



Full wwPDB EM Validation Report (i)

Dec 3, 2024 – 12:12 PM EST

PDB ID : 9AST
EMDB ID : EMD-43825
Title : Cryo-EM structure of XCR1 signaling complex
Authors : Zhang, X.; Zhang, C.
Deposited on : 2024-02-26
Resolution : 3.07 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 (i) 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 \(i\)](#)) were used in the production of this report:

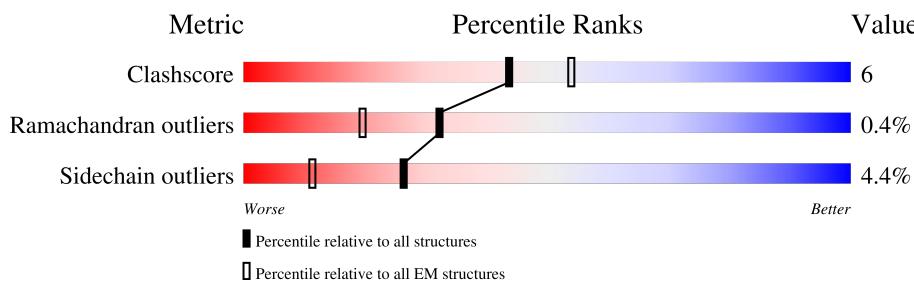
EMDB validation analysis : 0.0.1.dev113
MolProbity : 4.02b-467
Percentile statistics : 20231227.v01 (using entries in the PDB archive December 27th 2023)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.40

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 3.07 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)
Clashscore	210492	15764
Ramachandran outliers	207382	16835
Sidechain outliers	206894	16415

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 <=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.



2 Entry composition [\(i\)](#)

There are 6 unique types of molecules in this entry. The entry contains 8876 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 Guanine nucleotide-binding protein G(i) subunit alpha-1.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
1	A	218	1758	1119	294	332	13	0	0

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	47	ASN	SER	engineered mutation	UNP P63096
A	203	ALA	GLY	engineered mutation	UNP P63096
A	245	ALA	GLU	engineered mutation	UNP P63096
A	326	SER	ALA	engineered mutation	UNP P63096

- Molecule 2 is a protein called Lymphotactin.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
2	L	11	80	46	15	18	1	0	0

There are 42 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
L	21	CYS	VAL	conflict	UNP P47992
L	59	CYS	VAL	conflict	UNP P47992
L	94	GLY	-	expression tag	UNP P47992
L	95	SER	-	expression tag	UNP P47992
L	96	GLY	-	expression tag	UNP P47992
L	97	SER	-	expression tag	UNP P47992
L	98	GLY	-	expression tag	UNP P47992
L	99	SER	-	expression tag	UNP P47992
L	100	GLY	-	expression tag	UNP P47992
L	101	SER	-	expression tag	UNP P47992
L	102	GLY	-	expression tag	UNP P47992
L	103	SER	-	expression tag	UNP P47992
L	104	GLY	-	expression tag	UNP P47992

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Chain	Residue	Modelled	Actual	Comment	Reference
L	105	SER	-	expression tag	UNP P47992
L	106	GLY	-	expression tag	UNP P47992
L	107	SER	-	expression tag	UNP P47992
L	108	GLY	-	expression tag	UNP P47992
L	109	SER	-	expression tag	UNP P47992
L	110	GLY	-	expression tag	UNP P47992
L	111	SER	-	expression tag	UNP P47992
L	112	GLY	-	expression tag	UNP P47992
L	113	SER	-	expression tag	UNP P47992
L	114	GLY	-	expression tag	UNP P47992
L	115	SER	-	expression tag	UNP P47992
L	116	LEU	-	expression tag	UNP P47992
L	117	GLU	-	expression tag	UNP P47992
L	118	VAL	-	expression tag	UNP P47992
L	119	LEU	-	expression tag	UNP P47992
L	120	PHE	-	expression tag	UNP P47992
L	121	GLN	-	expression tag	UNP P47992
L	122	GLY	-	expression tag	UNP P47992
L	123	PRO	-	expression tag	UNP P47992
L	124	ASP	-	expression tag	UNP P47992
L	125	TYR	-	expression tag	UNP P47992
L	126	LYS	-	expression tag	UNP P47992
L	127	ASP	-	expression tag	UNP P47992
L	128	ASP	-	expression tag	UNP P47992
L	129	ASP	-	expression tag	UNP P47992
L	130	ASP	-	expression tag	UNP P47992
L	131	LYS	-	expression tag	UNP P47992
L	132	GLY	-	expression tag	UNP P47992
L	133	SER	-	expression tag	UNP P47992

- Molecule 3 is a protein called Chemokine XC receptor 1,Non structural polyprotein.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
3	R	283	2261	1518	354	375	14	0	0

There are 57 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
R	334	GLY	-	linker	UNP P46094
R	347	GLU	ARG	conflict	UNP A0A482LYE4
R	351	ALA	GLY	conflict	UNP A0A482LYE4

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Chain	Residue	Modelled	Actual	Comment	Reference
R	367	LEU	PHE	conflict	UNP A0A482LYE4
R	371	ALA	GLY	conflict	UNP A0A482LYE4
R	382	ARG	LEU	conflict	UNP A0A482LYE4
R	387	ALA	GLY	conflict	UNP A0A482LYE4
R	403	ALA	GLY	conflict	UNP A0A482LYE4
R	407	ALA	GLY	conflict	UNP A0A482LYE4
R	411	GLU	LYS	conflict	UNP A0A482LYE4
R	412	VAL	ILE	conflict	UNP A0A482LYE4
R	429	PRO	HIS	conflict	UNP A0A482LYE4
R	443	LEU	ILE	conflict	UNP A0A482LYE4
R	444	ASN	ASP	conflict	UNP A0A482LYE4
R	480	THR	ASN	conflict	UNP A0A482LYE4
R	485	MET	LEU	conflict	UNP A0A482LYE4
R	493	SER	-	expression tag	UNP A0A482LYE4
R	494	GLY	-	expression tag	UNP A0A482LYE4
R	495	GLY	-	expression tag	UNP A0A482LYE4
R	496	SER	-	expression tag	UNP A0A482LYE4
R	497	GLY	-	expression tag	UNP A0A482LYE4
R	498	HIS	-	expression tag	UNP A0A482LYE4
R	499	HIS	-	expression tag	UNP A0A482LYE4
R	500	HIS	-	expression tag	UNP A0A482LYE4
R	501	HIS	-	expression tag	UNP A0A482LYE4
R	502	HIS	-	expression tag	UNP A0A482LYE4
R	503	HIS	-	expression tag	UNP A0A482LYE4
R	504	HIS	-	expression tag	UNP A0A482LYE4
R	505	HIS	-	expression tag	UNP A0A482LYE4
R	506	TRP	-	expression tag	UNP A0A482LYE4
R	507	SER	-	expression tag	UNP A0A482LYE4
R	508	HIS	-	expression tag	UNP A0A482LYE4
R	509	PRO	-	expression tag	UNP A0A482LYE4
R	510	GLN	-	expression tag	UNP A0A482LYE4
R	511	PHE	-	expression tag	UNP A0A482LYE4
R	512	GLU	-	expression tag	UNP A0A482LYE4
R	513	LYS	-	expression tag	UNP A0A482LYE4
R	514	GLY	-	expression tag	UNP A0A482LYE4
R	515	GLY	-	expression tag	UNP A0A482LYE4
R	516	GLY	-	expression tag	UNP A0A482LYE4
R	517	SER	-	expression tag	UNP A0A482LYE4
R	518	GLY	-	expression tag	UNP A0A482LYE4
R	519	GLY	-	expression tag	UNP A0A482LYE4
R	520	GLY	-	expression tag	UNP A0A482LYE4
R	521	SER	-	expression tag	UNP A0A482LYE4

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Chain	Residue	Modelled	Actual	Comment	Reference
R	522	GLY	-	expression tag	UNP A0A482LYE4
R	523	GLY	-	expression tag	UNP A0A482LYE4
R	524	SER	-	expression tag	UNP A0A482LYE4
R	525	ALA	-	expression tag	UNP A0A482LYE4
R	526	TRP	-	expression tag	UNP A0A482LYE4
R	527	SER	-	expression tag	UNP A0A482LYE4
R	528	HIS	-	expression tag	UNP A0A482LYE4
R	529	PRO	-	expression tag	UNP A0A482LYE4
R	530	GLN	-	expression tag	UNP A0A482LYE4
R	531	PHE	-	expression tag	UNP A0A482LYE4
R	532	GLU	-	expression tag	UNP A0A482LYE4
R	533	LYS	-	expression tag	UNP A0A482LYE4

- Molecule 4 is a protein called Guanine nucleotide-binding protein G(I)/G(S)/G(T) subunit beta-1.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	B	336	Total	C	N	O	S	0	0
			2578	1590	462	505	21		

There are 12 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	-10	MET	-	expression tag	UNP P62873
B	-9	HIS	-	expression tag	UNP P62873
B	-8	HIS	-	expression tag	UNP P62873
B	-7	HIS	-	expression tag	UNP P62873
B	-6	HIS	-	expression tag	UNP P62873
B	-5	HIS	-	expression tag	UNP P62873
B	-4	HIS	-	expression tag	UNP P62873
B	-3	GLY	-	expression tag	UNP P62873
B	-2	SER	-	expression tag	UNP P62873
B	-1	LEU	-	expression tag	UNP P62873
B	0	LEU	-	expression tag	UNP P62873
B	1	GLN	-	expression tag	UNP P62873

- Molecule 5 is a protein called Guanine nucleotide-binding protein G(I)/G(S)/G(O) subunit gamma-2.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	G	54	Total	C	N	O	S	0	0
			418	263	76	76	3		

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
G	17	GLN	GLU	conflict	UNP P59768
G	58	GLN	GLU	conflict	UNP P59768

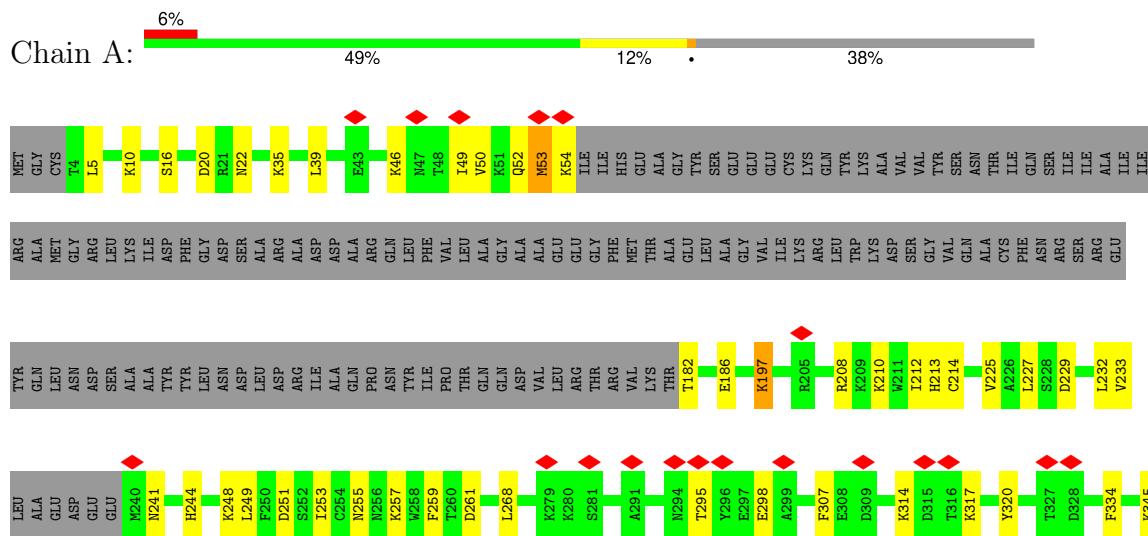
- Molecule 6 is a protein called scFv16.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	E	232	Total	C	N	O	S	0	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.

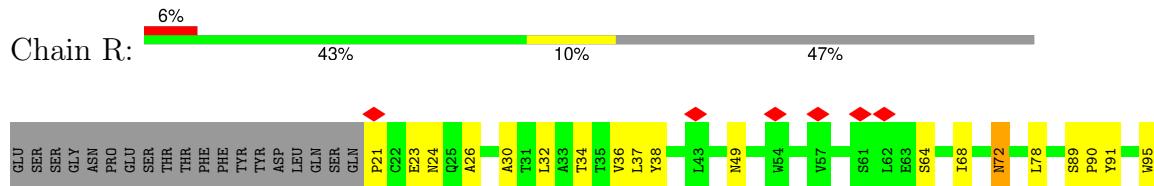
- Molecule 1: Guanine nucleotide-binding protein G(i) subunit alpha-1

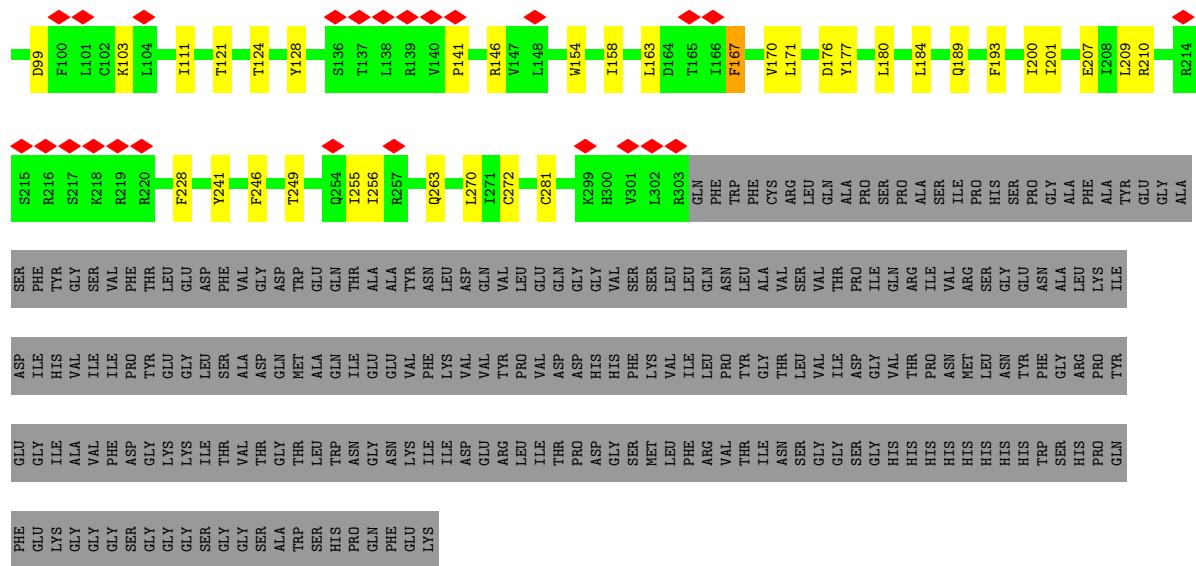


- Molecule 2: Lymphotactin



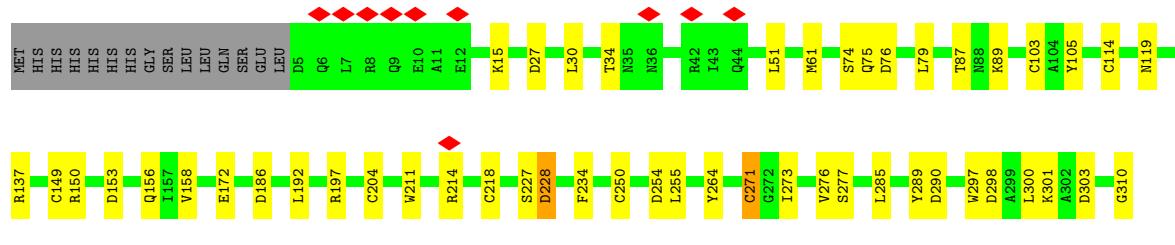
- Molecule 3: Chemokine XC receptor 1,Non structural polyprotein





- Molecule 4: Guanine nucleotide-binding protein G(I)/G(S)/G(T) subunit beta-1

Chain B: 78% 17% • •



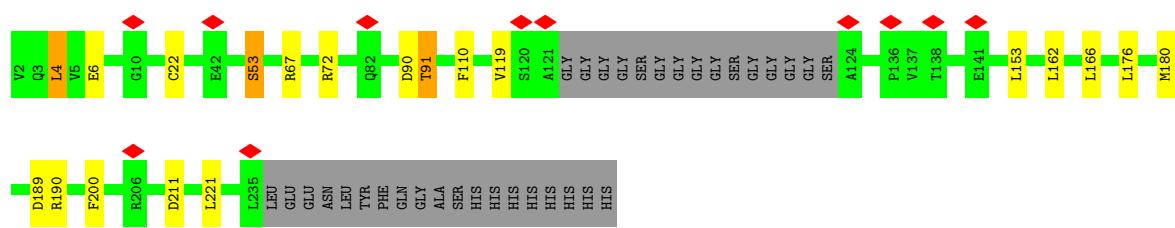
- Molecule 5: Guanine nucleotide-binding protein G(I)/G(S)/G(O) subunit gamma-2

Chain G: 42% 23% 10% • 24%



- Molecule 6: scFv16

Chain E: 80% 6% • 13%



4 Experimental information i

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	255110	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TECNAI SPIRIT	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	55	Depositor
Minimum defocus (nm)	1000	Depositor
Maximum defocus (nm)	2000	Depositor
Magnification	Not provided	
Image detector	GATAN K3 BIOQUANTUM (6k x 4k)	Depositor
Maximum map value	1.785	Depositor
Minimum map value	-0.033	Depositor
Average map value	0.002	Depositor
Map value standard deviation	0.026	Depositor
Recommended contour level	0.0465	Depositor
Map size (Å)	209.92, 209.92, 209.92	wwPDB
Map dimensions	256, 256, 256	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	0.82, 0.82, 0.82	Depositor

5 Model quality i

5.1 Standard geometry i

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	0.28	0/1787	0.47	0/2395
2	L	0.54	0/79	0.70	0/104
3	R	0.29	0/2324	0.47	0/3179
4	B	0.28	0/2625	0.54	0/3559
5	G	0.55	0/424	0.72	1/572 (0.2%)
6	E	0.27	0/1825	0.50	1/2475 (0.0%)
All	All	0.30	0/9064	0.51	2/12284 (0.0%)

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed($^{\circ}$)	Ideal($^{\circ}$)
5	G	51	LEU	CA-CB-CG	5.32	127.53	115.30
6	E	189	ASP	CB-CG-OD2	5.21	122.99	118.30

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	1758	0	1755	24	0
2	L	80	0	81	3	0
3	R	2261	0	2298	32	0
4	B	2578	0	2477	39	0
5	G	418	0	432	15	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
6	E	1781	0	1719	9	0
All	All	8876	0	8762	111	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 6.

All (111) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:G:55:PRO:O	5:G:57:SER:N	2.05	0.90
5:G:55:PRO:C	5:G:57:SER:H	1.87	0.77
4:B:271:CYS:HB2	4:B:290:ASP:HB2	1.75	0.69
3:R:163:LEU:O	3:R:167:PHE:HB2	1.94	0.68
3:R:36:VAL:HG23	3:R:37:LEU:HD22	1.78	0.66
3:R:176:ASP:OD1	3:R:177:TYR:N	2.31	0.63
1:A:244:HIS:O	1:A:248:LYS:HG2	1.99	0.63
4:B:320:VAL:HG22	4:B:327:VAL:HG22	1.81	0.61
5:G:57:SER:HB3	5:G:58:GLN:OE1	1.99	0.61
4:B:149:CYS:O	4:B:150:ARG:NH1	2.34	0.60
4:B:289:TYR:OH	4:B:297:TRP:NE1	2.31	0.60
3:R:255:ILE:HG13	3:R:256:ILE:HG13	1.82	0.60
1:A:227:LEU:HD21	1:A:268:LEU:HG	1.83	0.59
5:G:55:PRO:C	5:G:57:SER:N	2.53	0.59
4:B:158:VAL:HG11	4:B:192:LEU:HD11	1.84	0.59
1:A:259:PHE:O	1:A:317:LYS:NZ	2.35	0.58
4:B:51:LEU:HD23	4:B:87:THR:HG23	1.83	0.58
4:B:289:TYR:HH	4:B:297:TRP:HE1	1.50	0.58
5:G:11:GLN:HB3	5:G:14:LYS:HZ3	1.68	0.58
4:B:290:ASP:HA	4:B:314:ARG:HG3	1.86	0.57
3:R:30:ALA:HA	3:R:270:LEU:HD11	1.86	0.57
6:E:67:ARG:NH1	6:E:90:ASP:OD2	2.30	0.56
1:A:208:ARG:O	1:A:212:ILE:HB	2.06	0.56
3:R:207:GLU:OE2	3:R:210:ARG:NH2	2.39	0.56
3:R:241:TYR:HA	3:R:272:CYS:HB3	1.88	0.55
6:E:4:LEU:HD12	6:E:110:PHE:HD2	1.72	0.54
6:E:190:ARG:NH1	6:E:211:ASP:OD2	2.41	0.54
4:B:34:THR:O	4:B:301:LYS:NZ	2.40	0.54
2:L:5:VAL:HG23	3:R:91:TYR:CE1	2.43	0.54
1:A:251:ASP:OD1	1:A:255:ASN:ND2	2.42	0.53
4:B:318:LEU:HD12	4:B:329:THR:HG22	1.91	0.53
1:A:186:GLU:OE2	1:A:197:LYS:NZ	2.41	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:B:310:GLY:O	4:B:337:LYS:NZ	2.36	0.52
2:L:9:ARG:HH21	3:R:21:PRO:HB2	1.74	0.52
1:A:49:ILE:O	1:A:52:GLN:NE2	2.42	0.52
4:B:250:CYS:HB2	4:B:264:TYR:HB2	1.92	0.52
3:R:34:THR:O	3:R:38:TYR:HB2	2.10	0.51
6:E:91:THR:HB	6:E:119:VAL:HG22	1.91	0.51
3:R:24:ASN:C	3:R:26:ALA:N	2.65	0.51
5:G:18:GLN:HA	5:G:22:GLU:HB2	1.94	0.50
4:B:276:VAL:HG13	4:B:285:LEU:HD11	1.93	0.50
4:B:153:ASP:N	4:B:153:ASP:OD1	2.45	0.49
4:B:254:ASP:OD1	4:B:255:LEU:N	2.45	0.49
1:A:53:MET:HG2	1:A:54:LYS:HE3	1.95	0.49
5:G:11:GLN:HA	5:G:14:LYS:NZ	2.28	0.49
1:A:5:LEU:O	1:A:10:LYS:NZ	2.46	0.48
2:L:9:ARG:NH1	3:R:23:GLU:HB3	2.30	0.47
4:B:331:SER:OG	4:B:332:TRP:N	2.47	0.47
1:A:46:LYS:O	1:A:50:VAL:HG23	2.15	0.47
3:R:49:ASN:HB2	3:R:78:LEU:HD13	1.95	0.47
3:R:72:ASN:HD21	3:R:154:TRP:HE1	1.62	0.46
3:R:170:VAL:C	3:R:171:LEU:HD12	2.35	0.46
1:A:227:LEU:HD11	1:A:268:LEU:HB3	1.97	0.46
5:G:20:LYS:HB3	5:G:20:LYS:HE3	1.49	0.46
4:B:227:SER:OG	4:B:228:ASP:N	2.47	0.46
4:B:323:ASP:OD1	4:B:323:ASP:N	2.34	0.46
3:R:111:ILE:HD11	3:R:158:ILE:HA	1.96	0.46
3:R:141:PRO:O	3:R:146:ARG:NH1	2.46	0.46
1:A:210:LYS:O	1:A:213:HIS:NE2	2.49	0.46
1:A:249:LEU:O	1:A:253:ILE:HG23	2.15	0.46
3:R:32:LEU:O	3:R:36:VAL:HG22	2.16	0.46
4:B:277:SER:HB3	4:B:318:LEU:HD23	1.98	0.45
1:A:35:LYS:NZ	1:A:197:LYS:HD3	2.31	0.45
1:A:229:ASP:OD1	1:A:232:LEU:HB3	2.16	0.45
3:R:64:SER:O	3:R:68:ILE:HG13	2.17	0.45
3:R:189:GLN:HE21	3:R:193:PHE:HE2	1.65	0.45
3:R:209:LEU:HD23	3:R:209:LEU:HA	1.77	0.45
4:B:51:LEU:HB2	4:B:336:LEU:HB2	1.99	0.45
3:R:89:SER:OG	3:R:90:PRO:HD3	2.17	0.45
4:B:30:LEU:HD13	5:G:34:ALA:HB1	1.99	0.44
4:B:79:LEU:HD11	4:B:114:CYS:HB3	1.99	0.44
3:R:24:ASN:C	3:R:26:ALA:H	2.20	0.44
4:B:254:ASP:OD2	5:G:33:ALA:HB1	2.18	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:B:300:LEU:HD13	5:G:38:MET:HG3	2.00	0.44
4:B:211:TRP:CZ3	4:B:218:CYS:HB2	2.52	0.43
4:B:250:CYS:SG	4:B:273:ILE:HD13	2.58	0.43
6:E:53:SER:HA	6:E:72:ARG:NH1	2.34	0.43
1:A:320:TYR:HB3	1:A:334:PHE:CZ	2.53	0.43
3:R:90:PRO:HG3	3:R:95:TRP:HE3	1.84	0.43
1:A:295:THR:HG23	1:A:298:GLU:H	1.84	0.43
6:E:162:LEU:HD22	6:E:200:PHE:CG	2.54	0.43
3:R:34:THR:HG21	3:R:91:TYR:CE2	2.54	0.42
4:B:197:ARG:NH1	4:B:214:ARG:HG3	2.34	0.42
4:B:137:ARG:HH22	4:B:172:GLU:HA	1.84	0.42
4:B:186:ASP:HB2	4:B:204:CYS:SG	2.59	0.42
6:E:166:LEU:HB2	6:E:176:LEU:HD11	2.01	0.42
1:A:257:LYS:HB3	1:A:257:LYS:HE2	1.84	0.42
4:B:15:LYS:HG2	5:G:18:GLN:OE1	2.19	0.42
5:G:11:GLN:HB3	5:G:14:LYS:NZ	2.35	0.42
3:R:24:ASN:OD1	3:R:26:ALA:HB3	2.19	0.42
1:A:182:THR:HG23	4:B:119:ASN:HD22	1.85	0.41
4:B:153:ASP:OD1	4:B:156:GLN:HB2	2.19	0.41
1:A:214:CYS:SG	4:B:75:GLN:NE2	2.88	0.41
3:R:121:THR:HG23	3:R:200:ILE:HG21	2.03	0.41
1:A:16:SER:HB2	4:B:89:LYS:H	1.84	0.41
6:E:153:LEU:HA	6:E:221:LEU:HD22	2.03	0.41
3:R:99:ASP:OD1	3:R:103:LYS:NZ	2.53	0.41
5:G:46:LYS:H	5:G:46:LYS:HG3	1.42	0.41
3:R:23:GLU:OE1	3:R:23:GLU:N	2.54	0.41
4:B:311:HIS:ND1	4:B:331:SER:HB3	2.35	0.41
1:A:233:VAL:HA	1:A:241:ASN:HA	2.02	0.41
1:A:314:LYS:HE3	1:A:314:LYS:HB2	1.83	0.41
4:B:303:ASP:OD1	4:B:303:ASP:N	2.45	0.41
6:E:6:GLU:HA	6:E:22:CYS:HA	2.03	0.41
3:R:180:LEU:HD13	3:R:184:LEU:HG	2.02	0.41
1:A:225:VAL:HG11	1:A:307:PHE:CZ	2.57	0.41
4:B:27:ASP:OD1	4:B:27:ASP:N	2.51	0.41
3:R:124:THR:HG21	3:R:201:ILE:HA	2.01	0.40
4:B:76:ASP:OD1	4:B:76:ASP:N	2.54	0.40
4:B:15:LYS:HG3	5:G:18:GLN:HE22	1.85	0.40
3:R:246:PHE:HA	3:R:249:THR:HG22	2.03	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	212/354 (60%)	209 (99%)	3 (1%)	0	100 100
2	L	9/133 (7%)	9 (100%)	0	0	100 100
3	R	281/532 (53%)	278 (99%)	3 (1%)	0	100 100
4	B	334/351 (95%)	326 (98%)	8 (2%)	0	100 100
5	G	52/71 (73%)	40 (77%)	8 (15%)	4 (8%)	1 4
6	E	228/266 (86%)	223 (98%)	5 (2%)	0	100 100
All	All	1116/1707 (65%)	1085 (97%)	27 (2%)	4 (0%)	32 60

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
5	G	56	ALA
5	G	58	GLN
5	G	59	ASN
5	G	60	PRO

5.3.2 Protein sidechains [\(i\)](#)

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	194/305 (64%)	187 (96%)	7 (4%)	30 58
2	L	10/111 (9%)	10 (100%)	0	100 100
3	R	253/473 (54%)	247 (98%)	6 (2%)	44 67

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
4	B	278/293 (95%)	268 (96%)	10 (4%)	30 58
5	G	44/58 (76%)	28 (64%)	16 (36%)	0 0
6	E	195/215 (91%)	191 (98%)	4 (2%)	48 69
All	All	974/1455 (67%)	931 (96%)	43 (4%)	26 52

All (43) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	20	ASP
1	A	22	ASN
1	A	39	LEU
1	A	53	MET
1	A	197	LYS
1	A	261	ASP
1	A	345	LYS
3	R	72	ASN
3	R	128	TYR
3	R	167	PHE
3	R	228	PHE
3	R	263	GLN
3	R	281	CYS
4	B	61	MET
4	B	74	SER
4	B	103	CYS
4	B	105	TYR
4	B	228	ASP
4	B	234	PHE
4	B	271	CYS
4	B	298	ASP
4	B	323	ASP
4	B	340	ASN
5	G	11	GLN
5	G	13	ARG
5	G	17	GLN
5	G	19	LEU
5	G	20	LYS
5	G	22	GLU
5	G	24	ASN
5	G	28	ILE
5	G	42	GLU
5	G	46	LYS

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Mol	Chain	Res	Type
5	G	50	LEU
5	G	51	LEU
5	G	57	SER
5	G	58	GLN
5	G	59	ASN
5	G	62	ARG
6	E	4	LEU
6	E	53	SER
6	E	91	THR
6	E	180	MET

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (3) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	241	ASN
4	B	237	ASN
4	B	340	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 [\(i\)](#)

There are no ligands in this entry.

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.

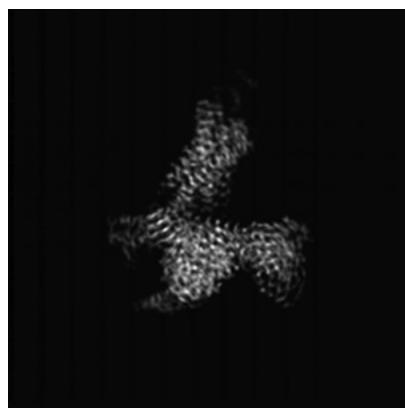
6 Map visualisation (i)

This section contains visualisations of the EMDB entry EMD-43825. 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)

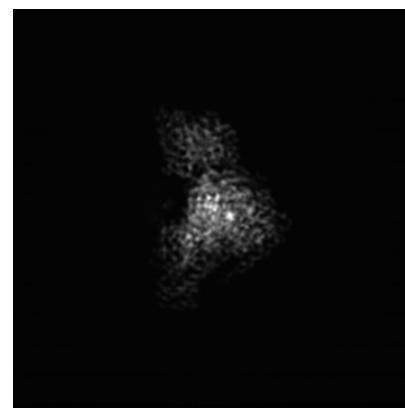
6.1.1 Primary map



X

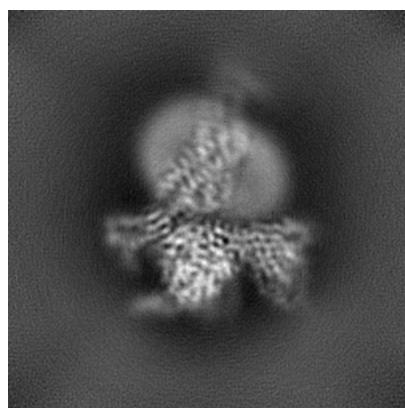


Y

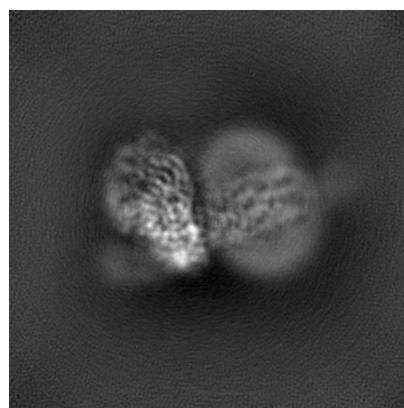


Z

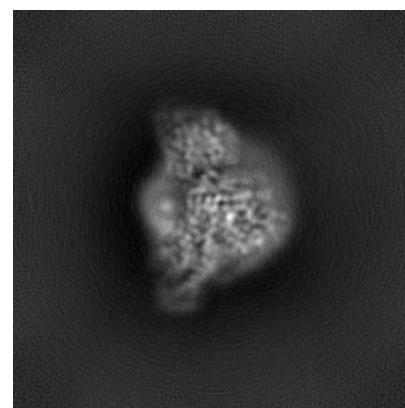
6.1.2 Raw map



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: 128

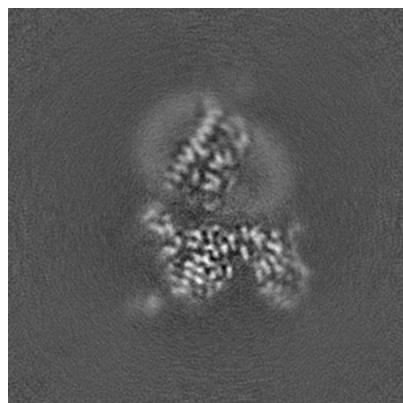


Y Index: 128

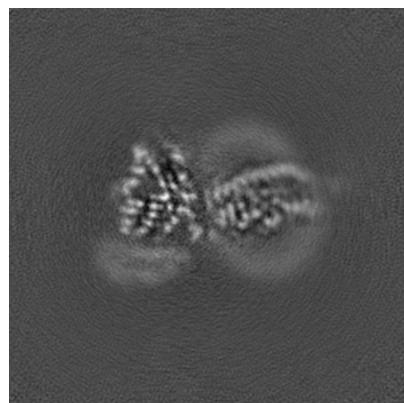


Z Index: 128

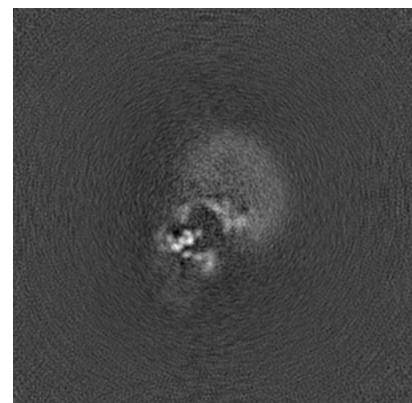
6.2.2 Raw map



X Index: 128



Y Index: 128



Z Index: 128

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: 124

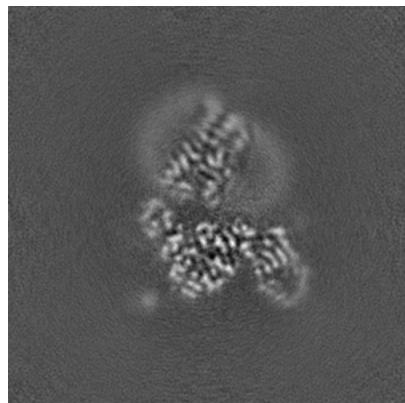


Y Index: 129

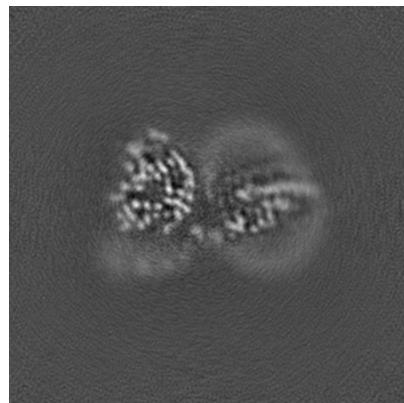


Z Index: 100

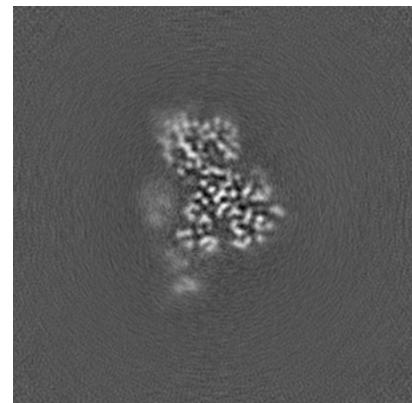
6.3.2 Raw map



X Index: 125



Y Index: 122

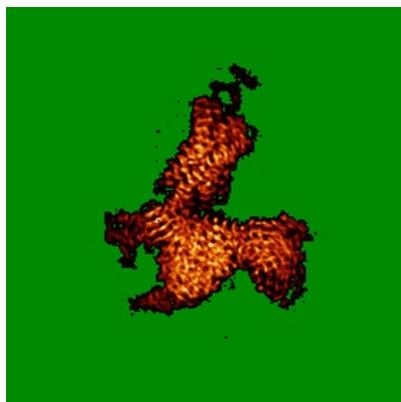


Z Index: 100

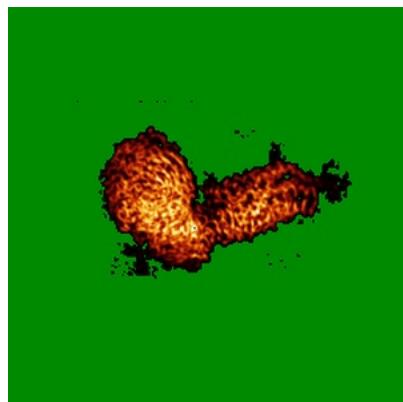
The images above show the largest variance slices of the map in three orthogonal directions.

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

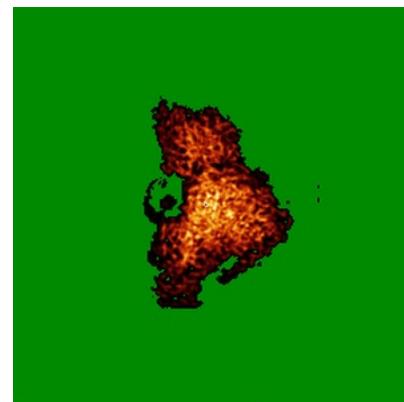
6.4.1 Primary map



X

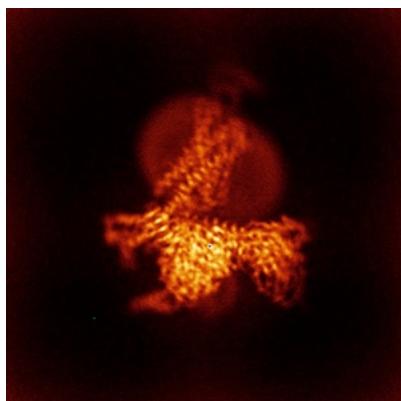


Y

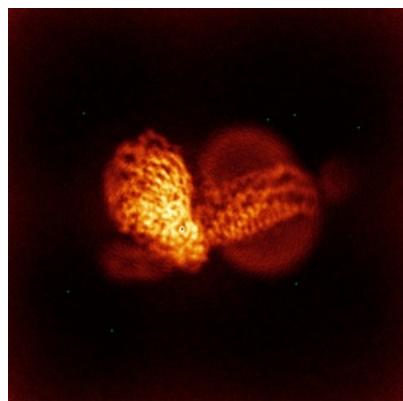


Z

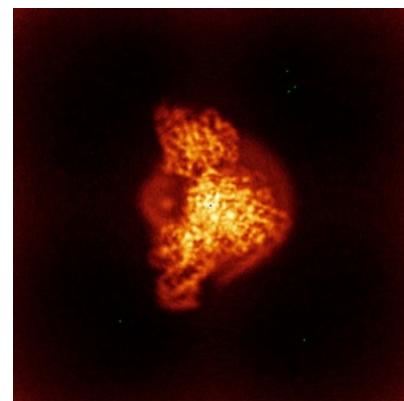
6.4.2 Raw map



X



Y

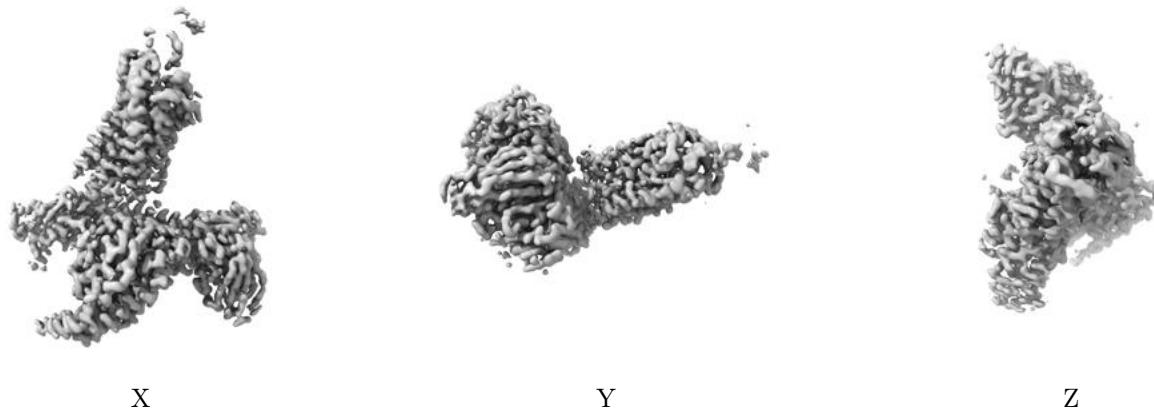


Z

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.

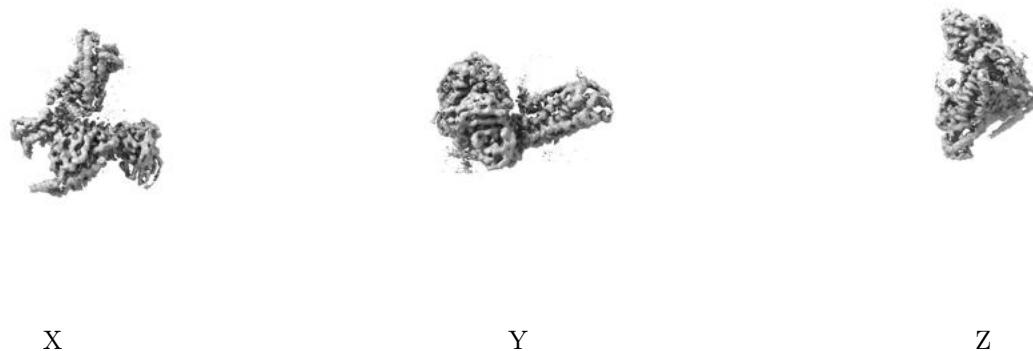
6.5 Orthogonal surface views (i)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.0465. 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.

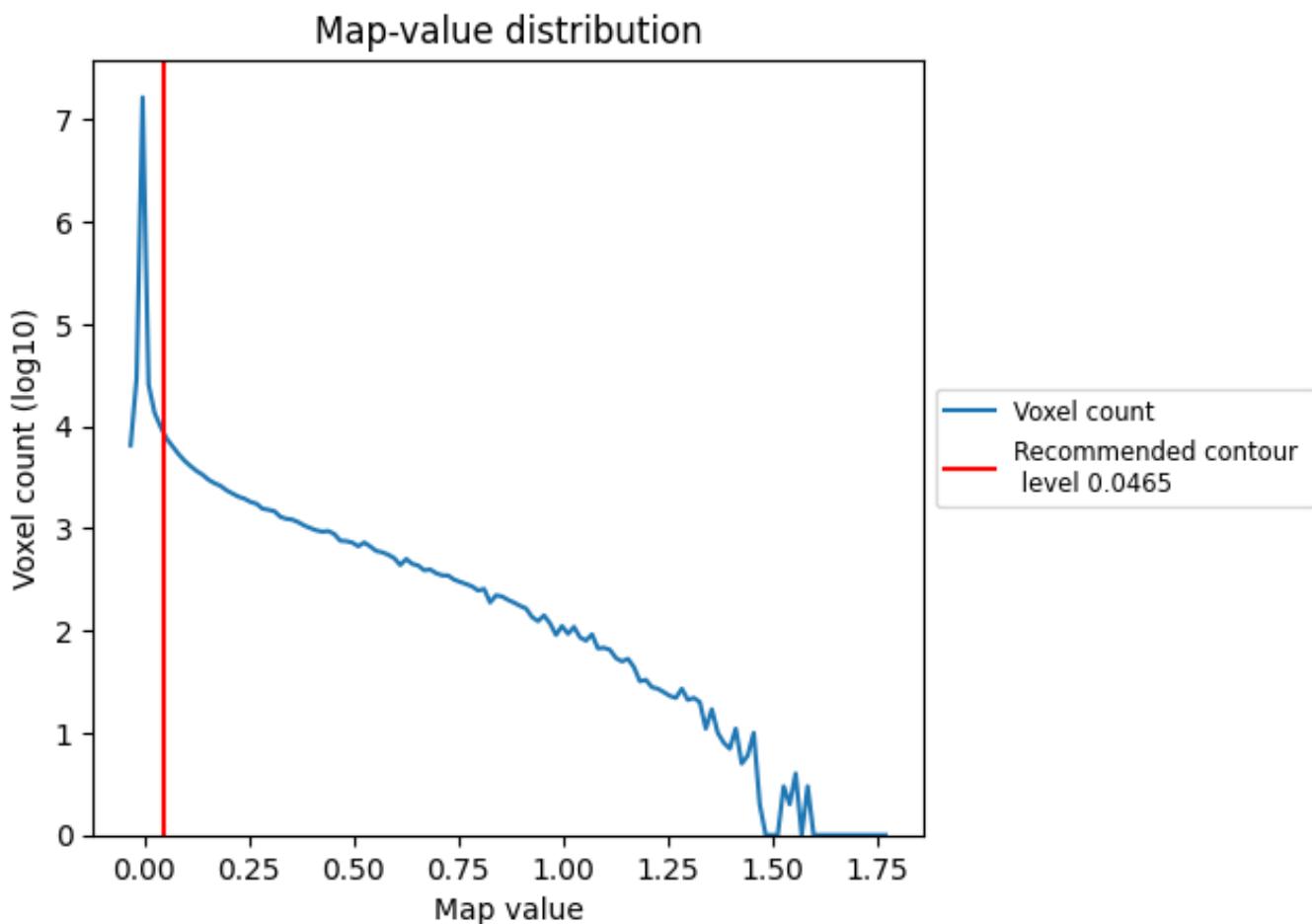
6.6 Mask visualisation (i)

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

7 Map analysis (i)

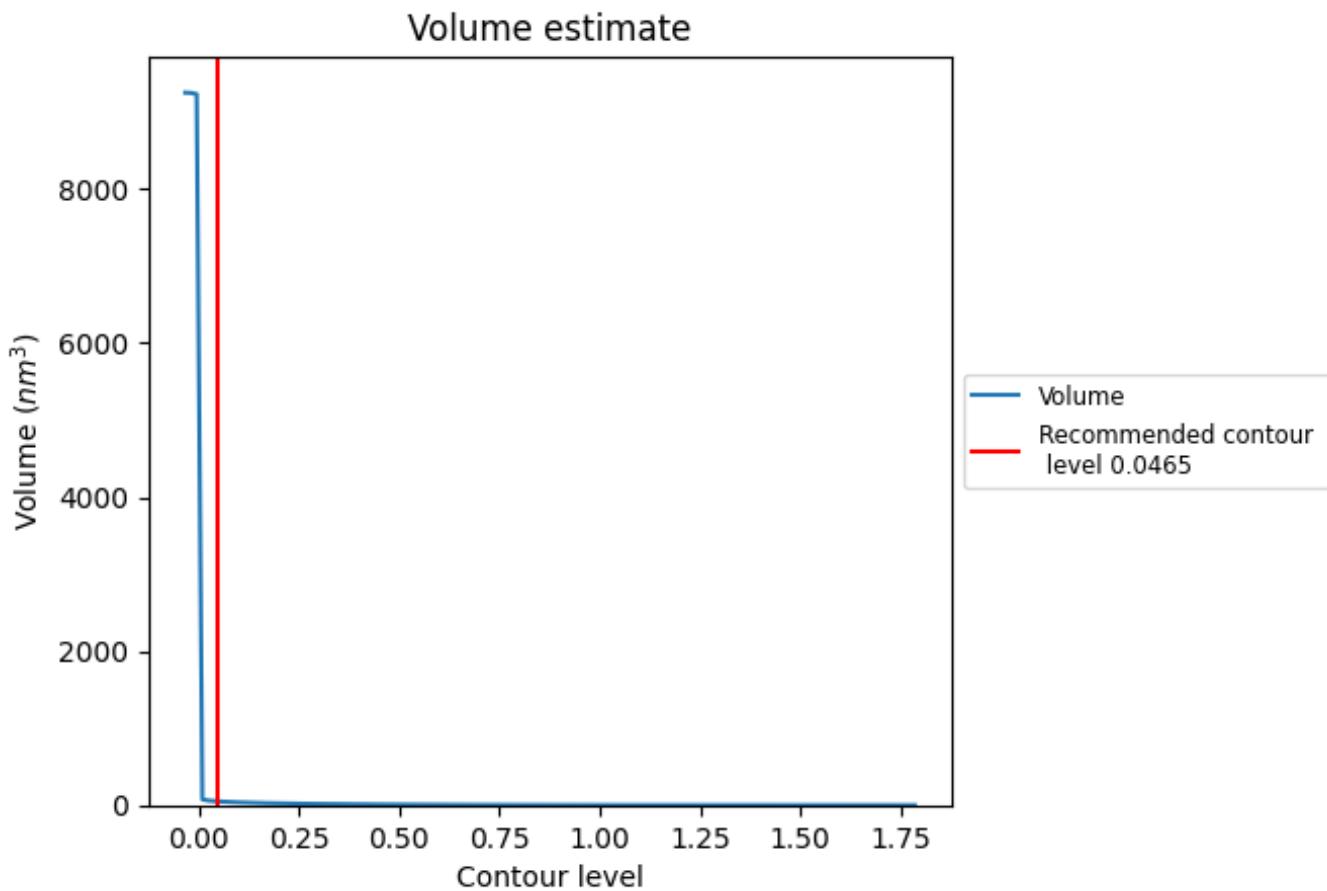
This section contains the results of statistical analysis of the map.

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.

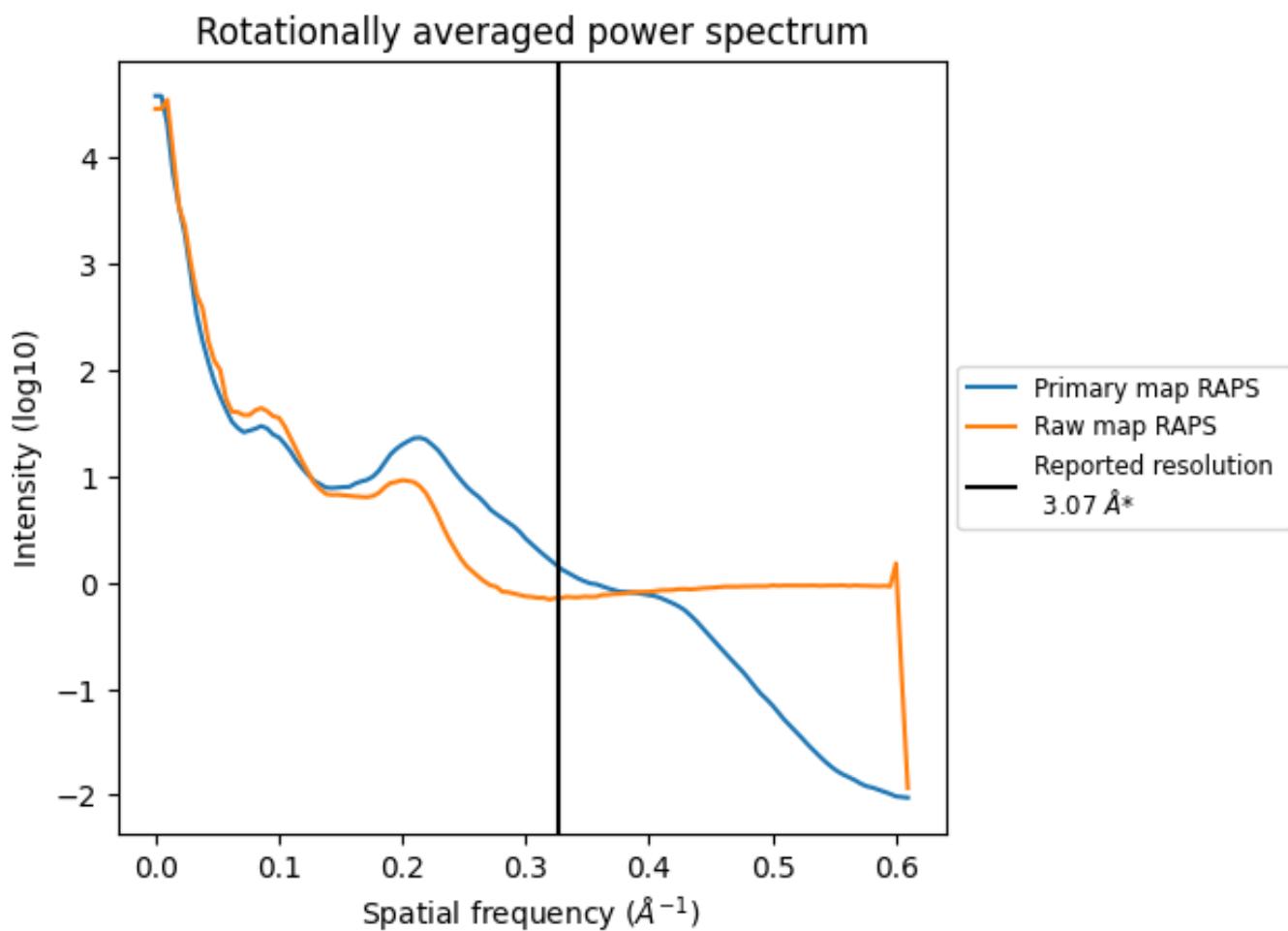
7.2 Volume estimate [\(i\)](#)



The volume at the recommended contour level is 50 nm^3 ; this corresponds to an approximate mass of 45 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 [\(i\)](#)

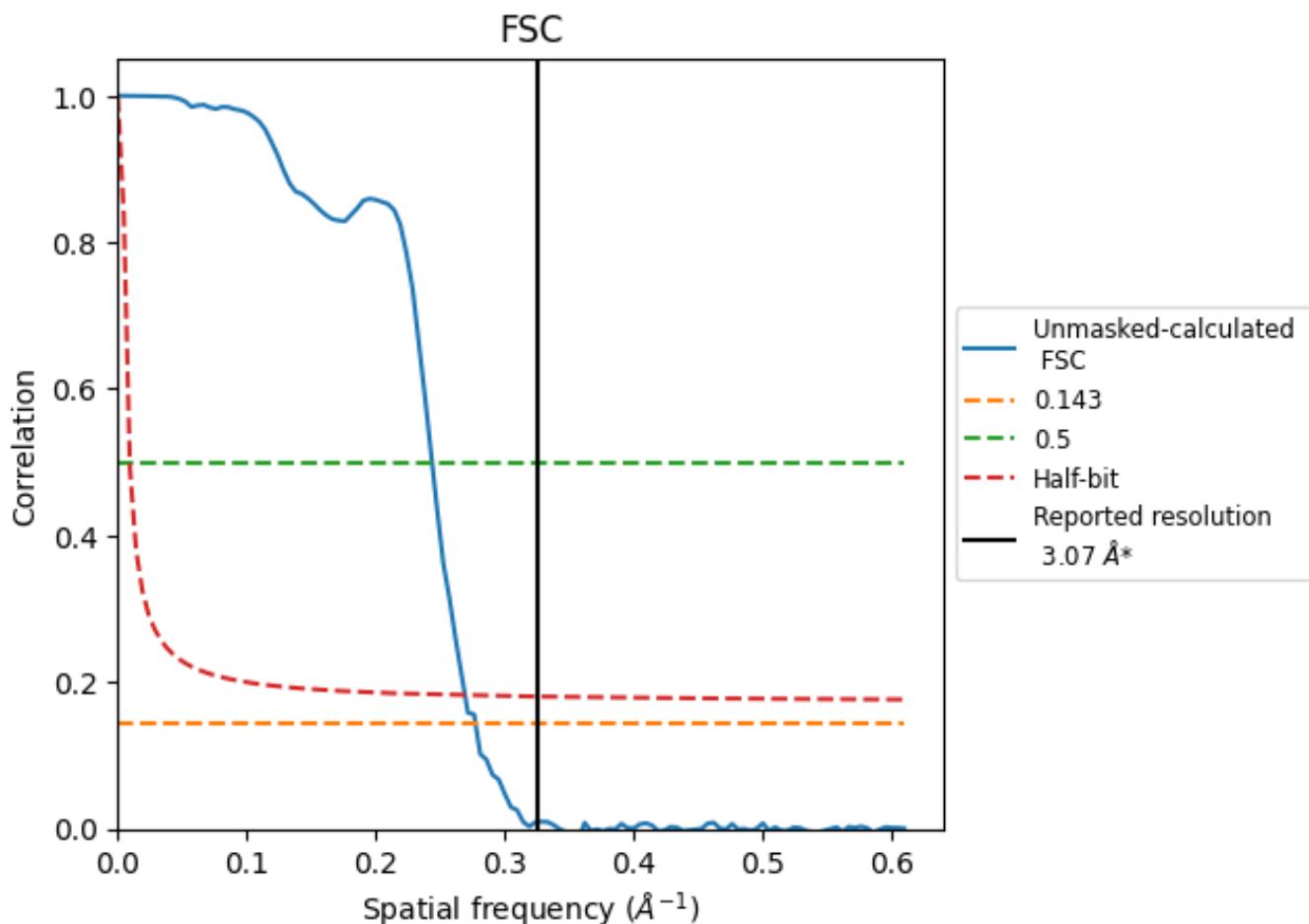


*Reported resolution corresponds to spatial frequency of 0.326 \AA^{-1}

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 0.326 \AA^{-1}

8.2 Resolution estimates [\(i\)](#)

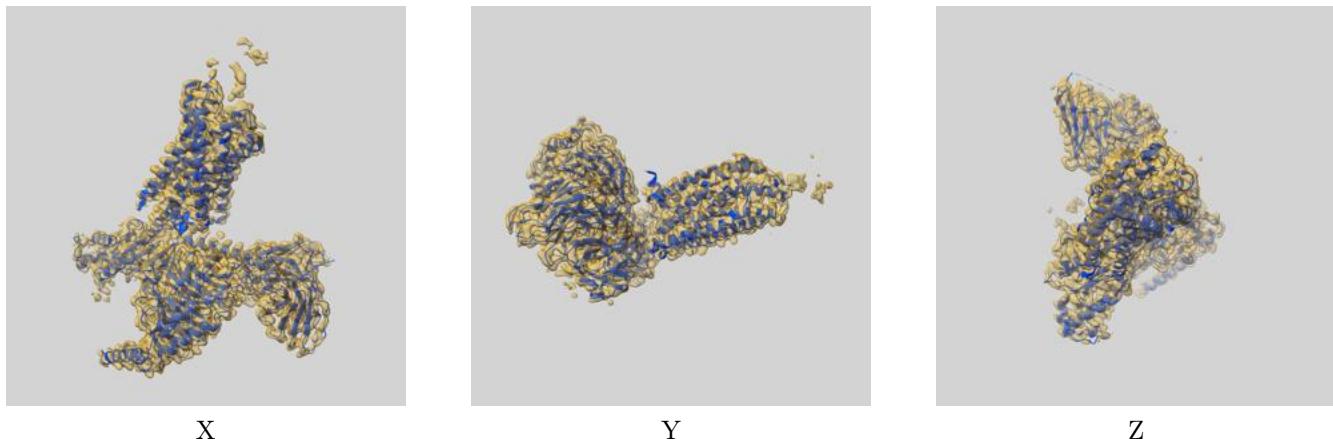
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.07	-	-
Author-provided FSC curve	-	-	-
Unmasked-calculated*	3.60	4.10	3.71

*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 3.60 differs from the reported value 3.07 by more than 10 %

9 Map-model fit (i)

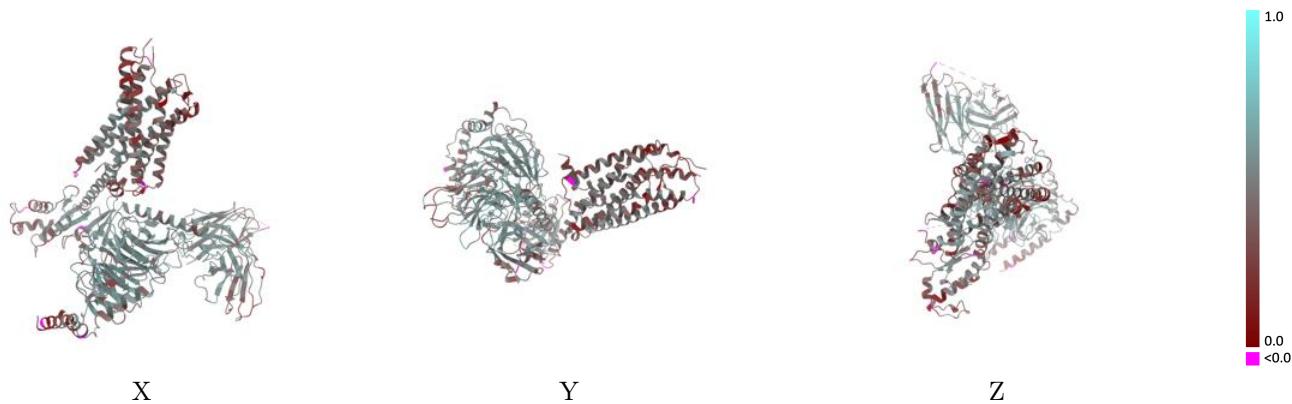
This section contains information regarding the fit between EMDB map EMD-43825 and PDB model 9AST. Per-residue inclusion information can be found in section 3 on page 8.

9.1 Map-model overlay (i)



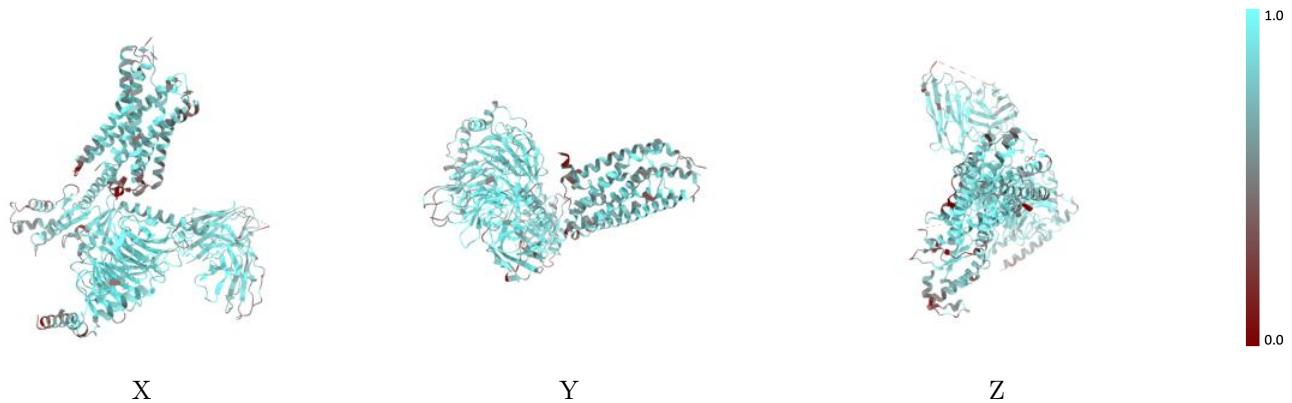
The images above show the 3D surface view of the map at the recommended contour level 0.0465 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



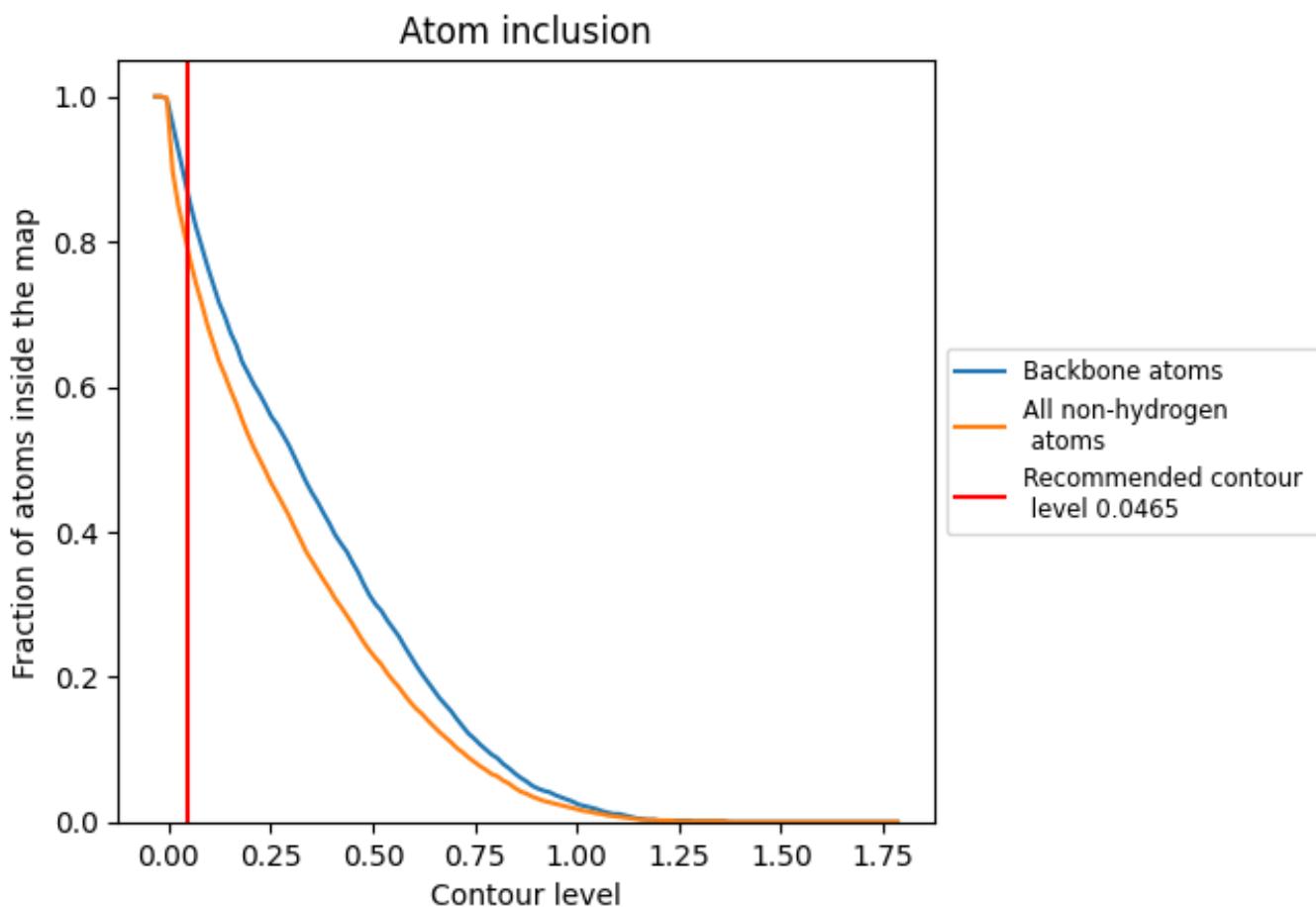
The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.0465).

9.4 Atom inclusion [\(i\)](#)



At the recommended contour level, 87% of all backbone atoms, 79% 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 (0.0465) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.7890	0.4550
A	0.7230	0.4220
B	0.8860	0.5280
E	0.8110	0.4890
G	0.6710	0.4100
L	0.6920	0.3160
R	0.7370	0.3820

