C6-O16-P6
15	B	501	IHP	C4-C3-O13-P3

There are no ring outliers.

1 monomer is involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
15	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.

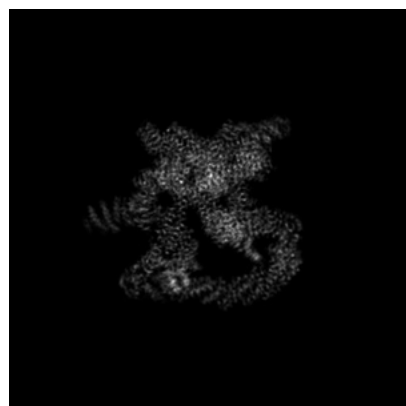
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-53256. These allow visual inspection of the internal detail of the map and identification of artifacts.

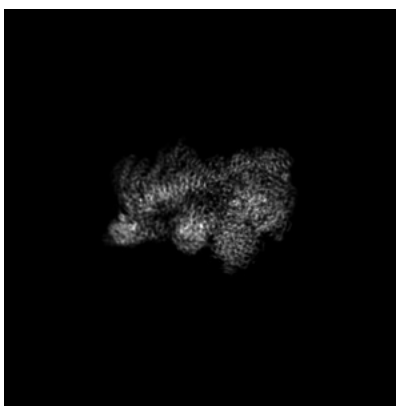
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

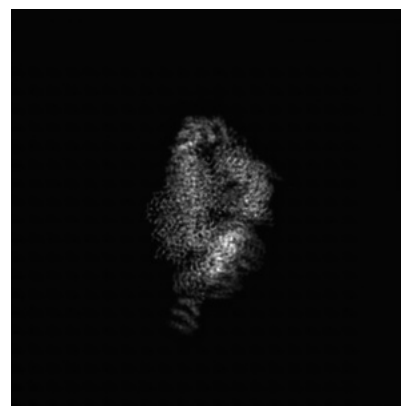
6.1.1 Primary map



X

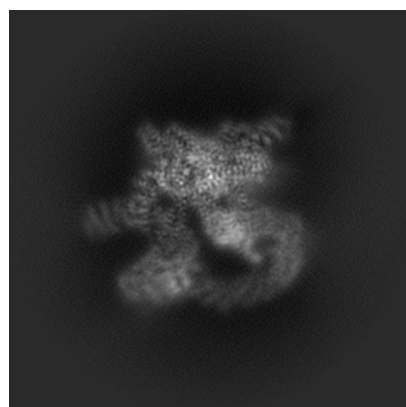


Y

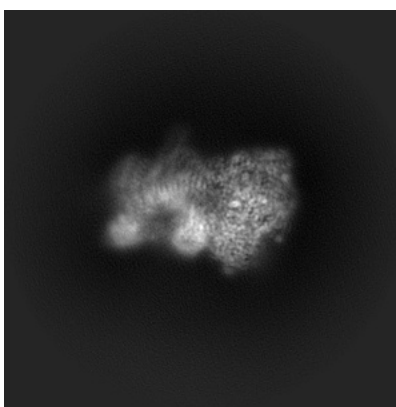


Z

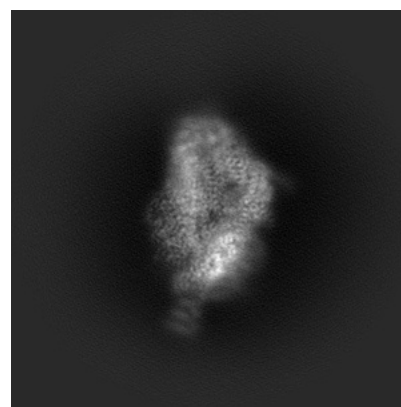
6.1.2 Raw map



X



Y



Z

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

6.2 Central slices [i](#)

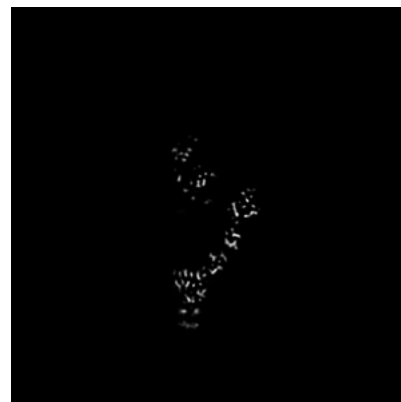
6.2.1 Primary map



X Index: 160

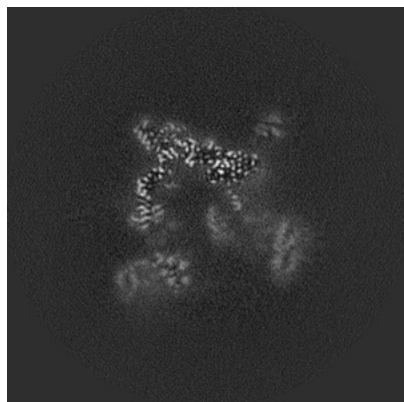


Y Index: 160

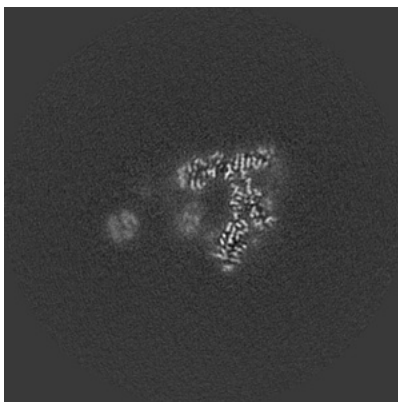


Z Index: 160

6.2.2 Raw map



X Index: 160



Y Index: 160



Z Index: 160

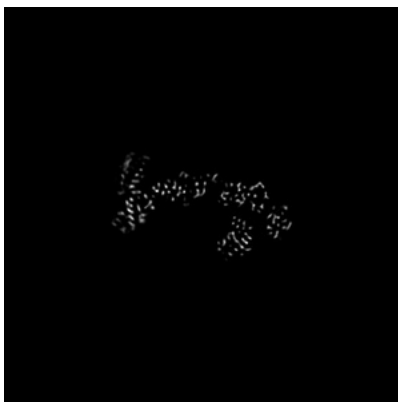
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

6.3.1 Primary map



X Index: 146

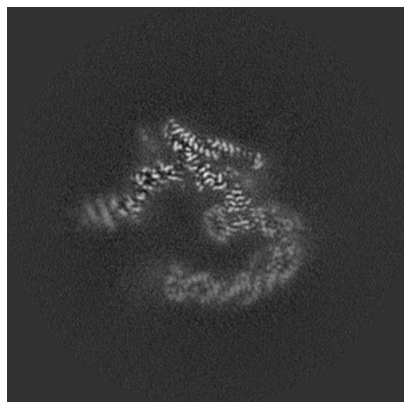


Y Index: 131

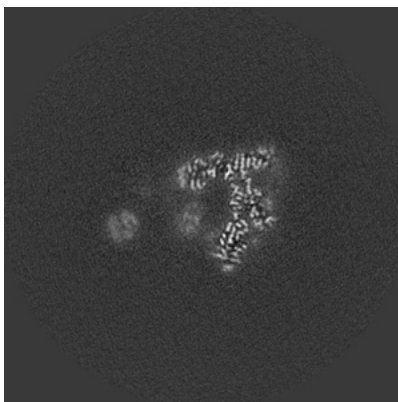


Z Index: 186

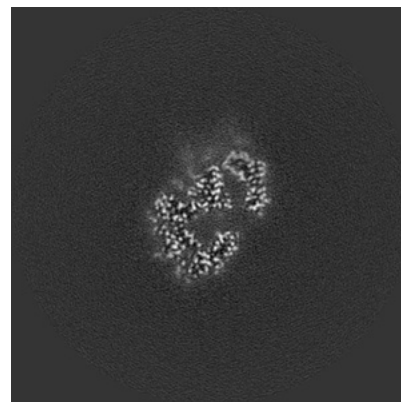
6.3.2 Raw map



X Index: 146



Y Index: 160

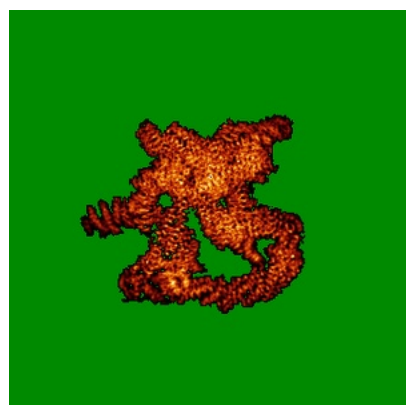


Z Index: 186

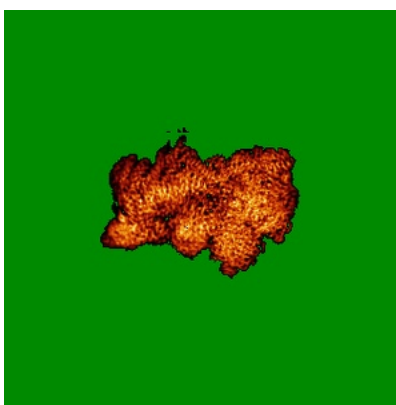
The images above show the largest variance slices of the map in three orthogonal directions.

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

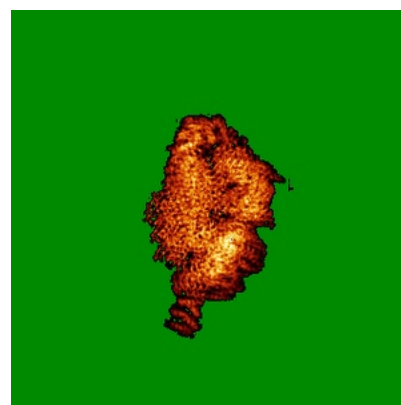
6.4.1 Primary map



X

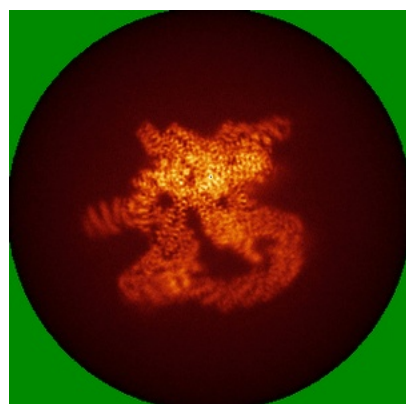


Y

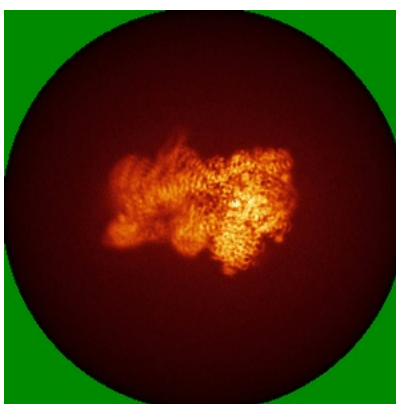


Z

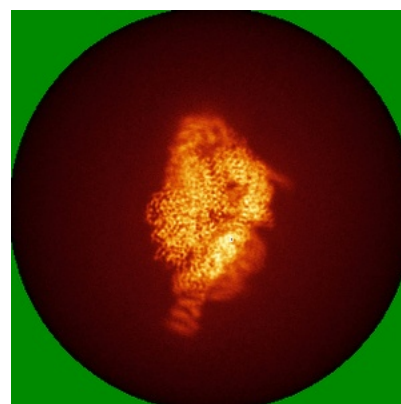
6.4.2 Raw map



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](#)

This section was not generated.

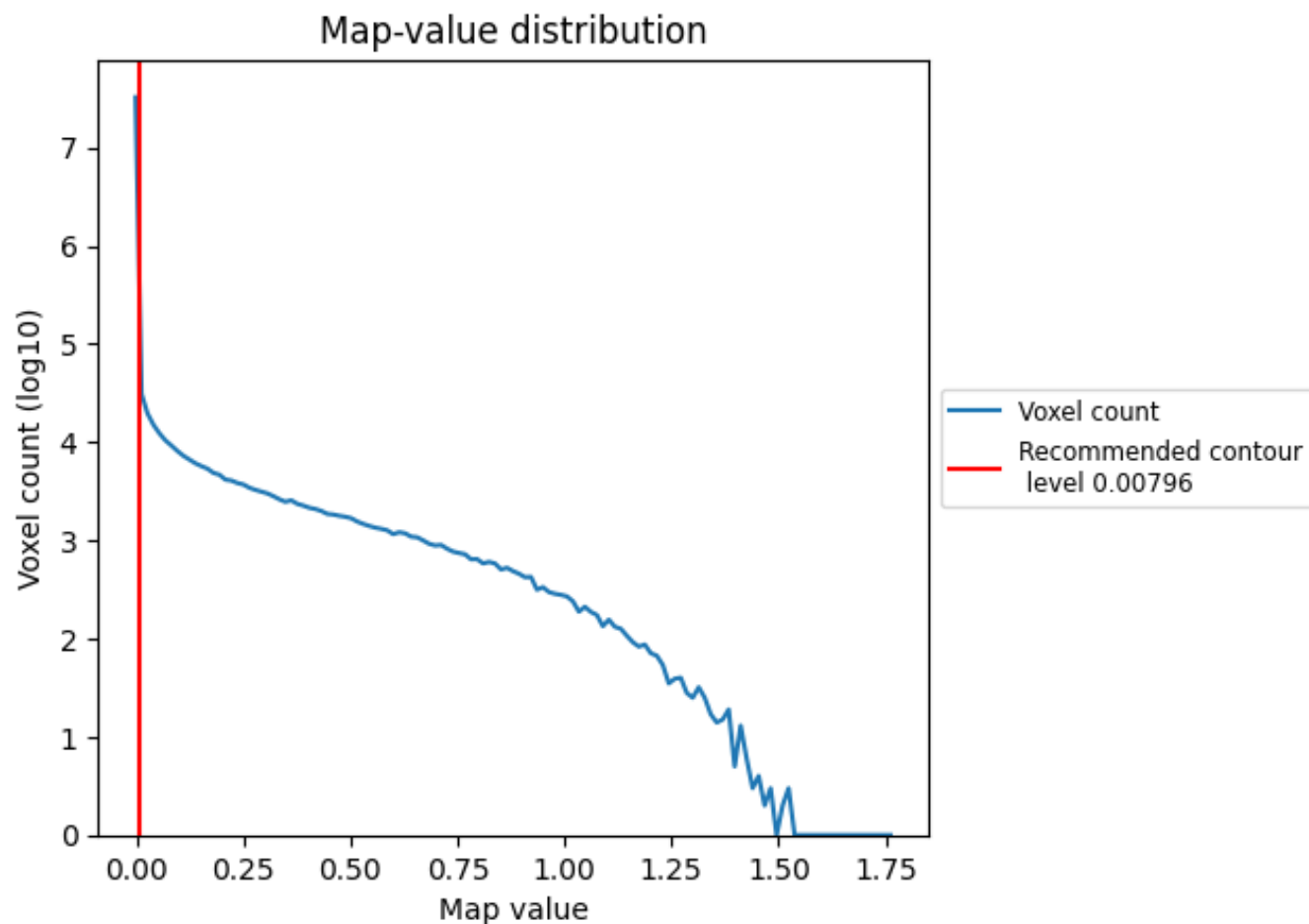
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

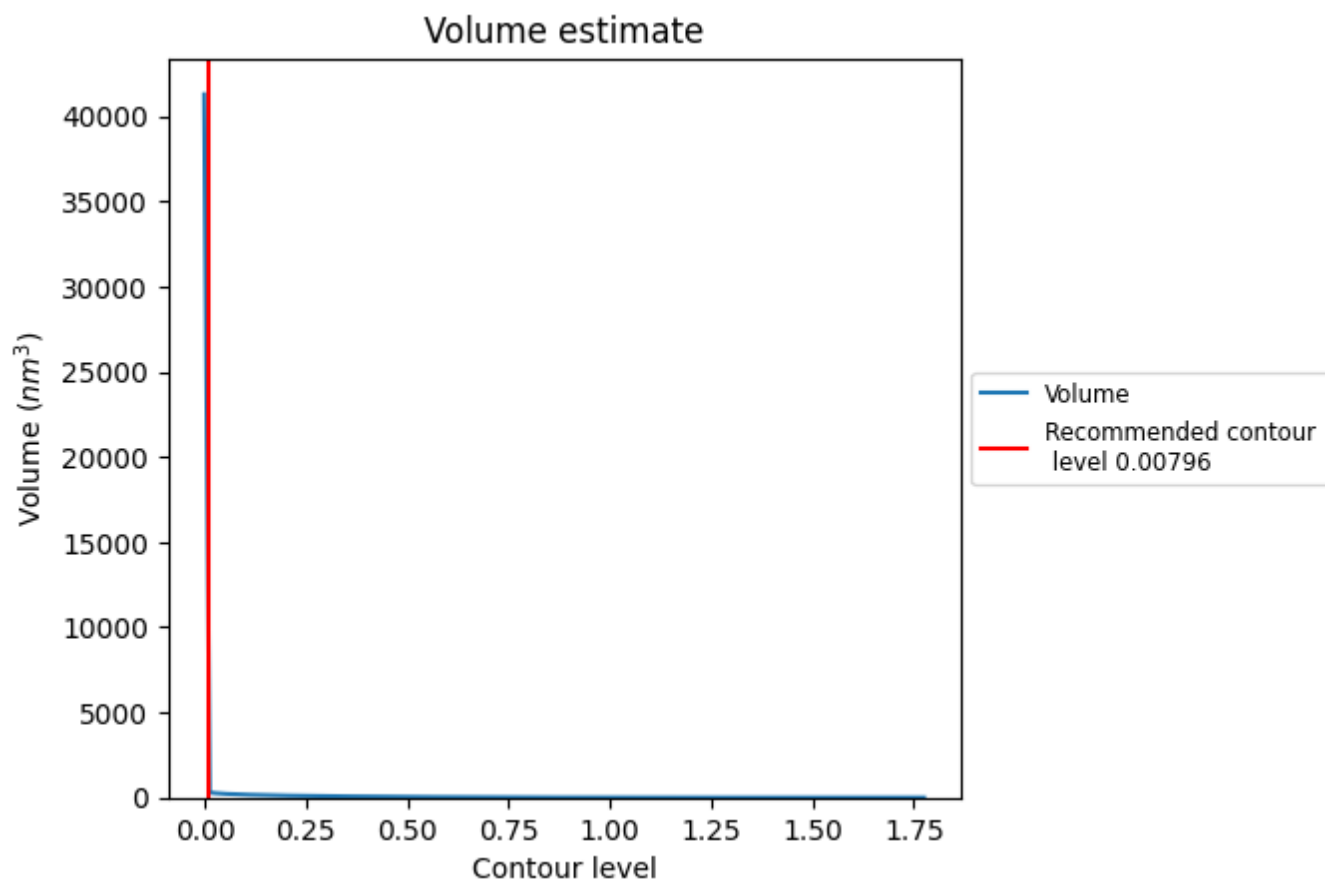
This section contains the results of statistical analysis of the map.

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.

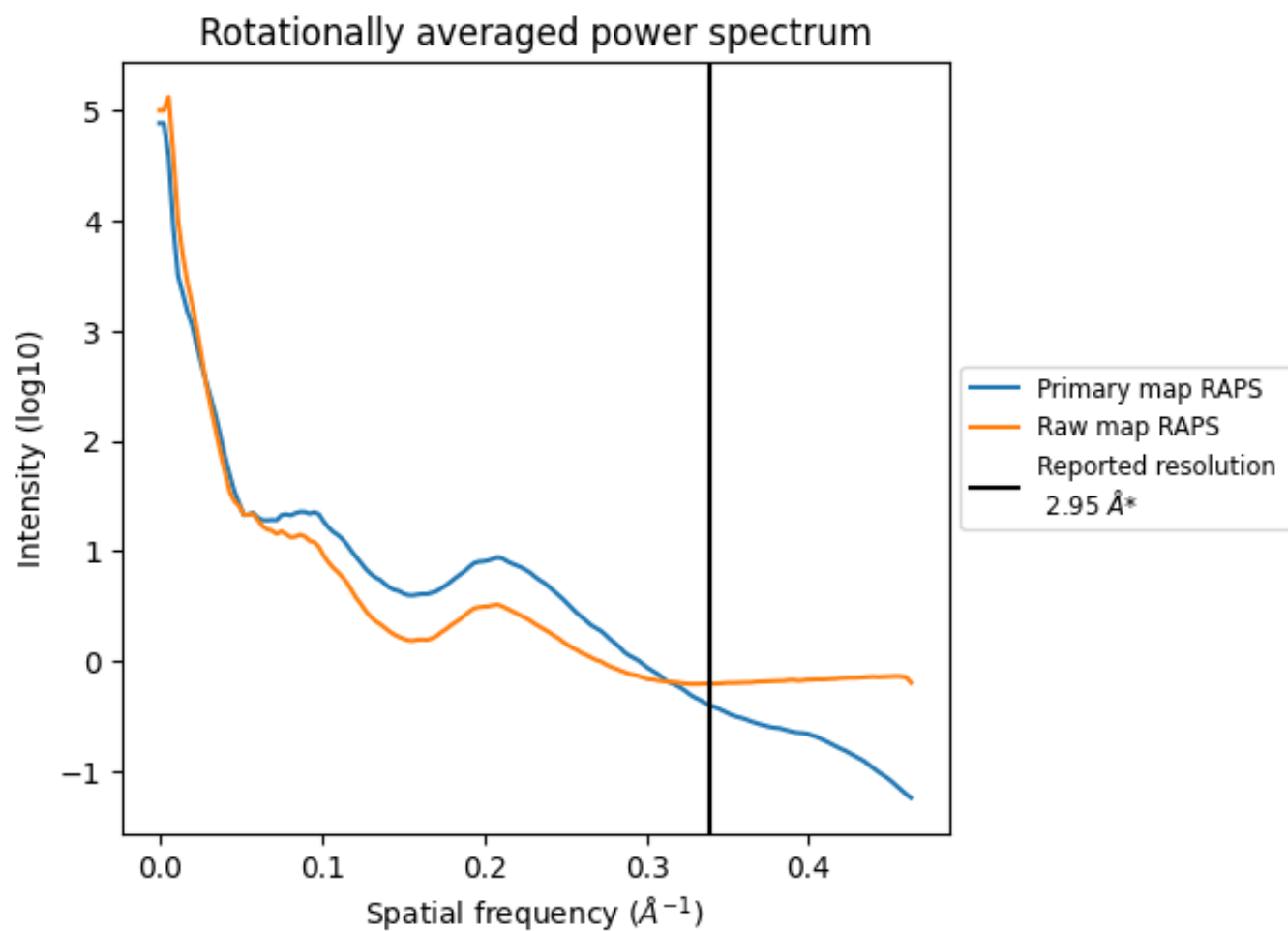
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 12748 nm^3 ; this corresponds to an approximate mass of 11516 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 ⓘ

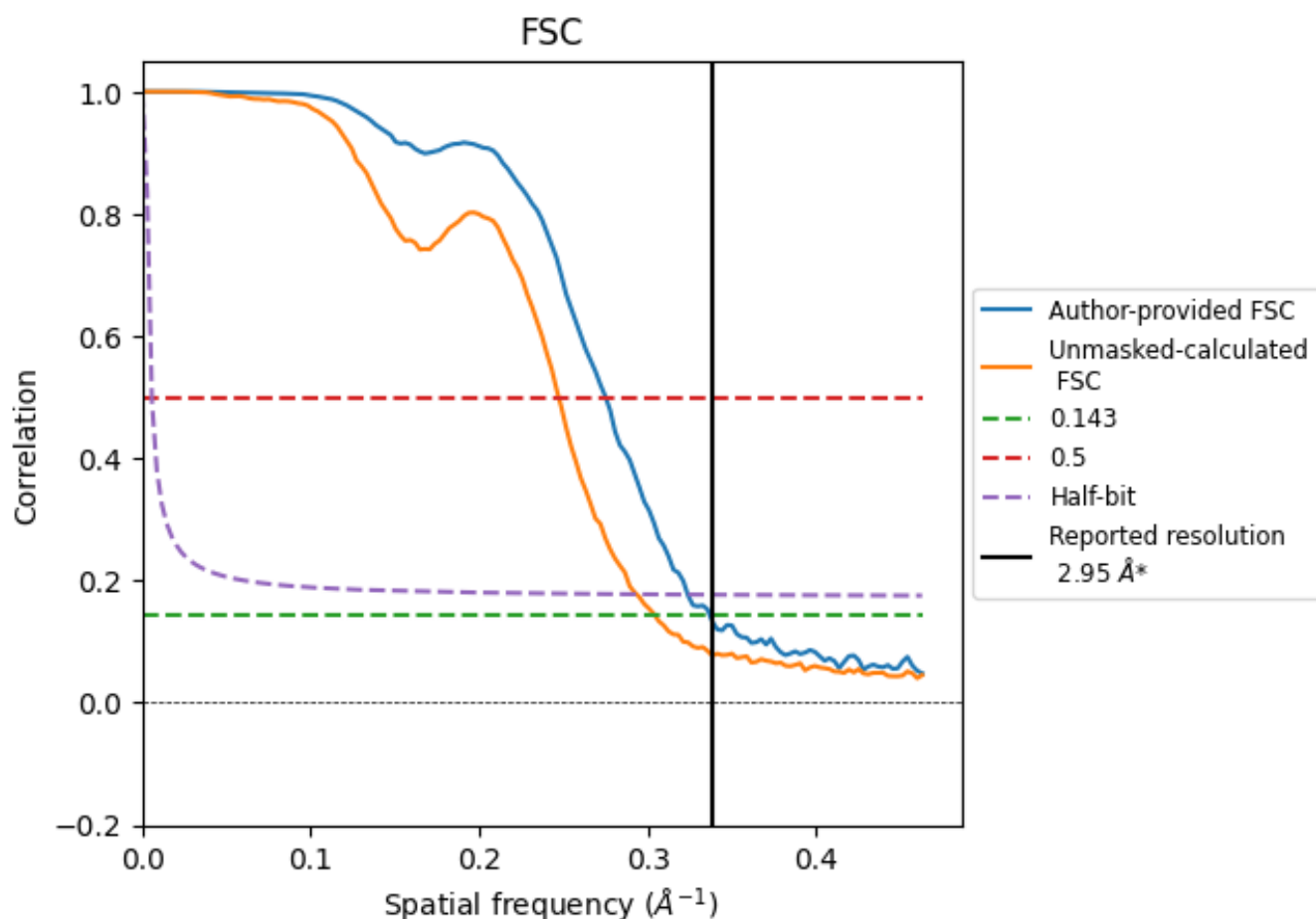


*Reported resolution corresponds to spatial frequency of 0.339 $\text{\AA}^{-1}$

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 0.339 $\text{\AA}^{-1}$

8.2 Resolution estimates [i](#)

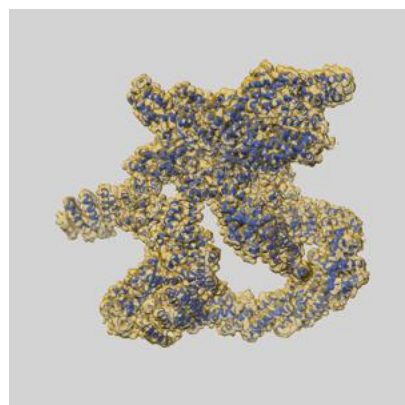
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	2.95	-	-
Author-provided FSC curve	2.97	3.64	3.09
Unmasked-calculated*	3.29	4.04	3.41

*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 3.29 differs from the reported value 2.95 by more than 10 %

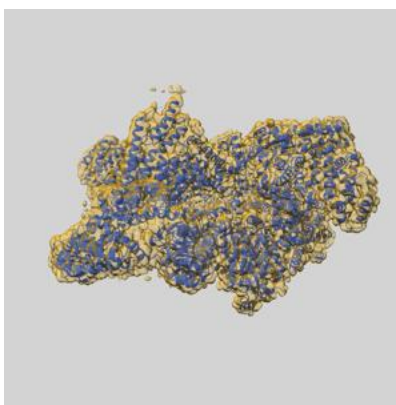
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-53256 and PDB model 9QO4. Per-residue inclusion information can be found in section [3](#) on page [8](#).

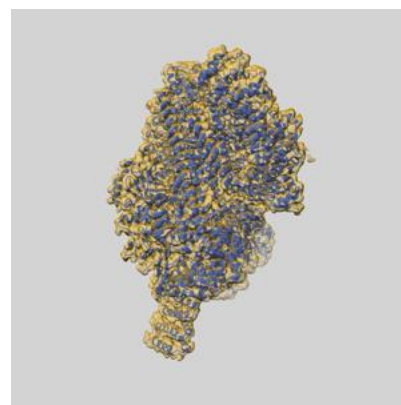
9.1 Map-model overlay [i](#)



X



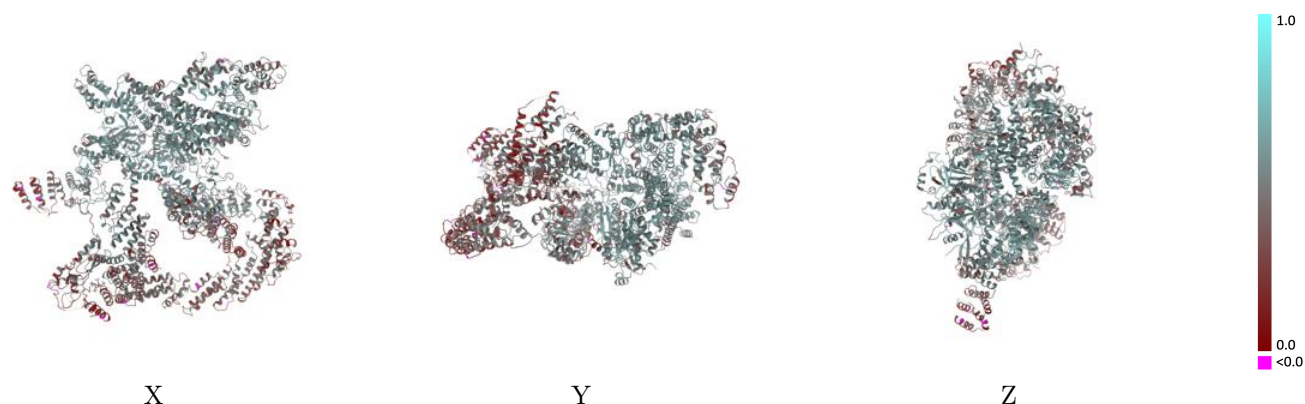
Y



Z

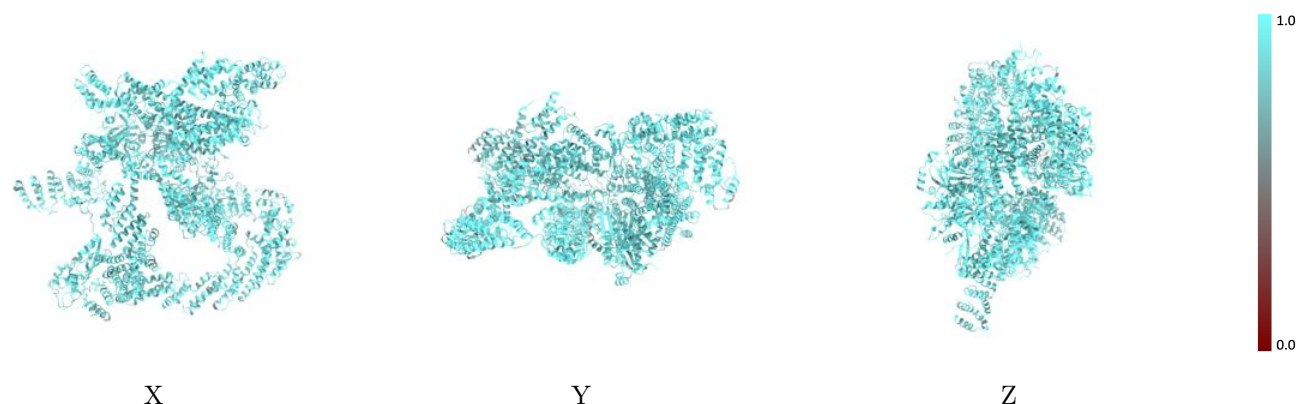
The images above show the 3D surface view of the map at the recommended contour level 0.00796 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



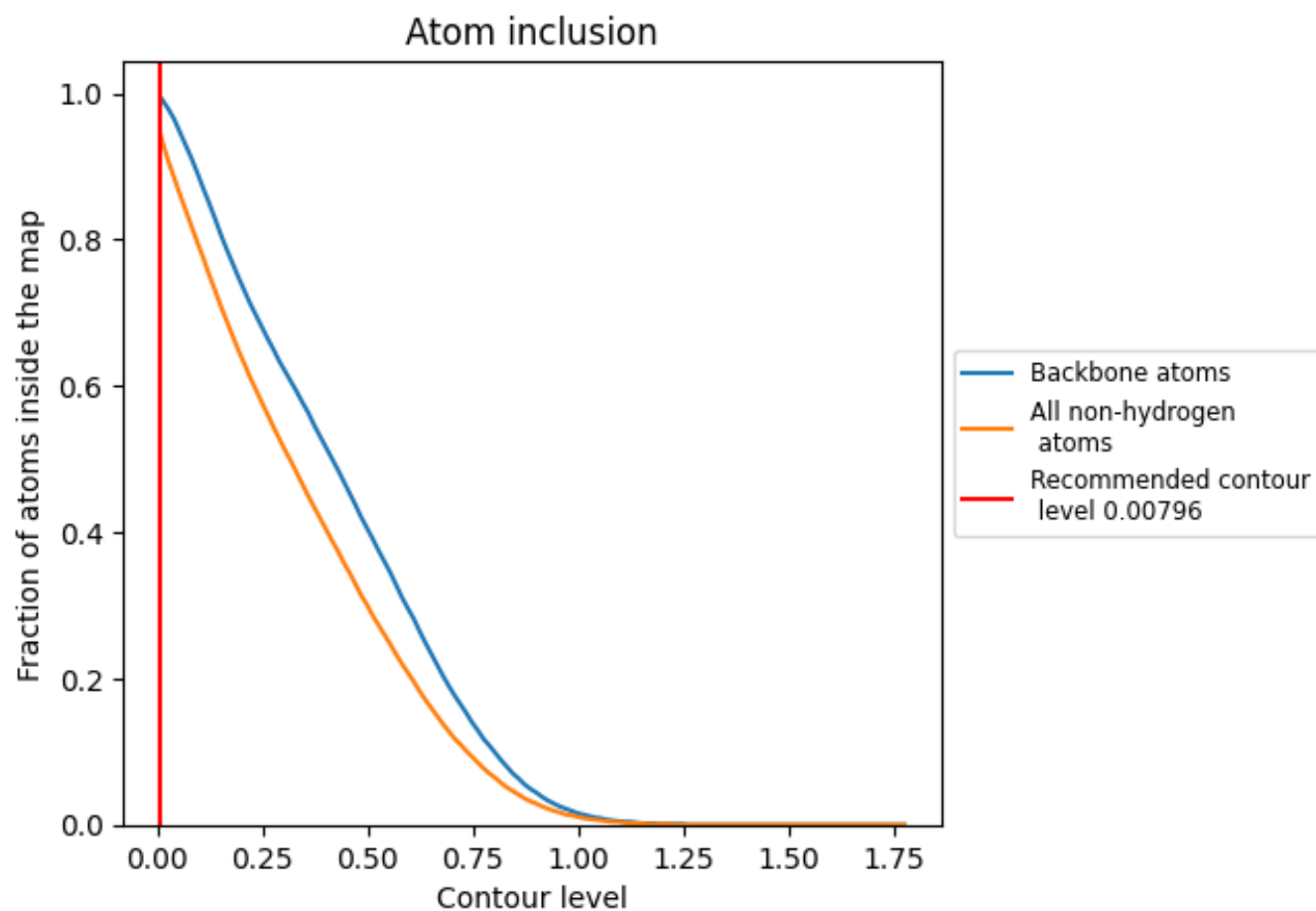
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.00796).

9.4 Atom inclusion ⓘ



At the recommended contour level, 99% 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 (0.00796) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.9430	 0.4650
A	 0.9460	 0.4570
B	 0.9110	 0.4220
C	 0.9710	 0.5290
D	 0.9350	 0.4560
E	 0.9450	 0.5360
F	 0.9700	 0.5490
G	 0.9640	 0.5320
H	 0.9640	 0.5030
I	 0.9360	 0.3810
J	 0.9260	 0.4500
L	 0.8750	 0.2910
M	 0.9680	 0.4800
N	 0.9320	 0.5250
P	 0.9230	 0.5030

