



Full wwPDB EM Validation Report ⓘ

Mar 30, 2026 – 03:23 AM UTC

PDB ID : 8ZH8 / pdb_00008zh8
EMDB ID : EMD-60096
Title : Human GPR103 -Gq complex bound to QRFP26
Authors : Iwama, A.; Akasaka, H.; Sano, F.K.; Oshima, H.S.; Shihoya, W.; Nureki, O.
Deposited on : 2024-05-10
Resolution : 3.19 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
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

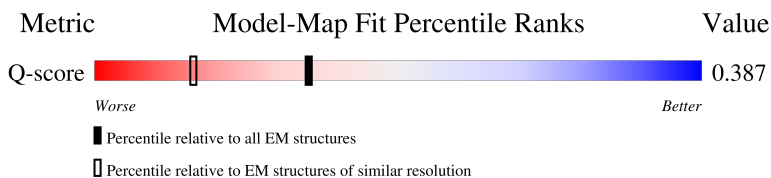
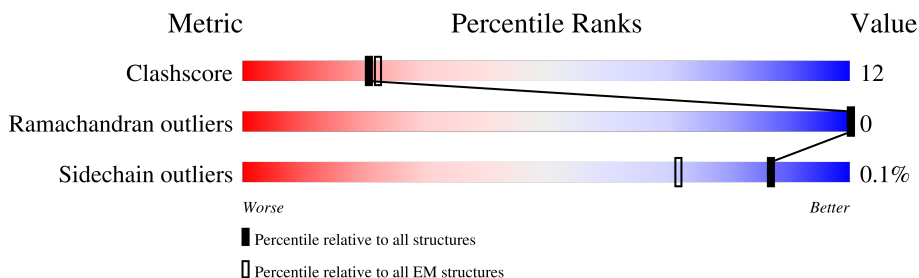
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 3.19 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	14455 (2.69 - 3.69)

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	R	402	
2	N	137	
3	B	351	
4	G	68	

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Mol	Chain	Length	Quality of chain
5	A	326	
6	S	260	
7	Q	27	

2 Entry composition

There are 7 unique types of molecules in this entry. The entry contains 10048 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 Pyroglutamylated RF-amide peptide receptor.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	R	325	Total	C	N	O	S	0	0
			2635	1751	426	435	23		

There are 37 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
R	-22	MET	-	initiating methionine	UNP Q96P65
R	-21	LYS	-	expression tag	UNP Q96P65
R	-20	THR	-	expression tag	UNP Q96P65
R	-19	ILE	-	expression tag	UNP Q96P65
R	-18	ILE	-	expression tag	UNP Q96P65
R	-17	ALA	-	expression tag	UNP Q96P65
R	-16	LEU	-	expression tag	UNP Q96P65
R	-15	SER	-	expression tag	UNP Q96P65
R	-14	TYR	-	expression tag	UNP Q96P65
R	-13	ILE	-	expression tag	UNP Q96P65
R	-12	PHE	-	expression tag	UNP Q96P65
R	-11	CYS	-	expression tag	UNP Q96P65
R	-10	LEU	-	expression tag	UNP Q96P65
R	-9	VAL	-	expression tag	UNP Q96P65
R	-8	PHE	-	expression tag	UNP Q96P65
R	-7	ALA	-	expression tag	UNP Q96P65
R	-6	ASP	-	expression tag	UNP Q96P65
R	-5	TYR	-	expression tag	UNP Q96P65
R	-4	LYS	-	expression tag	UNP Q96P65
R	-3	ASP	-	expression tag	UNP Q96P65
R	-2	ASP	-	expression tag	UNP Q96P65
R	-1	ASP	-	expression tag	UNP Q96P65
R	0	ASP	-	expression tag	UNP Q96P65
R	1	LYS	-	expression tag	UNP Q96P65
R	367	SER	-	expression tag	UNP Q96P65
R	368	GLY	-	expression tag	UNP Q96P65
R	369	GLY	-	expression tag	UNP Q96P65
R	370	GLY	-	expression tag	UNP Q96P65

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Chain	Residue	Modelled	Actual	Comment	Reference
R	371	GLY	-	expression tag	UNP Q96P65
R	372	SER	-	expression tag	UNP Q96P65
R	373	GLY	-	expression tag	UNP Q96P65
R	374	GLY	-	expression tag	UNP Q96P65
R	375	SER	-	expression tag	UNP Q96P65
R	376	SER	-	expression tag	UNP Q96P65
R	377	SER	-	expression tag	UNP Q96P65
R	378	GLY	-	expression tag	UNP Q96P65
R	379	GLY	-	expression tag	UNP Q96P65

- Molecule 2 is a protein called nanobody Nb35.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	N	128	Total	C	N	O	S	0	0
			968	603	170	189	6		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
3	B	337	Total	C	N	O	S	0	0
			2473	1541	439	473	20		

There are 12 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	-10	MET	-	expression tag	UNP P54311
B	-9	HIS	-	expression tag	UNP P54311
B	-8	HIS	-	expression tag	UNP P54311
B	-7	HIS	-	expression tag	UNP P54311
B	-6	HIS	-	expression tag	UNP P54311
B	-5	HIS	-	expression tag	UNP P54311
B	-4	HIS	-	expression tag	UNP P54311
B	-3	GLY	-	expression tag	UNP P54311
B	-2	SER	-	expression tag	UNP P54311
B	-1	LEU	-	expression tag	UNP P54311
B	0	LEU	-	expression tag	UNP P54311
B	1	GLN	-	expression tag	UNP P54311

- Molecule 4 is a protein called Guanine nucleotide-binding protein G(I)/G(S)/G(O) subunit gamma-2.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	G	51	Total	C	N	O	S	0	0
			350	221	60	67	2		

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
G	68	SER	-	expression tag	UNP P63212

- Molecule 5 is a protein called Guanine nucleotide-binding protein G(I)/G(S)/G(O) subunit gamma-2, Guanine nucleotide-binding protein G(i) subunit alpha-2, Guanine nucleotide-binding protein G(s) subunit alpha isoforms XLas.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	A	220	Total	C	N	O	S	0	0
			1704	1085	301	311	7		

There are 52 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-8	GLY	-	linker	UNP P59768
A	-7	SER	-	linker	UNP P59768
A	-6	ALA	-	linker	UNP P59768
A	-5	GLY	-	linker	UNP P59768
A	-4	SER	-	linker	UNP P59768
A	-3	ALA	-	linker	UNP P59768
A	-2	GLY	-	linker	UNP P59768
A	-1	SER	-	linker	UNP P59768
A	0	ALA	-	linker	UNP P59768
A	3	SER	CYS	engineered mutation	UNP P04899
A	31	ARG	ALA	engineered mutation	UNP P04899
A	33	THR	GLU	engineered mutation	UNP P04899
A	34	LEU	VAL	engineered mutation	UNP P04899
A	35	ARG	LYS	engineered mutation	UNP P04899
A	42	ASP	GLY	engineered mutation	UNP P04899
A	43	ASN	GLU	engineered mutation	UNP P04899
A	54	ARG	LYS	engineered mutation	UNP P04899
A	56	LEU	ILE	engineered mutation	UNP P04899
A	58	GLY	-	linker	UNP P04899
A	59	GLY	-	linker	UNP P04899
A	60	SER	-	linker	UNP P04899
A	61	GLY	-	linker	UNP P04899
A	62	GLY	-	linker	UNP P04899
A	63	SER	-	linker	UNP P04899

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Chain	Residue	Modelled	Actual	Comment	Reference
A	64	GLY	-	linker	UNP P04899
A	65	GLY	-	linker	UNP P04899
A	111	ASP	ALA	engineered mutation	UNP Q5JWF2
A	114	ASP	SER	engineered mutation	UNP Q5JWF2
A	?	-	ASN	deletion	UNP Q5JWF2
A	?	-	MET	deletion	UNP Q5JWF2
A	?	-	VAL	deletion	UNP Q5JWF2
A	?	-	ILE	deletion	UNP Q5JWF2
A	?	-	ARG	deletion	UNP Q5JWF2
A	?	-	GLU	deletion	UNP Q5JWF2
A	?	-	ASP	deletion	UNP Q5JWF2
A	?	-	ASN	deletion	UNP Q5JWF2
A	?	-	GLN	deletion	UNP Q5JWF2
A	?	-	THR	deletion	UNP Q5JWF2
A	124	ASP	LEU	engineered mutation	UNP Q5JWF2
A	195	LYS	ASP	engineered mutation	UNP Q5JWF2
A	198	VAL	LEU	engineered mutation	UNP Q5JWF2
A	199	ASP	ARG	engineered mutation	UNP Q5JWF2
A	210	ILE	TYR	engineered mutation	UNP Q5JWF2
A	224	ALA	ILE	engineered mutation	UNP Q5JWF2
A	227	ILE	VAL	engineered mutation	UNP Q5JWF2
A	232	LYS	ARG	engineered mutation	UNP Q5JWF2
A	236	LEU	GLN	engineered mutation	UNP Q5JWF2
A	237	GLN	ARG	engineered mutation	UNP Q5JWF2
A	239	ASN	HIS	engineered mutation	UNP Q5JWF2
A	242	GLU	GLN	engineered mutation	UNP Q5JWF2
A	244	ASN	GLU	engineered mutation	UNP Q5JWF2
A	246	VAL	LEU	engineered mutation	UNP Q5JWF2

- Molecule 6 is a protein called scFv16.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	S	231	Total	C	N	O	S	0	0
			1730	1101	289	330	10		

- Molecule 7 is a protein called QRF-amide.

Mol	Chain	Residues	Atoms				AltConf	Trace
7	Q	25	Total	C	N	O	0	1
			188	120	35	33		

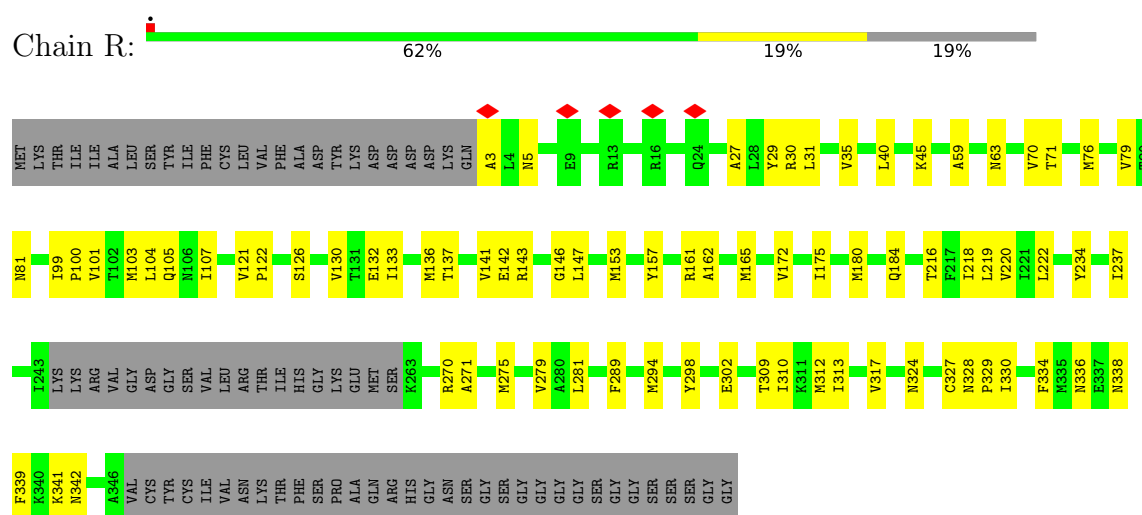
There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
Q	27	NH2	-	amidation	UNP P83859

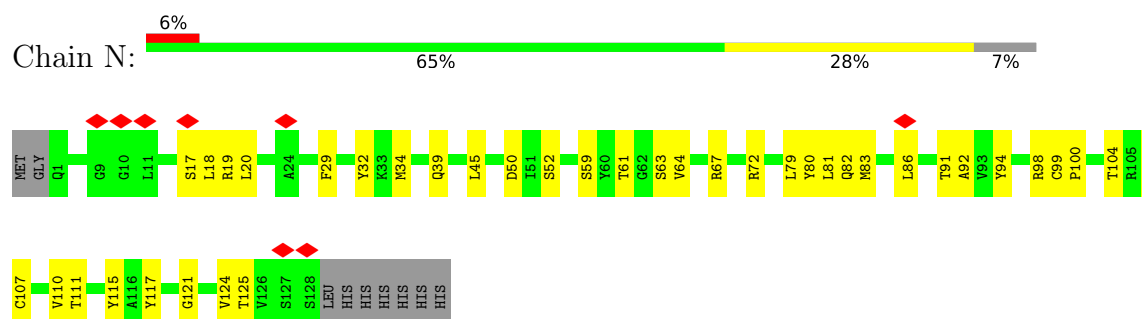
3 Residue-property plots [i](#)

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.

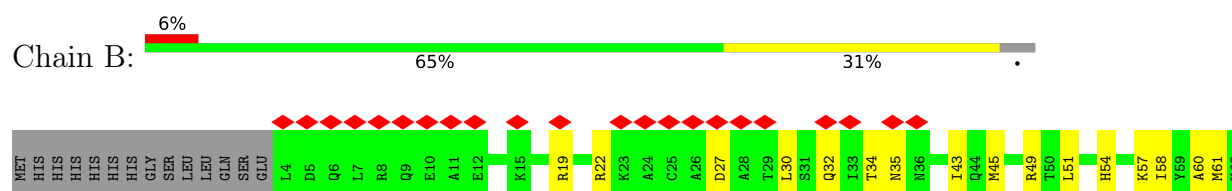
- Molecule 1: Pyroglutamylated RF-amide peptide receptor

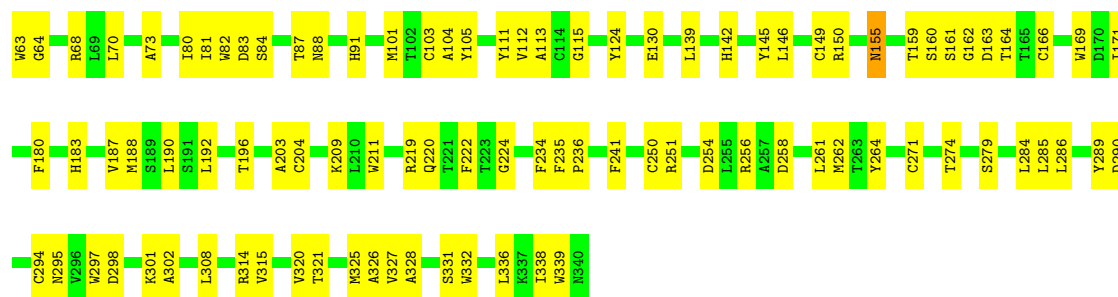


- Molecule 2: nanobody Nb35

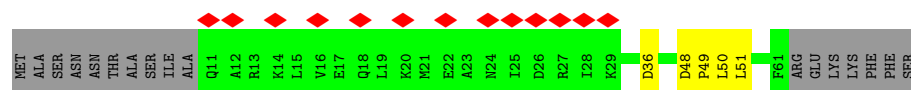


- Molecule 3: Guanine nucleotide-binding protein G(I)/G(S)/G(T) subunit beta-1

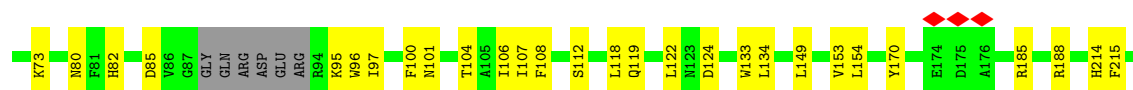
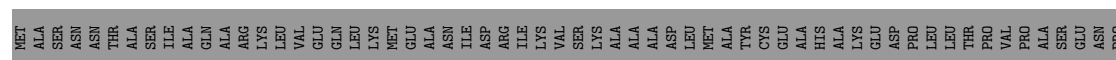




- Molecule 4: Guanine nucleotide-binding protein G(I)/G(S)/G(O) subunit gamma-2



- Molecule 5: Guanine nucleotide-binding protein G(I)/G(S)/G(O) subunit gamma-2, Guanine nucleotide-binding protein G(i) subunit alpha-2, Guanine nucleotide-binding protein G(s) subunit alpha isoforms XLas



- Molecule 6: scFv16



- Molecule 7: QRF-amide



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	142831	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	0.83	Depositor
Minimum defocus (nm)	800	Depositor
Maximum defocus (nm)	1600	Depositor
Magnification	Not provided	
Image detector	GATAN K3 (6k x 4k)	Depositor
Maximum map value	36.747	Depositor
Minimum map value	-19.046	Depositor
Average map value	-0.001	Depositor
Map value standard deviation	1.034	Depositor
Recommended contour level	4.2	Depositor
Map size ($\text{\AA}$)	265.59, 265.59, 265.59	wwPDB
Map dimensions	260, 260, 260	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing ($\text{\AA}$)	1.0215, 1.0215, 1.0215	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: NH2

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	R	0.21	0/2701	0.45	0/3671
2	N	0.13	0/988	0.37	0/1339
3	B	0.14	0/2520	0.43	0/3432
4	G	0.10	0/356	0.29	0/488
5	A	0.14	0/1735	0.38	0/2347
6	S	0.12	0/1774	0.37	0/2411
7	Q	0.29	0/191	0.46	0/252
All	All	0.16	0/10265	0.41	0/13940

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	R	2635	0	2735	54	0
2	N	968	0	931	28	0
3	B	2473	0	2303	80	0
4	G	350	0	315	4	0
5	A	1704	0	1637	45	0
6	S	1730	0	1628	44	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
7	Q	188	0	181	6	0
All	All	10048	0	9730	237	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 12.

All (237) 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:R:79:VAL:HG13	1:R:162:ALA:HB2	1.64	0.78
2:N:17:SER:HA	2:N:83:MET:O	1.87	0.73
3:B:155:ASN:O	3:B:155:ASN:ND2	2.23	0.72
2:N:63:SER:O	2:N:67:ARG:NH2	2.24	0.71
1:R:218:ILE:HG23	1:R:222:LEU:HD12	1.71	0.71
1:R:5:ASN:ND2	7:Q:15:TYR:OH	2.24	0.69
3:B:325:MET:HA	4:G:49:PRO:HG2	1.74	0.69
1:R:130:VAL:HG22	1:R:222:LEU:HD21	1.73	0.69
2:N:39:GLN:HB2	2:N:45:LEU:HD23	1.73	0.69
3:B:289:TYR:OH	3:B:297:TRP:NE1	2.25	0.69
3:B:150:ARG:HB2	3:B:192:LEU:HD13	1.76	0.68
6:S:9:GLY:O	6:S:18:ARG:NH1	2.27	0.68
2:N:20:LEU:HD12	2:N:81:LEU:HD23	1.77	0.67
6:S:94:TYR:O	6:S:114:GLY:CA	2.41	0.67
3:B:332:TRP:HZ3	5:A:101:ASN:HD22	1.43	0.67
1:R:281:LEU:HD21	1:R:327:CYS:HB3	1.76	0.66
1:R:147:LEU:HD12	1:R:237:ILE:HG23	1.75	0.66
2:N:52:SER:O	2:N:72:ARG:NH1	2.28	0.66
2:N:32:TYR:O	2:N:72:ARG:NH2	2.28	0.66
3:B:103:CYS:O	3:B:150:ARG:NH1	2.27	0.66
3:B:224:GLY:O	3:B:251:ARG:NH1	2.29	0.65
6:S:94:TYR:O	6:S:114:GLY:HA3	1.96	0.65
1:R:133:ILE:HD12	1:R:222:LEU:HD22	1.80	0.63
1:R:105:GLN:HG3	7:Q:22:PHE:HB2	1.81	0.63
5:A:170:TYR:O	5:A:188:ARG:NH1	2.32	0.63
3:B:58:ILE:HD13	3:B:336:LEU:HD12	1.82	0.62
6:S:128:MET:HG2	6:S:149:SER:HA	1.80	0.62
1:R:161:ARG:O	1:R:165:MET:HG3	2.00	0.62
2:N:29:PHE:HE1	2:N:34:MET:HE2	1.63	0.62
1:R:29:TYR:HB3	1:R:31:LEU:HG	1.82	0.62
2:N:83:MET:HE1	2:N:124:VAL:HG21	1.82	0.61
1:R:338:ASN:OD1	1:R:339:PHE:N	2.33	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:B:49:ARG:HD2	3:B:87:THR:HG23	1.81	0.61
3:B:104:ALA:HB3	3:B:113:ALA:HB3	1.83	0.61
1:R:143:ARG:HG2	5:A:245:LEU:HD21	1.83	0.60
1:R:146:GLY:HA3	5:A:243:TYR:HE2	1.66	0.60
6:S:167:GLN:NE2	6:S:168:ARG:O	2.30	0.60
1:R:324:ASN:ND2	1:R:328:ASN:OD1	2.34	0.60
3:B:60:ALA:HB3	3:B:73:ALA:HB3	1.84	0.60
5:A:28:GLU:OE2	5:A:32:ARG:NH1	2.27	0.60
3:B:145:TYR:O	3:B:162:GLY:N	2.35	0.60
3:B:234:PHE:HD1	3:B:241:PHE:HB3	1.67	0.60
3:B:279:SER:HA	3:B:320:VAL:HG11	1.84	0.59
1:R:142:GLU:OE1	1:R:157:TYR:OH	2.21	0.59
3:B:298:ASP:HB3	3:B:301:LYS:HB2	1.83	0.59
2:N:117:TYR:OH	3:B:204:CYS:O	2.22	0.58
1:R:122:PRO:HB2	1:R:180:MET:HB3	1.85	0.58
1:R:45:LYS:HE2	1:R:107:ILE:HA	1.84	0.57
6:S:9:GLY:HA3	6:S:116:THR:O	2.04	0.57
3:B:83:ASP:HB3	3:B:88:ASN:HB2	1.87	0.57
1:R:3:ALA:N	7:Q:11:GLU:OE2	2.37	0.57
5:A:73:LYS:HD3	5:A:82:HIS:HD2	1.70	0.56
6:S:6:GLU:OE2	6:S:96:CYS:N	2.36	0.56
5:A:106:ILE:HD11	5:A:134:LEU:HD22	1.88	0.56
3:B:294:CYS:HB2	3:B:308:LEU:HB2	1.87	0.56
3:B:51:LEU:HB2	3:B:336:LEU:HB2	1.89	0.55
6:S:22:CYS:HB3	6:S:79:LEU:HB3	1.89	0.54
3:B:166:CYS:HB2	3:B:180:PHE:HB2	1.88	0.54
1:R:275:MET:O	1:R:279:VAL:HG23	2.07	0.54
3:B:146:LEU:HD11	3:B:159:THR:HB	1.89	0.54
2:N:83:MET:SD	2:N:86:LEU:HD21	2.47	0.54
6:S:166:LEU:HB2	6:S:176:LEU:HD11	1.90	0.54
3:B:149:CYS:O	3:B:150:ARG:NH1	2.41	0.53
3:B:314:ARG:HD3	3:B:332:TRP:CE2	2.43	0.53
5:A:37:LEU:HD21	5:A:97:ILE:HD11	1.88	0.53
1:R:146:GLY:HA2	1:R:153:MET:HG3	1.89	0.53
1:R:234:TYR:HD1	1:R:237:ILE:HD12	1.74	0.53
6:S:38:ARG:N	6:S:46:GLU:O	2.41	0.53
3:B:271:CYS:HB2	3:B:290:ASP:HB2	1.90	0.53
3:B:54:HIS:CD2	3:B:80:ILE:HD12	2.43	0.52
3:B:61:MET:HE3	3:B:328:ALA:HB3	1.91	0.52
3:B:155:ASN:ND2	3:B:155:ASN:C	2.67	0.52
3:B:115:GLY:HA3	3:B:146:LEU:HD23	1.90	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:R:101:VAL:HG21	1:R:121:VAL:HG11	1.91	0.52
3:B:57:LYS:HZ3	5:A:101:ASN:HB3	1.74	0.52
2:N:110:VAL:HG23	2:N:111:THR:HG23	1.91	0.52
6:S:215:TYR:O	6:S:230:GLY:HA2	2.10	0.52
3:B:51:LEU:HD22	3:B:82:TRP:CE3	2.44	0.52
1:R:76:MET:SD	1:R:342:ASN:ND2	2.82	0.52
2:N:94:TYR:O	2:N:121:GLY:HA2	2.09	0.52
4:G:48:ASP:HB3	4:G:51:LEU:HB3	1.92	0.52
7:Q:16:SER:O	7:Q:17:ARG:HD3	2.09	0.51
3:B:57:LYS:NZ	5:A:101:ASN:HB3	2.25	0.51
6:S:38:ARG:HG3	6:S:46:GLU:HB3	1.92	0.51
1:R:100:PRO:HA	1:R:103:MET:HG2	1.93	0.51
2:N:104:THR:OG1	2:N:106:ASP:OD1	2.24	0.51
6:S:175:LEU:HD22	6:S:184:ALA:HB2	1.93	0.51
5:A:38:LEU:HD23	5:A:85:ASP:HB3	1.92	0.51
6:S:9:GLY:CA	6:S:116:THR:O	2.58	0.50
3:B:235:PHE:CD1	3:B:236:PRO:HD2	2.45	0.50
6:S:91:THR:HG23	6:S:118:THR:HA	1.92	0.50
5:A:214:HIS:CD2	5:A:226:ARG:HD3	2.45	0.50
5:A:95:LYS:C	5:A:97:ILE:H	2.19	0.50
2:N:61:THR:O	5:A:119:GLN:NE2	2.44	0.50
3:B:222:PHE:HE2	3:B:258:ASP:HA	1.75	0.50
1:R:35:VAL:HG22	7:Q:18:LYS:HB3	1.93	0.50
2:N:34:MET:HE3	2:N:79:LEU:HD22	1.94	0.50
3:B:264:TYR:HD1	3:B:302:ALA:HA	1.77	0.50
5:A:215:PHE:O	5:A:226:ARG:NH1	2.33	0.50
5:A:34:LEU:HD23	5:A:104:THR:HG21	1.93	0.49
5:A:108:PHE:HZ	5:A:124:ASP:HB3	1.77	0.49
1:R:76:MET:O	1:R:81:ASN:ND2	2.43	0.49
1:R:302:GLU:HA	1:R:310:ILE:HD11	1.93	0.49
2:N:91:THR:OG1	2:N:125:THR:HA	2.13	0.49
6:S:94:TYR:O	6:S:114:GLY:HA2	2.11	0.49
6:S:24:ALA:HB1	6:S:27:PHE:CE1	2.48	0.49
6:S:61:ALA:HB3	6:S:64:VAL:HG22	1.95	0.49
3:B:45:MET:HB3	3:B:339:TRP:HB3	1.93	0.49
3:B:286:LEU:HD13	3:B:327:VAL:HG21	1.94	0.48
5:A:49:ILE:HG22	5:A:50:VAL:HG23	1.95	0.48
6:S:161:TYR:HD2	6:S:221:LEU:HA	1.78	0.48
3:B:81:ILE:HD11	3:B:112:VAL:HG11	1.96	0.48
1:R:122:PRO:HG2	1:R:184:GLN:HG3	1.95	0.48
3:B:111:TYR:HA	3:B:124:TYR:O	2.13	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:A:8:GLU:OE2	6:S:163:TYR:OH	2.31	0.48
1:R:219:LEU:HD12	1:R:294:MET:SD	2.53	0.48
3:B:30:LEU:HD23	3:B:262:MET:HB2	1.96	0.48
6:S:167:GLN:HE22	6:S:171:GLN:C	2.20	0.48
1:R:147:LEU:HD11	5:A:245:LEU:HD13	1.97	0.47
1:R:271:ALA:O	1:R:275:MET:HG2	2.14	0.47
6:S:68:PHE:CZ	6:S:83:MET:HG2	2.50	0.47
1:R:40:LEU:HD22	1:R:312:MET:HG2	1.97	0.47
3:B:164:THR:HA	3:B:187:VAL:HG23	1.97	0.47
2:N:50:ASP:OD1	2:N:59:SER:HB2	2.15	0.47
1:R:289:PHE:HA	1:R:317:VAL:HB	1.96	0.46
2:N:29:PHE:CE1	2:N:34:MET:HE2	2.49	0.46
6:S:93:MET:HE1	6:S:95:TYR:OH	2.15	0.46
6:S:47:TRP:CD1	6:S:225:LEU:HD12	2.50	0.46
1:R:70:VAL:HG13	1:R:71:THR:HG23	1.97	0.46
6:S:162:LEU:HD13	6:S:200:PHE:CD2	2.50	0.46
1:R:172:VAL:HA	1:R:175:ILE:HG12	1.98	0.46
3:B:43:ILE:HD13	3:B:284:LEU:HD21	1.97	0.46
3:B:256:ARG:NH2	4:G:36:ASP:OD2	2.49	0.46
6:S:168:ARG:NH1	6:S:171:GLN:OE1	2.41	0.46
5:A:73:LYS:HD3	5:A:82:HIS:CD2	2.51	0.46
2:N:29:PHE:HE2	2:N:72:ARG:HG3	1.80	0.46
5:A:37:LEU:HD23	5:A:106:ILE:HG12	1.97	0.46
1:R:59:ALA:O	1:R:63:ASN:ND2	2.48	0.46
2:N:39:GLN:O	2:N:92:ALA:HB1	2.16	0.46
3:B:315:VAL:HA	3:B:331:SER:HA	1.98	0.46
5:A:154:LEU:HG	5:A:185:ARG:HH21	1.80	0.46
1:R:103:MET:HG3	1:R:104:LEU:HD12	1.98	0.45
1:R:218:ILE:HD12	7:Q:26:PHE:HZ	1.82	0.45
1:R:281:LEU:HD21	1:R:327:CYS:CB	2.46	0.45
3:B:219:ARG:HG3	3:B:220:GLN:NE2	2.32	0.45
6:S:219:GLN:HE21	6:S:226:THR:H	1.63	0.45
3:B:274:THR:CG2	3:B:314:ARG:HE	2.30	0.45
5:A:36:LEU:HD13	5:A:107:ILE:HD11	1.97	0.45
6:S:32:PHE:O	6:S:72:ARG:NH2	2.39	0.45
1:R:336:ASN:ND2	5:A:244:ASN:O	2.48	0.45
6:S:142:SER:HA	6:S:204:ILE:O	2.17	0.45
1:R:330:ILE:O	1:R:334:PHE:HD1	1.99	0.45
1:R:132:GLU:HG2	1:R:136:MET:HE3	1.98	0.45
3:B:219:ARG:HG3	3:B:220:GLN:CD	2.42	0.45
5:A:95:LYS:O	5:A:96:TRP:CG	2.71	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:A:240:LEU:HA	5:A:245:LEU:HD12	1.98	0.44
1:R:103:MET:O	1:R:107:ILE:HG12	2.17	0.44
1:R:338:ASN:O	1:R:341:LYS:HG3	2.17	0.44
3:B:27:ASP:OD1	3:B:27:ASP:N	2.50	0.44
6:S:105:SER:O	6:S:179:ARG:NH1	2.41	0.44
2:N:19:ARG:HG3	2:N:80:TYR:HE1	1.82	0.44
3:B:63:TRP:CE3	3:B:321:THR:HG22	2.52	0.44
3:B:180:PHE:HB3	3:B:211:TRP:CE3	2.52	0.44
5:A:119:GLN:HA	5:A:122:LEU:HD12	1.97	0.44
1:R:324:ASN:HA	1:R:327:CYS:SG	2.56	0.44
5:A:112:SER:HA	5:A:118:LEU:HD13	1.99	0.44
6:S:38:ARG:O	6:S:46:GLU:N	2.39	0.44
3:B:285:LEU:HB3	3:B:297:TRP:O	2.17	0.44
5:A:112:SER:O	5:A:149:LEU:HD12	2.18	0.44
5:A:235:ILE:HA	5:A:238:MET:HG2	1.99	0.44
3:B:70:LEU:HD23	3:B:84:SER:HB3	2.00	0.44
1:R:216:THR:O	1:R:220:VAL:HG23	2.18	0.44
1:R:216:THR:HG1	1:R:298:TYR:HH	1.54	0.44
1:R:309:THR:O	1:R:313:ILE:HG12	2.18	0.44
1:R:270:ARG:HD3	5:A:246:VAL:HG23	1.99	0.44
5:A:33:THR:HG22	5:A:80:ASN:HB2	2.00	0.43
6:S:39:GLN:HB2	6:S:45:LEU:HD23	2.00	0.43
6:S:60:TYR:OH	6:S:69:THR:HA	2.18	0.43
1:R:137:THR:O	1:R:141:VAL:HG23	2.17	0.43
2:N:80:TYR:CE2	2:N:82:GLN:HB2	2.54	0.43
3:B:250:CYS:HB2	3:B:264:TYR:HB2	2.00	0.43
1:R:328:ASN:O	1:R:329:PRO:C	2.61	0.43
2:N:98:ARG:HH21	2:N:100:PRO:HA	1.84	0.43
3:B:264:TYR:CD1	3:B:302:ALA:HA	2.54	0.43
2:N:18:LEU:HB3	2:N:83:MET:HE2	2.01	0.43
2:N:61:THR:HG22	2:N:64:VAL:HG22	2.01	0.43
3:B:139:LEU:HD11	3:B:171:ILE:HG13	2.00	0.43
5:A:234:ILE:HG22	5:A:238:MET:HE3	2.00	0.43
6:S:68:PHE:CE1	6:S:83:MET:HG2	2.54	0.43
3:B:81:ILE:HB	3:B:91:HIS:HB2	2.01	0.43
3:B:163:ASP:CG	3:B:163:ASP:O	2.62	0.43
3:B:290:ASP:HB3	5:A:133:TRP:HH2	1.83	0.42
2:N:99:CYS:HB3	2:N:107:CYS:HB3	1.83	0.42
3:B:326:ALA:HA	4:G:50:LEU:HD21	2.01	0.42
3:B:19:ARG:HA	3:B:22:ARG:HG2	2.02	0.42
3:B:68:ARG:HD3	6:S:103:TYR:CZ	2.55	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:B:64:GLY:HA2	3:B:105:TYR:CD2	2.54	0.42
1:R:27:ALA:HA	1:R:30:ARG:HE	1.84	0.42
3:B:61:MET:HE1	3:B:63:TRP:CD1	2.54	0.42
5:A:85:ASP:OD1	5:A:85:ASP:N	2.52	0.42
3:B:196:THR:HG22	3:B:196:THR:O	2.19	0.42
3:B:222:PHE:CE2	3:B:258:ASP:HA	2.54	0.42
2:N:98:ARG:O	2:N:115:TYR:OH	2.31	0.42
3:B:187:VAL:HA	3:B:203:ALA:HA	2.01	0.42
6:S:32:PHE:CD2	6:S:100:ILE:HB	2.55	0.42
6:S:93:MET:HE1	6:S:95:TYR:CZ	2.55	0.42
3:B:234:PHE:CD1	3:B:241:PHE:HB3	2.51	0.42
3:B:188:MET:SD	5:A:95:LYS:HD3	2.60	0.41
3:B:274:THR:HG21	3:B:314:ARG:HE	1.84	0.41
5:A:235:ILE:HD12	5:A:238:MET:SD	2.60	0.41
6:S:52:SER:O	6:S:72:ARG:NH1	2.52	0.41
1:R:99:ILE:HB	1:R:100:PRO:HD3	2.02	0.41
2:N:19:ARG:HG3	2:N:80:TYR:CE1	2.55	0.41
5:A:37:LEU:HD22	5:A:100:PHE:HB2	2.02	0.41
3:B:142:HIS:CG	3:B:161:SER:HB2	2.56	0.41
5:A:240:LEU:HA	5:A:245:LEU:HB2	2.02	0.41
3:B:130:GLU:HG3	6:S:27:PHE:HA	2.03	0.41
5:A:149:LEU:O	5:A:153:VAL:HG23	2.20	0.41
1:R:126:SER:O	1:R:130:VAL:HG23	2.19	0.41
6:S:52:SER:OG	6:S:53:SER:N	2.54	0.41
3:B:289:TYR:HE1	3:B:295:ASN:HB2	1.86	0.41
6:S:86:LEU:HD13	6:S:117:LEU:HD21	2.02	0.41
3:B:139:LEU:HB3	3:B:169:TRP:CE3	2.56	0.41
3:B:160:SER:HB3	3:B:190:LEU:HD23	2.02	0.41
3:B:254:ASP:HB2	3:B:261:LEU:HD22	2.03	0.41
3:B:183:HIS:CE1	3:B:209:LYS:HG3	2.56	0.41
5:A:15:ARG:NH1	6:S:100:ILE:HD11	2.36	0.41
5:A:154:LEU:HG	5:A:185:ARG:NH2	2.35	0.41
5:A:232:LYS:O	5:A:235:ILE:HG22	2.21	0.41
6:S:175:LEU:HD11	6:S:178:TYR:HB3	2.03	0.41
3:B:314:ARG:O	3:B:332:TRP:N	2.48	0.41
3:B:32:GLN:HA	3:B:35:ASN:ND2	2.36	0.40
3:B:49:ARG:HB2	3:B:338:ILE:HD13	2.02	0.40
3:B:101:MET:HE2	3:B:101:MET:HB3	1.98	0.40
5:A:233:ASP:O	5:A:237:GLN:HG2	2.21	0.40
6:S:47:TRP:HZ2	6:S:50:TYR:HB3	1.86	0.40
3:B:34:THR:O	3:B:301:LYS:NZ	2.30	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	R	321/402 (80%)	313 (98%)	8 (2%)	0	100	100
2	N	126/137 (92%)	122 (97%)	4 (3%)	0	100	100
3	B	335/351 (95%)	318 (95%)	17 (5%)	0	100	100
4	G	49/68 (72%)	49 (100%)	0	0	100	100
5	A	214/326 (66%)	209 (98%)	5 (2%)	0	100	100
6	S	227/260 (87%)	226 (100%)	1 (0%)	0	100	100
7	Q	23/27 (85%)	20 (87%)	3 (13%)	0	100	100
All	All	1295/1571 (82%)	1257 (97%)	38 (3%)	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	R	292/354 (82%)	292 (100%)	0	100	100
2	N	104/114 (91%)	104 (100%)	0	100	100
3	B	247/293 (84%)	246 (100%)	1 (0%)	84	86
4	G	30/56 (54%)	30 (100%)	0	100	100
5	A	172/274 (63%)	172 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
6	S	182/209 (87%)	182 (100%)	0	100	100
7	Q	18/20 (90%)	18 (100%)	0	100	100
All	All	1045/1320 (79%)	1044 (100%)	1 (0%)	87	91

All (1) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
3	B	155	ASN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (17) such sidechains are listed below:

Mol	Chain	Res	Type
1	R	5	ASN
1	R	63	ASN
1	R	81	ASN
1	R	125	GLN
1	R	145	GLN
1	R	156	GLN
1	R	336	ASN
1	R	342	ASN
2	N	123	GLN
3	B	88	ASN
3	B	176	GLN
4	G	18	GLN
5	A	101	ASN
5	A	123	ASN
6	S	3	GLN
6	S	82	GLN
6	S	219	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

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.

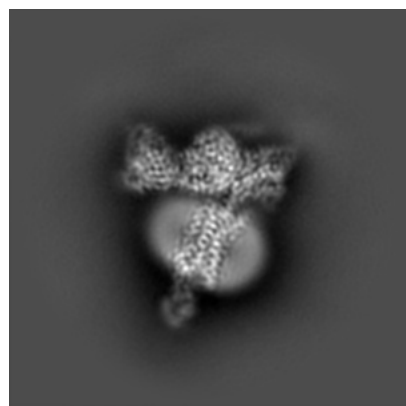
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-60096. These allow visual inspection of the internal detail of the map and identification of artifacts.

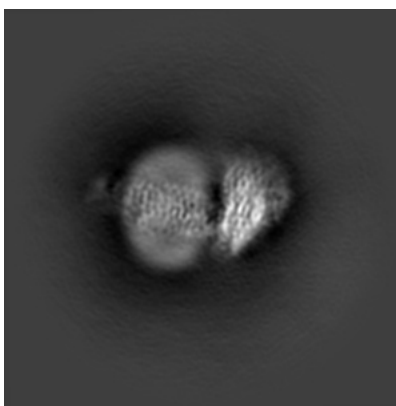
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

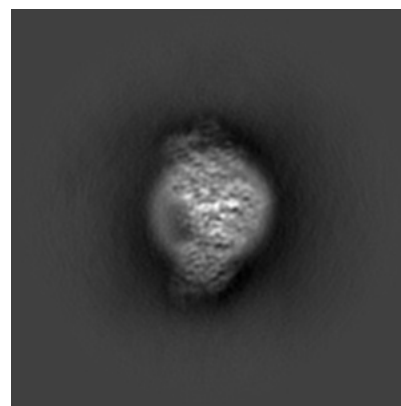
6.1.1 Primary map



X

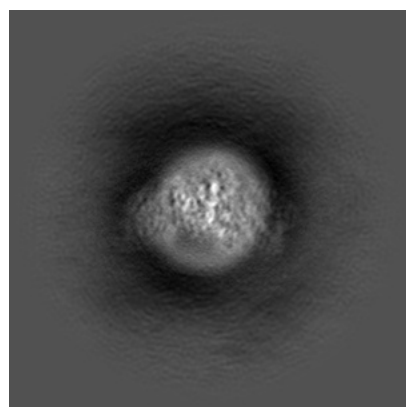


Y

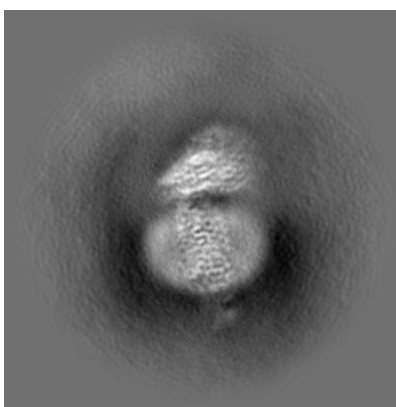


Z

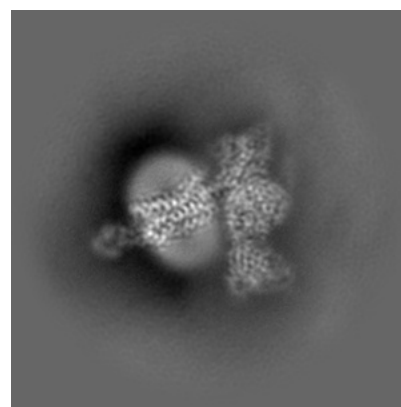
6.1.2 Raw map



X



Y

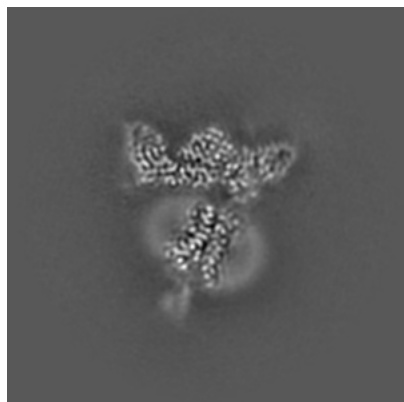


Z

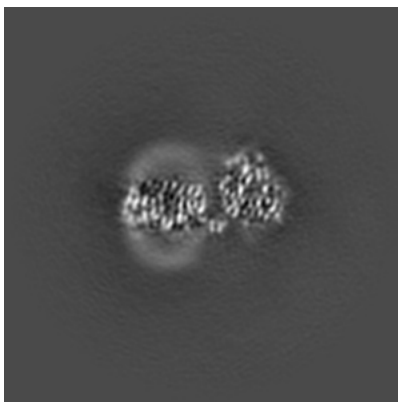
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

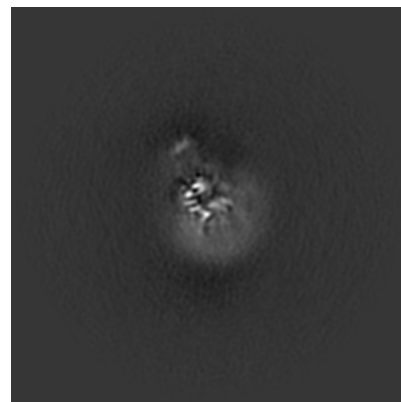
6.2.1 Primary map



X Index: 130

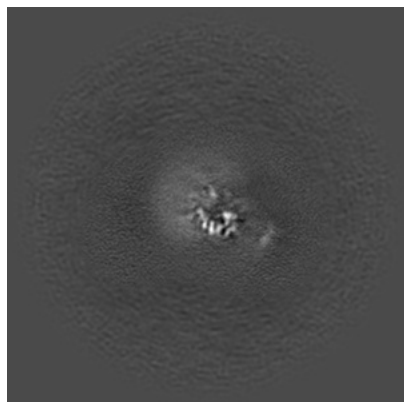


Y Index: 130

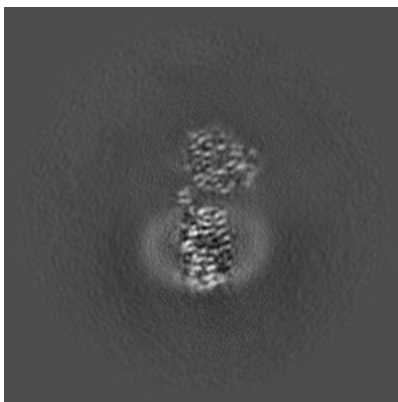


Z Index: 130

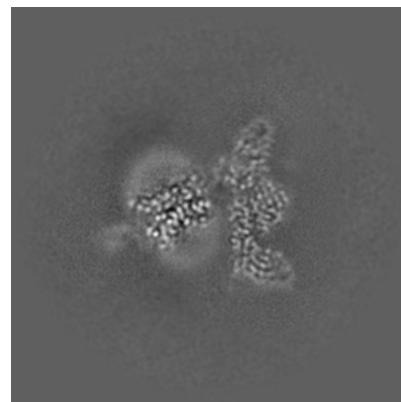
6.2.2 Raw map



X Index: 130



Y Index: 130

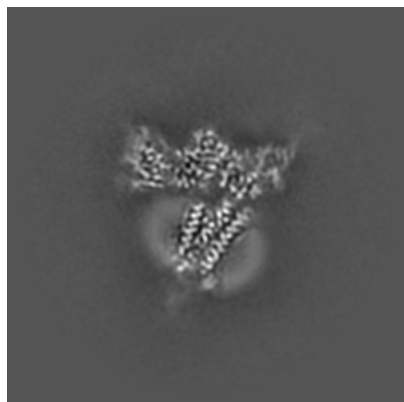


Z Index: 130

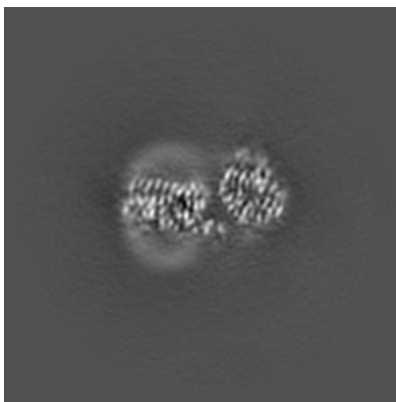
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

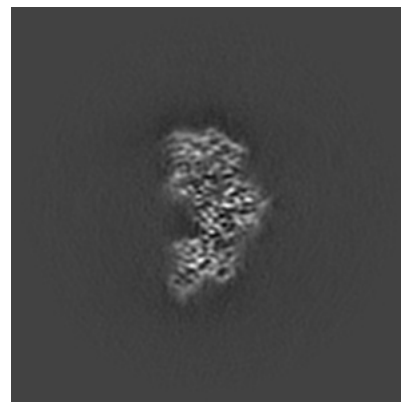
6.3.1 Primary map



X Index: 125

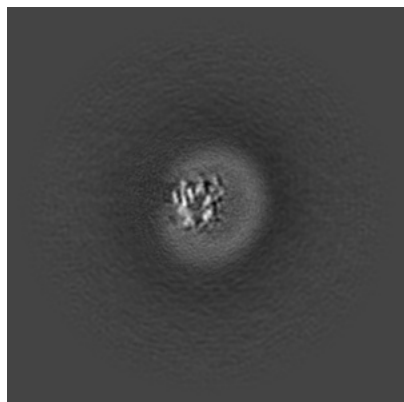


Y Index: 132

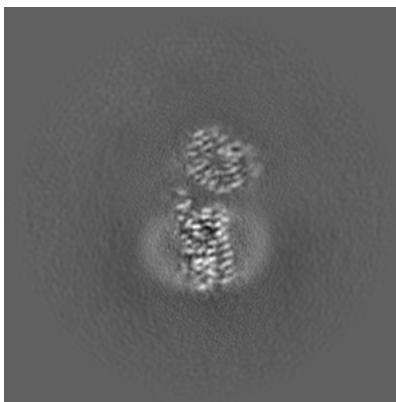


Z Index: 153

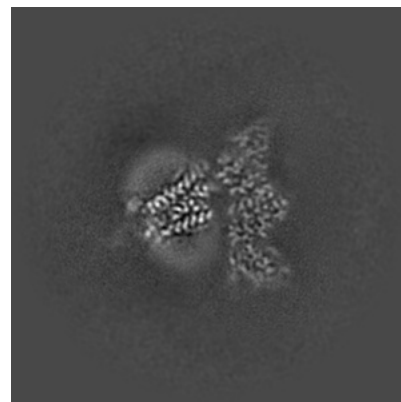
6.3.2 Raw map



X Index: 90



Y Index: 132

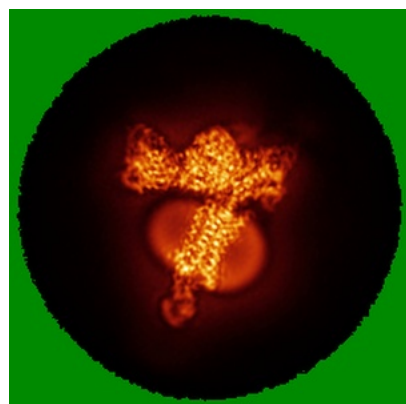


Z Index: 126

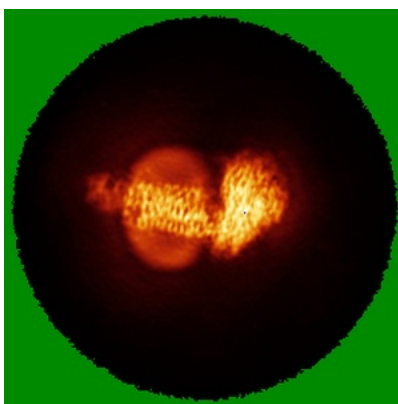
The images above show the largest variance slices of the map in three orthogonal directions.

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

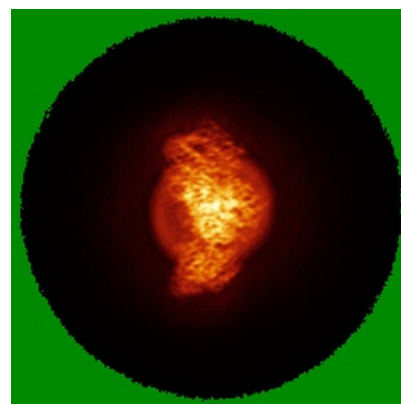
6.4.1 Primary map



X

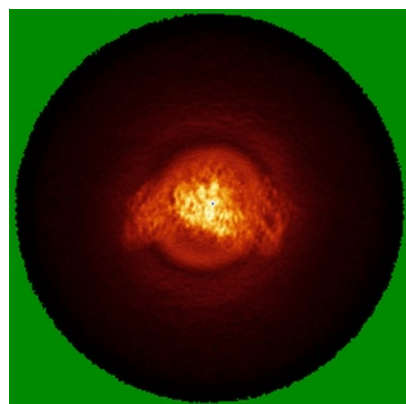


Y

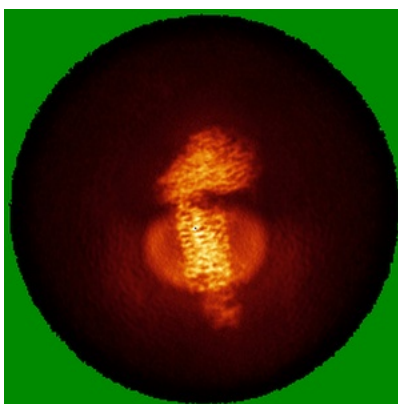


Z

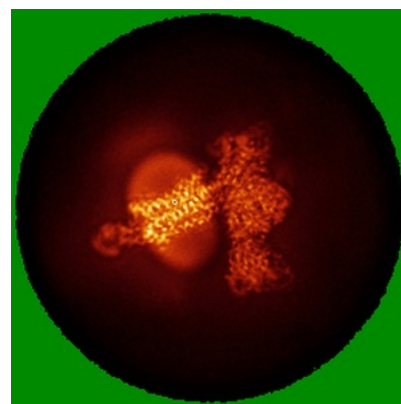
6.4.2 Raw map



X



Y

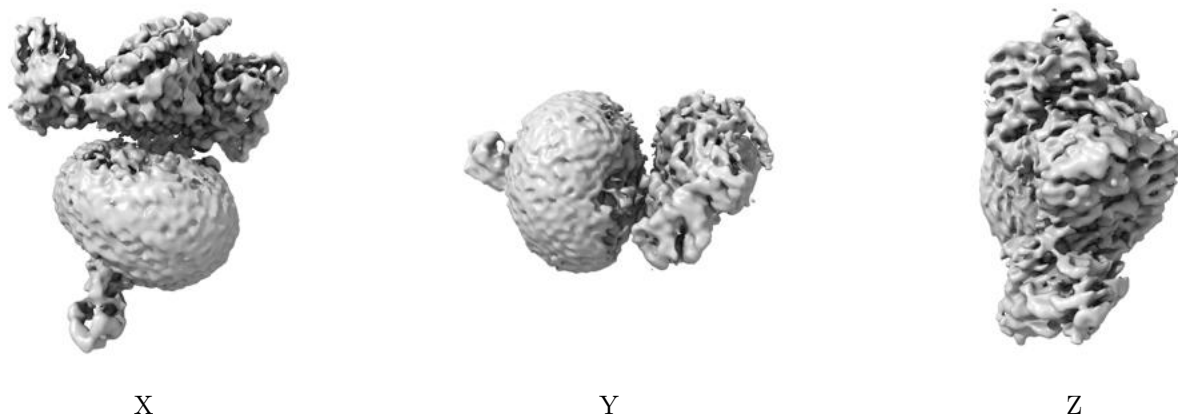


Z

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.

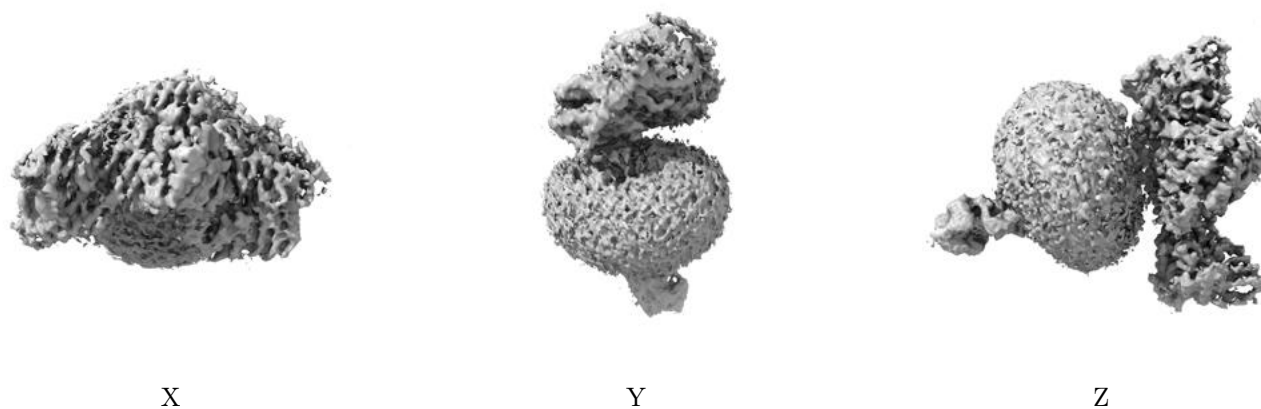
6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 4.2. 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.

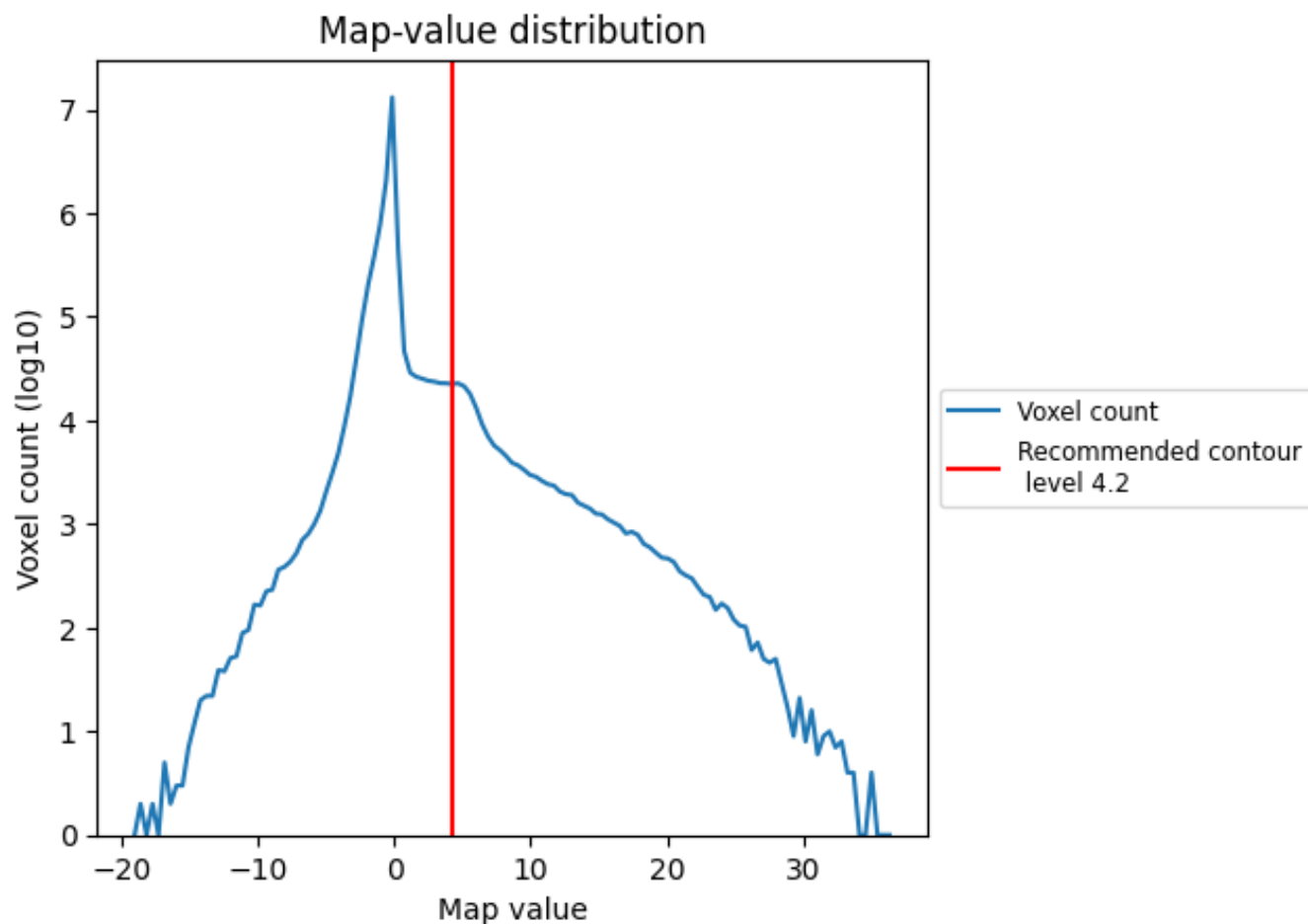
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

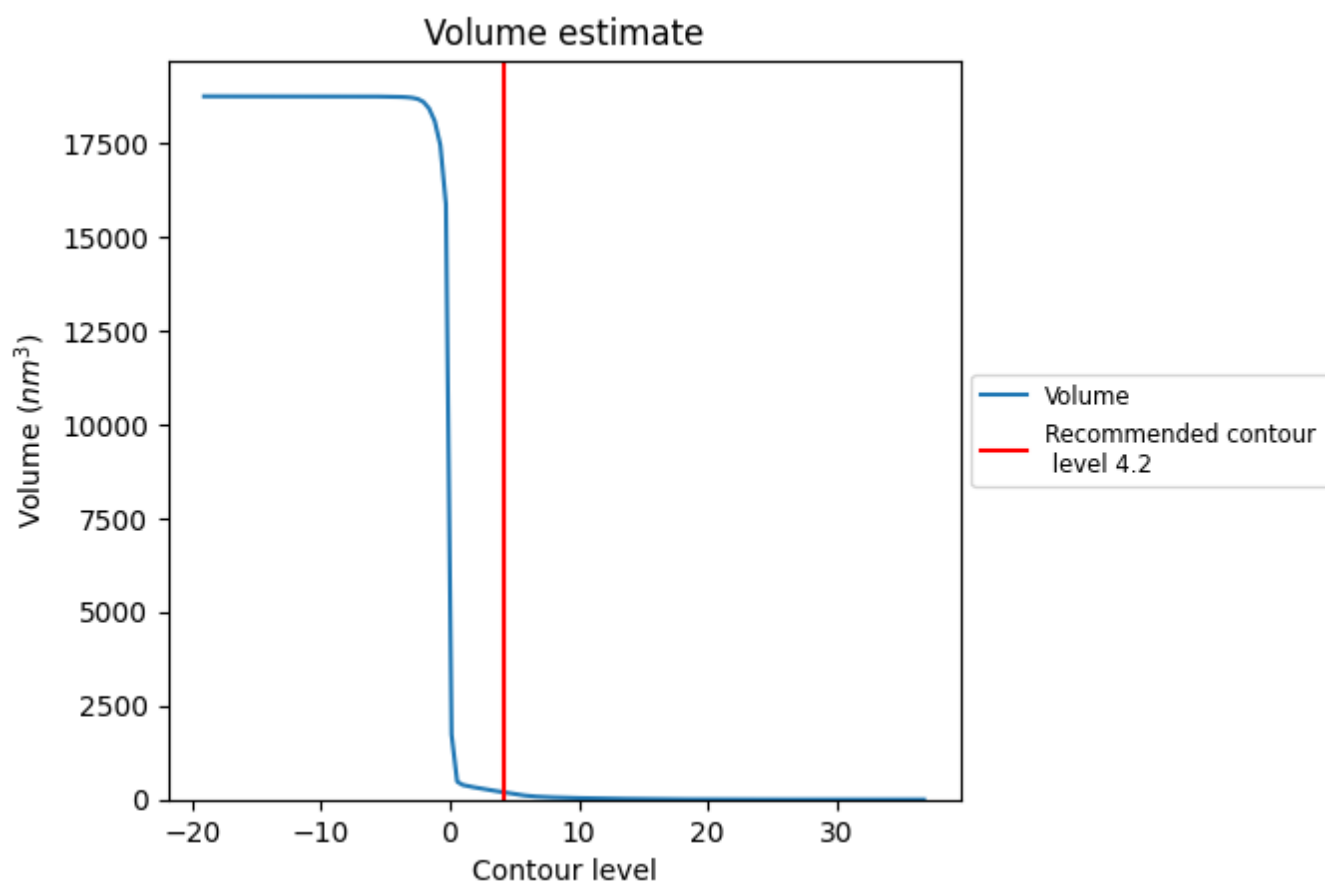
This section contains the results of statistical analysis of the map.

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.

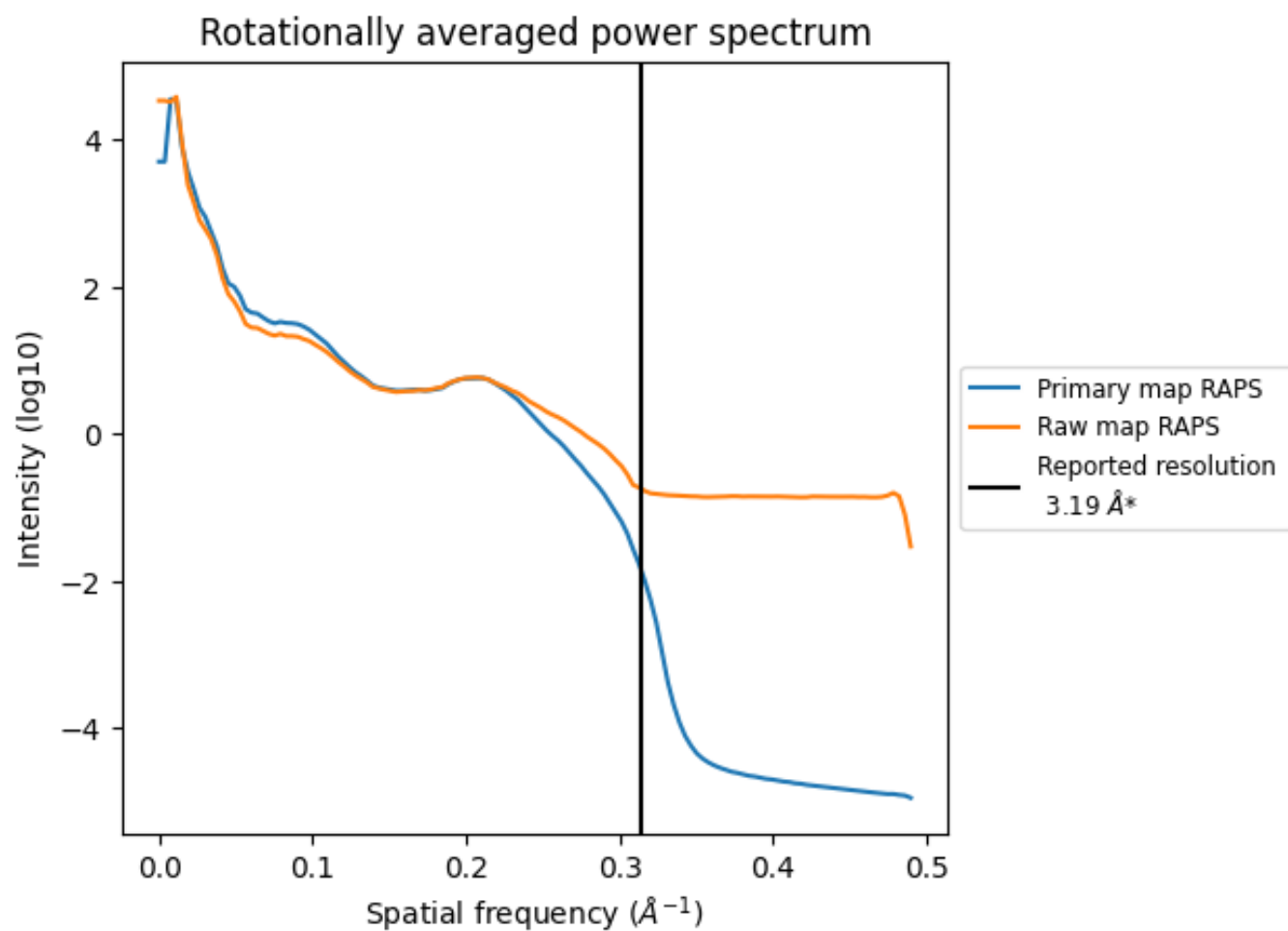
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 192 nm³; this corresponds to an approximate mass of 174 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 ⓘ

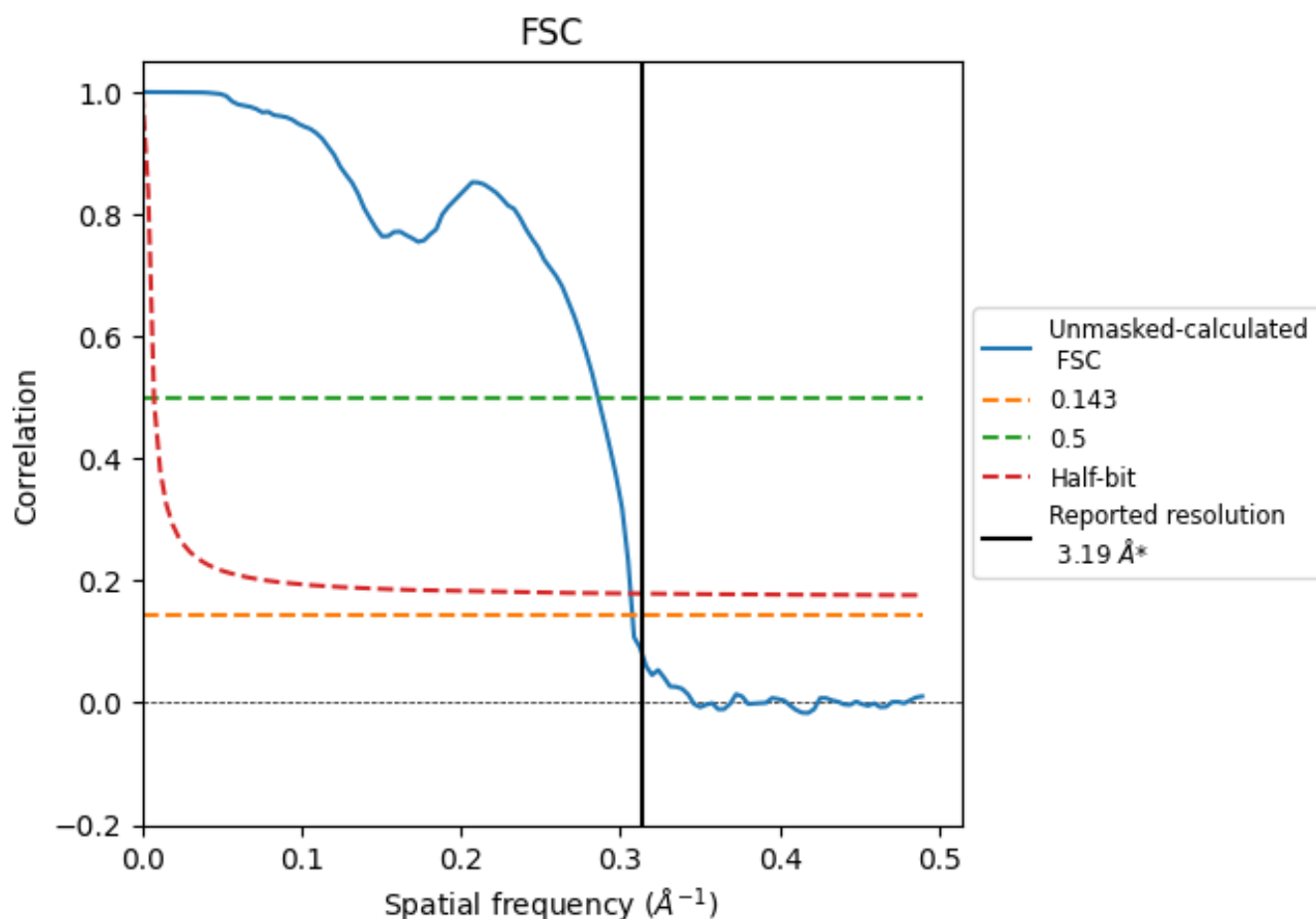


*Reported resolution corresponds to spatial frequency of $0.313 \text{ \AA}^{-1}$

8 Fourier-Shell correlation [i](#)

Fourier-Shell Correlation (FSC) is the most commonly used method to estimate the resolution of single-particle and subtomogram-averaged maps. The shape of the curve depends on the imposed symmetry, mask and whether or not the two 3D reconstructions used were processed from a common reference. The reported resolution is shown as a black line. A curve is displayed for the half-bit criterion in addition to lines showing the 0.143 gold standard cut-off and 0.5 cut-off.

8.1 FSC [i](#)



*Reported resolution corresponds to spatial frequency of 0.313 Å⁻¹

8.2 Resolution estimates [i](#)

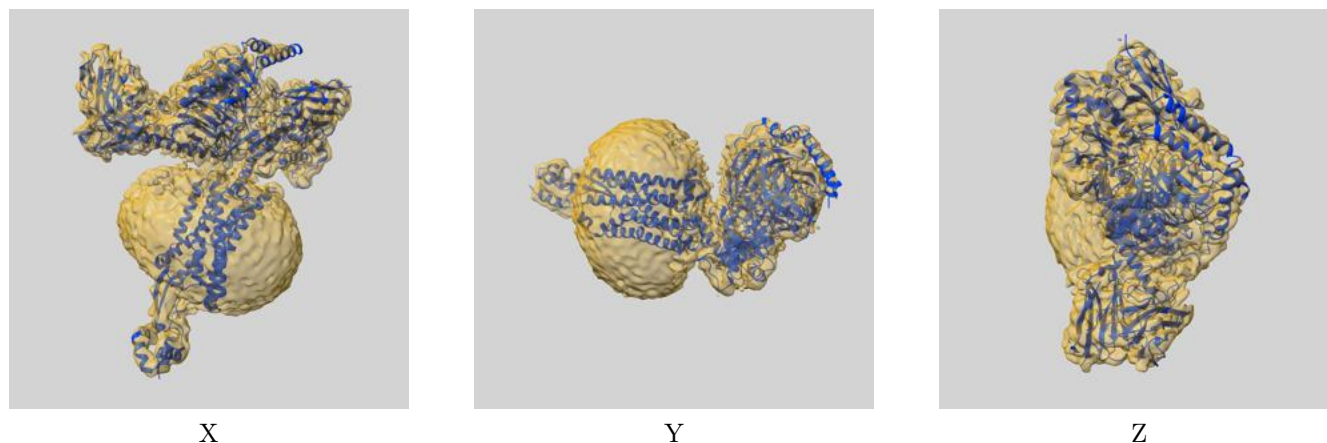
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.19	-	-
Author-provided FSC curve	-	-	-
Unmasked-calculated*	3.25	3.50	3.26

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps.

9 Map-model fit [i](#)

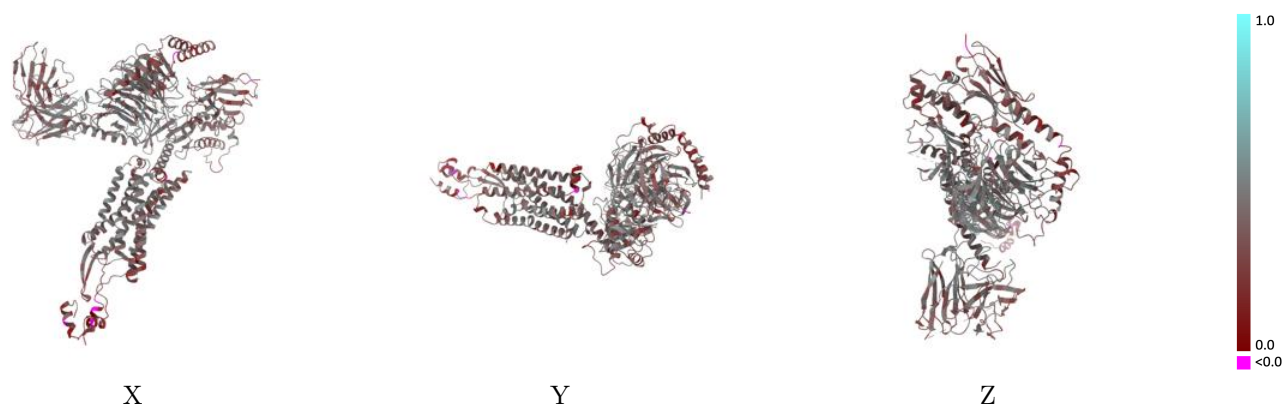
This section contains information regarding the fit between EMDB map EMD-60096 and PDB model 8ZH8. Per-residue inclusion information can be found in section [3](#) on page [9](#).

9.1 Map-model overlay [i](#)



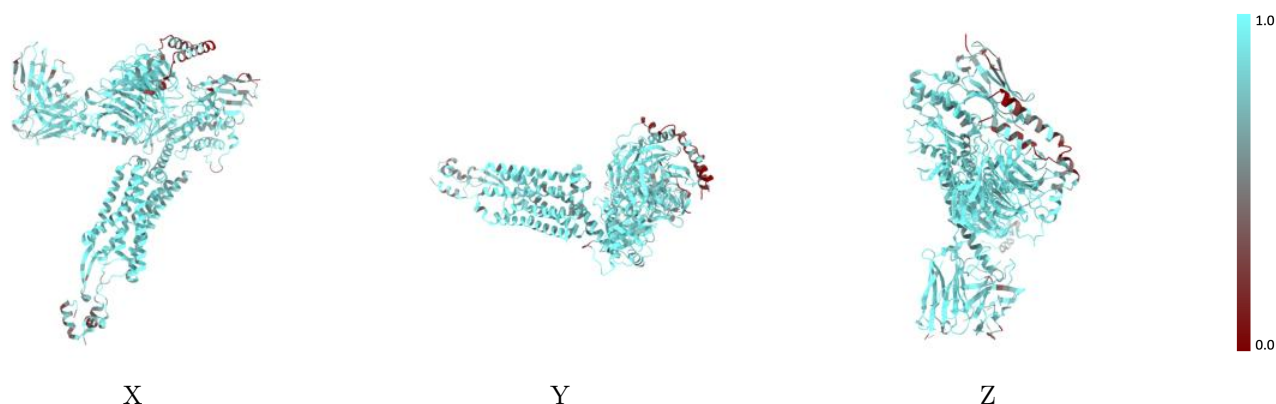
The images above show the 3D surface view of the map at the recommended contour level 4.2 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



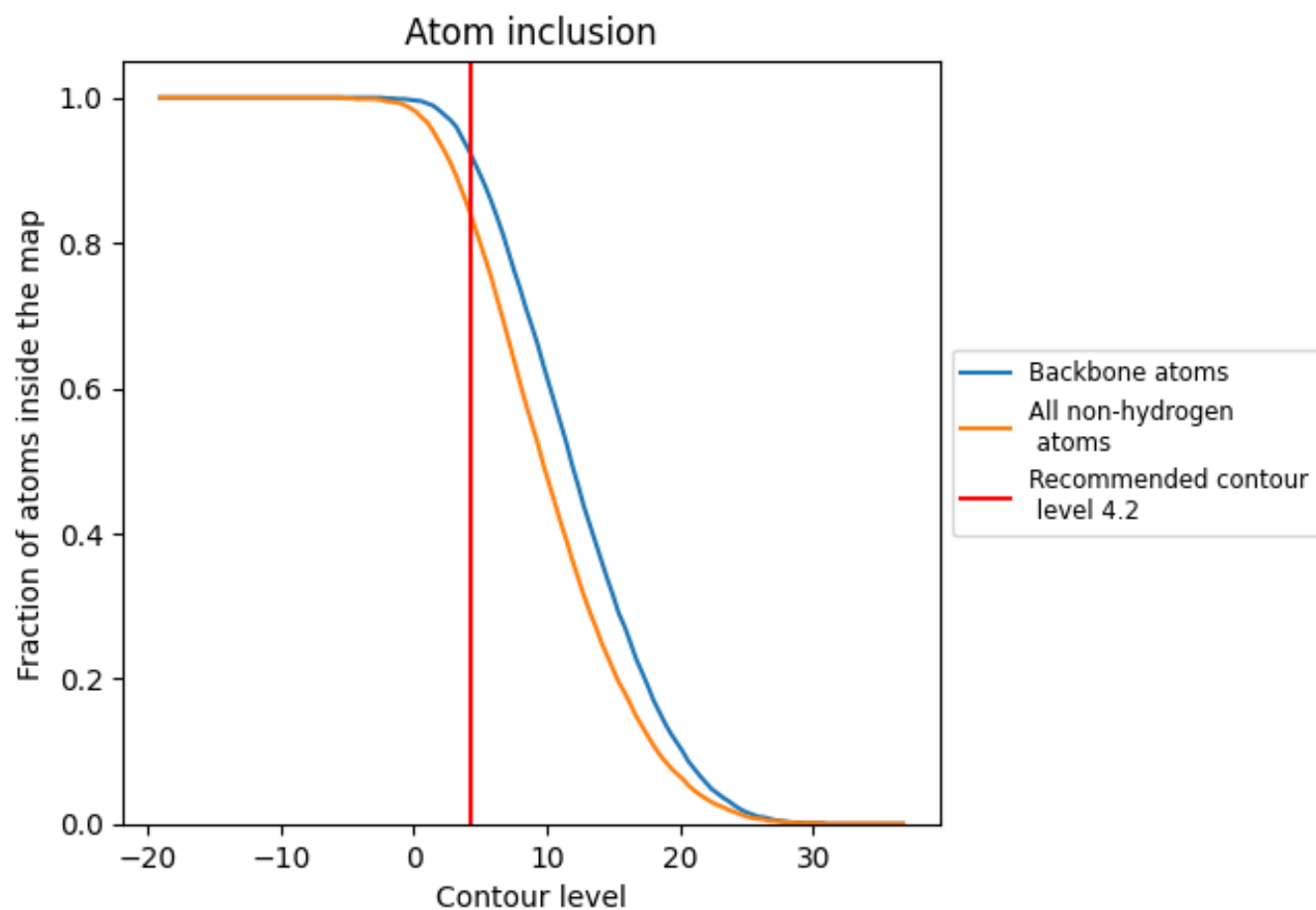
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (4.2).

9.4 Atom inclusion [i](#)



At the recommended contour level, 92% of all backbone atoms, 84% 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 (4.2) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.8430	0.3870
A	0.8730	0.3940
B	0.8680	0.4330
G	0.6800	0.3200
N	0.7530	0.3690
Q	0.7320	0.2620
R	0.8580	0.3620
S	0.8520	0.3880

1.0

0.0

<0.0