



Full wwPDB EM Validation Report ⓘ

Mar 5, 2026 – 04:08 PM UTC

PDB ID : 7YSW / pdb_00007ysw
EMDB ID : EMD-34084
Title : Cryo-EM Structure of FGF23-FGFR4-aKlotho-HS Quaternary Complex
Authors : Mohammadi, M.; Chen, L.
Deposited on : 2022-08-13
Resolution : 3.03 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

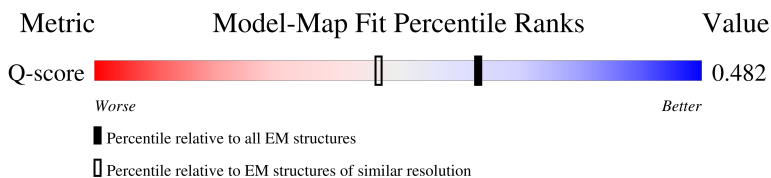
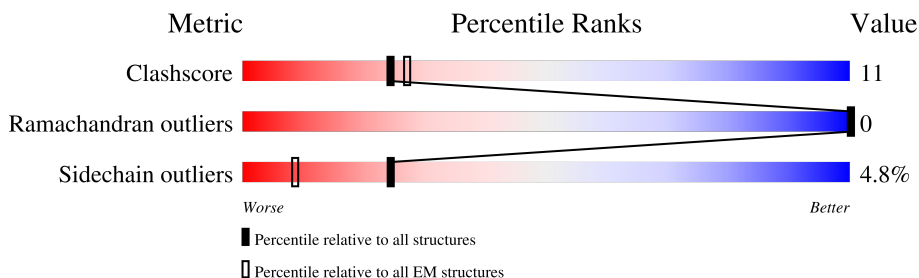
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 3.03 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	13929 (2.53 - 3.53)

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	C	213	
1	E	213	
2	A	942	
3	B	179	

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
4	F	10	

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
4	IDS	F	1	X	-	-	-
4	SGN	F	4	X	-	-	-
4	IDS	F	5	X	-	-	-
4	IDS	F	7	X	-	-	-
4	SGN	F	8	X	-	-	-

2 Entry composition [i](#)

There are 6 unique types of molecules in this entry. The entry contains 12407 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 Fibroblast growth factor receptor 4.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	C	213	Total	C	N	O	S	0	0
			1667	1058	294	309	6		
1	E	204	Total	C	N	O	S	0	0
			1597	1018	284	289	6		

- Molecule 2 is a protein called Klotho.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	A	921	Total	C	N	O	S	0	0
			7523	4875	1281	1338	29		

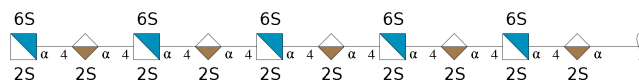
- Molecule 3 is a protein called Fibroblast growth factor 23.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	B	179	Total	C	N	O	S	0	0
			1442	913	265	257	7		

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	176	GLN	ARG	variant	UNP Q9GZV9
B	179	GLN	ARG	variant	UNP Q9GZV9

- Molecule 4 is an oligosaccharide called 2-deoxy-6-O-sulfo-2-(sulfoamino)-alpha-D-glucopyranose-(1-4)-2-O-sulfo-alpha-L-idopyranuronic acid-(1-4)-2-deoxy-6-O-sulfo-2-(sulfoamino)-alpha-D-glucopyranose-(1-4)-2-O-sulfo-alpha-L-idopyranuronic acid-(1-4)-2-deoxy-6-O-sulfo-2-(sulfoamino)-alpha-D-glucopyranose-(1-4)-2-O-sulfo-alpha-L-idopyranuronic acid-(1-4)-2-deoxy-6-O-sulfo-2-(sulfoamino)-alpha-D-glucopyranose-(1-4)-2-O-sulfo-alpha-L-idopyranuronic acid-(1-4)-2-deoxy-6-O-sulfo-2-(sulfoamino)-alpha-D-glucopyranose-(1-4)-2-O-sulfo-alpha-L-idopyranuronic acid.



Mol	Chain	Residues	Atoms				AltConf	Trace
4	F	10	Total	C	N	O	S	
			176	60	5	96	15	
								0
								0

- Molecule 5 is COPPER (II) ION (CCD ID: CU) (formula: Cu).

Mol	Chain	Residues	Atoms		AltConf
5	E	1	Total	Cu	
			1	1	
					0

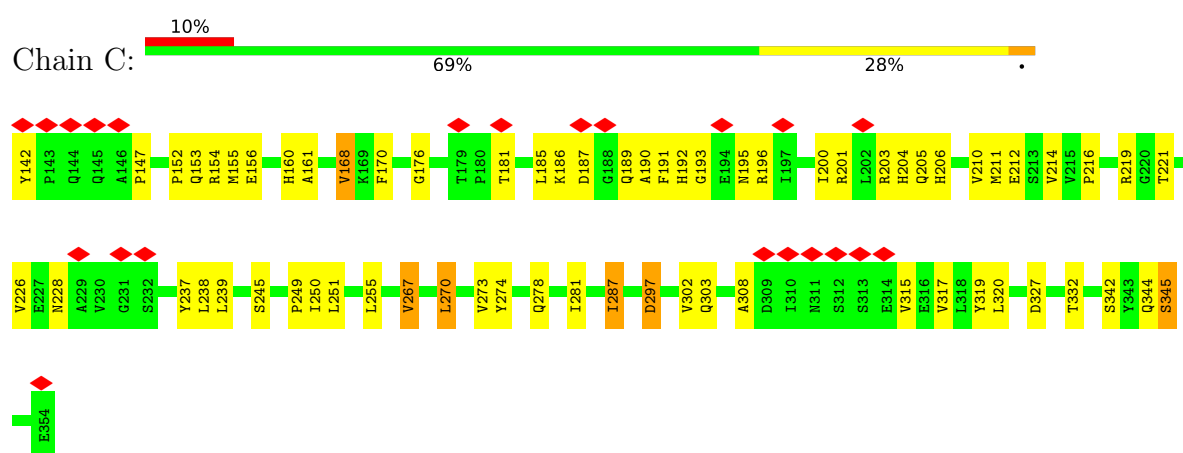
- Molecule 6 is ZINC ION (CCD ID: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		AltConf
6	A	1	Total	Zn	
			1	1	
					0

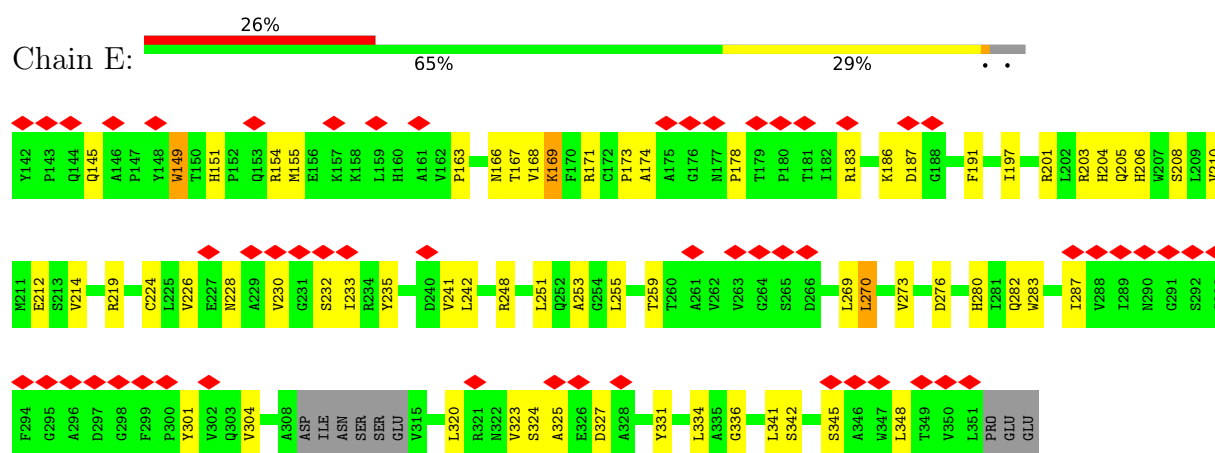
3 Residue-property plots

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.

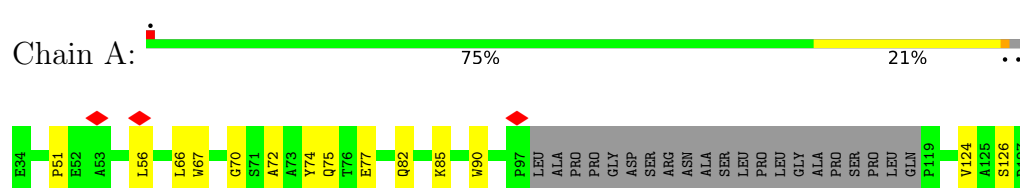
• Molecule 1: Fibroblast growth factor receptor 4

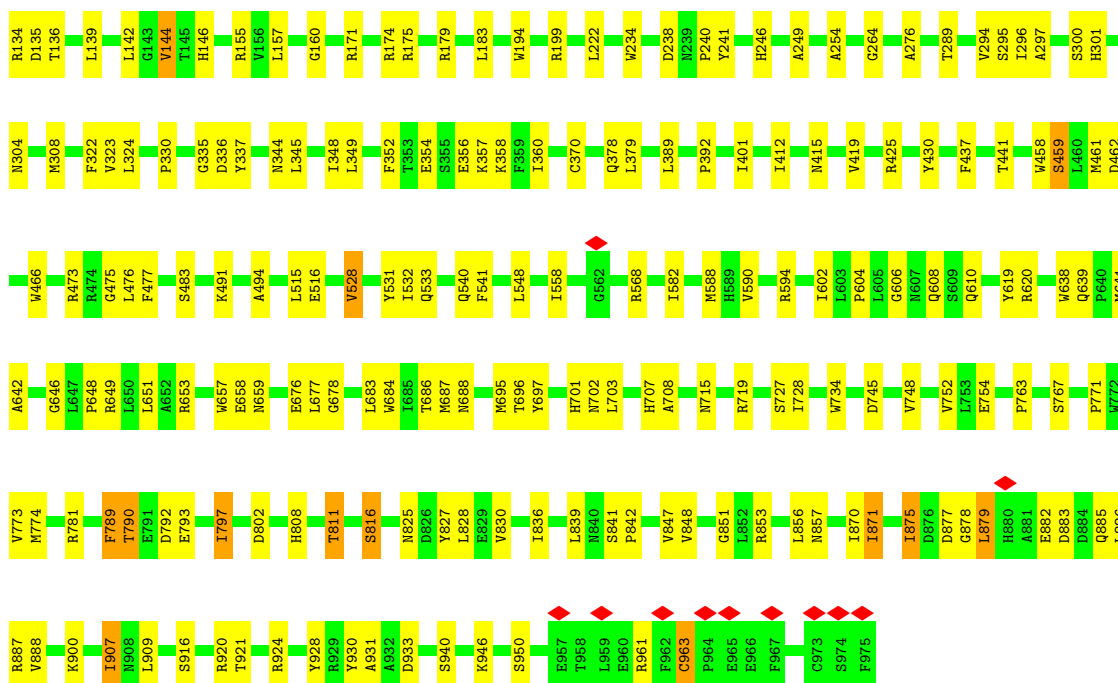


• Molecule 1: Fibroblast growth factor receptor 4

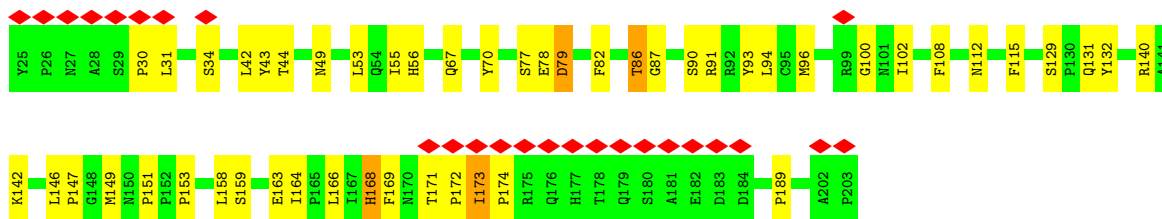


• Molecule 2: Klotho

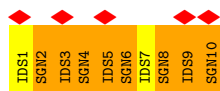




• Molecule 3: Fibroblast growth factor 23



• Molecule 4: 2-deoxy-6-O-sulfo-2-(sulfoamino)-alpha-D-glucopyranose-(1-4)-2-O-sulfo-alpha-L-idopyranuronic acid-(1-4)-2-deoxy-6-O-sulfo-2-(sulfoamino)-alpha-D-glucopyranose-(1-4)-2-O-sulfo-alpha-L-idopyranuronic acid-(1-4)-2-deoxy-6-O-sulfo-2-(sulfoamino)-alpha-D-glucopyranose-(1-4)-2-O-sulfo-alpha-L-idopyranuronic acid-(1-4)-2-deoxy-6-O-sulfo-2-(sulfoamino)-alpha-D-glucopyranose-(1-4)-2-O-sulfo-alpha-L-idopyranuronic acid-(1-4)-2-deoxy-6-O-sulfo-2-(sulfoamino)-alpha-D-glucopyranose-(1-4)-2-O-sulfo-alpha-L-idopyranuronic acid



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	856877	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	NONE	Depositor
Microscope	FEI TALOS ARCTICA	Depositor
Voltage (kV)	200	Depositor
Electron dose ($e^-/\text{\AA}^2$)	53.84	Depositor
Minimum defocus (nm)	700	Depositor
Maximum defocus (nm)	2800	Depositor
Magnification	Not provided	
Image detector	GATAN K3 (6k x 4k)	Depositor
Maximum map value	6.228	Depositor
Minimum map value	-4.266	Depositor
Average map value	-0.000	Depositor
Map value standard deviation	0.068	Depositor
Recommended contour level	0.5	Depositor
Map size ($\text{\AA}$)	438.4, 438.4, 438.4	wwPDB
Map dimensions	400, 400, 400	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing ($\text{\AA}$)	1.096, 1.096, 1.096	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: SGN, IDS, CU, 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	C	0.12	0/1712	0.29	0/2338
1	E	0.11	0/1640	0.29	0/2238
2	A	0.13	0/7764	0.28	0/10562
3	B	0.12	0/1489	0.31	0/2025
All	All	0.12	0/12605	0.29	0/17163

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

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	C	1667	0	1621	45	0
1	E	1597	0	1563	41	0
2	A	7523	0	7255	143	0
3	B	1442	0	1379	38	0
4	F	176	0	53	11	0
5	E	1	0	0	0	0
6	A	1	0	0	0	0
All	All	12407	0	11871	259	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 11.

All (259) 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:B:173:ILE:HD12	3:B:174:PRO:HD3	1.66	0.78
3:B:55:ILE:HD11	3:B:94:LEU:HD12	1.68	0.74
2:A:246:HIS:NE2	2:A:379:LEU:O	2.22	0.73
2:A:131:ASN:HB3	2:A:134:ARG:HG2	1.69	0.72
3:B:146:LEU:HD22	3:B:147:PRO:HD2	1.69	0.72
1:C:201:ARG:HH22	4:F:10:SGN:H5	1.54	0.72
3:B:153:PRO:HG2	4:F:2:SGN:H4	1.72	0.71
2:A:337:TYR:HD2	2:A:349:LEU:HD21	1.56	0.70
2:A:134:ARG:NH1	2:A:135:ASP:OD1	2.23	0.70
2:A:842:PRO:HG2	2:A:878:GLY:H	1.58	0.69
2:A:324:LEU:HD21	2:A:401:ILE:HD11	1.73	0.69
2:A:126:SER:O	2:A:134:ARG:NH2	2.25	0.68
1:C:205:GLN:OE1	1:C:205:GLN:N	2.27	0.68
2:A:336:ASP:HB2	2:A:357:LYS:HE2	1.76	0.67
3:B:96:MET:O	3:B:112:ASN:ND2	2.28	0.67
2:A:128:SER:OG	2:A:135:ASP:OD2	2.12	0.67
2:A:781:ARG:HB2	2:A:781:ARG:HH11	1.58	0.66
1:E:248:ARG:NH2	3:B:30:PRO:O	2.27	0.66
2:A:619:TYR:HB3	2:A:677:LEU:HD21	1.78	0.65
1:E:203:ARG:HH21	1:E:210:VAL:HG11	1.61	0.65
1:E:163:PRO:HD2	1:E:166:ASN:HD22	1.61	0.64
2:A:528:VAL:HG22	2:A:916:SER:H	1.60	0.64
2:A:462:ASP:OD2	2:A:473:ARG:NH1	2.30	0.64
1:E:145:GLN:NE2	1:E:178:PRO:O	2.31	0.63
2:A:540:GLN:HG2	2:A:541:PHE:HD1	1.62	0.63
2:A:653:ARG:HG3	2:A:653:ARG:HH11	1.64	0.63
2:A:719:ARG:NH2	2:A:802:ASP:OD2	2.31	0.63
1:E:331:TYR:H	1:E:348:LEU:HD12	1.64	0.63
2:A:238:ASP:HA	2:A:297:ALA:HB3	1.82	0.62
2:A:412:ILE:HG21	2:A:415:ASN:HD22	1.64	0.62
2:A:697:TYR:OH	2:A:827:TYR:OH	2.10	0.62
2:A:961:ARG:NH1	2:A:963:CYS:SG	2.71	0.62
1:E:201:ARG:NH1	4:F:4:SGN:O1S	2.33	0.62
3:B:100:GLY:O	3:B:142:LYS:NZ	2.30	0.62
1:C:201:ARG:HB3	1:C:210:VAL:HB	1.82	0.61
1:C:147:PRO:HD3	1:C:228:ASN:HD22	1.64	0.61
2:A:337:TYR:CD2	2:A:349:LEU:HD21	2.36	0.61
3:B:129:SER:HB3	3:B:132:TYR:HB2	1.83	0.61

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:249:PRO:O	1:C:342:SER:OG	2.18	0.60
2:A:771:PRO:HG2	2:A:774:MET:HB2	1.85	0.59
2:A:763:PRO:HB3	2:A:789:PHE:HE1	1.67	0.59
1:E:171:ARG:HG3	1:E:208:SER:HB3	1.84	0.58
2:A:847:VAL:HG21	2:A:886:LEU:HD11	1.86	0.58
2:A:459:SER:O	2:A:475:GLY:HA2	2.03	0.58
2:A:781:ARG:HB2	2:A:781:ARG:NH1	2.18	0.58
1:C:273:VAL:HG11	1:C:281:ILE:HD11	1.85	0.57
1:C:168:VAL:HG13	1:C:214:VAL:HG21	1.86	0.57
1:C:278:GLN:HB3	3:B:77:SER:HB2	1.86	0.57
2:A:686:THR:HG21	2:A:707:HIS:HA	1.87	0.57
2:A:392:PRO:HG3	3:B:189:PRO:HB2	1.86	0.57
2:A:425:ARG:HA	2:A:491:LYS:HG2	1.87	0.57
1:E:282:GLN:HE22	1:E:304:VAL:HA	1.71	0.56
2:A:77:GLU:HA	2:A:128:SER:HB3	1.88	0.56
2:A:51:PRO:HD2	2:A:885:GLN:HG3	1.85	0.56
2:A:839:LEU:HB2	2:A:847:VAL:HB	1.85	0.56
1:C:142:TYR:OH	1:C:176:GLY:O	2.24	0.56
2:A:686:THR:HG22	2:A:687:MET:SD	2.46	0.56
2:A:533:GLN:OE1	2:A:533:GLN:HA	2.05	0.56
3:B:171:THR:HB	3:B:173:ILE:HG13	1.86	0.56
1:E:149:TRP:HA	1:E:174:ALA:HA	1.88	0.55
2:A:234:TRP:HB2	2:A:294:VAL:HG22	1.89	0.55
1:E:282:GLN:O	1:E:334:LEU:N	2.38	0.54
2:A:82:GLN:NE2	2:A:130:ASN:OD1	2.33	0.54
1:C:153:GLN:HG2	1:C:154:ARG:HG3	1.88	0.54
1:C:216:PRO:O	1:C:219:ARG:NH1	2.41	0.54
2:A:532:ILE:HD11	2:A:619:TYR:HE1	1.72	0.54
3:B:166:LEU:HA	3:B:169:PHE:HD2	1.73	0.54
2:A:715:ASN:OD1	2:A:719:ARG:NH1	2.40	0.54
2:A:678:GLY:HA2	2:A:684:TRP:HZ2	1.73	0.54
1:C:185:LEU:HA	1:C:191:PHE:H	1.73	0.54
2:A:701:HIS:CD2	2:A:789:PHE:HE2	2.27	0.53
2:A:594:ARG:NH1	2:A:688:ASN:OD1	2.35	0.53
2:A:792:ASP:OD1	2:A:793:GLU:N	2.41	0.52
2:A:825:ASN:HB3	2:A:830:VAL:HG12	1.91	0.52
1:C:203:ARG:NH2	4:F:9:IDS:O2S	2.42	0.52
2:A:657:TRP:O	2:A:702:ASN:ND2	2.35	0.52
1:C:267:VAL:HG12	1:C:320:LEU:HB2	1.90	0.52
2:A:157:LEU:O	2:A:199:ARG:NH1	2.43	0.51
2:A:649:ARG:NH1	2:A:649:ARG:HB3	2.25	0.51

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:877:ASP:OD1	2:A:887:ARG:NH2	2.43	0.51
1:C:156:GLU:HB2	3:B:49:ASN:HB3	1.92	0.51
2:A:708:ALA:HB2	2:A:797:ILE:HG23	1.91	0.51
3:B:131:GLN:HG3	3:B:132:TYR:HD2	1.75	0.51
2:A:877:ASP:HB2	2:A:883:ASP:HB2	1.93	0.51
1:E:324:SER:OG	1:E:325:ALA:N	2.43	0.51
1:E:327:ASP:OD1	1:E:327:ASP:N	2.44	0.51
1:E:336:GLY:HA3	1:E:341:LEU:HG	1.93	0.51
2:A:687:MET:HG2	2:A:703:LEU:HD21	1.93	0.51
2:A:322:PHE:HZ	2:A:344:ASN:HD21	1.58	0.51
3:B:79:ASP:HB3	3:B:82:PHE:HD2	1.76	0.51
1:C:189:GLN:HE22	1:C:195:ASN:HD21	1.57	0.51
2:A:606:GLY:HA2	2:A:648:PRO:HG2	1.94	0.50
2:A:653:ARG:HG3	2:A:653:ARG:NH1	2.27	0.50
3:B:67:GLN:NE2	3:B:163:GLU:OE1	2.39	0.50
2:A:75:GLN:HE21	2:A:466:TRP:NE1	2.09	0.50
2:A:745:ASP:OD1	2:A:816:SER:OG	2.26	0.50
3:B:42:LEU:HD12	3:B:53:LEU:HD23	1.94	0.50
1:C:319:TYR:O	2:A:540:GLN:NE2	2.44	0.49
2:A:642:ALA:HB3	2:A:646:GLY:H	1.76	0.49
2:A:72:ALA:HB3	2:A:75:GLN:HB2	1.95	0.49
2:A:90:TRP:NE1	2:A:254:ALA:HB2	2.28	0.49
3:B:172:PRO:C	3:B:174:PRO:HD2	2.37	0.49
1:E:204:HIS:NE2	4:F:5:IDS:O6B	2.46	0.49
3:B:173:ILE:HD12	3:B:174:PRO:CD	2.38	0.49
1:C:287:ILE:HD11	1:C:303:GLN:HB3	1.94	0.49
2:A:160:GLY:HA2	2:A:199:ARG:NE	2.28	0.49
2:A:74:TYR:CZ	2:A:90:TRP:HB3	2.49	0.48
2:A:136:THR:HA	2:A:139:LEU:HD12	1.94	0.48
2:A:588:MET:HB3	2:A:590:VAL:HG13	1.95	0.48
2:A:920:ARG:HB2	2:A:930:TYR:CG	2.48	0.48
2:A:933:ASP:OD1	3:B:91:ARG:NH2	2.45	0.48
3:B:78:GLU:OE2	3:B:78:GLU:HA	2.14	0.48
1:C:161:ALA:HB3	3:B:43:TYR:CE1	2.49	0.48
1:C:332:THR:HG22	1:C:345:SER:HB2	1.94	0.48
2:A:249:ALA:HB2	2:A:264:GLY:HA3	1.96	0.48
2:A:300:SER:HB2	2:A:324:LEU:HD13	1.96	0.48
2:A:604:PRO:HG2	2:A:610:GLN:HE22	1.79	0.48
2:A:66:LEU:HD22	2:A:146:HIS:CE1	2.48	0.48
2:A:878:GLY:HA2	2:A:924:ARG:HD3	1.96	0.48
2:A:961:ARG:NH1	2:A:961:ARG:O	2.47	0.48

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:85:LYS:HG2	2:A:155:ARG:HA	1.96	0.47
2:A:90:TRP:CE2	2:A:254:ALA:HB2	2.49	0.47
2:A:946:LYS:HD3	2:A:946:LYS:N	2.29	0.47
2:A:352:PHE:HB3	2:A:357:LYS:HG3	1.96	0.47
2:A:659:ASN:OD1	2:A:659:ASN:N	2.45	0.47
2:A:142:LEU:HD22	2:A:477:PHE:HE1	1.78	0.47
2:A:658:GLU:OE2	2:A:658:GLU:N	2.48	0.47
1:E:151:HIS:HB3	1:E:154:ARG:HB3	1.96	0.47
2:A:620:ARG:HH21	2:A:676:GLU:HB3	1.80	0.47
1:C:196:ARG:NE	1:C:211:MET:HE1	2.30	0.47
1:E:145:GLN:NE2	1:E:228:ASN:OD1	2.48	0.47
2:A:240:PRO:HG3	2:A:296:ILE:HD11	1.97	0.47
2:A:330:PRO:O	2:A:335:GLY:HA2	2.14	0.47
2:A:540:GLN:HG2	2:A:541:PHE:CD1	2.47	0.47
4:F:4:SGN:O5S	4:F:5:IDS:O2S	2.33	0.47
1:E:183:ARG:NH1	1:E:191:PHE:O	2.45	0.47
2:A:297:ALA:HB1	2:A:370:CYS:SG	2.55	0.47
1:C:193:GLY:HA2	1:C:200:ILE:HD12	1.97	0.47
2:A:437:PHE:O	2:A:441:THR:HG23	2.15	0.46
1:C:154:ARG:NE	4:F:6:SGN:O3S	2.48	0.46
1:E:205:GLN:HG3	1:E:206:HIS:CD2	2.49	0.46
2:A:276:ALA:HB2	2:A:360:ILE:HG23	1.97	0.46
1:C:327:ASP:OD1	2:A:568:ARG:NH2	2.49	0.46
2:A:75:GLN:HE21	2:A:466:TRP:HE1	1.63	0.46
2:A:301:HIS:CE1	2:A:323:VAL:HG11	2.50	0.46
1:C:152:PRO:HA	1:C:155:MET:HG3	1.98	0.46
1:E:255:LEU:HB3	1:E:270:LEU:O	2.16	0.46
2:A:841:SER:HB3	2:A:875:ILE:HD11	1.98	0.46
1:E:224:CYS:SG	1:E:235:TYR:HB2	2.56	0.46
1:C:205:GLN:H	1:C:205:GLN:CD	2.22	0.46
1:E:167:THR:HG23	1:E:212:GLU:HA	1.98	0.46
2:A:811:THR:HG23	2:A:848:VAL:HB	1.97	0.46
2:A:354:GLU:O	2:A:358:LYS:NZ	2.49	0.46
1:E:197:ILE:HD12	3:B:151:PRO:HD3	1.97	0.45
1:E:248:ARG:NE	1:E:342:SER:OG	2.49	0.45
3:B:56:HIS:HA	3:B:70:TYR:HE1	1.81	0.45
1:E:203:ARG:NH2	1:E:210:VAL:HG11	2.28	0.45
2:A:136:THR:HB	2:A:183:LEU:HD11	1.97	0.45
2:A:345:LEU:H	2:A:345:LEU:HD23	1.80	0.45
1:C:191:PHE:O	1:C:192:HIS:ND1	2.49	0.45
2:A:515:LEU:HD23	2:A:900:LYS:HA	1.98	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:548:LEU:HB2	2:A:558:ILE:HB	1.97	0.45
2:A:642:ALA:HB3	2:A:646:GLY:N	2.32	0.45
2:A:308:MET:HE3	2:A:308:MET:O	2.16	0.45
2:A:638:TRP:CE3	2:A:687:MET:HG3	2.51	0.45
2:A:639:GLN:HG3	2:A:688:ASN:HD22	1.82	0.45
2:A:604:PRO:HD2	2:A:610:GLN:OE1	2.17	0.45
2:A:649:ARG:HH22	2:A:653:ARG:HH21	1.63	0.45
1:E:287:ILE:HG13	1:E:301:TYR:HB3	1.98	0.44
3:B:49:ASN:OD1	3:B:49:ASN:N	2.50	0.44
2:A:734:TRP:H	2:A:808:HIS:HE1	1.64	0.44
2:A:931:ALA:HB1	3:B:169:PHE:HB2	1.99	0.44
3:B:67:GLN:HB3	3:B:164:ILE:HD11	1.99	0.44
1:C:205:GLN:HG2	1:C:206:HIS:ND1	2.32	0.44
1:C:308:ALA:HB2	1:C:315:VAL:HG11	1.99	0.44
1:E:280:HIS:CE1	1:E:282:GLN:HG2	2.53	0.44
1:C:196:ARG:NH2	1:C:212:GLU:O	2.51	0.44
2:A:430:TYR:HE2	2:A:476:LEU:HD23	1.83	0.44
2:A:790:THR:OG1	2:A:793:GLU:OE1	2.34	0.44
3:B:140:ARG:HA	3:B:140:ARG:HD3	1.60	0.44
2:A:134:ARG:HH11	2:A:134:ARG:HG3	1.83	0.44
4:F:2:SGN:H62	4:F:3:IDS:H2	2.00	0.43
2:A:588:MET:HE2	2:A:928:TYR:CE1	2.53	0.43
2:A:695:MET:HE1	2:A:703:LEU:HD13	2.01	0.43
1:E:251:LEU:HB3	1:E:273:VAL:HG12	2.00	0.43
2:A:532:ILE:O	2:A:532:ILE:HD12	2.17	0.43
2:A:330:PRO:HG3	2:A:337:TYR:HD1	1.82	0.43
1:E:169:LYS:HE3	1:E:169:LYS:HB3	1.82	0.43
1:E:169:LYS:HG3	4:F:8:SGN:O6S	2.18	0.43
3:B:55:ILE:O	3:B:90:SER:OG	2.37	0.43
3:B:86:THR:OG1	3:B:87:GLY:N	2.51	0.43
1:C:170:PHE:HZ	1:C:239:LEU:HB2	1.84	0.43
1:E:331:TYR:O	1:E:345:SER:OG	2.36	0.42
2:A:67:TRP:O	2:A:144:VAL:HG22	2.19	0.42
2:A:734:TRP:H	2:A:808:HIS:CE1	2.37	0.42
1:C:221:THR:HB	1:C:238:LEU:HG	2.01	0.42
2:A:304:ASN:N	2:A:389:LEU:O	2.42	0.42
2:A:649:ARG:HH22	2:A:653:ARG:NH2	2.17	0.42
1:C:250:ILE:O	1:C:250:ILE:HG13	2.18	0.42
1:C:274:TYR:HE1	1:E:253:ALA:HB2	1.84	0.42
2:A:853:ARG:O	2:A:857:ASN:ND2	2.51	0.42
2:A:752:VAL:HG21	2:A:830:VAL:HG21	2.02	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:B:131:GLN:HG3	3:B:132:TYR:CD2	2.53	0.42
1:C:189:GLN:NE2	1:C:190:ALA:O	2.53	0.42
2:A:132:VAL:HG21	2:A:175:ARG:HH21	1.85	0.42
3:B:168:HIS:ND1	3:B:168:HIS:N	2.67	0.42
4:F:9:IDS:O3	4:F:10:SGN:N2	2.53	0.42
1:E:171:ARG:HG2	1:E:173:PRO:HD3	2.00	0.42
2:A:356:GLU:O	2:A:360:ILE:HG13	2.20	0.42
2:A:870:ILE:HG13	2:A:909:LEU:HD11	2.02	0.42
3:B:96:MET:HB2	3:B:115:PHE:HE1	1.84	0.42
1:C:168:VAL:HG22	1:C:211:MET:HB2	2.01	0.41
1:C:186:LYS:HG2	1:C:187:ASP:OD2	2.19	0.41
2:A:136:THR:HG21	2:A:179:ARG:HB3	2.01	0.41
2:A:811:THR:HG21	2:A:851:GLY:HA3	2.02	0.41
1:C:297:ASP:OD1	1:C:297:ASP:N	2.53	0.41
1:E:226:VAL:HG13	1:E:233:ILE:HB	2.03	0.41
1:C:181:THR:HA	1:C:204:HIS:CE1	2.56	0.41
1:C:270:LEU:HD23	1:C:317:VAL:HG22	2.02	0.41
2:A:879:LEU:HD23	2:A:882:GLU:HB2	2.02	0.41
2:A:241:TYR:CE2	2:A:323:VAL:HG23	2.55	0.41
2:A:378:GLN:HG3	2:A:379:LEU:HG	2.02	0.41
2:A:476:LEU:O	2:A:494:ALA:HB2	2.20	0.41
1:C:251:LEU:HB2	1:C:344:GLN:HG3	2.03	0.41
1:E:219:ARG:HE	1:E:219:ARG:HB3	1.60	0.41
2:A:295:SER:OG	2:A:296:ILE:N	2.52	0.41
2:A:727:SER:OG	2:A:728:ILE:N	2.52	0.41
1:E:154:ARG:NE	4:F:10:SGN:O2S	2.54	0.41
2:A:649:ARG:O	2:A:653:ARG:HG2	2.20	0.41
2:A:126:SER:OG	2:A:461:MET:SD	2.68	0.41
2:A:171:ARG:HA	2:A:174:ARG:HG2	2.02	0.41
2:A:531:TYR:O	2:A:921:THR:HB	2.21	0.41
3:B:149:MET:HE2	3:B:149:MET:C	2.46	0.41
1:E:269:LEU:HD23	1:E:283:TRP:CZ3	2.55	0.41
2:A:344:ASN:OD1	2:A:344:ASN:N	2.54	0.41
2:A:651:LEU:HD23	2:A:651:LEU:HA	1.97	0.41
2:A:300:SER:OG	2:A:301:HIS:N	2.54	0.41
2:A:515:LEU:HD12	2:A:516:GLU:N	2.36	0.41
2:A:754:GLU:HG3	2:A:773:VAL:HB	2.03	0.41
1:E:155:MET:HG3	1:E:173:PRO:HD2	2.02	0.40
1:E:163:PRO:HA	1:E:242:LEU:HG	2.03	0.40
1:C:186:LYS:N	1:C:189:GLN:O	2.54	0.40
1:C:255:LEU:HD23	1:C:255:LEU:HA	1.89	0.40

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:186:LYS:HG3	1:E:187:ASP:OD2	2.22	0.40
2:A:748:VAL:CG1	2:A:830:VAL:HG23	2.51	0.40
3:B:56:HIS:HA	3:B:70:TYR:CE1	2.56	0.40
3:B:93:TYR:CE2	3:B:108:PHE:HB2	2.57	0.40
1:C:201:ARG:HG3	1:C:203:ARG:HG3	2.03	0.40
1:E:280:HIS:HE1	1:E:282:GLN:HG2	1.86	0.40
2:A:70:GLY:HA3	2:A:458:TRP:CE3	2.56	0.40
2:A:194:TRP:CD1	2:A:194:TRP:N	2.89	0.40
2:A:856:LEU:HB3	2:A:907:ILE:HD12	2.02	0.40
2:A:871:ILE:HD12	2:A:871:ILE:HA	1.86	0.40
3:B:43:TYR:O	3:B:158:LEU:N	2.54	0.40
3:B:100:GLY:C	3:B:142:LYS:HG3	2.46	0.40
1:C:160:HIS:CG	1:C:170:PHE:HE2	2.39	0.40
2:A:77:GLU:OE2	2:A:155:ARG:NE	2.55	0.40
1:E:149:TRP:CD1	1:E:149:TRP:H	2.40	0.40
2:A:419:VAL:HG13	2:A:430:TYR:HB2	2.02	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	C	211/213 (99%)	200 (95%)	11 (5%)	0	100	100
1	E	200/213 (94%)	181 (90%)	19 (10%)	0	100	100
2	A	917/942 (97%)	861 (94%)	56 (6%)	0	100	100
3	B	177/179 (99%)	166 (94%)	11 (6%)	0	100	100
All	All	1505/1547 (97%)	1408 (94%)	97 (6%)	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	C	180/180 (100%)	170 (94%)	10 (6%)	19	49
1	E	171/180 (95%)	159 (93%)	12 (7%)	14	41
2	A	792/809 (98%)	761 (96%)	31 (4%)	28	59
3	B	156/156 (100%)	147 (94%)	9 (6%)	18	48
All	All	1299/1325 (98%)	1237 (95%)	62 (5%)	24	54

All (62) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	C	168	VAL
1	C	226	VAL
1	C	237	TYR
1	C	245	SER
1	C	267	VAL
1	C	270	LEU
1	C	287	ILE
1	C	297	ASP
1	C	302	VAL
1	C	345	SER
1	E	149	TRP
1	E	168	VAL
1	E	169	LYS
1	E	214	VAL
1	E	230	VAL
1	E	232	SER
1	E	241	VAL
1	E	259	THR
1	E	270	LEU
1	E	276	ASP
1	E	320	LEU
1	E	323	VAL
2	A	56	LEU
2	A	124	VAL

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
2	A	144	VAL
2	A	222	LEU
2	A	289	THR
2	A	348	ILE
2	A	459	SER
2	A	483	SER
2	A	528	VAL
2	A	582	ILE
2	A	602	ILE
2	A	608	GLN
2	A	641	MET
2	A	683	LEU
2	A	696	THR
2	A	767	SER
2	A	789	PHE
2	A	790	THR
2	A	797	ILE
2	A	811	THR
2	A	816	SER
2	A	828	LEU
2	A	836	ILE
2	A	871	ILE
2	A	875	ILE
2	A	879	LEU
2	A	888	VAL
2	A	907	ILE
2	A	940	SER
2	A	950	SER
2	A	963	CYS
3	B	31	LEU
3	B	34	SER
3	B	44	THR
3	B	79	ASP
3	B	86	THR
3	B	102	ILE
3	B	159	SER
3	B	168	HIS
3	B	173	ILE

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

Mol	Chain	Res	Type
1	C	189	GLN
1	C	286	HIS
1	E	145	GLN
1	E	160	HIS
1	E	166	ASN
1	E	206	HIS
1	E	228	ASN
1	E	282	GLN
2	A	40	GLN
2	A	75	GLN
2	A	146	HIS
2	A	290	GLN
2	A	388	GLN
2	A	553	HIS
2	A	592	HIS
2	A	831	GLN
2	A	844	GLN
3	B	128	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 ⓘ

10 monosaccharides 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	$\# Z > 2$
4	IDS	F	1	4	17,17,17	1.76	6 (35%)	22,26,26	2.57	4 (18%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
4	SGN	F	10	4	19,19,20	2.51	2 (10%)	23,29,31	1.89	3 (13%)
4	SGN	F	2	4	19,19,20	1.51	2 (10%)	23,29,31	1.92	5 (21%)
4	IDS	F	3	4	16,16,17	2.10	4 (25%)	16,24,26	2.85	2 (12%)
4	SGN	F	4	4	19,19,20	2.61	3 (15%)	23,29,31	2.03	4 (17%)
4	IDS	F	5	4	16,16,17	2.07	4 (25%)	16,24,26	2.30	4 (25%)
4	SGN	F	6	4	19,19,20	2.60	3 (15%)	23,29,31	2.97	4 (17%)
4	IDS	F	7	4	16,16,17	2.05	4 (25%)	16,24,26	3.16	3 (18%)
4	SGN	F	8	4	19,19,20	2.50	2 (10%)	23,29,31	3.00	7 (30%)
4	IDS	F	9	4	16,16,17	2.04	5 (31%)	16,24,26	3.35	6 (37%)

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
4	IDS	F	1	4	1/1/7/7	0/9/29/29	0/1/1/1
4	SGN	F	10	4	-	6/11/28/31	0/1/1/1
4	SGN	F	2	4	-	3/11/28/31	0/1/1/1
4	IDS	F	3	4	-	0/9/26/29	0/1/1/1
4	SGN	F	4	4	1/1/6/8	7/11/28/31	0/1/1/1
4	IDS	F	5	4	1/1/6/7	2/9/26/29	0/1/1/1
4	SGN	F	6	4	-	5/11/28/31	0/1/1/1
4	IDS	F	7	4	1/1/6/7	0/9/26/29	0/1/1/1
4	SGN	F	8	4	1/1/6/8	4/11/28/31	0/1/1/1
4	IDS	F	9	4	-	1/9/26/29	0/1/1/1

All (35) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	F	4	SGN	O1S-S1	9.20	1.52	1.42
4	F	6	SGN	O2S-S1	9.13	1.52	1.42
4	F	10	SGN	O1S-S1	9.12	1.52	1.42
4	F	8	SGN	O2S-S1	9.06	1.52	1.42
4	F	10	SGN	S1-N2	5.32	1.66	1.59
4	F	4	SGN	S1-N2	5.31	1.66	1.59
4	F	6	SGN	S1-N2	5.28	1.66	1.59
4	F	2	SGN	S1-N2	5.22	1.66	1.59
4	F	8	SGN	S1-N2	4.92	1.65	1.59

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	F	3	IDS	O5-C1	-4.84	1.35	1.43
4	F	5	IDS	O5-C1	-4.83	1.35	1.43
4	F	7	IDS	O5-C1	-4.75	1.35	1.43
4	F	9	IDS	O5-C1	-4.61	1.36	1.43
4	F	3	IDS	O2-C2	-4.07	1.41	1.47
4	F	5	IDS	O2-C2	-3.89	1.41	1.47
4	F	7	IDS	O2-C2	-3.83	1.41	1.47
4	F	1	IDS	C1-C2	-3.70	1.49	1.52
4	F	9	IDS	O2-C2	-3.38	1.42	1.47
4	F	7	IDS	C3-C2	-3.22	1.46	1.53
4	F	3	IDS	C3-C2	-3.17	1.46	1.53
4	F	9	IDS	C3-C2	-3.08	1.46	1.53
4	F	5	IDS	C3-C2	-3.08	1.46	1.53
4	F	9	IDS	O6A-C6	3.00	1.31	1.22
4	F	1	IDS	O5-C1	-2.97	1.35	1.42
4	F	1	IDS	O5-C5	-2.27	1.39	1.43
4	F	1	IDS	O2-C2	-2.24	1.41	1.46
4	F	1	IDS	C3-C2	-2.12	1.46	1.52
4	F	4	SGN	O4-C4	-2.07	1.37	1.43
4	F	2	SGN	O4-C4	-2.07	1.37	1.43
4	F	9	IDS	O4-C4	-2.05	1.37	1.43
4	F	5	IDS	O4-C4	-2.05	1.37	1.43
4	F	1	IDS	O4-C4	-2.04	1.37	1.43
4	F	3	IDS	O4-C4	-2.04	1.37	1.43
4	F	7	IDS	O4-C4	-2.03	1.37	1.43
4	F	6	SGN	O4-C4	-2.03	1.37	1.43

All (42) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	F	9	IDS	O4-C4-C5	11.75	136.59	109.76
4	F	1	IDS	O4-C4-C3	10.78	135.78	110.38
4	F	7	IDS	O4-C4-C3	10.63	135.42	110.38
4	F	6	SGN	O4-C4-C3	10.56	135.26	110.38
4	F	3	IDS	O4-C4-C5	10.38	133.47	109.76
4	F	8	SGN	O4-C4-C5	9.95	133.83	109.32
4	F	5	IDS	O4-C4-C3	6.84	126.50	110.38
4	F	6	SGN	O1S-S1-O2S	-6.62	105.63	120.36
4	F	10	SGN	O1S-S1-O2S	-6.61	105.66	120.36
4	F	4	SGN	O1S-S1-O2S	-6.49	105.93	120.36
4	F	8	SGN	O1S-S1-O2S	-6.44	106.02	120.36
4	F	7	IDS	O4-C4-C5	-5.27	97.72	109.76

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	F	6	SGN	O6S-S2-O4S	4.87	125.59	108.56
4	F	2	SGN	O4-C4-C3	-4.86	98.92	110.38
4	F	2	SGN	O6S-S2-O5S	4.80	125.34	108.56
4	F	4	SGN	O6S-S2-O4S	4.78	125.28	108.56
4	F	5	IDS	O4-C4-C5	-3.94	100.76	109.76
4	F	8	SGN	C4-C3-C2	-3.79	105.46	111.02
4	F	8	SGN	O5-C1-C2	-3.67	105.61	111.29
4	F	10	SGN	O5S-S2-O4S	3.39	125.30	112.24
4	F	10	SGN	C1-O5-C5	-3.36	107.68	112.19
4	F	6	SGN	C1-O5-C5	-3.29	107.78	112.19
4	F	8	SGN	O5S-S2-O4S	3.28	124.90	112.24
4	F	9	IDS	O2S-S-O1S	-3.07	100.39	112.24
4	F	9	IDS	O4-C4-C3	-2.92	103.50	110.38
4	F	9	IDS	O3S-S-O2	2.50	112.12	106.37
4	F	2	SGN	O4-C4-C5	-2.44	103.31	109.32
4	F	2	SGN	C1-O5-C5	-2.42	108.95	112.19
4	F	4	SGN	C4-C3-C2	-2.37	107.54	111.02
4	F	2	SGN	O1S-S1-O2S	2.23	125.33	120.36
4	F	1	IDS	O3S-S-O2	2.16	111.33	106.37
4	F	5	IDS	O3S-S-O2	2.16	111.33	106.37
4	F	9	IDS	O2-C2-C3	2.14	109.94	106.95
4	F	8	SGN	O1S-S1-N2	-2.14	105.31	108.88
4	F	8	SGN	C6-C5-C4	-2.13	107.59	112.07
4	F	7	IDS	O3S-S-O2	2.13	111.27	106.37
4	F	4	SGN	C1-O5-C5	-2.10	109.38	112.19
4	F	3	IDS	O3S-S-O1S	-2.08	101.28	108.56
4	F	1	IDS	O4-C4-C5	2.08	114.50	109.76
4	F	1	IDS	O3S-S-O1S	-2.07	101.30	108.56
4	F	5	IDS	O3S-S-O2S	-2.07	101.33	108.56
4	F	9	IDS	O5-C1-C2	2.02	113.60	109.51

All (5) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
4	F	1	IDS	C4
4	F	4	SGN	C4
4	F	5	IDS	C4
4	F	7	IDS	C4
4	F	8	SGN	C4

All (28) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	F	4	SGN	C4-C5-C6-O6
4	F	4	SGN	C2-N2-S1-O2S
4	F	5	IDS	C4-C5-C6-O6A
4	F	5	IDS	C4-C5-C6-O6B
4	F	6	SGN	C1-C2-N2-S1
4	F	6	SGN	C3-C2-N2-S1
4	F	6	SGN	C2-N2-S1-O3S
4	F	8	SGN	C2-N2-S1-O2S
4	F	8	SGN	C2-N2-S1-O3S
4	F	9	IDS	C1-C2-O2-S
4	F	10	SGN	C2-N2-S1-O2S
4	F	10	SGN	C6-O6-S2-O6S
4	F	2	SGN	C6-O6-S2-O5S
4	F	10	SGN	C6-O6-S2-O5S
4	F	2	SGN	C2-N2-S1-O2S
4	F	8	SGN	C2-N2-S1-O1S
4	F	4	SGN	C6-O6-S2-O6S
4	F	2	SGN	C6-O6-S2-O4S
4	F	10	SGN	C6-O6-S2-O4S
4	F	4	SGN	O5-C5-C6-O6
4	F	10	SGN	O5-C5-C6-O6
4	F	8	SGN	C6-O6-S2-O5S
4	F	4	SGN	C1-C2-N2-S1
4	F	4	SGN	C3-C2-N2-S1
4	F	6	SGN	C2-N2-S1-O2S
4	F	4	SGN	C6-O6-S2-O5S
4	F	10	SGN	C5-C6-O6-S2
4	F	6	SGN	O5-C5-C6-O6

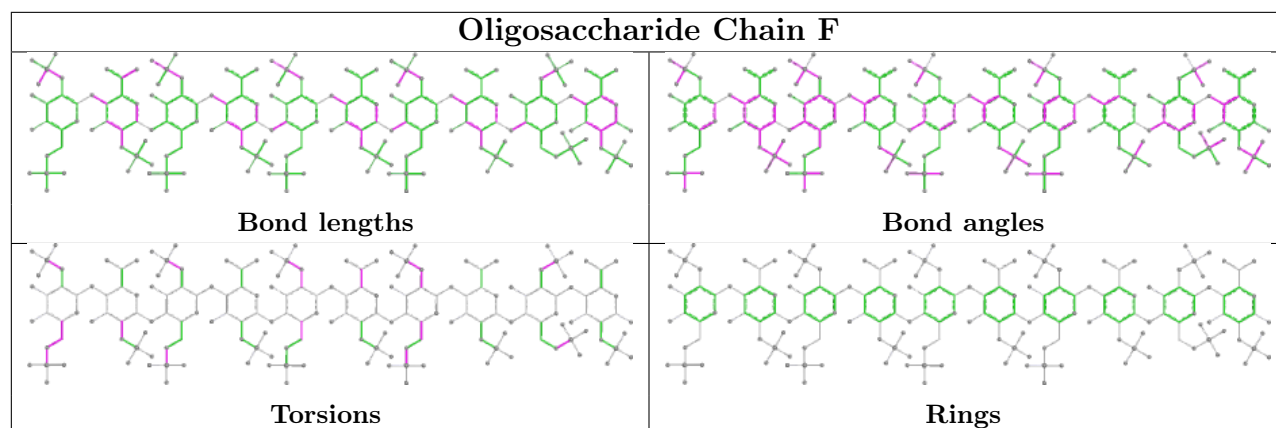
There are no ring outliers.

8 monomers are involved in 11 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	F	2	SGN	2	0
4	F	4	SGN	2	0
4	F	10	SGN	3	0
4	F	6	SGN	1	0
4	F	8	SGN	1	0
4	F	3	IDS	1	0
4	F	9	IDS	2	0
4	F	5	IDS	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 oligosaccharide.



5.6 Ligand geometry [i](#)

Of 2 ligands modelled in this entry, 2 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.

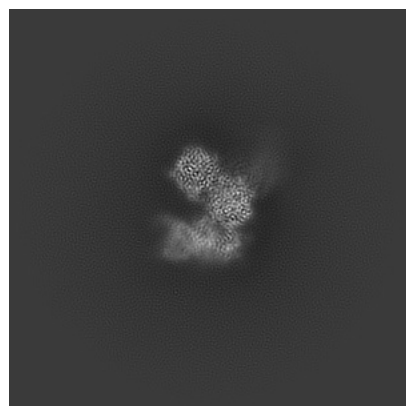
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-34084. These allow visual inspection of the internal detail of the map and identification of artifacts.

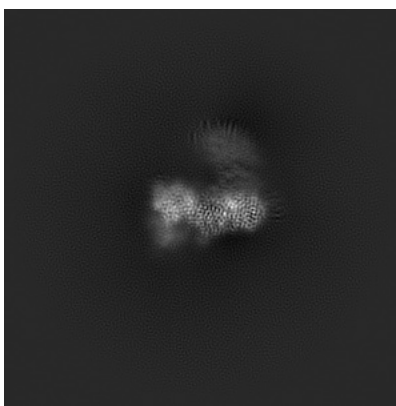
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

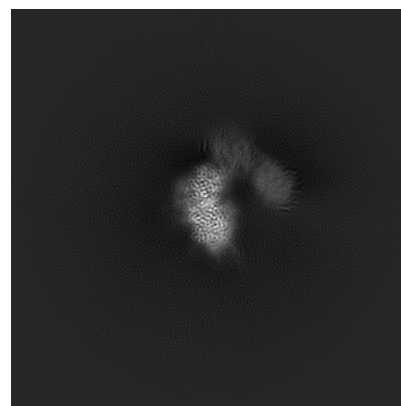
6.1.1 Primary map



X

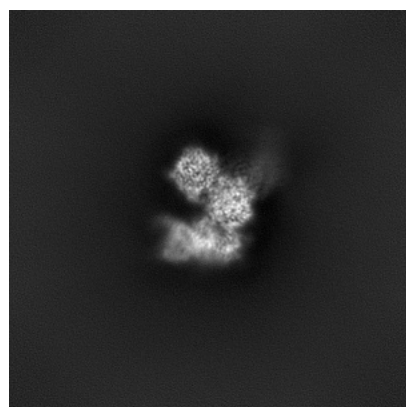


Y

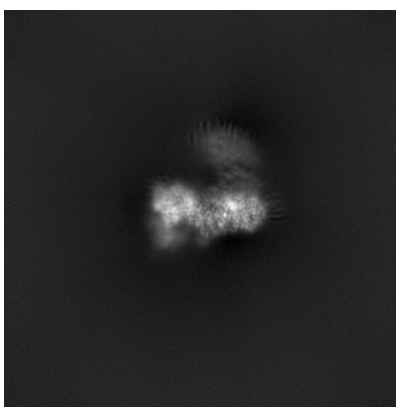


Z

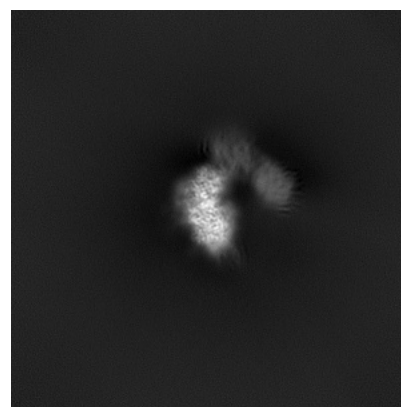
6.1.2 Raw map



X



Y

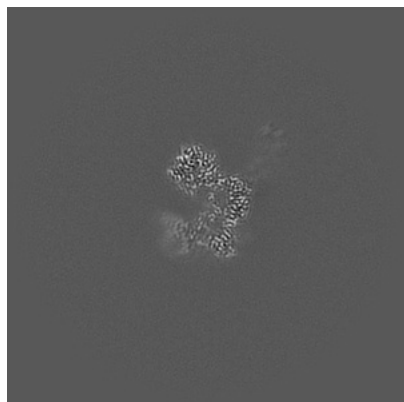


Z

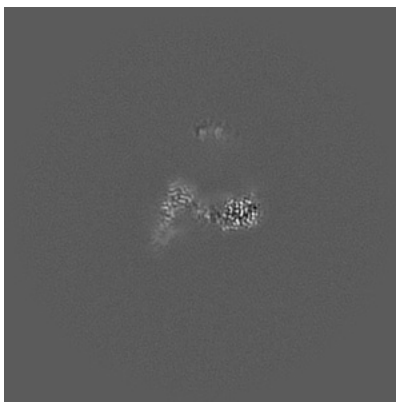
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

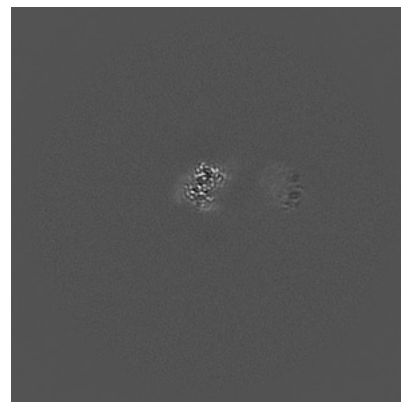
6.2.1 Primary map



X Index: 200

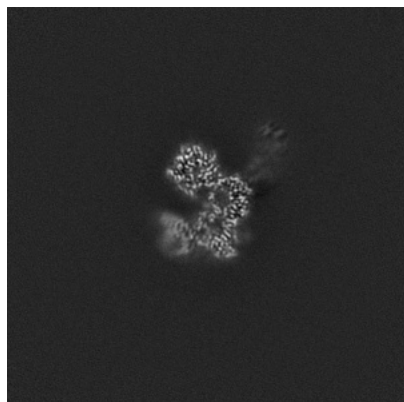


Y Index: 200

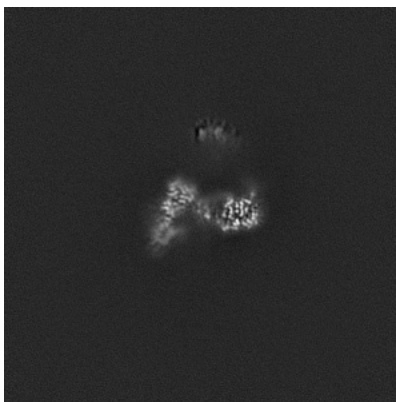


Z Index: 200

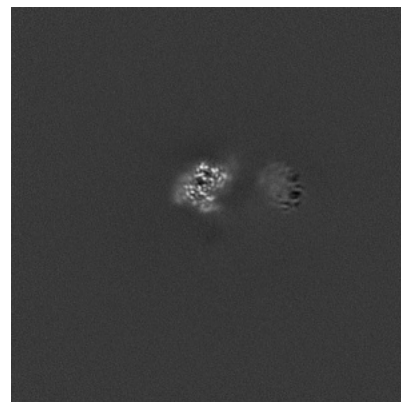
6.2.2 Raw map



X Index: 200



Y Index: 200

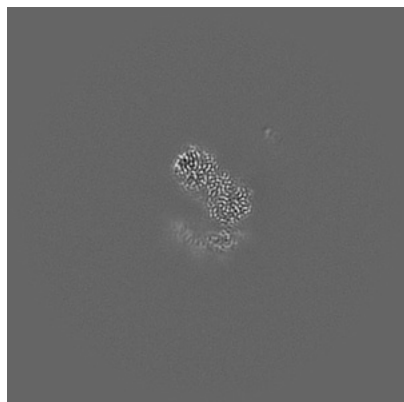


Z Index: 200

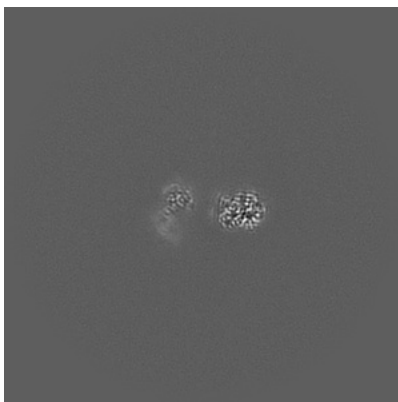
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

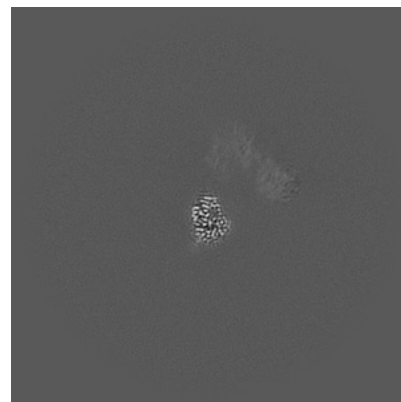
6.3.1 Primary map



X Index: 192

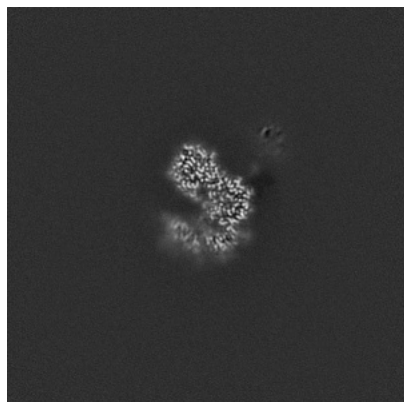


Y Index: 190

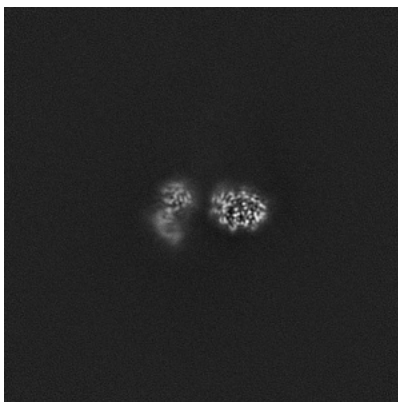


Z Index: 238

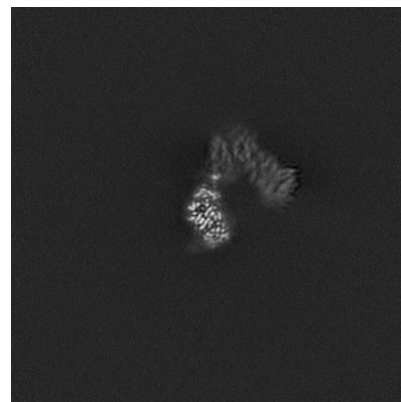
6.3.2 Raw map



X Index: 195



Y Index: 187

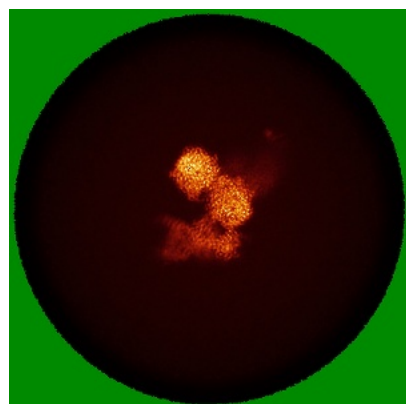


Z Index: 231

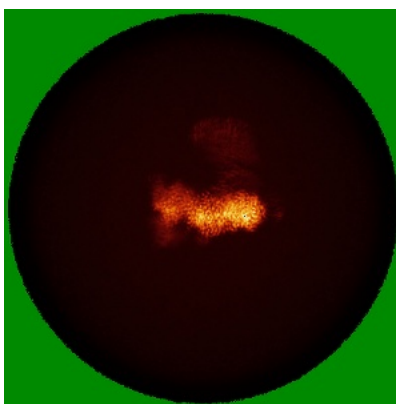
The images above show the largest variance slices of the map in three orthogonal directions.

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

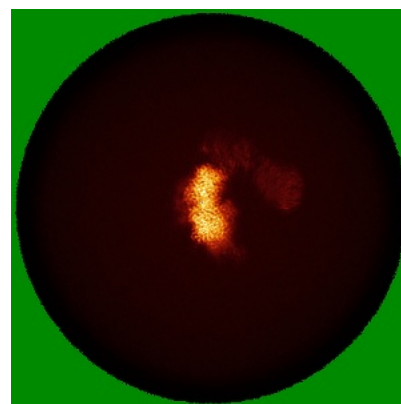
6.4.1 Primary map



X

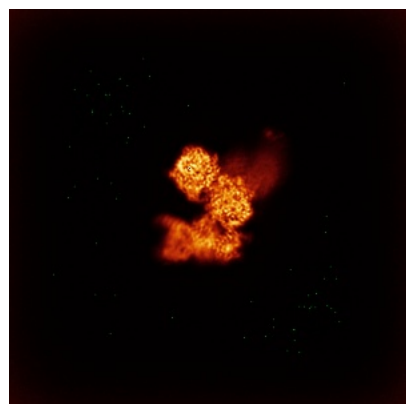


Y

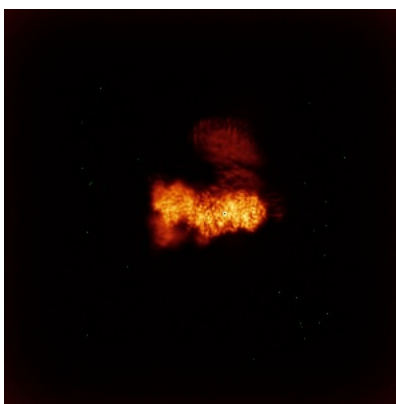


Z

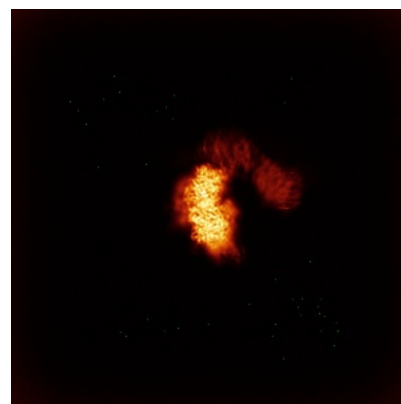
6.4.2 Raw map



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.

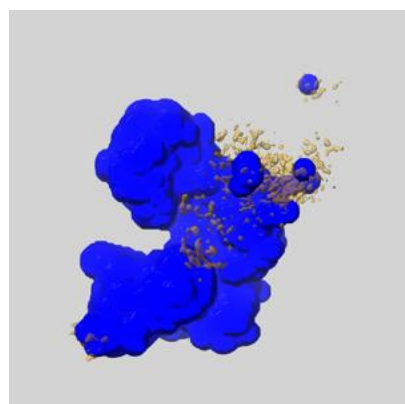
6.6 Mask visualisation [i](#)

This section shows the 3D surface view of the primary map at 50% transparency overlaid with the specified mask at 0% transparency

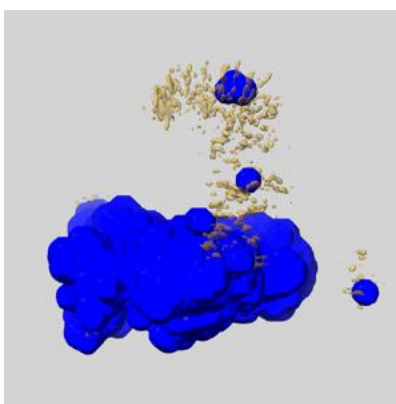
A mask typically either:

- Encompasses the whole structure
- Separates out a domain, a functional unit, a monomer or an area of interest from a larger structure

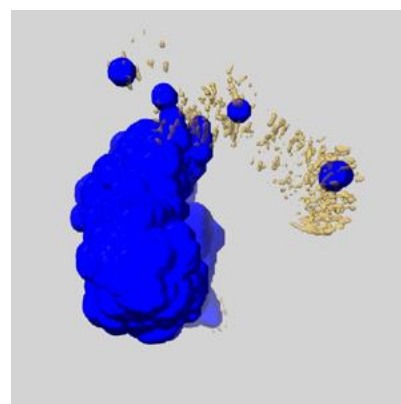
6.6.1 emd_34084_msk_1.map [i](#)



X



Y

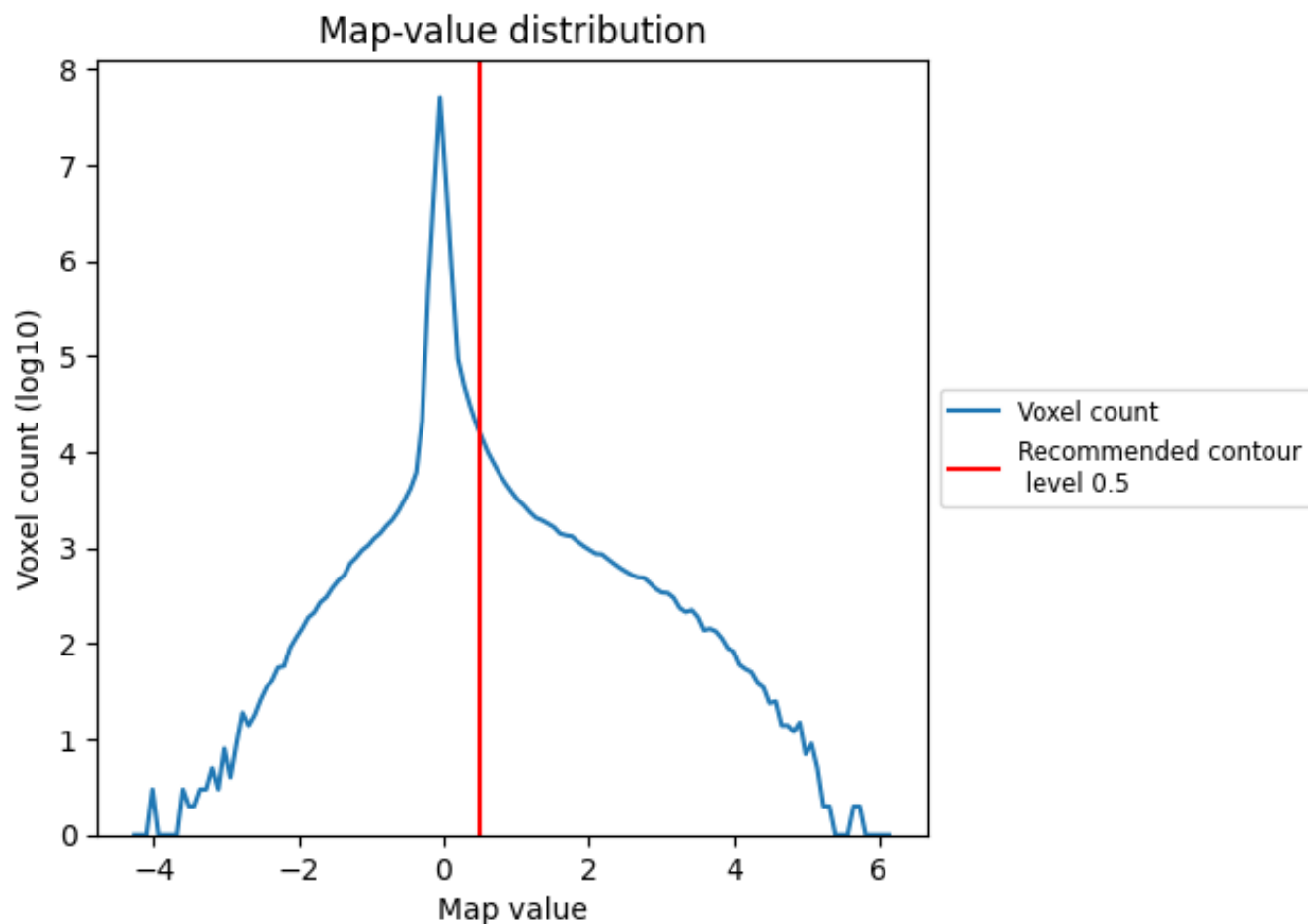


Z

7 Map analysis [i](#)

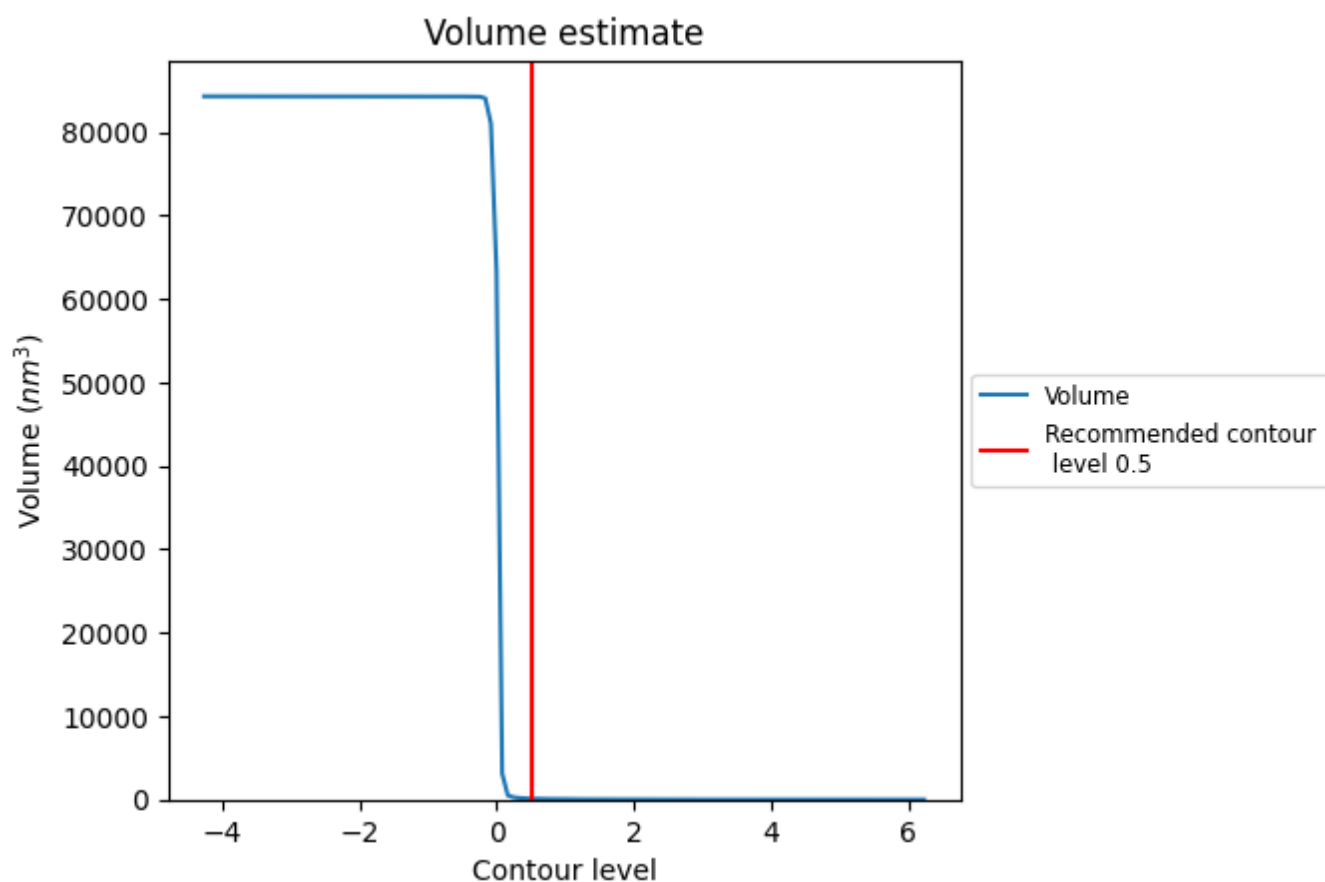
This section contains the results of statistical analysis of the map.

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.

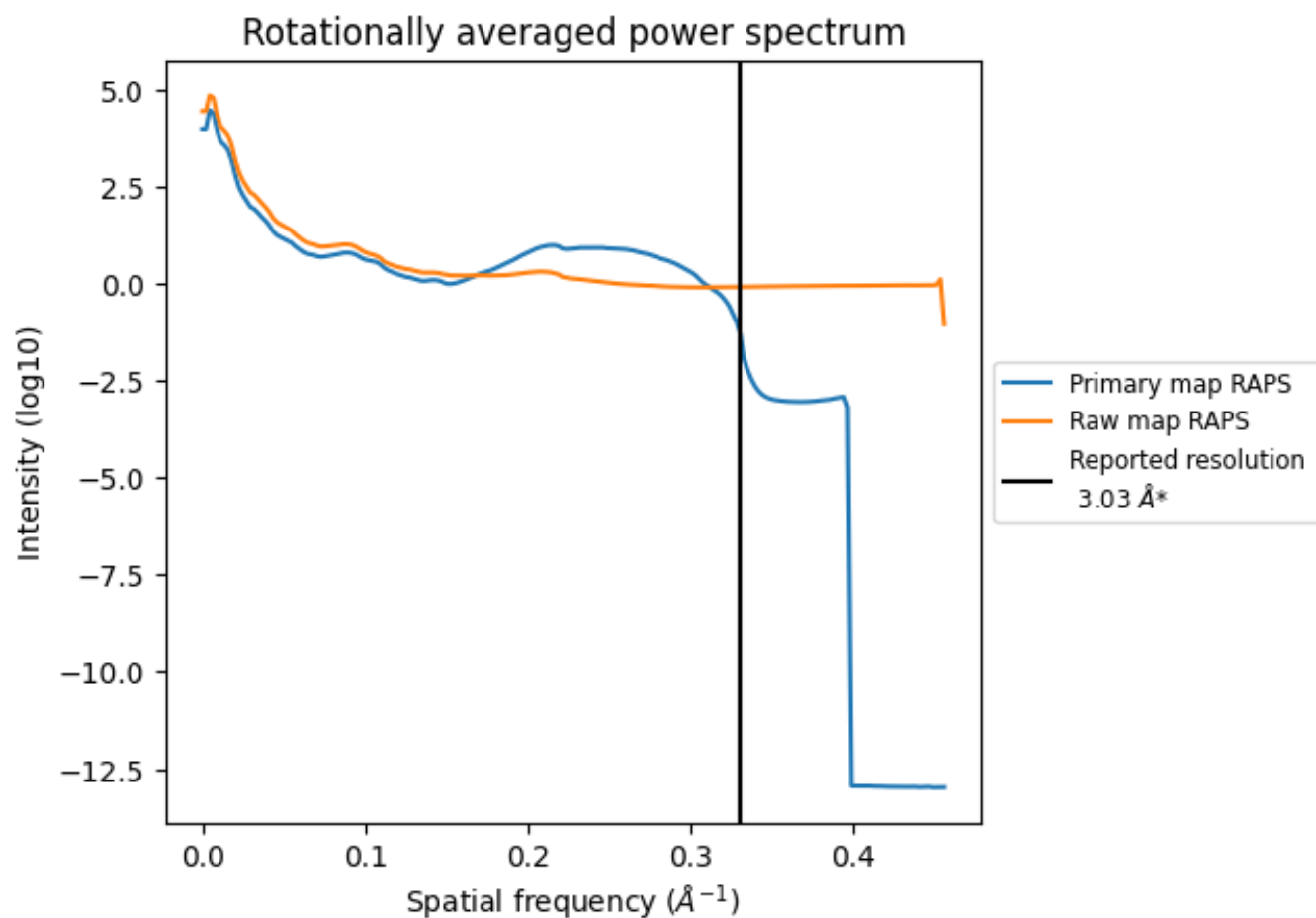
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 110 nm³; this corresponds to an approximate mass of 100 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 ⓘ

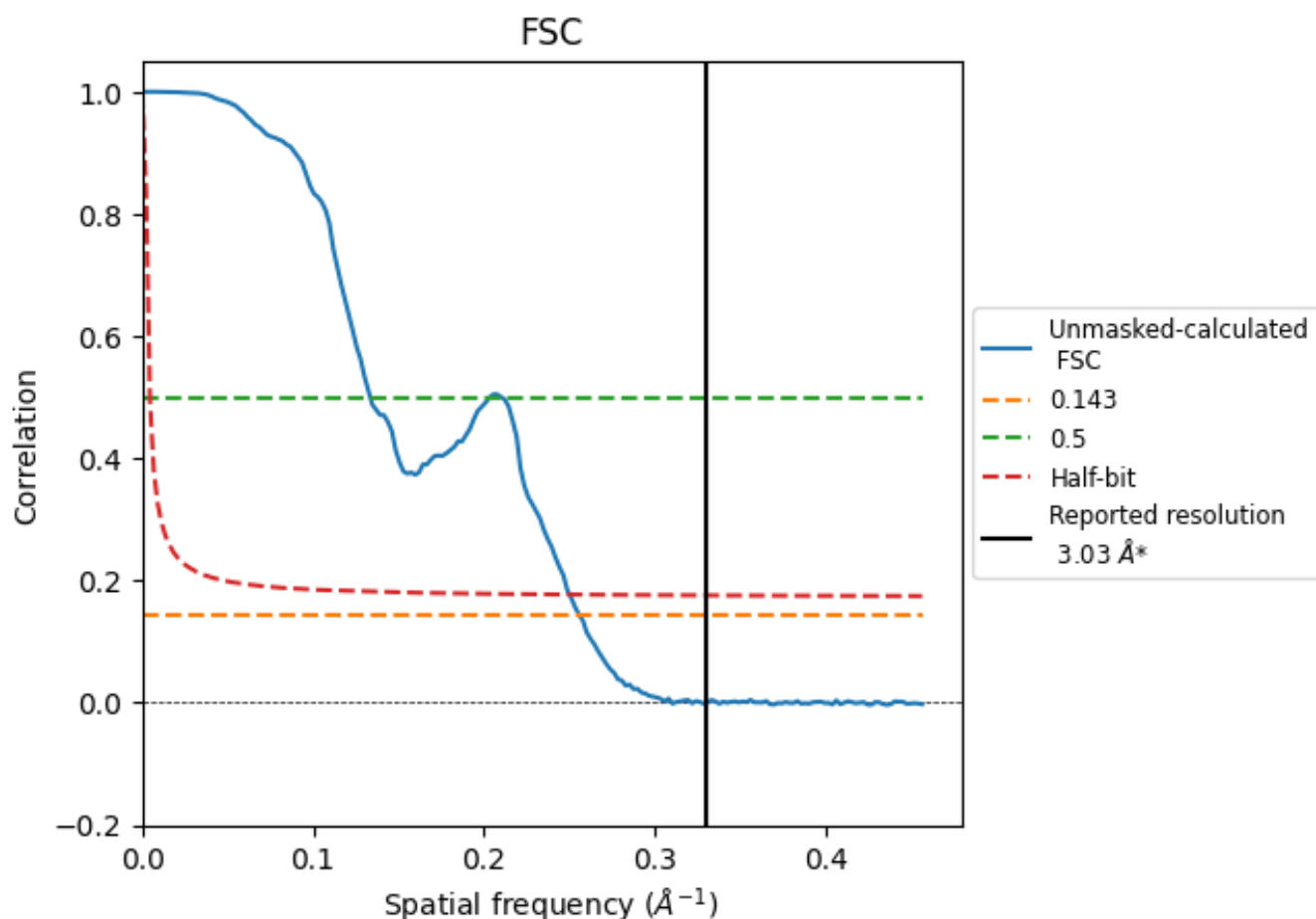


*Reported resolution corresponds to spatial frequency of 0.330 Å⁻¹

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 0.330 $\text{\AA}^{-1}$

8.2 Resolution estimates [i](#)

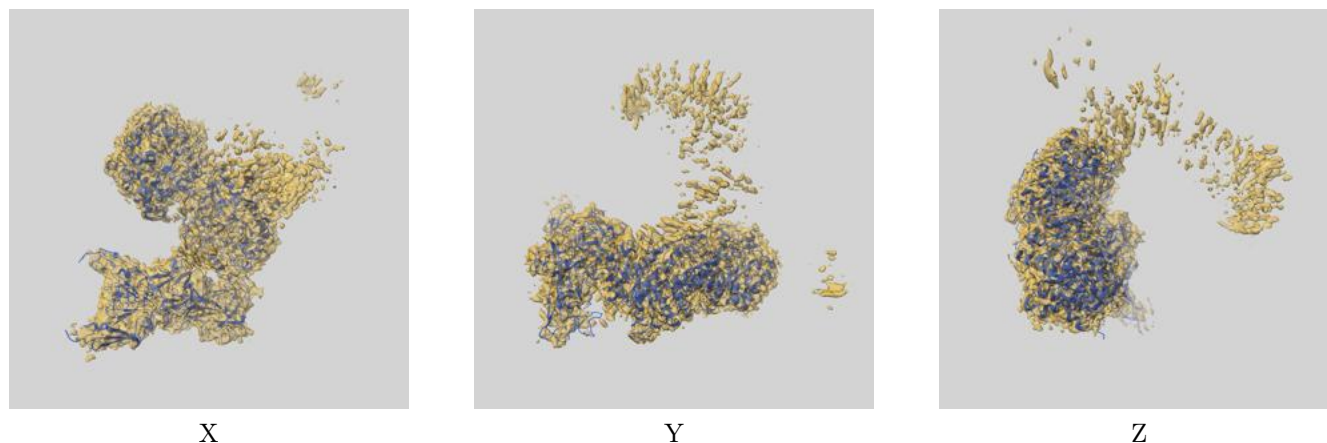
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.03	-	-
Author-provided FSC curve	-	-	-
Unmasked-calculated*	3.91	7.50	4.00

*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 3.91 differs from the reported value 3.03 by more than 10 %

9 Map-model fit [i](#)

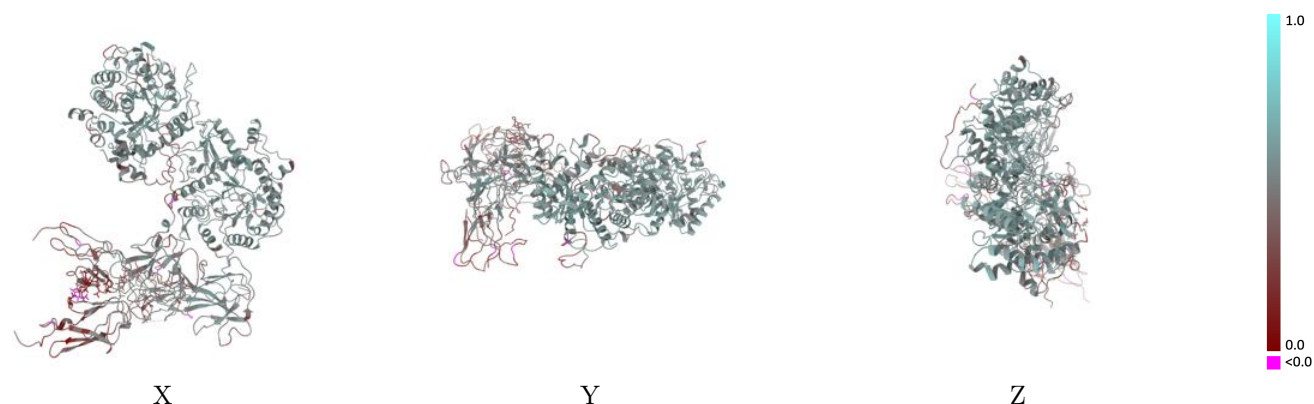
This section contains information regarding the fit between EMDB map EMD-34084 and PDB model 7YSW. Per-residue inclusion information can be found in [section 3](#) on [page 6](#).

9.1 Map-model overlay [i](#)



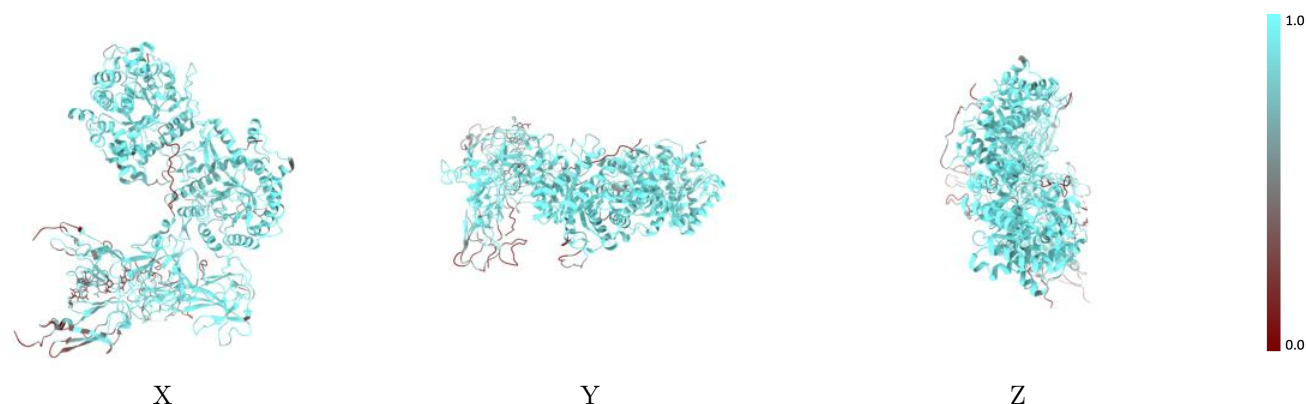
The images above show the 3D surface view of the map at the recommended contour level 0.5 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



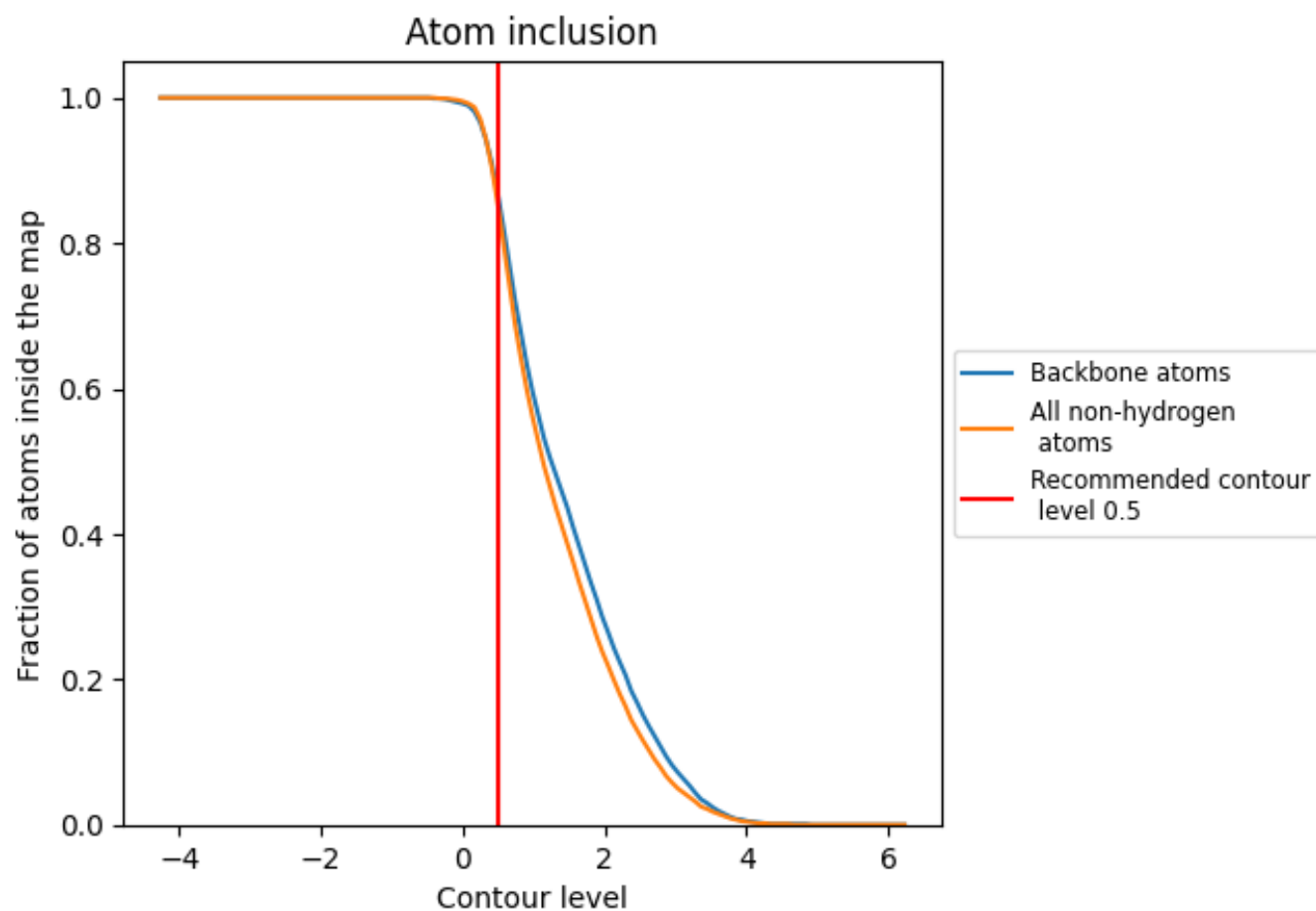
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.5).

9.4 Atom inclusion [i](#)



At the recommended contour level, 86% of all backbone atoms, 85% 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 (0.5) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.8480	0.4820
A	0.9230	0.5410
B	0.7670	0.4400
C	0.8330	0.4430
E	0.6260	0.3200
F	0.5000	0.1650

