



Full wwPDB EM Validation Report ⓘ

Jul 6, 2026 – 07:56 PM JST

PDB ID : 9VV6 / pdb_00009vv6
EMDB ID : EMD-65376
Title : The structure of ITN bound OXGR1
Authors : Su, Q.; Liang, E.Y.; Ma, T.S.; Chen, Z.Y.; Tang, X.F.
Deposited on : 2025-07-14
Resolution : 2.62 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.dev133
Mogul : 1.8.5 (274361), CSD as541be (2020)
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) : 2.50

Continued from previous page...

Mol	Chain	Length	Quality of chain
5	E	547	 A horizontal bar chart showing the quality of chain 5. The bar is divided into three segments: a red segment at the beginning (0-34%), a yellow segment (34-58%), and a grey segment (58-100%). The percentages 34%, 8%, and 58% are labeled below the segments.

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
6	ITN	A	1301	-	X	-	-

2 Entry composition [i](#)

There are 6 unique types of molecules in this entry. The entry contains 9047 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 Soluble cytochrome b562,2-oxoglutarate receptor 1,Soluble cytochrome b562,2-oxoglutarate receptor 1,Soluble cytochrome b562,2-oxoglutarate receptor 1,Fusion protein,Maltose/maltodextrin-binding periplasmic protein,Maltose/maltodextrin-binding periplasmic protein,Maltose/maltodextrin-binding periplasmic protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	291	Total	C	N	O	S	0	0
			2337	1546	375	395	21		

There are 50 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-141	MET	-	initiating methionine	UNP P0ABE7
A	-140	ASP	-	expression tag	UNP P0ABE7
A	-139	MET	-	expression tag	UNP P0ABE7
A	-138	ARG	-	expression tag	UNP P0ABE7
A	-137	VAL	-	expression tag	UNP P0ABE7
A	-136	PRO	-	expression tag	UNP P0ABE7
A	-135	ALA	-	expression tag	UNP P0ABE7
A	-134	GLN	-	expression tag	UNP P0ABE7
A	-133	LEU	-	expression tag	UNP P0ABE7
A	-132	LEU	-	expression tag	UNP P0ABE7
A	-131	GLY	-	expression tag	UNP P0ABE7
A	-130	LEU	-	expression tag	UNP P0ABE7
A	-129	LEU	-	expression tag	UNP P0ABE7
A	-128	LEU	-	expression tag	UNP P0ABE7
A	-127	LEU	-	expression tag	UNP P0ABE7
A	-126	TRP	-	expression tag	UNP P0ABE7
A	-125	LEU	-	expression tag	UNP P0ABE7
A	-124	SER	-	expression tag	UNP P0ABE7
A	-123	GLY	-	expression tag	UNP P0ABE7
A	-122	ALA	-	expression tag	UNP P0ABE7
A	-121	ARG	-	expression tag	UNP P0ABE7
A	-120	CYS	-	expression tag	UNP P0ABE7
A	-119	MET	-	expression tag	UNP P0ABE7
A	-118	ASP	-	expression tag	UNP P0ABE7
A	-117	TYR	-	expression tag	UNP P0ABE7

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
A	-116	LYS	-	expression tag	UNP P0ABE7
A	-115	ASP	-	expression tag	UNP P0ABE7
A	-114	ASP	-	expression tag	UNP P0ABE7
A	-113	ASP	-	expression tag	UNP P0ABE7
A	-112	ASP	-	expression tag	UNP P0ABE7
A	-111	LYS	-	expression tag	UNP P0ABE7
A	-110	GLY	-	expression tag	UNP P0ABE7
A	-109	GLY	-	expression tag	UNP P0ABE7
A	-108	SER	-	expression tag	UNP P0ABE7
A	-101	TRP	MET	conflict	UNP P0ABE7
A	-6	ILE	HIS	conflict	UNP P0ABE7
A	-2	LEU	-	linker	UNP P0ABE7
A	-1	GLY	-	linker	UNP P0ABE7
A	0	SER	-	linker	UNP P0ABE7
A	879	GLY	-	linker	UNP P0AEX9
A	880	GLY	-	linker	UNP P0AEX9
A	881	GLY	-	linker	UNP P0AEX9
A	882	GLY	-	linker	UNP P0AEX9
A	883	SER	-	linker	UNP P0AEX9
A	884	GLY	-	linker	UNP P0AEX9
A	885	GLY	-	linker	UNP P0AEX9
A	886	GLY	-	linker	UNP P0AEX9
A	887	GLY	-	linker	UNP P0AEX9
A	888	SER	-	linker	UNP P0AEX9
A	889	MET	-	linker	UNP P0AEX9

- Molecule 2 is a protein called Guanine nucleotide-binding protein G(I)/G(S)/G(O) subunit gamma-2.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	C	53	Total	C	N	O	S	0	0
			399	249	69	78	3		

- Molecule 3 is a protein called Fusion protein, Guanine nucleotide-binding protein G(I)/G(S)/G(T) subunit beta-1, Guanine nucleotide-binding protein G(I)/G(S)/G(T) subunit beta-1, Guanine nucleotide-binding protein G(I)/G(S)/G(T) subunit beta-1.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	D	337	Total	C	N	O	S	0	0
			2591	1599	466	505	21		

There are 26 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
D	341	GLY	-	expression tag	UNP P62873
D	342	SER	-	expression tag	UNP P62873
D	343	SER	-	expression tag	UNP P62873
D	344	GLY	-	expression tag	UNP P62873
D	345	GLY	-	expression tag	UNP P62873
D	346	GLY	-	expression tag	UNP P62873
D	347	GLY	-	expression tag	UNP P62873
D	348	SER	-	expression tag	UNP P62873
D	349	GLY	-	expression tag	UNP P62873
D	350	GLY	-	expression tag	UNP P62873
D	351	GLY	-	expression tag	UNP P62873
D	352	GLY	-	expression tag	UNP P62873
D	353	SER	-	expression tag	UNP P62873
D	354	SER	-	expression tag	UNP P62873
D	355	GLY	-	expression tag	UNP P62873
D	356	VAL	-	expression tag	UNP P62873
D	357	SER	-	expression tag	UNP P62873
D	358	GLY	-	expression tag	UNP P62873
D	359	TRP	-	expression tag	UNP P62873
D	360	ARG	-	expression tag	UNP P62873
D	361	LEU	-	expression tag	UNP P62873
D	362	PHE	-	expression tag	UNP P62873
D	363	LYS	-	expression tag	UNP P62873
D	364	LYS	-	expression tag	UNP P62873
D	365	ILE	-	expression tag	UNP P62873
D	366	SER	-	expression tag	UNP P62873

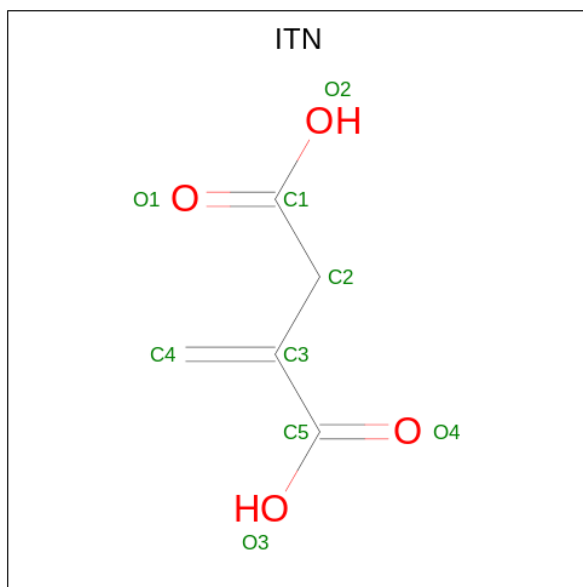
- Molecule 4 is a protein called Gq alpha.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	B	234	Total	C	N	O	S	0	0
			1932	1224	342	358	8		

- Molecule 5 is a protein called scFv-16.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	E	231	Total	C	N	O	S	0	0
			1779	1129	294	346	10		

- Molecule 6 is 2-methylidenebutanedioic acid (CCD ID: ITN) (formula: C₅H₆O₄).

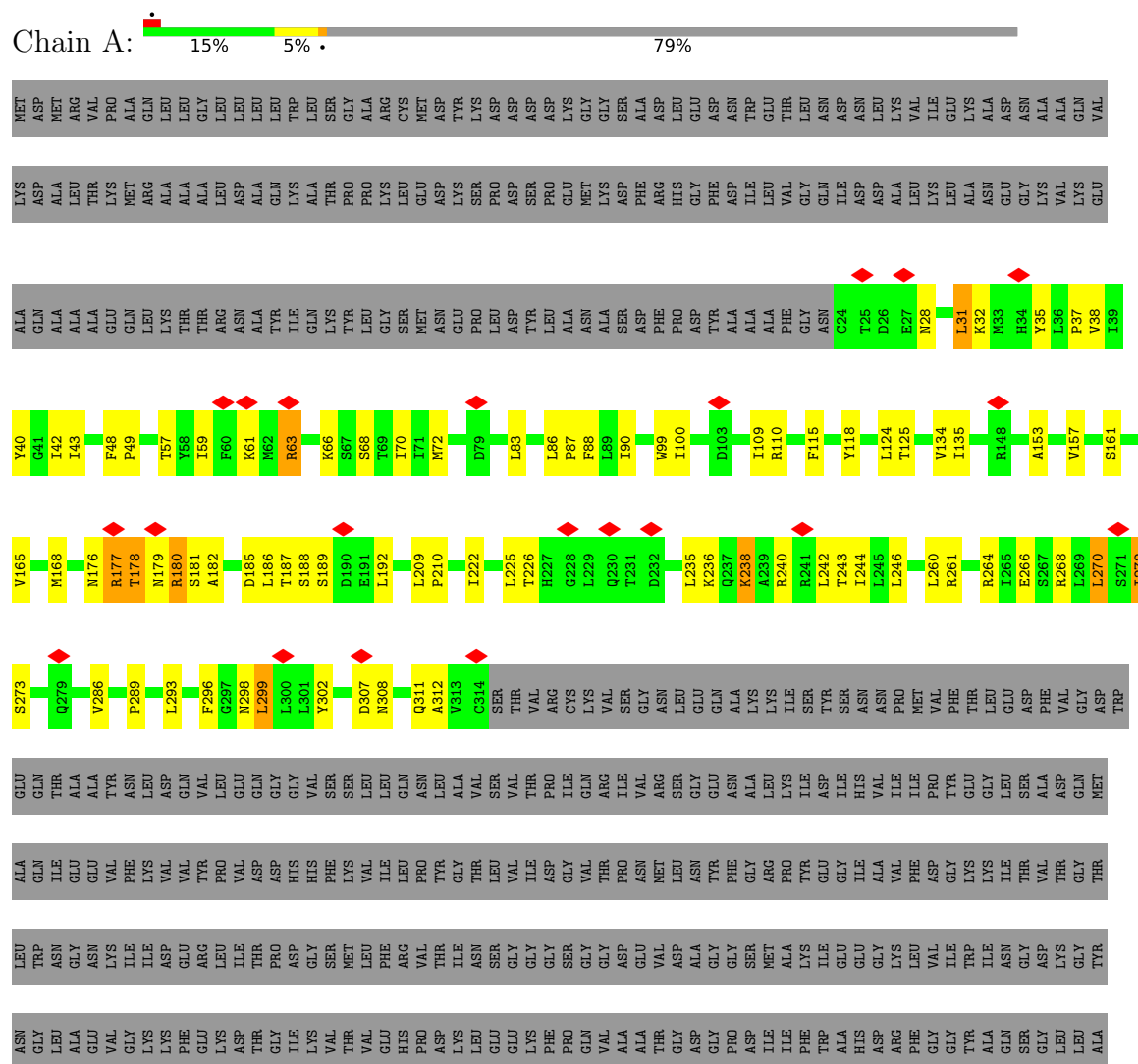


Mol	Chain	Residues	Atoms			AltConf
			Total	C	O	
6	A	1	9	5	4	0

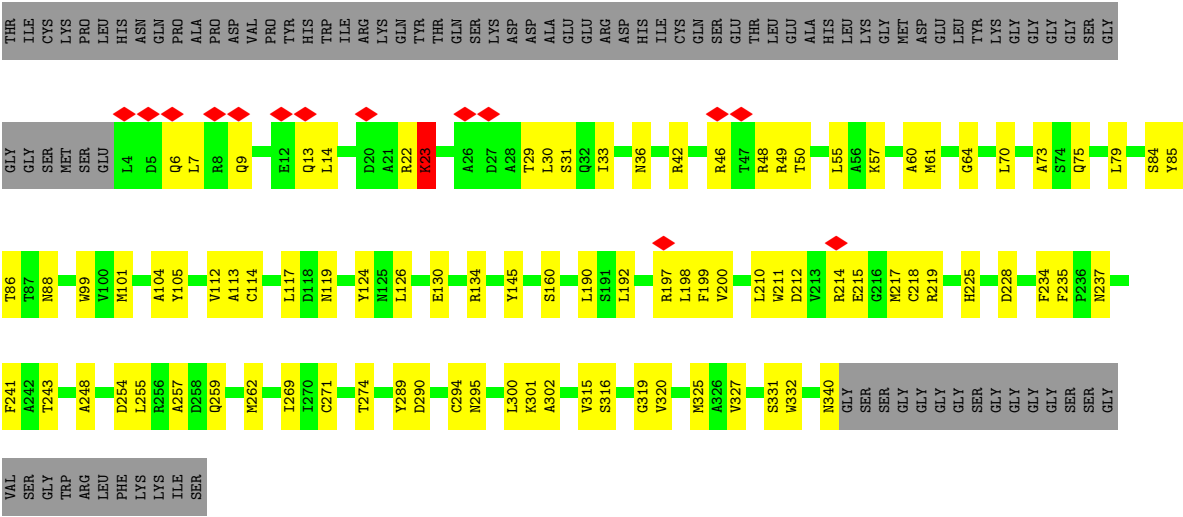
3 Residue-property plots

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.

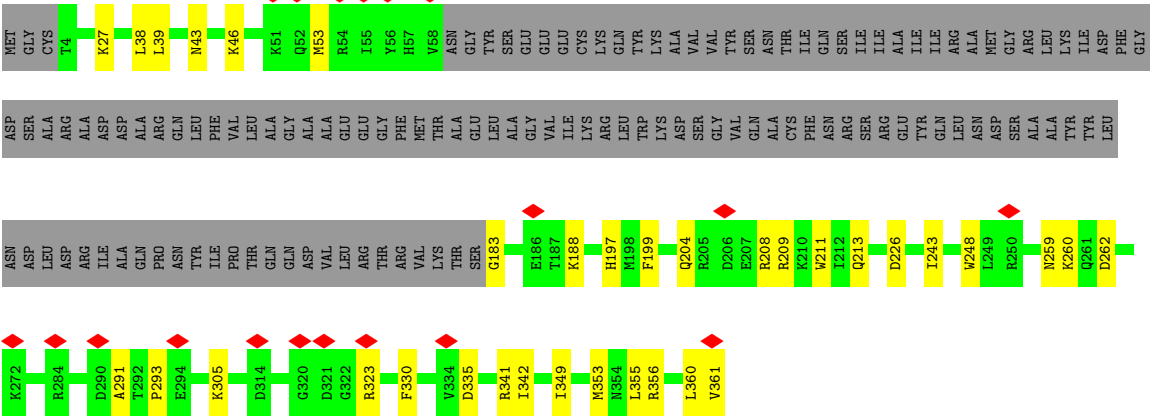
- Molecule 1: Soluble cytochrome b562,2-oxoglutarate receptor 1,Soluble cytochrome b562,2-oxoglutarate receptor 1,Soluble cytochrome b562,2-oxoglutarate receptor 1,Fusion protein,Maltose/maltodextrin-binding periplasmic protein,Maltose/maltodextrin-binding periplasmic protein ,Maltose/maltodextrin-binding periplasmic protein



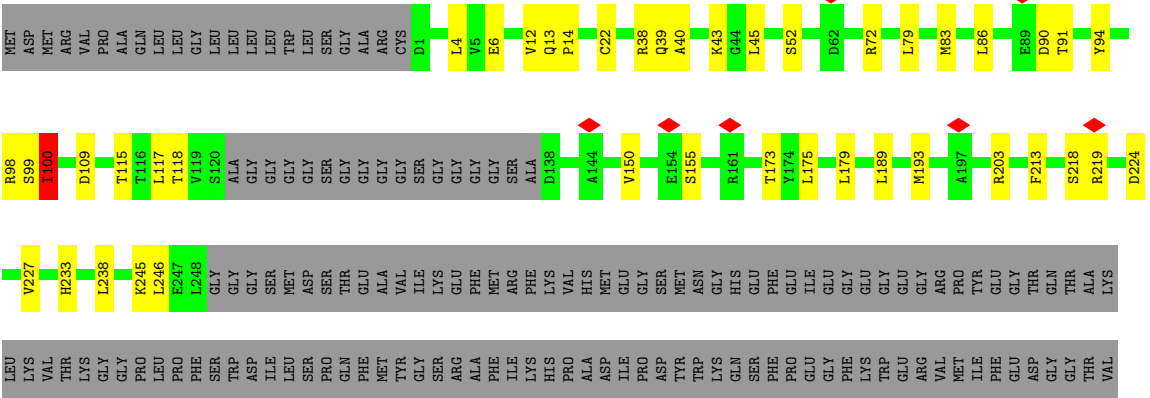




• Molecule 4: Gq alpha



• Molecule 5: scFv-16



[illegible]

4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	334276	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	NONE	Depositor
Microscope	FEI POLARA 300	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	50	Depositor
Minimum defocus (nm)	1000	Depositor
Maximum defocus (nm)	2000	Depositor
Magnification	Not provided	
Image detector	FEI FALCON I (4k x 4k)	Depositor
Maximum map value	1.786	Depositor
Minimum map value	-0.002	Depositor
Average map value	0.001	Depositor
Map value standard deviation	0.018	Depositor
Recommended contour level	0.143	Depositor
Map size ($\text{\AA}$)	303.264, 303.264, 303.264	wwPDB
Map dimensions	324, 324, 324	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing ($\text{\AA}$)	0.93600005, 0.93600005, 0.93600005	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: ITN

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	0.35	0/2397	0.49	0/3269
2	C	0.15	0/403	0.42	0/544
3	D	0.19	0/2638	0.36	1/3577 (0.0%)
4	B	0.17	0/1968	0.33	0/2649
5	E	0.25	0/1823	0.35	0/2472
All	All	0.25	0/9229	0.39	1/12511 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed($^{\circ}$)	Ideal($^{\circ}$)
3	D	23	LYS	N-CA-C	-8.21	100.31	110.65

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	A	2337	0	2407	72	0
2	C	399	0	413	10	0
3	D	2591	0	2499	70	0
4	B	1932	0	1925	28	0
5	E	1779	0	1714	24	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
6	A	9	0	0	0	0
All	All	9047	0	8958	186	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 10.

All (186) 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)
1:A:43:ILE:HG23	1:A:296:PHE:CZ	1.53	1.41
1:A:43:ILE:HG12	1:A:296:PHE:HE2	1.16	1.05
1:A:43:ILE:CG2	1:A:296:PHE:CZ	2.40	1.04
1:A:43:ILE:CG2	1:A:296:PHE:HZ	1.71	1.03
1:A:43:ILE:HG12	1:A:296:PHE:CE2	1.98	0.99
1:A:43:ILE:HG23	1:A:296:PHE:HZ	1.12	0.90
3:D:225:HIS:HE2	3:D:243:THR:HG1	1.22	0.84
5:E:173:THR:HG21	5:E:193:MET:HE2	1.60	0.81
1:A:43:ILE:HA	1:A:296:PHE:CZ	2.21	0.76
1:A:235:LEU:HG	4:B:361:VAL:HG11	1.70	0.73
1:A:243:THR:HA	1:A:246:LEU:HD12	1.68	0.73
3:D:49:ARG:HH12	3:D:85:TYR:HA	1.55	0.72
3:D:130:GLU:OE2	3:D:134:ARG:NH1	2.23	0.71
3:D:48:ARG:HD3	3:D:49:ARG:HD3	1.73	0.70
4:B:53:MET:HE1	4:B:342:ILE:HD12	1.74	0.69
1:A:43:ILE:CA	1:A:296:PHE:HZ	2.06	0.69
1:A:293:LEU:HD23	1:A:296:PHE:CD2	2.29	0.69
3:D:160:SER:HB3	3:D:190:LEU:HD23	1.74	0.69
4:B:38:LEU:HD21	4:B:46:LYS:HB2	1.75	0.67
1:A:83:LEU:HA	1:A:86:LEU:HD23	1.77	0.67
3:D:325:MET:O	3:D:340:ASN:ND2	2.28	0.66
2:C:20:LYS:HG3	3:D:14:LEU:HD21	1.77	0.66
1:A:43:ILE:CA	1:A:296:PHE:CZ	2.79	0.66
5:E:22:CYS:HB3	5:E:79:LEU:HB3	1.77	0.65
1:A:192:LEU:HD13	1:A:268:ARG:HH11	1.62	0.65
3:D:320:VAL:HG22	3:D:327:VAL:HG22	1.79	0.65
5:E:98:ARG:NH2	5:E:109:ASP:OD2	2.30	0.65
3:D:215:GLU:HB3	3:D:217:MET:HE3	1.79	0.63
4:B:335:ASP:OD2	4:B:341:ARG:NH2	2.32	0.62
1:A:225:LEU:HD22	1:A:236:LYS:HG2	1.80	0.62
1:A:293:LEU:HD23	1:A:296:PHE:HD2	1.66	0.61
1:A:72:MET:HE1	1:A:302:TYR:HB3	1.83	0.60

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:9:GLN:O	3:D:13:GLN:HG3	2.02	0.60
1:A:43:ILE:CB	1:A:296:PHE:HZ	2.14	0.60
5:E:83:MET:HE1	5:E:117:LEU:HD21	1.83	0.59
3:D:197:ARG:HH22	3:D:214:ARG:HB2	1.66	0.59
3:D:60:ALA:HB3	3:D:73:ALA:HB3	1.85	0.59
3:D:271:CYS:HB2	3:D:290:ASP:HB2	1.83	0.59
4:B:259:ASN:OD1	4:B:260:LYS:N	2.34	0.58
3:D:294:CYS:SG	3:D:295:ASN:N	2.76	0.58
1:A:134:VAL:HG23	1:A:135:ILE:HD12	1.86	0.58
1:A:185:ASP:OD1	1:A:188:SER:OG	2.22	0.58
5:E:38:ARG:NH1	5:E:90:ASP:OD1	2.37	0.57
5:E:150:VAL:HG11	5:E:246:LEU:HD23	1.86	0.57
2:C:49:PRO:HD3	3:D:42:ARG:HH22	1.68	0.57
3:D:49:ARG:NH2	3:D:85:TYR:O	2.39	0.56
2:C:46:LYS:HE3	3:D:327:VAL:HG23	1.88	0.56
1:A:99:TRP:O	1:A:181:SER:OG	2.21	0.56
3:D:57:LYS:HZ1	3:D:75:GLN:HG3	1.71	0.56
1:A:43:ILE:CB	1:A:296:PHE:CZ	2.88	0.55
3:D:212:ASP:OD2	3:D:219:ARG:NH1	2.40	0.55
5:E:203:ARG:NH1	5:E:224:ASP:OD2	2.33	0.55
2:C:37:LEU:HA	2:C:40:TYR:CE1	2.43	0.54
3:D:262:MET:SD	3:D:302:ALA:HB2	2.48	0.53
5:E:6:GLU:HG2	5:E:115:THR:HG23	1.90	0.53
5:E:91:THR:HG23	5:E:118:THR:HA	1.90	0.53
1:A:43:ILE:HG23	1:A:296:PHE:CE2	2.31	0.53
3:D:86:THR:O	3:D:88:ASN:N	2.41	0.53
4:B:349:ILE:HG22	4:B:353:MET:HE3	1.90	0.53
1:A:192:LEU:HD21	1:A:268:ARG:HB3	1.90	0.53
3:D:48:ARG:O	3:D:49:ARG:HD2	2.07	0.53
4:B:208:ARG:HG3	4:B:211:TRP:CZ2	2.44	0.53
1:A:168:MET:HE1	1:A:186:LEU:HD22	1.90	0.52
1:A:311:GLN:O	1:A:312:ALA:C	2.52	0.52
5:E:227:VAL:HG22	5:E:245:LYS:HG3	1.90	0.52
3:D:210:LEU:HD22	3:D:255:LEU:HD22	1.91	0.52
3:D:49:ARG:NH1	3:D:85:TYR:HA	2.24	0.52
1:A:57:THR:HG23	1:A:61:LYS:HD2	1.91	0.52
3:D:235:PHE:HD2	3:D:237:ASN:OD1	1.93	0.51
5:E:39:GLN:HB2	5:E:45:LEU:HD23	1.91	0.51
1:A:110:ARG:NH1	1:A:185:ASP:HB3	2.26	0.51
3:D:197:ARG:NH2	3:D:212:ASP:OD1	2.43	0.51
1:A:270:LEU:HB2	1:A:272:ILE:HD13	1.91	0.51

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:49:ARG:NH1	3:D:84:SER:O	2.44	0.51
3:D:192:LEU:HD23	3:D:199:PHE:HB3	1.92	0.51
5:E:13:GLN:O	5:E:14:PRO:C	2.51	0.50
4:B:39:LEU:HD13	4:B:243:ILE:HD13	1.94	0.50
1:A:238:LYS:HE3	4:B:361:VAL:OXT	2.11	0.50
1:A:37:PRO:HB3	1:A:90:ILE:HG23	1.93	0.49
1:A:38:VAL:O	1:A:42:ILE:HG13	2.12	0.49
5:E:52:SER:O	5:E:72:ARG:NH1	2.39	0.49
3:D:79:LEU:HD11	3:D:114:CYS:HB3	1.94	0.49
3:D:48:ARG:C	3:D:49:ARG:HD2	2.38	0.49
1:A:31:LEU:HD12	1:A:35:TYR:HB3	1.95	0.49
1:A:180:ARG:HH22	1:A:182:ALA:HB2	1.77	0.49
2:C:52:THR:HA	2:C:58:GLU:HA	1.95	0.49
3:D:48:ARG:HD3	3:D:49:ARG:CD	2.41	0.49
1:A:238:LYS:HD2	4:B:361:VAL:HA	1.95	0.49
3:D:112:VAL:HG23	3:D:124:TYR:HB2	1.94	0.49
3:D:145:TYR:HB3	4:B:204:GLN:HE22	1.79	0.48
3:D:254:ASP:HB3	3:D:257:ALA:HB3	1.95	0.48
1:A:61:LYS:HD3	1:A:312:ALA:HB1	1.94	0.48
3:D:104:ALA:HB3	3:D:113:ALA:HB3	1.95	0.48
1:A:177:ARG:CZ	1:A:178:THR:H	2.27	0.48
3:D:101:MET:HE1	3:D:145:TYR:HB2	1.96	0.48
3:D:61:MET:SD	3:D:70:LEU:HD11	2.54	0.48
3:D:200:VAL:HG22	3:D:234:PHE:CE2	2.48	0.48
1:A:66:LYS:O	1:A:70:ILE:HG13	2.14	0.48
3:D:46:ARG:NH1	3:D:50:THR:OG1	2.26	0.48
5:E:99:SER:OG	5:E:100:ILE:N	2.43	0.48
5:E:40:ALA:HB3	5:E:43:LYS:HB2	1.96	0.47
1:A:115:PHE:HA	1:A:165:VAL:HG21	1.95	0.47
2:C:38:MET:O	2:C:42:GLU:HB3	2.14	0.47
3:D:22:ARG:O	3:D:259:GLN:NE2	2.47	0.47
1:A:293:LEU:CD2	1:A:296:PHE:HD2	2.27	0.47
3:D:228:ASP:OD1	4:B:209:ARG:NH2	2.47	0.47
1:A:87:PRO:HA	1:A:90:ILE:HD12	1.96	0.47
3:D:119:ASN:ND2	4:B:183:GLY:HA2	2.30	0.47
4:B:188:LYS:HG2	4:B:197:HIS:CD2	2.50	0.47
3:D:112:VAL:HG13	3:D:126:LEU:HD11	1.97	0.47
1:A:124:LEU:HD22	1:A:302:TYR:CZ	2.50	0.47
4:B:213:GLN:HG2	4:B:248:TRP:CD1	2.51	0.46
2:C:49:PRO:HG3	3:D:42:ARG:HH12	1.80	0.46
3:D:64:GLY:HA2	3:D:105:TYR:CD2	2.50	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:43:ILE:HA	1:A:296:PHE:CE2	2.51	0.46
1:A:298:ASN:O	1:A:302:TYR:HB2	2.16	0.46
5:E:100:ILE:HD13	5:E:100:ILE:HA	1.57	0.46
3:D:6:GLN:O	3:D:9:GLN:HG3	2.15	0.45
4:B:291:ALA:O	4:B:293:PRO:HD3	2.15	0.45
4:B:305:LYS:HB3	4:B:330:PHE:CZ	2.51	0.45
3:D:117:LEU:HD21	4:B:211:TRP:HB2	1.97	0.45
4:B:43:ASN:ND2	4:B:226:ASP:OD2	2.49	0.45
5:E:175:LEU:HD13	5:E:213:PHE:CG	2.51	0.45
5:E:38:ARG:HD3	5:E:94:TYR:CZ	2.52	0.45
1:A:307:ASP:O	1:A:308:ASN:C	2.60	0.45
3:D:33:ILE:HD11	3:D:300:LEU:HB3	1.99	0.45
5:E:83:MET:HB3	5:E:86:LEU:HD21	1.99	0.44
1:A:125:THR:OG1	1:A:210:PRO:HB3	2.17	0.44
3:D:29:THR:HG22	3:D:31:SER:H	1.80	0.44
5:E:233:HIS:HA	5:E:238:LEU:HD22	2.00	0.44
3:D:99:TRP:HB3	3:D:117:LEU:HD12	1.99	0.44
4:B:323:ARG:HA	4:B:356:ARG:NH2	2.32	0.44
3:D:197:ARG:HG3	3:D:198:LEU:HG	2.00	0.44
1:A:161:SER:O	1:A:165:VAL:HG23	2.18	0.44
1:A:189:SER:O	1:A:268:ARG:NH1	2.50	0.44
3:D:331:SER:OG	3:D:332:TRP:N	2.51	0.44
1:A:59:ILE:HG23	1:A:63:ARG:HH21	1.83	0.43
3:D:30:LEU:O	3:D:33:ILE:HG12	2.18	0.43
1:A:40:TYR:CG	1:A:86:LEU:HD12	2.52	0.43
1:A:246:LEU:HD22	1:A:302:TYR:CE1	2.53	0.43
2:C:51:LEU:HD12	2:C:51:LEU:O	2.19	0.43
4:B:262:ASP:N	4:B:262:ASP:OD1	2.49	0.43
3:D:9:GLN:OE1	3:D:13:GLN:NE2	2.52	0.43
1:A:222:ILE:O	1:A:226:THR:HG23	2.19	0.43
3:D:248:ALA:HB1	3:D:269:ILE:HG22	2.01	0.43
3:D:99:TRP:HZ2	4:B:199:PHE:CE1	2.37	0.43
1:A:48:PHE:HB3	1:A:49:PRO:HD3	2.00	0.42
3:D:61:MET:HE1	3:D:319:GLY:N	2.33	0.42
1:A:88:PHE:HD2	1:A:109:ILE:HD11	1.83	0.42
1:A:209:LEU:HB3	1:A:210:PRO:HD3	2.00	0.42
1:A:266:GLU:O	1:A:270:LEU:HG	2.18	0.42
4:B:355:LEU:HB3	4:B:361:VAL:HG23	2.02	0.42
1:A:72:MET:CE	1:A:302:TYR:HB3	2.47	0.42
2:C:16:VAL:HG21	3:D:7:LEU:HD22	2.02	0.42
1:A:235:LEU:HD11	4:B:356:ARG:NH2	2.34	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:316:SER:HB3	3:D:332:TRP:HE1	1.83	0.42
1:A:68:SER:O	1:A:72:MET:HG2	2.20	0.42
1:A:118:TYR:OH	1:A:261:ARG:NH2	2.53	0.42
3:D:316:SER:HB3	3:D:332:TRP:NE1	2.35	0.42
3:D:274:THR:OG1	3:D:315:VAL:O	2.29	0.42
1:A:299:LEU:HD12	1:A:299:LEU:HA	1.79	0.42
1:A:242:LEU:O	1:A:246:LEU:HG	2.20	0.42
1:A:43:ILE:CG1	1:A:296:PHE:CE2	2.85	0.41
3:D:36:ASN:HB2	3:D:301:LYS:HE2	2.02	0.41
5:E:155:SER:HA	5:E:218:SER:O	2.20	0.41
1:A:185:ASP:O	1:A:189:SER:OG	2.37	0.41
1:A:238:LYS:CE	4:B:361:VAL:OXT	2.68	0.41
3:D:289:TYR:CE1	3:D:295:ASN:HB2	2.54	0.41
1:A:260:LEU:HD23	1:A:260:LEU:HA	1.86	0.41
3:D:289:TYR:HE1	3:D:295:ASN:HB2	1.84	0.41
4:B:360:LEU:HD23	4:B:360:LEU:HA	1.89	0.41
3:D:23:LYS:HA	3:D:23:LYS:HD2	1.74	0.41
3:D:55:LEU:CD2	4:B:27:LYS:HB2	2.51	0.41
1:A:28:ASN:O	1:A:32:LYS:NZ	2.51	0.41
1:A:187:THR:HB	1:A:264:ARG:HD2	2.03	0.41
1:A:240:ARG:O	1:A:244:ILE:HG12	2.20	0.41
2:C:35:ALA:HA	3:D:300:LEU:HD11	2.03	0.41
3:D:200:VAL:HG11	3:D:241:PHE:CD2	2.55	0.41
5:E:179:LEU:HB2	5:E:189:LEU:HD11	2.03	0.41
5:E:4:LEU:HD11	5:E:98:ARG:HG3	2.03	0.41
1:A:286:VAL:O	1:A:289:PRO:HD2	2.20	0.40
3:D:211:TRP:CZ3	3:D:218:CYS:HB2	2.56	0.40
1:A:153:ALA:O	1:A:157:VAL:HG23	2.21	0.40
3:D:55:LEU:HD22	4:B:27:LYS:HB2	2.03	0.40
1:A:178:THR:C	1:A:180:ARG:H	2.29	0.40
5:E:219:ARG:HG2	5:E:219:ARG:O	2.21	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	289/1398 (21%)	274 (95%)	15 (5%)	0	100	100
2	C	51/71 (72%)	44 (86%)	7 (14%)	0	100	100
3	D	335/609 (55%)	320 (96%)	15 (4%)	0	100	100
4	B	230/361 (64%)	227 (99%)	3 (1%)	0	100	100
5	E	227/547 (42%)	214 (94%)	12 (5%)	1 (0%)	30	49
All	All	1132/2986 (38%)	1079 (95%)	52 (5%)	1 (0%)	49	69

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
5	E	100	ILE

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	269/1157 (23%)	256 (95%)	13 (5%)	23	45
2	C	42/58 (72%)	42 (100%)	0	100	100
3	D	280/504 (56%)	279 (100%)	1 (0%)	84	92
4	B	212/316 (67%)	212 (100%)	0	100	100
5	E	196/440 (44%)	194 (99%)	2 (1%)	68	85
All	All	999/2475 (40%)	983 (98%)	16 (2%)	54	78

All (16) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	31	LEU
1	A	63	ARG
1	A	100	ILE
1	A	176	ASN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	177	ARG
1	A	178	THR
1	A	179	ASN
1	A	180	ARG
1	A	238	LYS
1	A	270	LEU
1	A	272	ILE
1	A	273	SER
1	A	299	LEU
3	D	23	LYS
5	E	12	VAL
5	E	100	ILE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (2) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	28	ASN
1	A	176	ASN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains [i](#)

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](#)

1 ligand is 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	$\# Z > 2$
6	ITN	A	1301	-	8,8,8	3.32	2 (25%)	10,10,10	9.91	4 (40%)

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
6	ITN	A	1301	-	-	6/8/8/8	-

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	A	1301	ITN	C5-C3	7.04	1.54	1.49
6	A	1301	ITN	C2-C3	5.26	1.54	1.50

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	A	1301	ITN	C2-C3-C5	-26.16	96.30	115.76
6	A	1301	ITN	C4-C3-C5	12.52	131.76	120.61
6	A	1301	ITN	C2-C3-C4	10.83	131.94	123.09
6	A	1301	ITN	O3-C5-C3	3.91	119.32	115.05

There are no chirality outliers.

All (6) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
6	A	1301	ITN	C1-C2-C3-C5
6	A	1301	ITN	C1-C2-C3-C4
6	A	1301	ITN	O2-C1-C2-C3
6	A	1301	ITN	C4-C3-C5-O3
6	A	1301	ITN	C4-C3-C5-O4
6	A	1301	ITN	O1-C1-C2-C3

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-65376. 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](#)

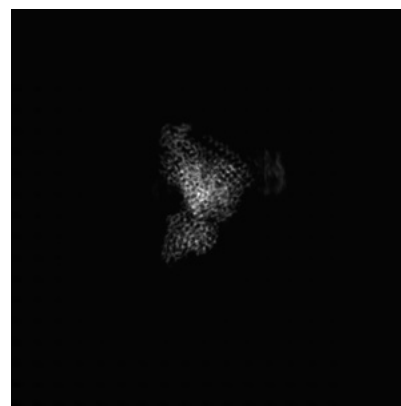
6.1.1 Primary map



X

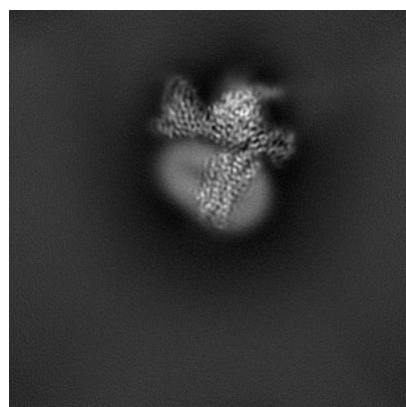


Y

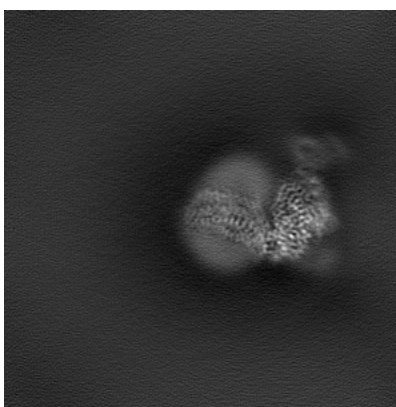


Z

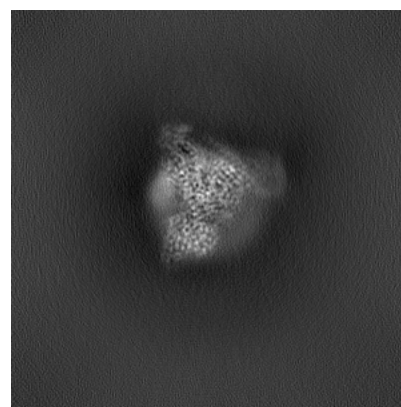
6.1.2 Raw map



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: 162

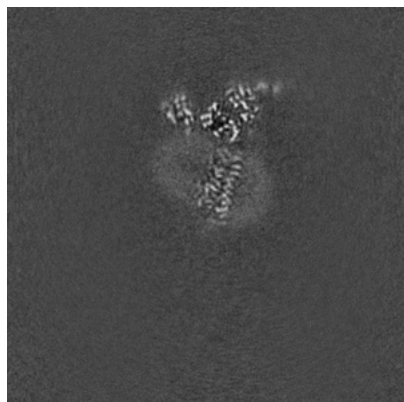


Y Index: 162

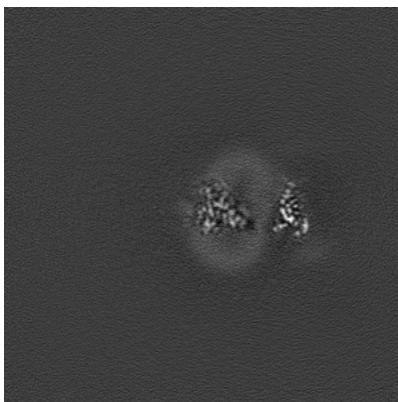


Z Index: 162

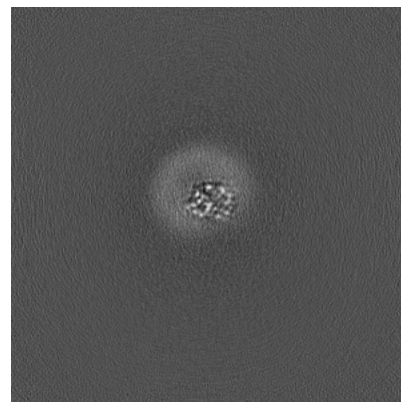
6.2.2 Raw map



X Index: 162



Y Index: 162



Z Index: 162

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: 151

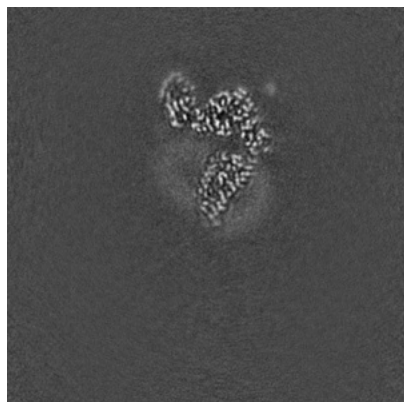


Y Index: 178

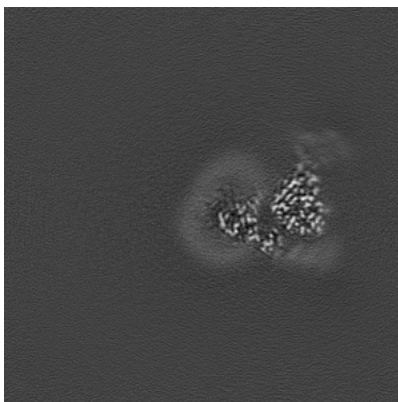


Z Index: 241

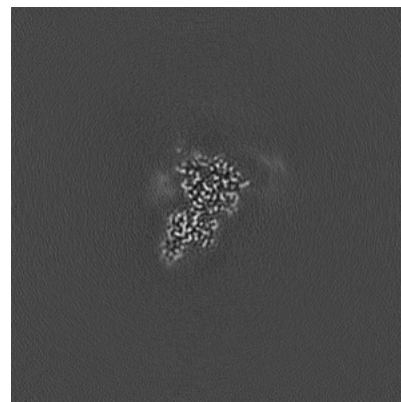
6.3.2 Raw map



X Index: 151



Y Index: 184

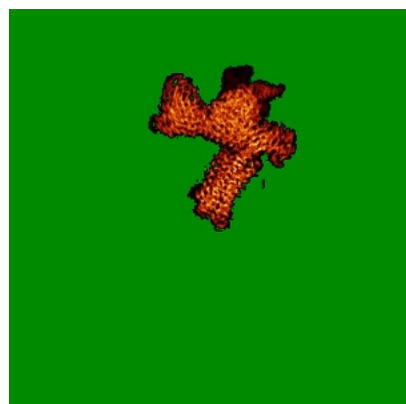


Z Index: 233

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

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

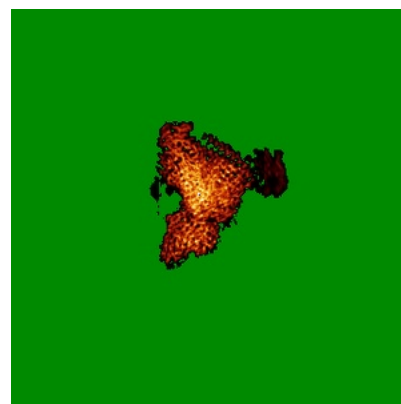
6.4.1 Primary map



X

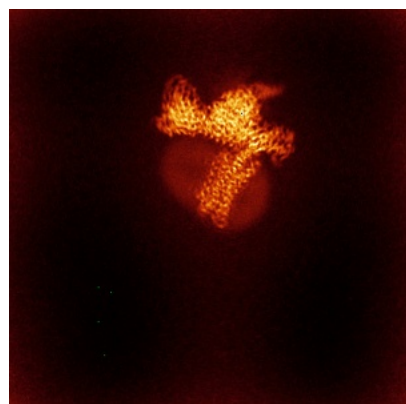


Y

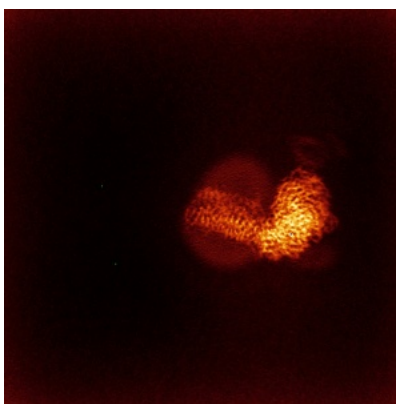


Z

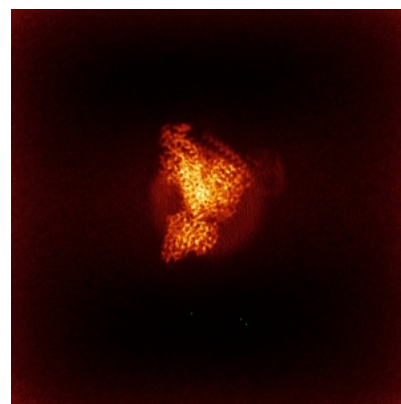
6.4.2 Raw map



X



Y

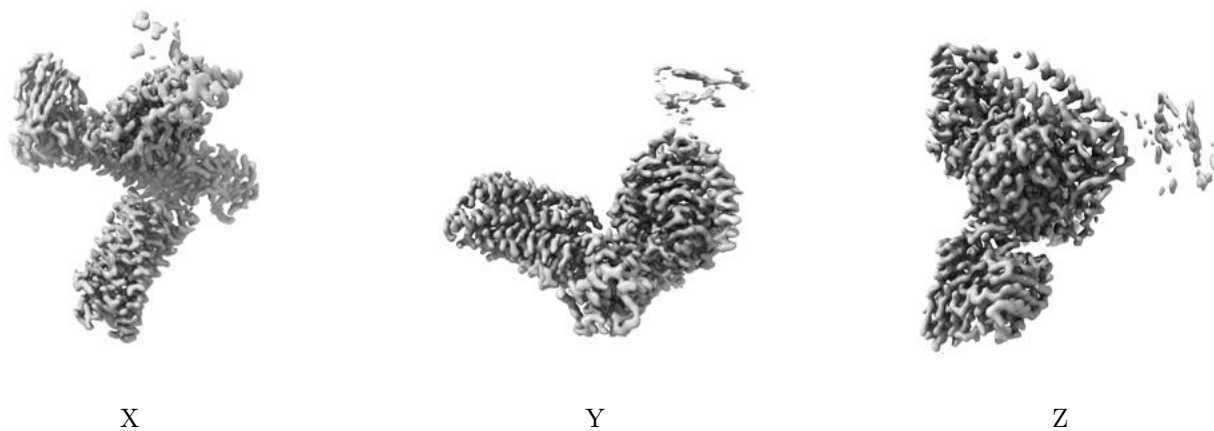


Z

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.

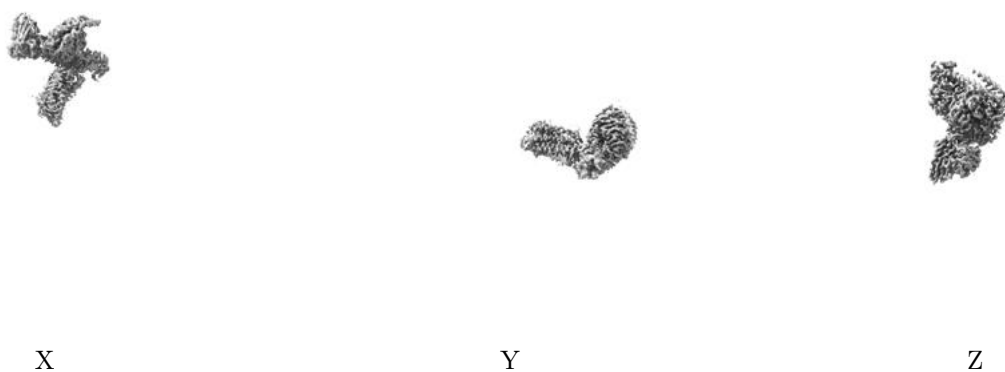
6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.143. 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.

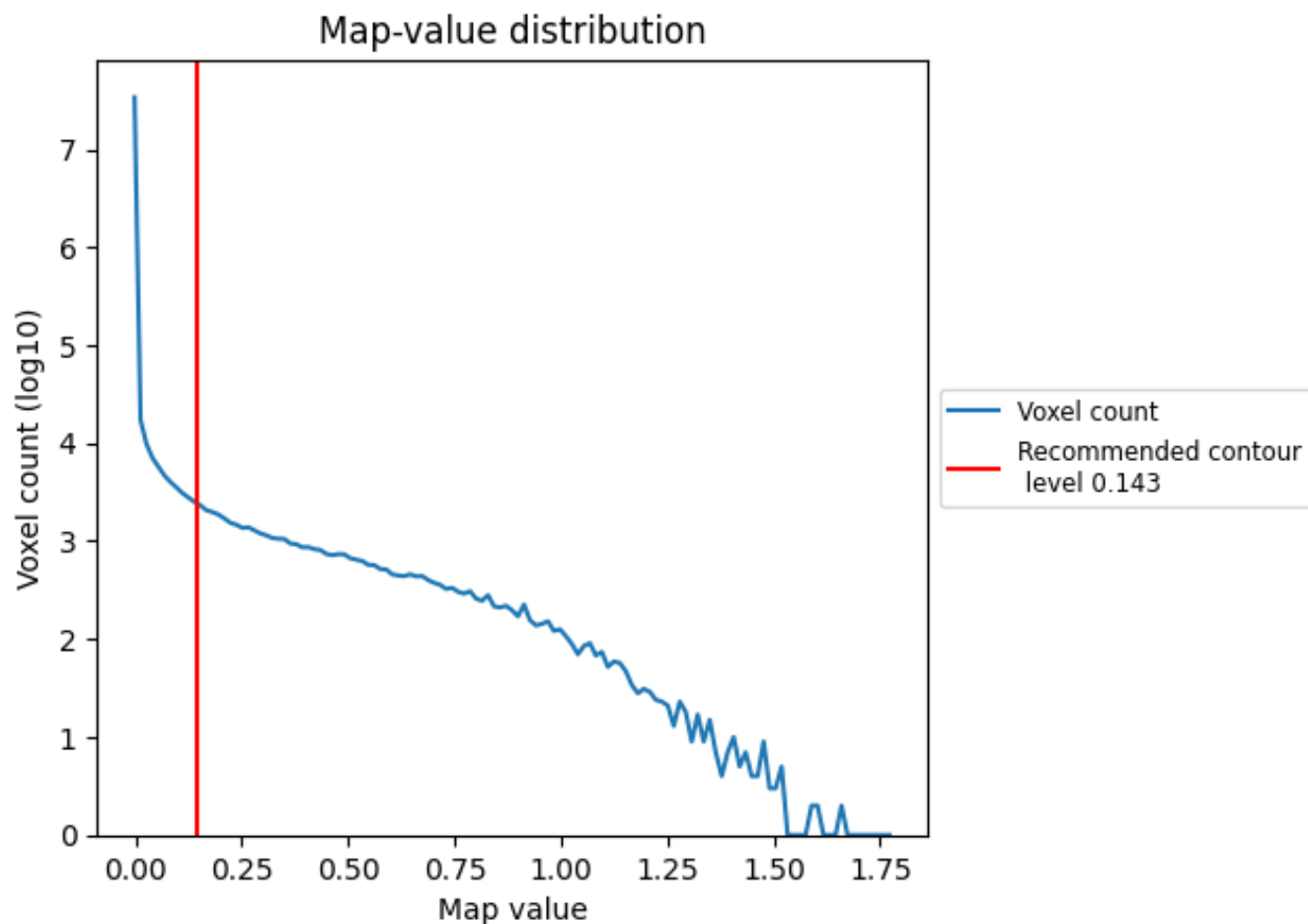
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

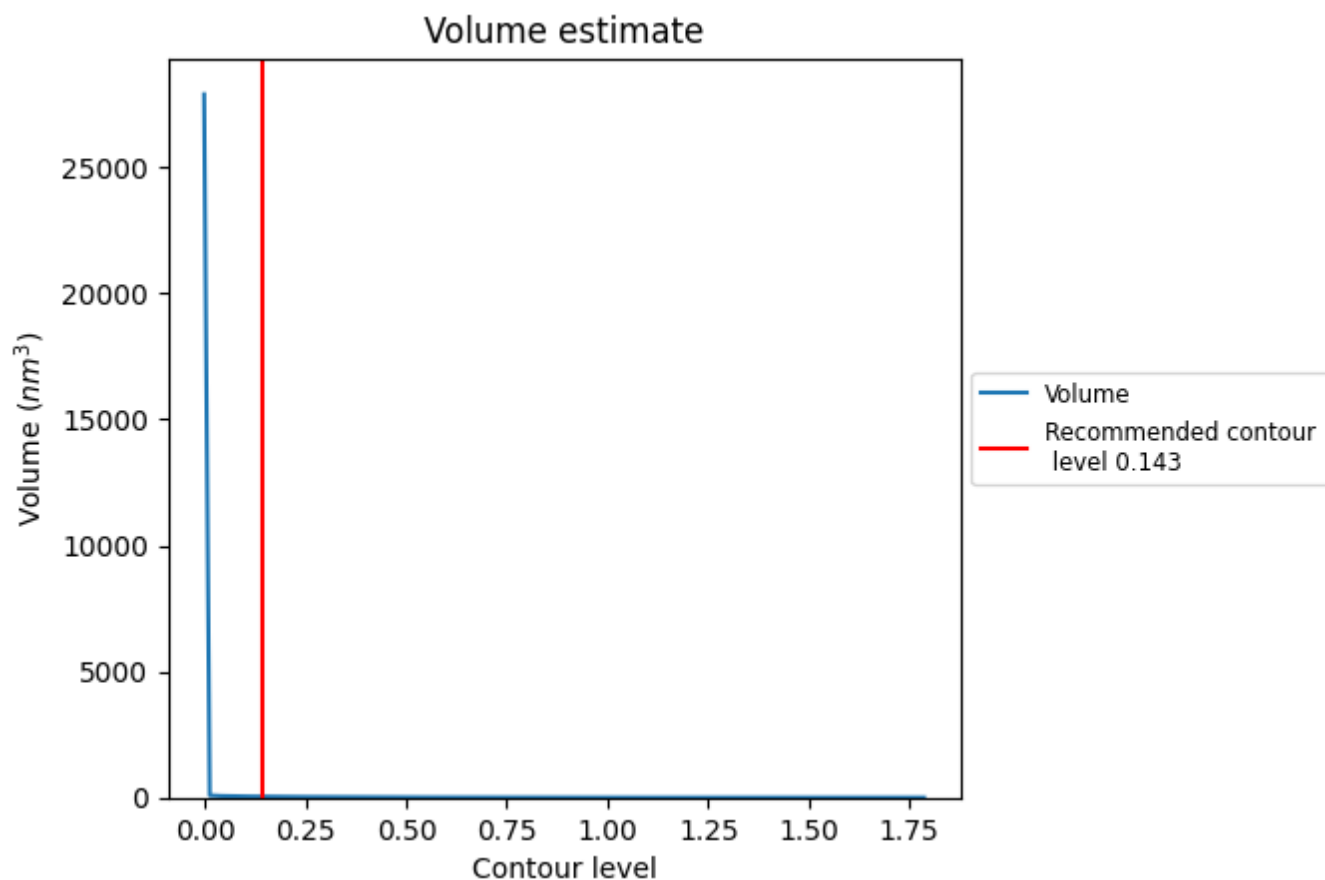
This section contains the results of statistical analysis of the map.

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.

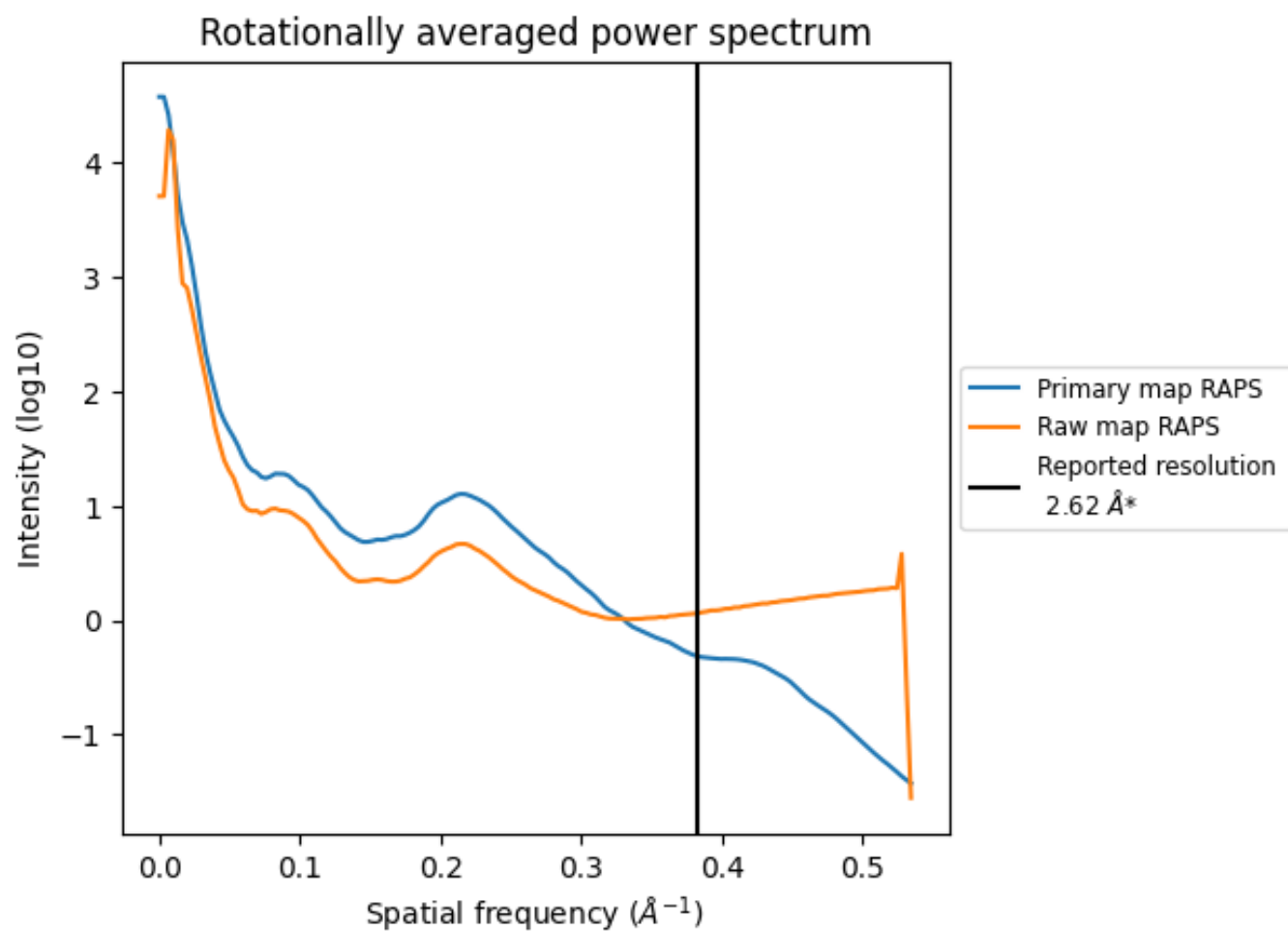
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 38 nm³; this corresponds to an approximate mass of 34 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 ⓘ

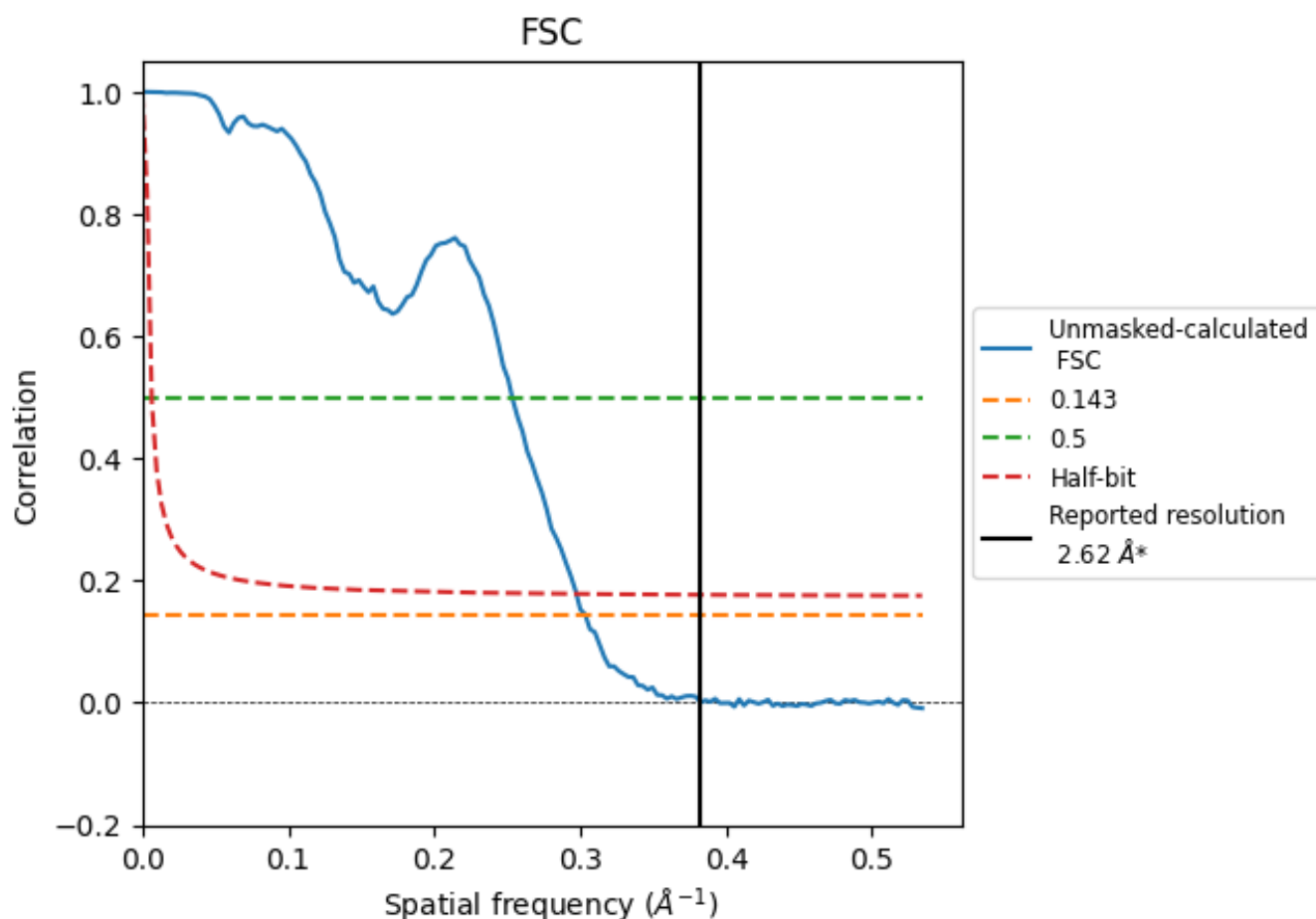


*Reported resolution corresponds to spatial frequency of 0.382 Å⁻¹

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 0.382 $\text{\AA}^{-1}$

8.2 Resolution estimates [i](#)

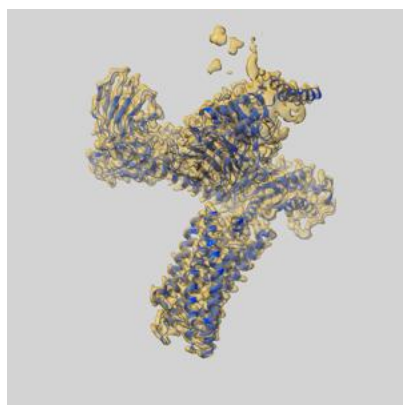
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	2.62	-	-
Author-provided FSC curve	-	-	-
Unmasked-calculated*	3.29	3.95	3.36

*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 2.62 by more than 10 %

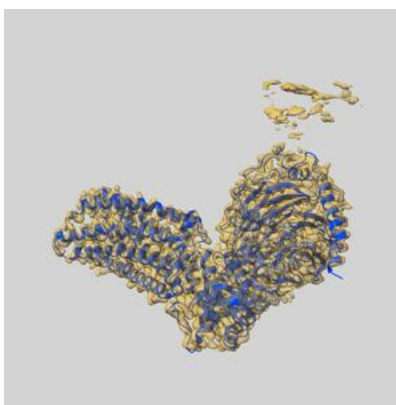
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-65376 and PDB model 9VV6. Per-residue inclusion information can be found in section [3](#) on page [8](#).

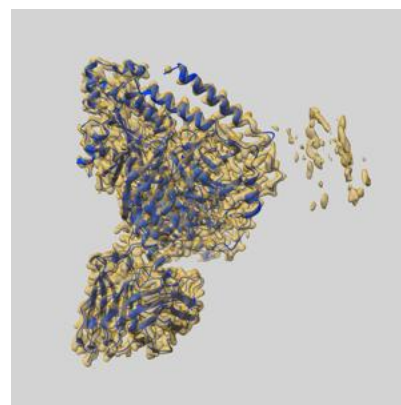
9.1 Map-model overlay [i](#)



X



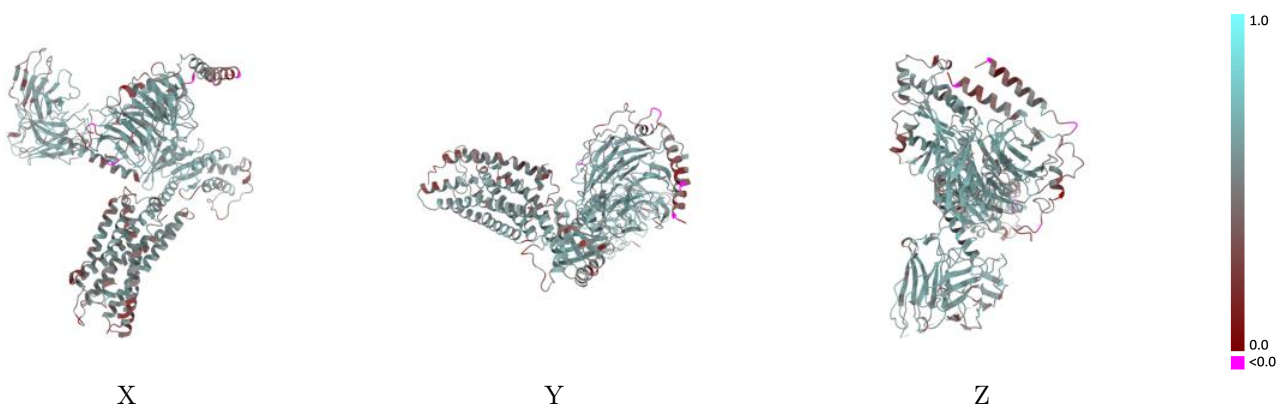
Y



Z

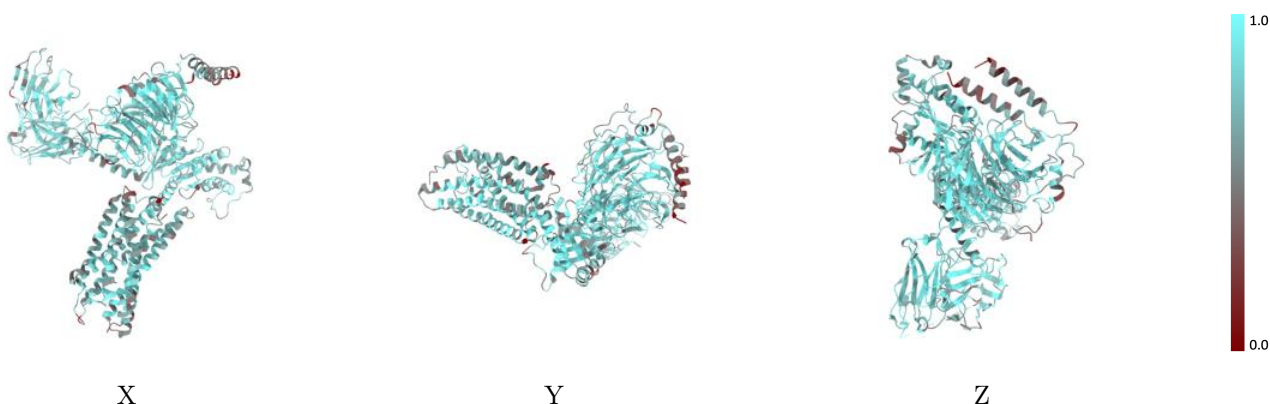
The images above show the 3D surface view of the map at the recommended contour level 0.143 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



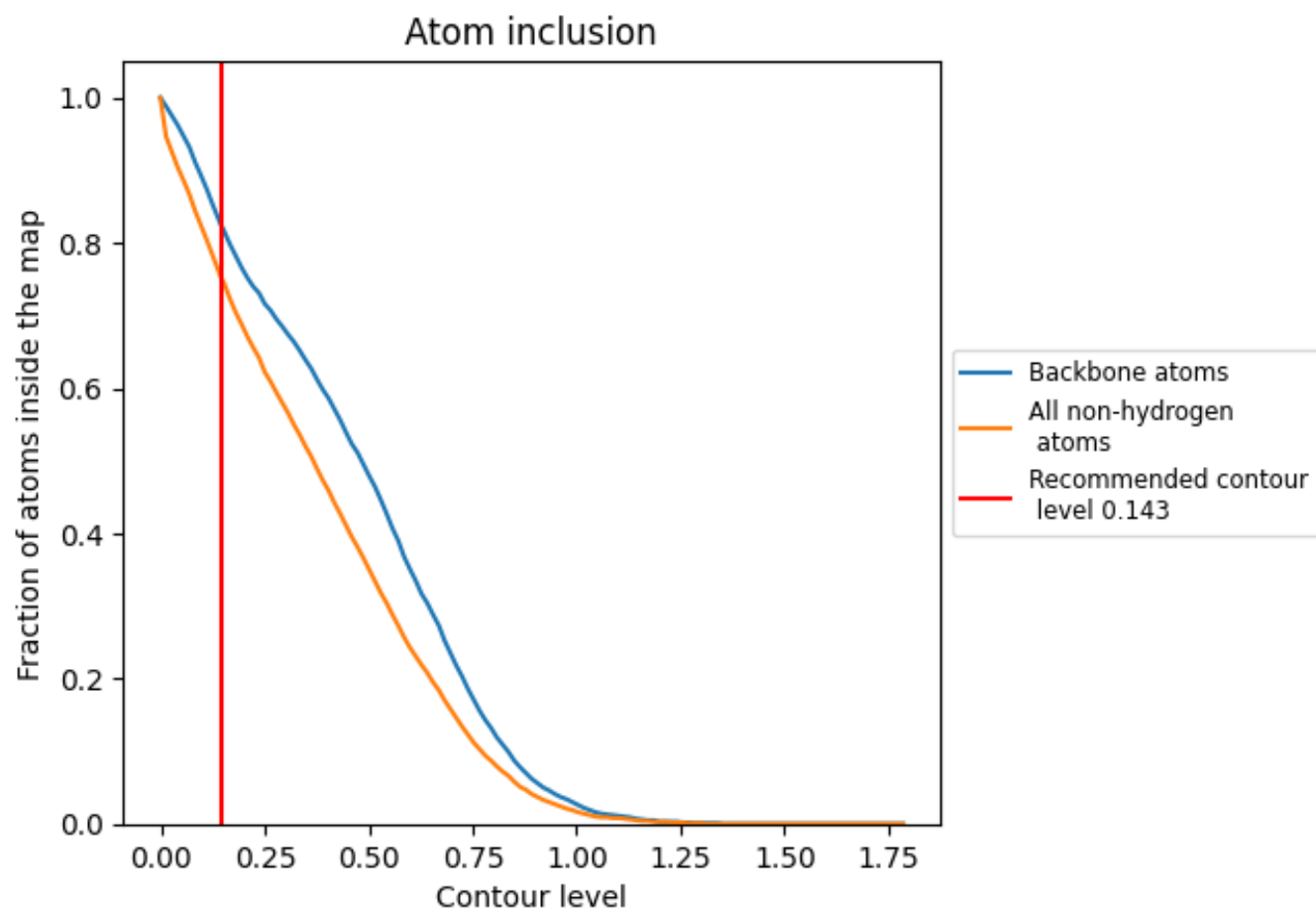
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.143).

9.4 Atom inclusion ⓘ



At the recommended contour level, 83% of all backbone atoms, 75% 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 (0.143) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.7540	0.5310
A	0.7290	0.5030
B	0.7520	0.5320
C	0.5250	0.3520
D	0.7890	0.5600
E	0.7920	0.5640

