



Full wwPDB EM Validation Report ⓘ

Mar 14, 2026 – 06:26 AM UTC

PDB ID : 8ZD1 / pdb_00008zd1
EMDB ID : EMD-39946
Title : Cryo-EM structure of the xGPR4-Gs complex in pH6.2
Authors : Rong, N.K.; Wen, X.; Yang, F.; Sun, J.P.
Deposited on : 2024-04-30
Resolution : 2.60 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

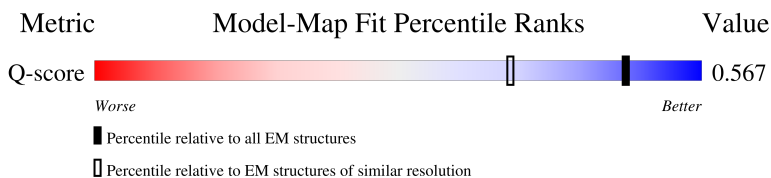
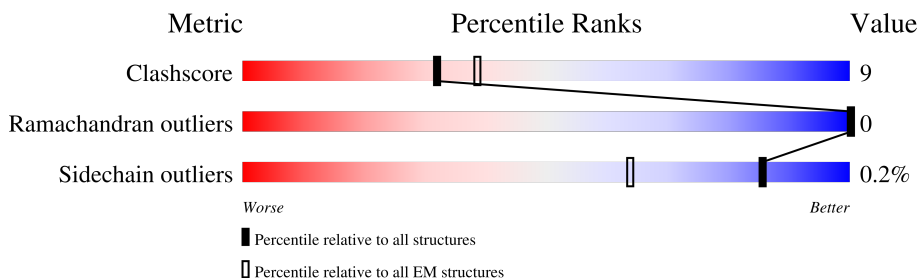
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 2.60 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	8728 (2.10 - 3.10)

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

Mol	Chain	Length	Quality of chain
1	A	374	 57% 7% 36%
2	B	338	 79% 21%
3	G	52	 87% 13%
4	R	289	 79% 18% .

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Mol	Chain	Length	Quality of chain
5	S	250	71% 19% • 8%

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 8364 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(s) subunit alpha isoforms short.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	238	Total	C	N	O	S	0	0
			1865	1188	338	332	7		

There are 37 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	4	THR	-	expression tag	UNP P63092
A	5	LEU	-	expression tag	UNP P63092
A	6	SER	-	expression tag	UNP P63092
A	7	ALA	-	expression tag	UNP P63092
A	8	GLU	-	expression tag	UNP P63092
A	9	ASP	-	expression tag	UNP P63092
A	10	LYS	-	expression tag	UNP P63092
A	11	ALA	-	expression tag	UNP P63092
A	12	ALA	-	expression tag	UNP P63092
A	13	VAL	-	expression tag	UNP P63092
A	14	GLU	-	expression tag	UNP P63092
A	15	ARG	-	expression tag	UNP P63092
A	16	SER	-	expression tag	UNP P63092
A	17	LYS	-	expression tag	UNP P63092
A	18	MET	-	expression tag	UNP P63092
A	49	ASP	GLY	conflict	UNP P63092
A	50	ASN	GLU	conflict	UNP P63092
A	63	TYR	LEU	conflict	UNP P63092
A	213	LYS	LEU	conflict	UNP P63092
A	236	ALA	GLY	conflict	UNP P63092
A	259	ASP	ALA	conflict	UNP P63092
A	262	ASP	SER	conflict	UNP P63092
A	?	-	ASN	deletion	UNP P63092
A	?	-	MET	deletion	UNP P63092
A	?	-	VAL	deletion	UNP P63092
A	?	-	ILE	deletion	UNP P63092
A	?	-	ARG	deletion	UNP P63092

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Chain	Residue	Modelled	Actual	Comment	Reference
A	?	-	GLU	deletion	UNP P63092
A	?	-	ASP	deletion	UNP P63092
A	?	-	ASN	deletion	UNP P63092
A	?	-	GLN	deletion	UNP P63092
A	?	-	THR	deletion	UNP P63092
A	264	ALA	ASN	conflict	UNP P63092
A	272	ASP	LEU	conflict	UNP P63092
A	366	SER	ALA	conflict	UNP P63092
A	372	ALA	ILE	conflict	UNP P63092
A	375	ILE	VAL	conflict	UNP P63092

- Molecule 2 is a protein called Guanine nucleotide-binding protein G(I)/G(S)/G(T) subunit beta-1.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	B	338	Total	C	N	O	S	0	0
			2484	1539	441	483	21		

- Molecule 3 is a protein called Guanine nucleotide-binding protein G(I)/G(S)/G(O) subunit gamma-2.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	G	52	Total	C	N	O	S	0	0
			355	225	61	67	2		

- Molecule 4 is a protein called G-protein coupled receptor 4.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	R	281	Total	C	N	O	S	0	0
			1953	1272	339	330	12		

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
R	155	ALA	GLY	conflict	UNP A0A6I8PUB9

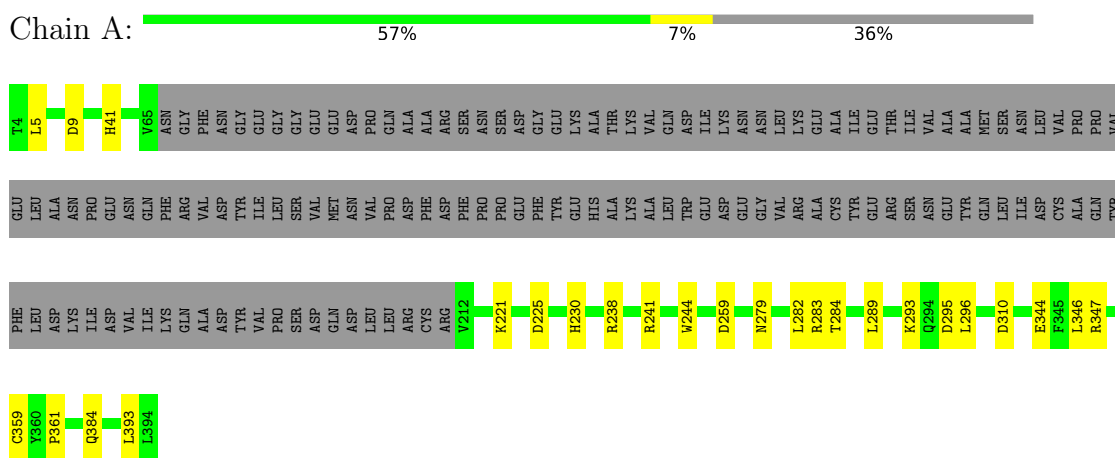
- Molecule 5 is a protein called scFv16.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	S	231	Total	C	N	O	S	0	0
			1707	1088	283	326	10		

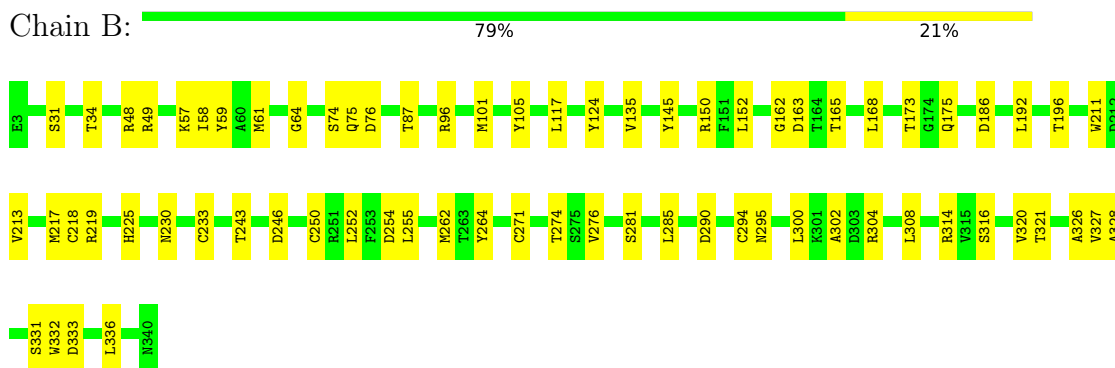
3 Residue-property plots

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.

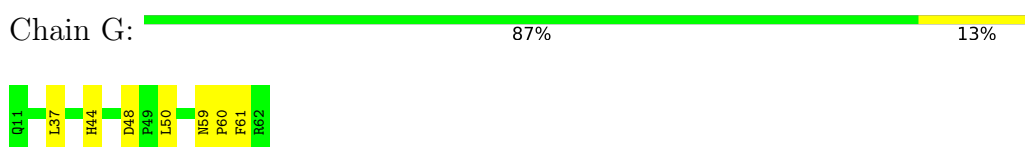
- Molecule 1: Guanine nucleotide-binding protein G(s) subunit alpha isoforms short



- Molecule 2: Guanine nucleotide-binding protein G(I)/G(S)/G(T) subunit beta-1

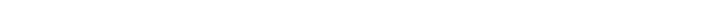


- Molecule 3: Guanine nucleotide-binding protein G(I)/G(S)/G(O) subunit gamma-2



- Molecule 4: G-protein coupled receptor 4

R20	S13
L230	D16
P231	L19
L244	P20
R248	Y24
S249	A42
L250	V46
V251	E51
F252	L52
L253	L52
V254	P71
GLY	P72
GLY	W73
GLY	T74
SER	P75
VAL	Y76
ASP	Y77
ALA	W83
GLY	C90
G283	F97
L267	V111
E288	V119
L271	L123
F272	R124
H276	P130
L279	N149
A280	P152
T283	A155
L292	Y163
R301	N162
	H165
	C168
	Y169
	R177
	L193
	P194
	L205
	T209

Chain S:  71% 19% 8%

ASP	ASP	PRO	ASP	V2	Q3	L4	V5	E6	L20	S21	C22	F32	Q39	L45	Y60	T63	V64	R67	F68	T69	D73	N77	T78	L79	Q82	H83	R87	D90	V97	I100	F108	D109	F110	T115	L116	L117	T118	V119	S120	S121	GLY	GLY	GLY	GLY	
SER	GLY	GLY	GLY	GLY	GLY	SER	GLY	GLY	GLY	S136	M140	T141	Q142	A143	T144	S145	S146	V147	P148	V149	T150	P151	G152	E153	C159	R160	S161	S162	K163	S164	L165	T172	Y173	L174	R191	M192	F212	L219	V224	T243	K244	L245	E246	LEU	LYS

4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	640581	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	NONE	Depositor
Microscope	TFS KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	1.875	Depositor
Minimum defocus (nm)	1000	Depositor
Maximum defocus (nm)	2000	Depositor
Magnification	Not provided	
Image detector	FEI FALCON IV (4k x 4k)	Depositor
Maximum map value	2.051	Depositor
Minimum map value	-0.007	Depositor
Average map value	0.001	Depositor
Map value standard deviation	0.029	Depositor
Recommended contour level	0.1	Depositor
Map size ($\text{\AA}$)	279.0, 279.0, 279.0	wwPDB
Map dimensions	300, 300, 300	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing ($\text{\AA}$)	0.93, 0.93, 0.93	Depositor

5 Model quality

5.1 Standard geometry

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	0.38	0/1903	0.42	0/2578
2	B	0.42	0/2531	0.46	0/3446
3	G	0.30	0/361	0.40	0/497
4	R	0.26	0/2008	0.52	1/2760 (0.0%)
5	S	0.74	4/1751 (0.2%)	0.79	11/2384 (0.5%)
All	All	0.47	4/8554 (0.0%)	0.54	12/11665 (0.1%)

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	S	151	PRO	C-O	-6.57	1.14	1.23
5	S	151	PRO	CA-C	-6.42	1.44	1.52
5	S	140	MET	C-O	-5.10	1.17	1.24
5	S	144	THR	CA-C	-5.05	1.46	1.52

All (12) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	S	153	GLU	CB-CA-C	-14.12	83.69	110.24
5	S	148	PRO	N-CA-C	-7.51	96.99	112.47
5	S	150	THR	CA-C-N	7.35	127.79	119.93
5	S	150	THR	C-N-CA	7.35	127.79	119.93
5	S	143	ALA	N-CA-C	6.78	118.67	111.28
5	S	147	VAL	N-CA-C	-6.10	104.19	109.19
5	S	148	PRO	CB-CA-C	5.96	121.40	111.56
5	S	144	THR	N-CA-C	-5.75	99.76	108.67
4	R	71	PRO	N-CA-C	5.22	117.07	110.70
5	S	151	PRO	CB-CA-C	-5.14	105.11	111.64
5	S	191	ARG	CA-C-N	5.02	131.12	121.54
5	S	191	ARG	C-N-CA	5.02	131.12	121.54

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	1865	0	1791	28	0
2	B	2484	0	2305	43	0
3	G	355	0	322	6	0
4	R	1953	0	1777	40	0
5	S	1707	0	1582	34	0
All	All	8364	0	7777	139	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 9.

All (139) 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)
4:R:77:TYR:HE1	4:R:276:HIS:ND1	1.44	1.16
1:A:225:ASP:O	4:R:124:ARG:NH2	2.02	0.92
5:S:149:VAL:HG21	5:S:219:LEU:HD13	1.59	0.83
4:R:77:TYR:CE1	4:R:276:HIS:ND1	2.34	0.81
1:A:289:LEU:HD12	1:A:289:LEU:O	1.81	0.80
5:S:172:THR:OG1	5:S:192:MET:SD	2.38	0.79
2:B:96:ARG:HH12	2:B:135:VAL:HG21	1.49	0.78
1:A:289:LEU:CD1	1:A:361:PRO:HA	2.15	0.77
1:A:238:ARG:NH1	2:B:186:ASP:OD1	2.17	0.76
4:R:77:TYR:HE1	4:R:276:HIS:HD1	0.77	0.75
1:A:289:LEU:HD23	1:A:359:CYS:SG	2.27	0.73
5:S:20:LEU:HD13	5:S:83:MET:HE2	1.70	0.73
2:B:217:MET:SD	2:B:219:ARG:NH1	2.63	0.71
2:B:331:SER:OG	2:B:333:ASP:OD1	2.09	0.70
2:B:271:CYS:HB2	2:B:290:ASP:HB2	1.73	0.70
2:B:320:VAL:HG22	2:B:327:VAL:HG22	1.73	0.69
2:B:281:SER:OG	3:G:48:ASP:OD2	2.12	0.68
5:S:63:THR:HG23	5:S:64:VAL:HG13	1.75	0.68
1:A:344:GLU:OE1	1:A:347:ARG:NH2	2.27	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:R:24:TYR:HE1	4:R:283:THR:HG21	1.59	0.67
5:S:6:GLU:HG2	5:S:115:THR:HG23	1.77	0.66
4:R:177:ARG:H	4:R:252:PHE:HE2	1.42	0.65
4:R:19:LEU:HB3	4:R:20:PRO:HD3	1.79	0.65
1:A:393:LEU:HD11	4:R:205:LEU:HD11	1.79	0.64
5:S:140:MET:HE1	5:S:165:LEU:HD11	1.80	0.63
4:R:52:LEU:HD11	4:R:111:VAL:HG13	1.80	0.62
4:R:83:TRP:CE2	4:R:90:CYS:HB3	2.35	0.62
1:A:289:LEU:HD11	1:A:361:PRO:HA	1.81	0.61
1:A:295:ASP:OD2	1:A:296:LEU:N	2.34	0.60
2:B:276:VAL:HG13	2:B:285:LEU:HD11	1.83	0.60
4:R:51:GLU:HG2	4:R:130:PRO:HB2	1.83	0.60
2:B:145:TYR:O	2:B:162:GLY:N	2.34	0.60
4:R:193:LEU:HB3	4:R:194:PRO:HD3	1.84	0.60
1:A:221:LYS:HD3	1:A:230:HIS:CE1	2.37	0.60
4:R:209:LEU:O	4:R:220:ARG:NH1	2.34	0.60
2:B:152:LEU:HD22	2:B:196:THR:HB	1.85	0.59
2:B:64:GLY:HA2	2:B:105:TYR:CD2	2.39	0.58
2:B:58:ILE:HD13	2:B:336:LEU:HD12	1.86	0.57
4:R:76:TYR:HD2	4:R:83:TRP:HE3	1.52	0.57
5:S:22:CYS:HB3	5:S:79:LEU:HB3	1.87	0.57
5:S:144:THR:O	5:S:243:THR:HG22	2.05	0.57
5:S:149:VAL:CG2	5:S:219:LEU:HD13	2.31	0.57
5:S:149:VAL:HG21	5:S:219:LEU:CD1	2.33	0.56
5:S:67:ARG:NH1	5:S:90:ASP:OD1	2.24	0.56
2:B:163:ASP:O	2:B:165:THR:N	2.39	0.55
1:A:393:LEU:CD1	4:R:205:LEU:HD11	2.36	0.55
1:A:289:LEU:HD11	1:A:361:PRO:HB3	1.88	0.55
2:B:74:SER:OG	2:B:76:ASP:OD1	2.24	0.54
1:A:289:LEU:HD12	1:A:361:PRO:HA	1.88	0.54
4:R:244:LEU:HD22	4:R:271:LEU:HD12	1.88	0.54
2:B:274:THR:HG21	2:B:314:ARG:NH2	2.23	0.53
1:A:41:HIS:NE2	4:R:123:LEU:HD22	2.24	0.53
4:R:71:PRO:HD2	4:R:72:PRO:CD	2.39	0.53
1:A:310:ASP:N	1:A:310:ASP:OD1	2.41	0.53
5:S:174:LEU:HD22	5:S:212:PHE:CG	2.44	0.53
5:S:68:PHE:CE1	5:S:83:MET:HB3	2.44	0.53
2:B:233:CYS:SG	2:B:276:VAL:HG12	2.50	0.52
2:B:252:LEU:HD21	3:G:37:LEU:HD21	1.92	0.52
2:B:225:HIS:NE2	2:B:243:THR:OG1	2.37	0.51
5:S:159:CYS:SG	5:S:160:ARG:N	2.83	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:281:SER:HB3	3:G:44:HIS:O	2.11	0.51
4:R:24:TYR:CE1	4:R:283:THR:HG21	2.43	0.51
2:B:168:LEU:HD22	2:B:213:VAL:HG13	1.92	0.50
1:A:289:LEU:HD11	1:A:361:PRO:CA	2.42	0.50
4:R:42:ALA:O	4:R:46:VAL:HG23	2.11	0.50
2:B:295:ASN:OD1	2:B:304:ARG:HD2	2.11	0.49
4:R:83:TRP:NE1	4:R:90:CYS:HB3	2.27	0.49
4:R:152:PRO:O	4:R:155:ALA:HB2	2.11	0.49
2:B:254:ASP:OD1	2:B:255:LEU:N	2.44	0.49
2:B:124:TYR:CE2	2:B:135:VAL:HG22	2.48	0.49
2:B:294:CYS:HB2	2:B:308:LEU:HB2	1.95	0.48
1:A:289:LEU:CD2	1:A:359:CYS:SG	2.98	0.48
5:S:83:MET:HE1	5:S:117:LEU:CD1	2.44	0.48
2:B:230:ASN:ND2	2:B:246:ASP:OD1	2.47	0.48
2:B:262:MET:SD	2:B:302:ALA:HB2	2.54	0.48
1:A:289:LEU:HD11	1:A:361:PRO:CB	2.44	0.48
5:S:20:LEU:CD1	5:S:83:MET:HE2	2.42	0.48
5:S:32:PHE:CE1	5:S:100:ILE:HB	2.49	0.47
2:B:57:LYS:HE2	2:B:75:GLN:HG3	1.97	0.47
4:R:280:ALA:HA	4:R:283:THR:HG22	1.98	0.46
1:A:384:GLN:HG3	4:R:119:VAL:O	2.15	0.46
2:B:31:SER:HA	2:B:34:THR:HG22	1.97	0.46
2:B:58:ILE:O	2:B:316:SER:OG	2.26	0.46
2:B:321:THR:CG2	2:B:326:ALA:H	2.29	0.46
4:R:244:LEU:O	4:R:248:ARG:HG3	2.15	0.46
5:S:109:ASP:OD2	5:S:109:ASP:N	2.46	0.46
1:A:295:ASP:OD2	1:A:296:LEU:HD12	2.16	0.46
1:A:346:LEU:HD11	1:A:361:PRO:HG2	1.98	0.45
4:R:71:PRO:HD2	4:R:72:PRO:HD3	1.97	0.45
4:R:97:PHE:HE2	4:R:279:LEU:HD11	1.80	0.45
4:R:73:TRP:O	4:R:77:TYR:HD2	2.00	0.45
4:R:268:GLU:HA	4:R:271:LEU:HD23	1.98	0.45
2:B:49:ARG:HD2	2:B:87:THR:HG23	1.97	0.45
2:B:61:MET:HE3	2:B:328:ALA:HB3	1.97	0.45
2:B:59:TYR:HD2	2:B:101:MET:HB2	1.82	0.45
4:R:16:ASP:HA	4:R:20:PRO:HD2	1.99	0.45
1:A:283:ARG:O	1:A:284:THR:OG1	2.26	0.45
1:A:346:LEU:HD21	1:A:361:PRO:HG3	1.99	0.44
5:S:32:PHE:CD1	5:S:100:ILE:HB	2.53	0.44
5:S:87:ARG:O	5:S:119:VAL:HG21	2.18	0.44
1:A:244:TRP:HB2	2:B:117:LEU:HD21	2.00	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:R:230:LEU:HD13	4:R:292:LEU:HD23	1.99	0.44
5:S:22:CYS:N	5:S:79:LEU:O	2.50	0.44
5:S:39:GLN:HB3	5:S:45:LEU:HD23	1.98	0.43
2:B:173:THR:O	2:B:175:GLN:N	2.51	0.43
5:S:174:LEU:HD22	5:S:212:PHE:CD1	2.53	0.43
2:B:211:TRP:CZ3	2:B:218:CYS:HB2	2.53	0.43
5:S:4:LEU:HD12	5:S:110:PHE:HD2	1.83	0.43
5:S:97:VAL:HG11	5:S:108:PHE:CD2	2.53	0.43
4:R:149:ASN:C	4:R:152:PRO:HD2	2.43	0.43
5:S:60:TYR:OH	5:S:69:THR:HA	2.18	0.43
4:R:249:SER:O	4:R:253:LEU:HB2	2.19	0.42
5:S:69:THR:HG23	5:S:82:GLN:HB3	2.01	0.42
5:S:147:VAL:HG12	5:S:148:PRO:O	2.19	0.42
4:R:251:VAL:HA	4:R:254:VAL:HG23	2.01	0.42
5:S:161:SER:OG	5:S:163:LYS:O	2.33	0.42
5:S:224:VAL:HG23	5:S:245:LEU:O	2.20	0.42
4:R:267:LEU:O	4:R:271:LEU:HD23	2.20	0.42
1:A:241:ARG:HG3	1:A:244:TRP:CZ2	2.55	0.41
1:A:279:ASN:HB3	1:A:282:LEU:HB2	2.02	0.41
2:B:152:LEU:HD23	2:B:192:LEU:HD13	2.02	0.41
4:R:13:SER:HB3	4:R:272:PHE:HE2	1.86	0.41
4:R:230:LEU:HB3	4:R:231:PRO:HD3	2.03	0.41
1:A:259:ASP:CG	1:A:293:LYS:HD2	2.46	0.41
2:B:250:CYS:HB2	2:B:264:TYR:HB2	2.02	0.41
2:B:314:ARG:HD3	2:B:332:TRP:CZ2	2.56	0.41
4:R:163:TYR:O	4:R:165:HIS:ND1	2.53	0.41
4:R:168:CYS:SG	4:R:169:TYR:N	2.93	0.41
5:S:64:VAL:HB	5:S:68:PHE:CD2	2.55	0.41
5:S:73:ASP:O	5:S:77:ASN:N	2.54	0.41
2:B:34:THR:HG21	2:B:300:LEU:O	2.21	0.41
2:B:150:ARG:HA	2:B:150:ARG:HD3	1.88	0.41
3:G:59:ASN:HA	3:G:60:PRO:HD3	1.89	0.40
1:A:5:LEU:HD12	1:A:9:ASP:HB3	2.04	0.40
5:S:191:ARG:O	5:S:192:MET:HG2	2.21	0.40
2:B:48:ARG:HD2	3:G:61:PHE:O	2.21	0.40
4:R:71:PRO:HA	4:R:74:THR:HB	2.03	0.40
5:S:148:PRO:O	5:S:148:PRO:CD	2.66	0.40
2:B:327:VAL:HG23	3:G:50:LEU:HD11	2.02	0.40

There are no symmetry-related clashes.

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	234/374 (63%)	228 (97%)	6 (3%)	0	100	100
2	B	336/338 (99%)	322 (96%)	14 (4%)	0	100	100
3	G	50/52 (96%)	44 (88%)	6 (12%)	0	100	100
4	R	277/289 (96%)	260 (94%)	17 (6%)	0	100	100
5	S	227/250 (91%)	217 (96%)	10 (4%)	0	100	100
All	All	1124/1303 (86%)	1071 (95%)	53 (5%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	188/332 (57%)	188 (100%)	0	100	100
2	B	252/281 (90%)	252 (100%)	0	100	100
3	G	31/43 (72%)	31 (100%)	0	100	100
4	R	160/221 (72%)	160 (100%)	0	100	100
5	S	175/203 (86%)	173 (99%)	2 (1%)	65	84
All	All	806/1080 (75%)	804 (100%)	2 (0%)	85	95

All (2) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
5	S	141	THR
5	S	146	SER

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (8) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	371	ASN
2	B	220	GLN
2	B	237	ASN
2	B	268	ASN
4	R	58	ASN
4	R	121	HIS
4	R	159	HIS
5	S	13	GLN

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.

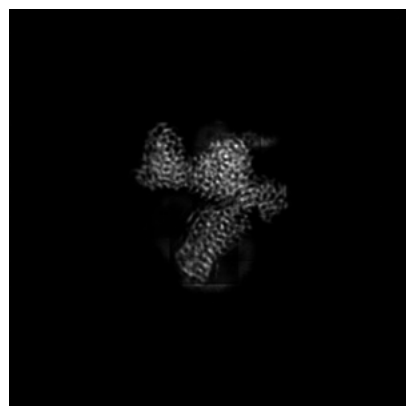
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-39946. These allow visual inspection of the internal detail of the map and identification of artifacts.

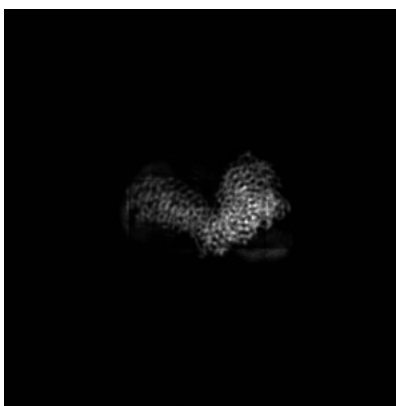
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

6.1.1 Primary map



X

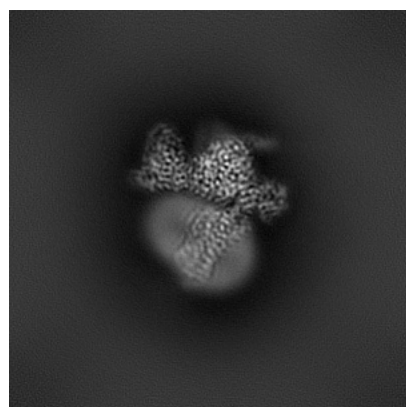


Y

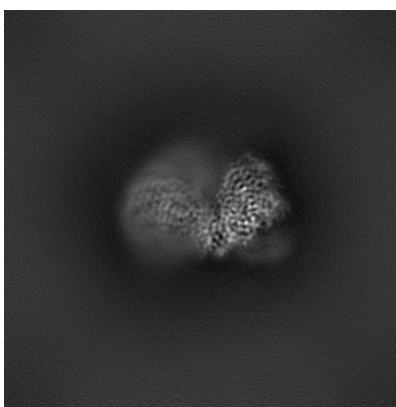


Z

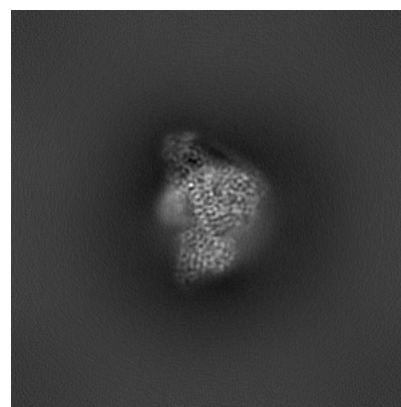
6.1.2 Raw map



X



Y



Z

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

6.2 Central slices [i](#)

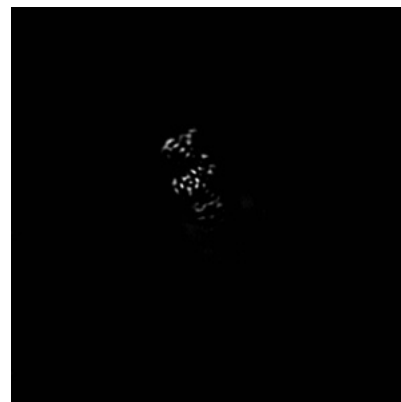
6.2.1 Primary map



X Index: 150

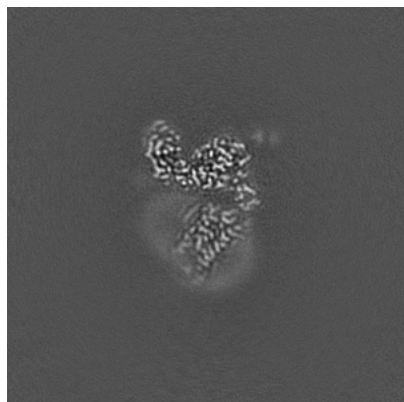


Y Index: 150

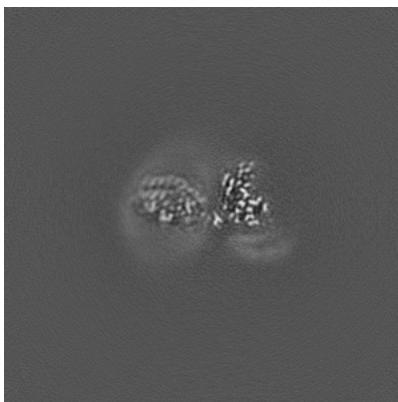


Z Index: 150

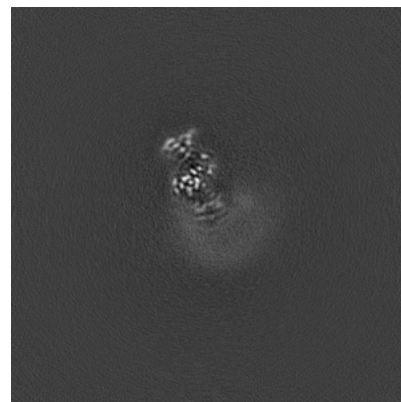
6.2.2 Raw map



X Index: 150



Y Index: 150



Z Index: 150

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: 149

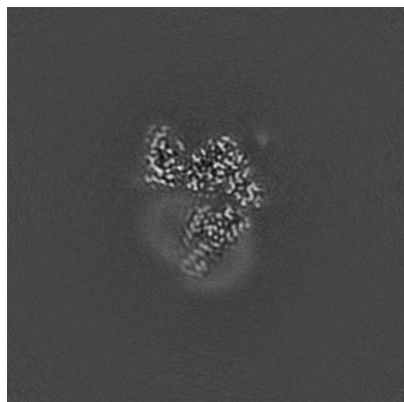


Y Index: 159

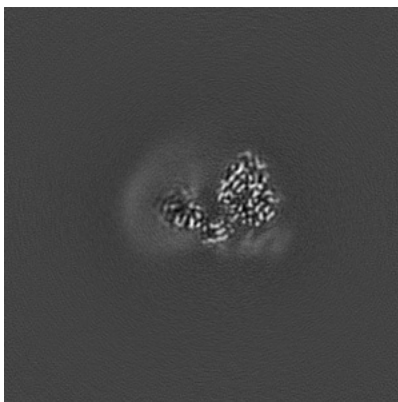


Z Index: 181

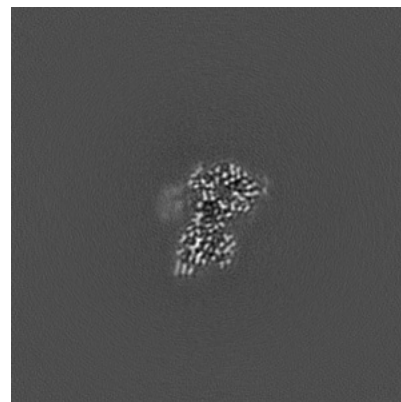
6.3.2 Raw map



X Index: 145



Y Index: 163

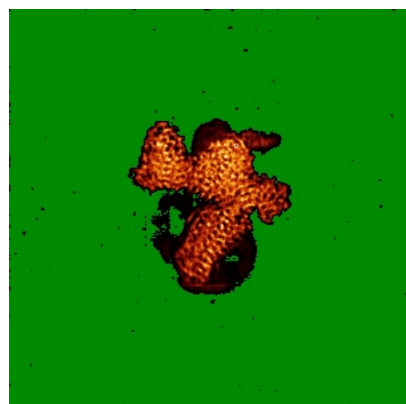


Z Index: 181

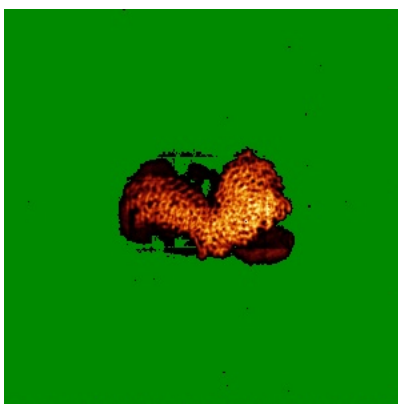
The images above show the largest variance slices of the map in three orthogonal directions.

6.4 Orthogonal standard-deviation projections (False-color) ⓘ

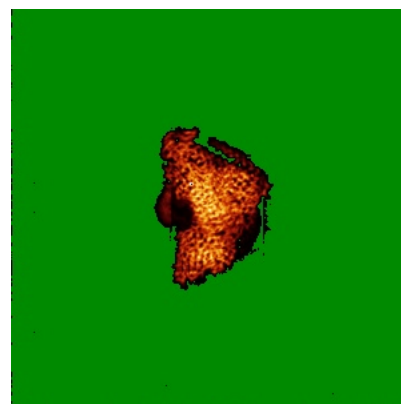
6.4.1 Primary map



X

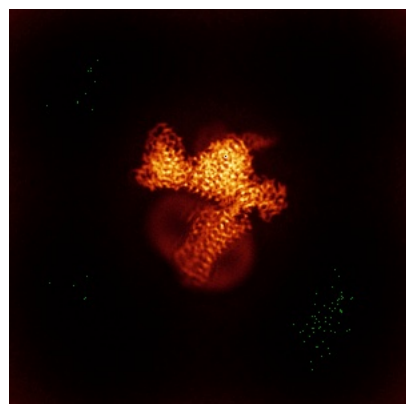


Y

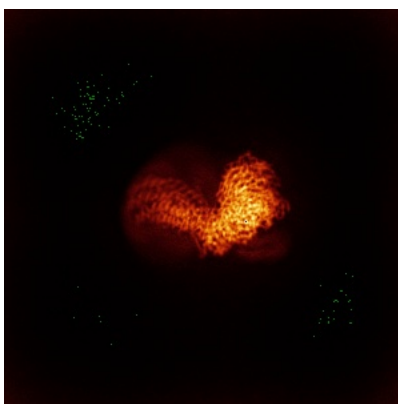


Z

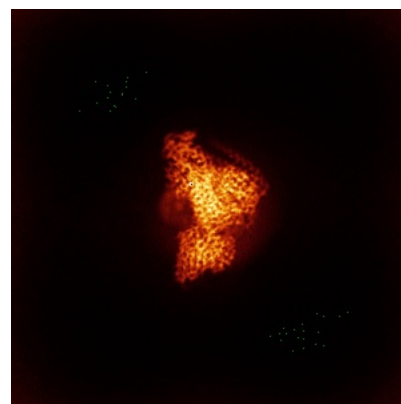
6.4.2 Raw map



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 0.1. 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.

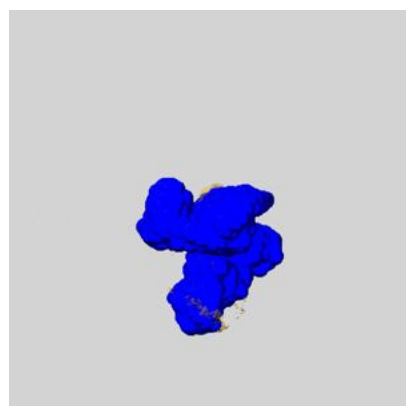
6.6 Mask visualisation [i](#)

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

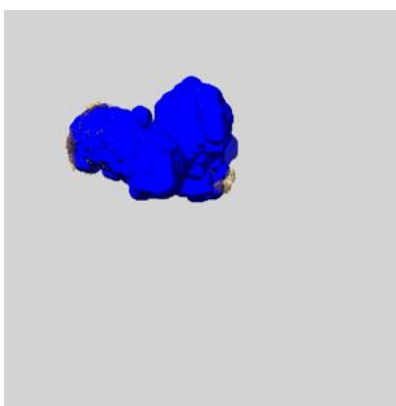
A mask typically either:

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

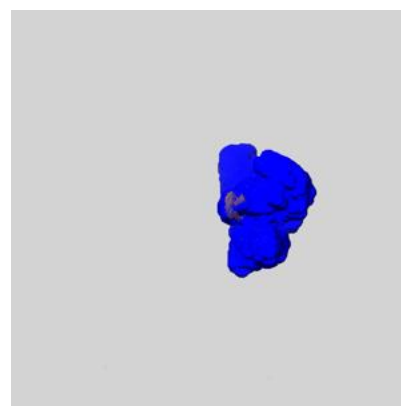
6.6.1 emd_39946_msk_1.map [i](#)



X



Y

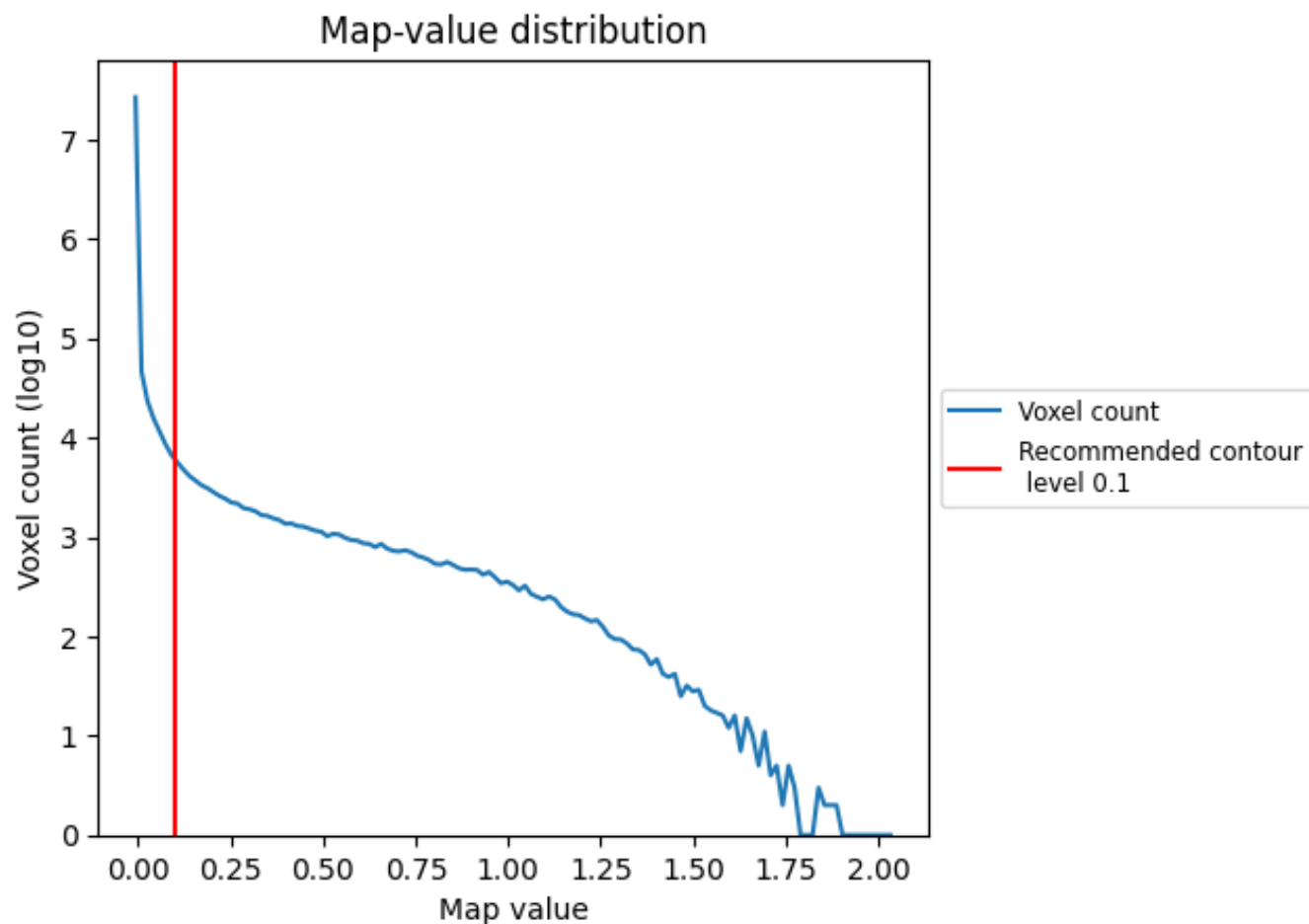


Z

7 Map analysis [i](#)

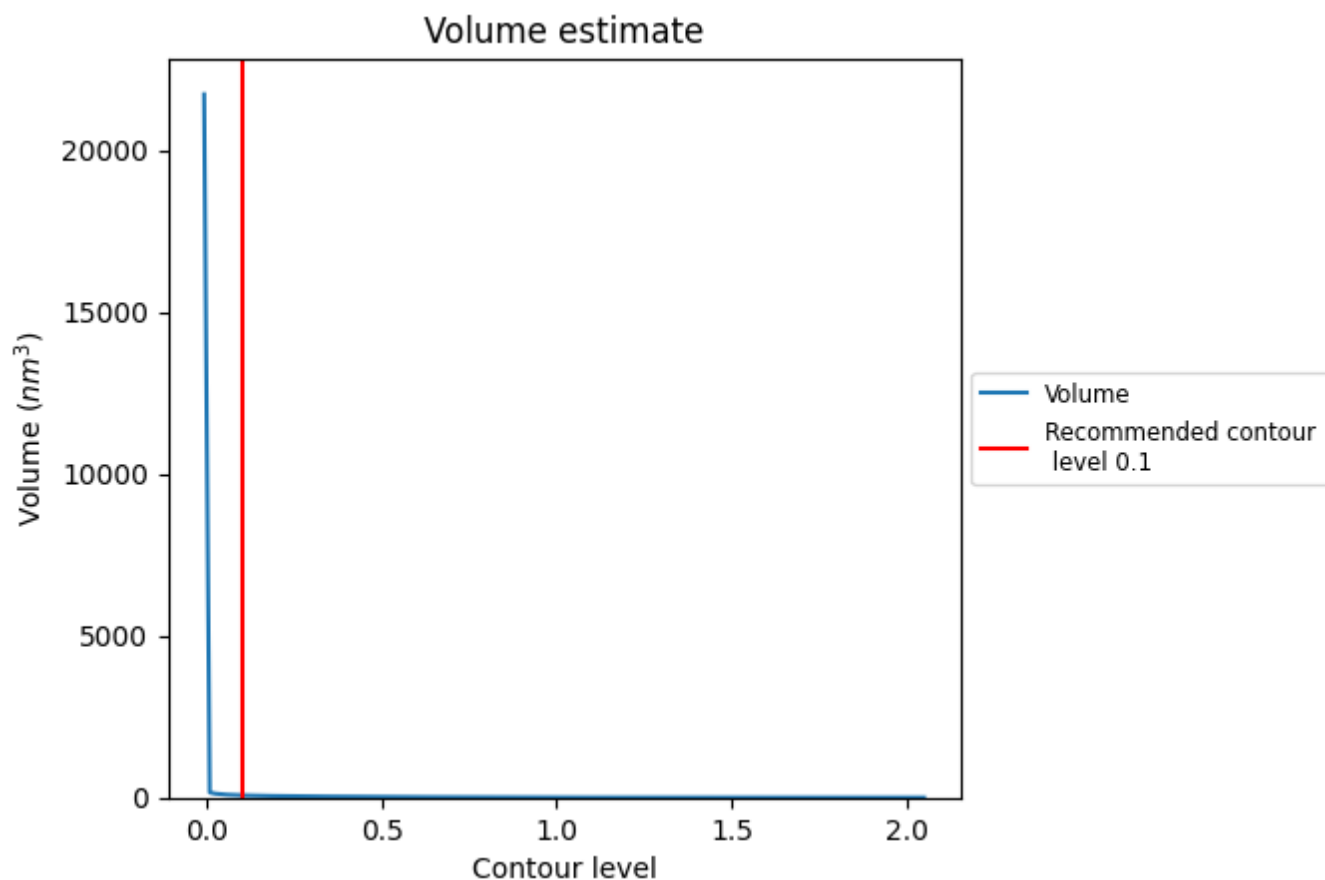
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution [i](#)



The map-value distribution is plotted in 128 intervals along the x-axis. The y-axis is logarithmic. A spike in this graph at zero usually indicates that the volume has been masked.

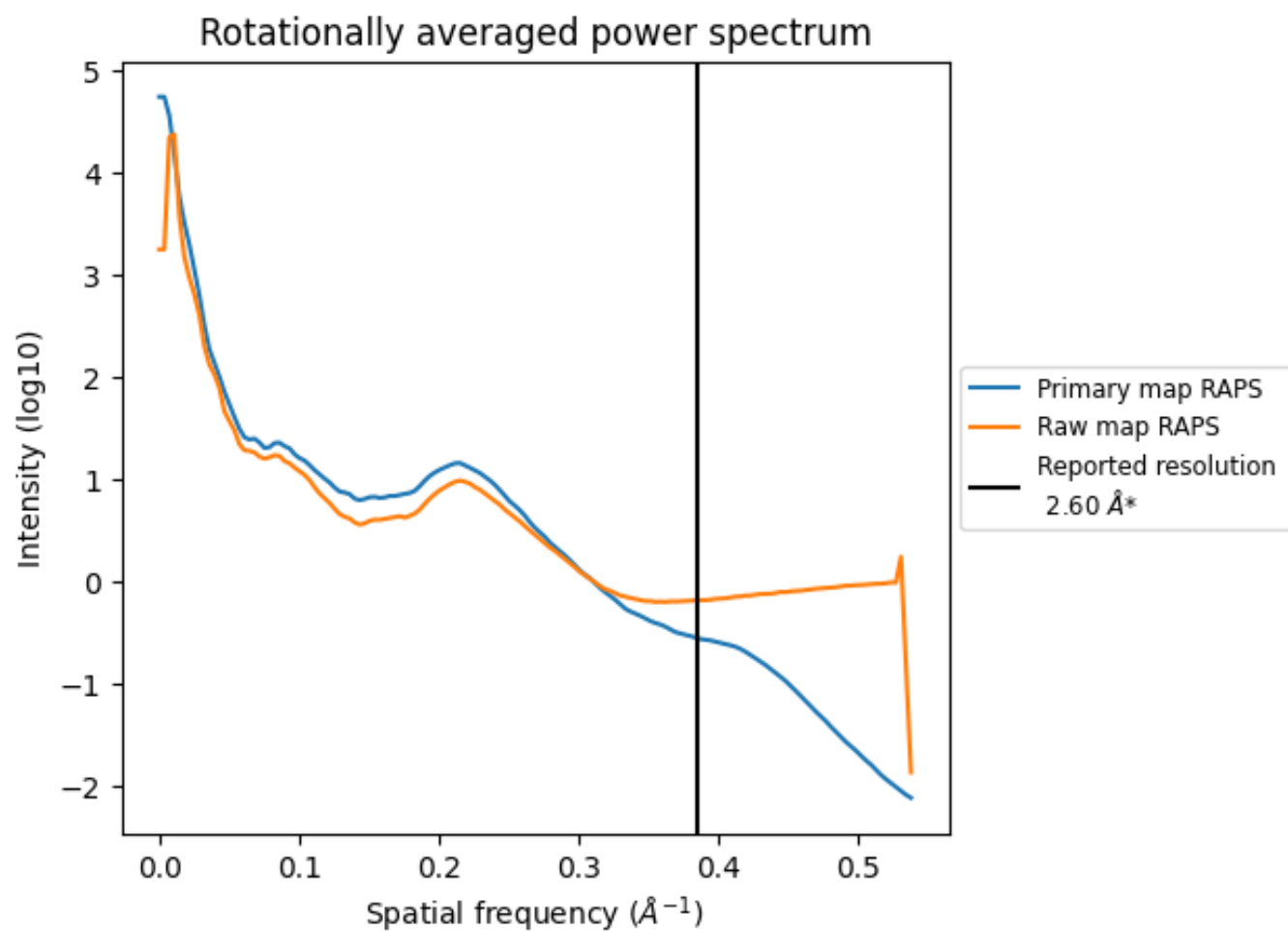
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 69 nm³; this corresponds to an approximate mass of 62 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 ⓘ

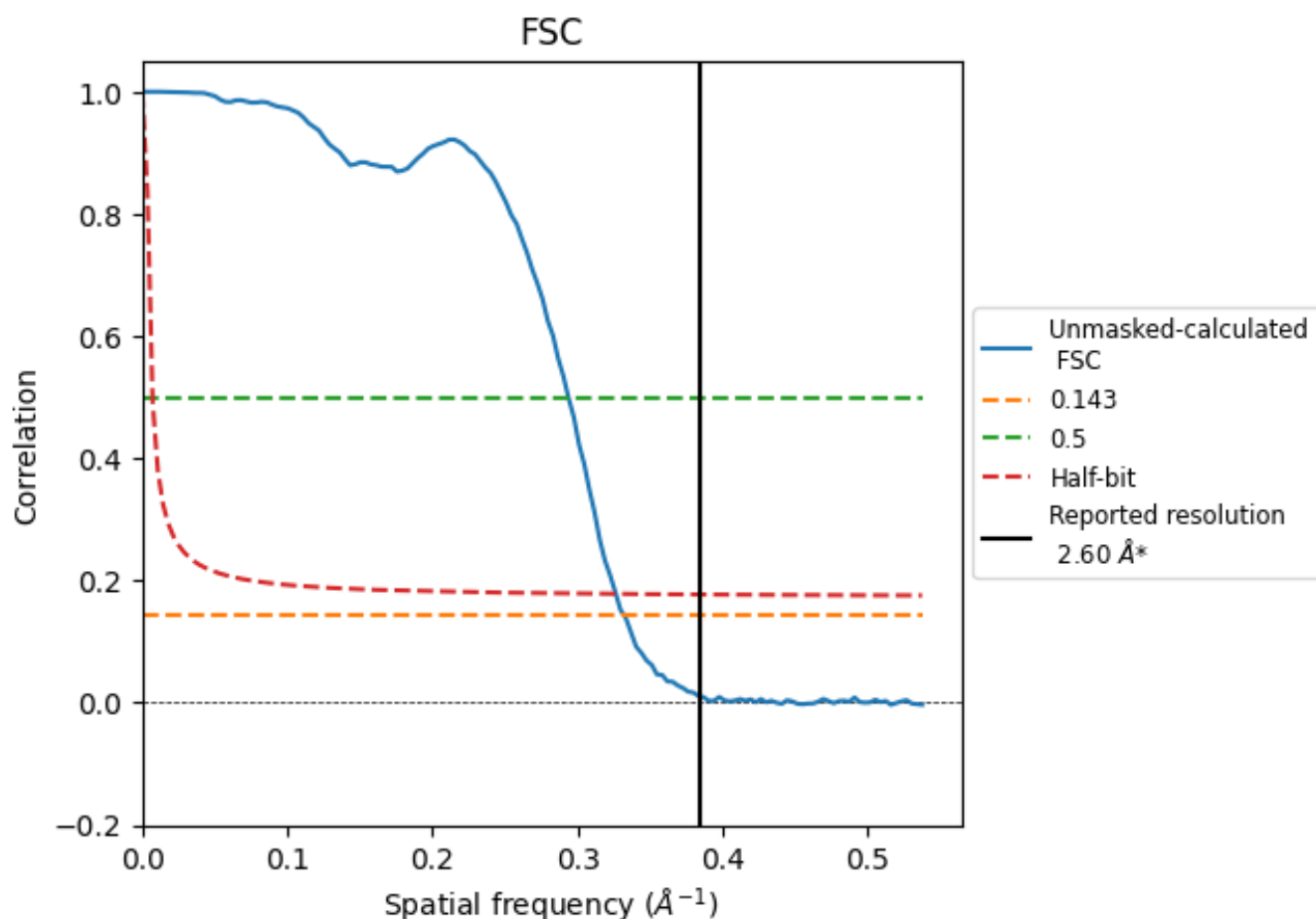


*Reported resolution corresponds to spatial frequency of 0.385 Å⁻¹

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 $0.385 \text{ \AA}^{-1}$

8.2 Resolution estimates [i](#)

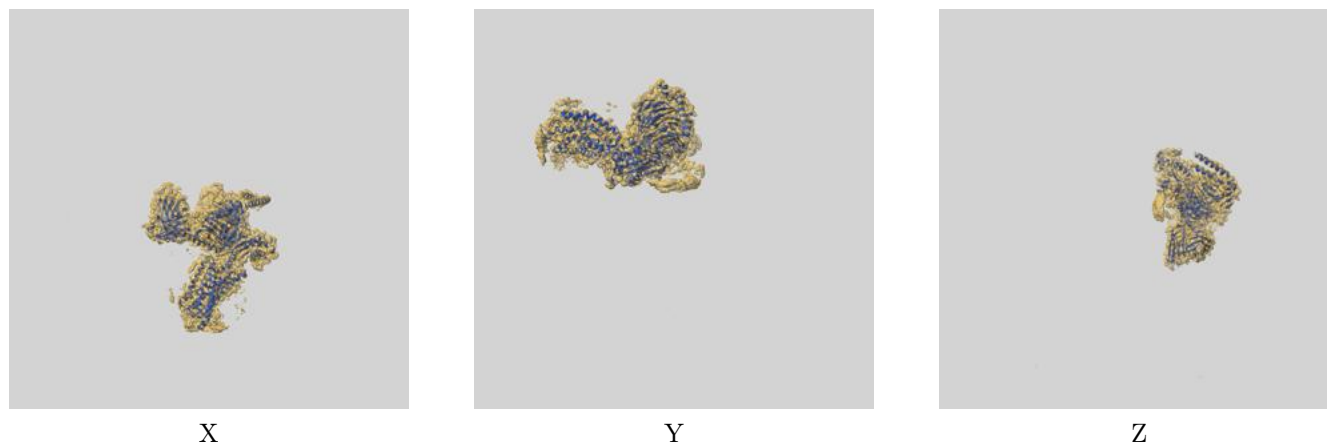
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	2.60	-	-
Author-provided FSC curve	-	-	-
Unmasked-calculated*	3.01	3.40	3.06

*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 3.01 differs from the reported value 2.6 by more than 10 %

9 Map-model fit [i](#)

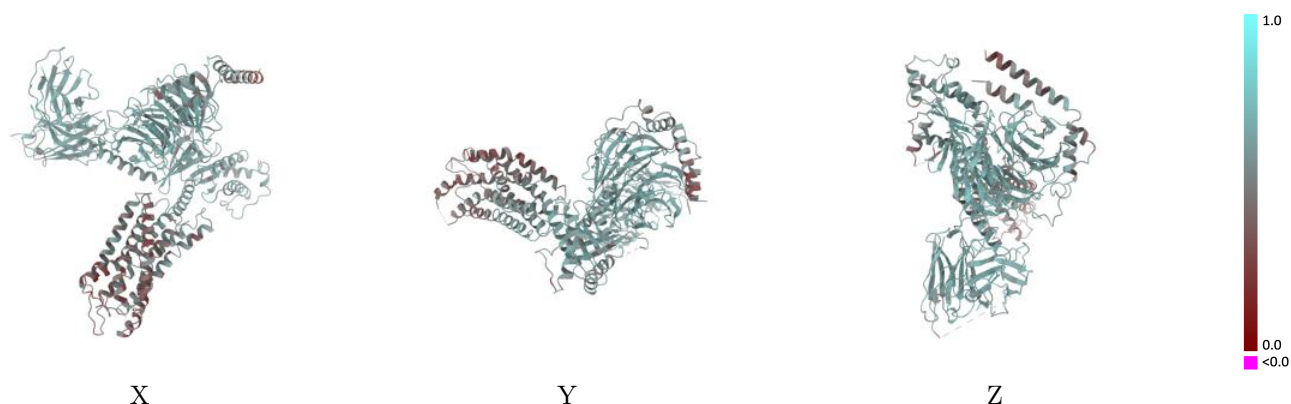
This section contains information regarding the fit between EMDB map EMD-39946 and PDB model 8ZD1. Per-residue inclusion information can be found in section [3](#) on page [6](#).

9.1 Map-model overlay [i](#)



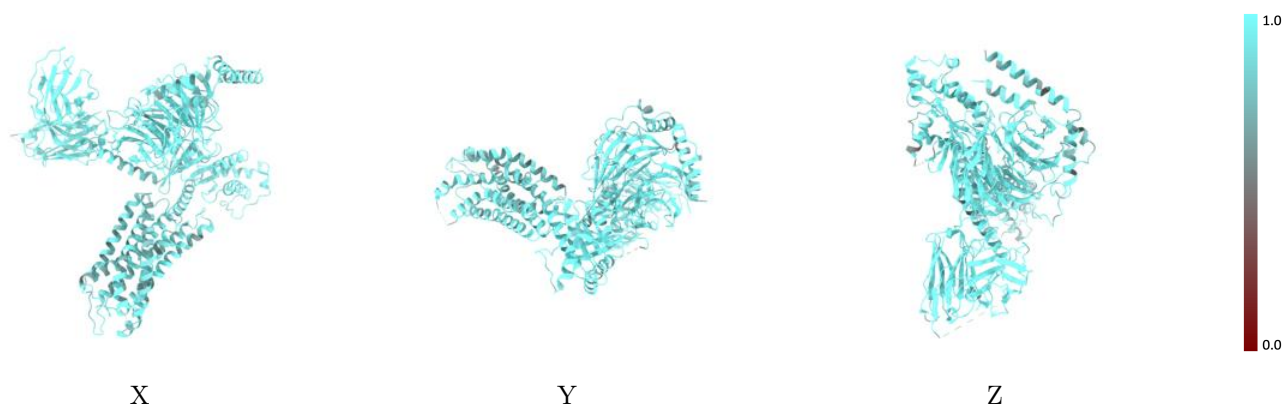
The images above show the 3D surface view of the map at the recommended contour level 0.1 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



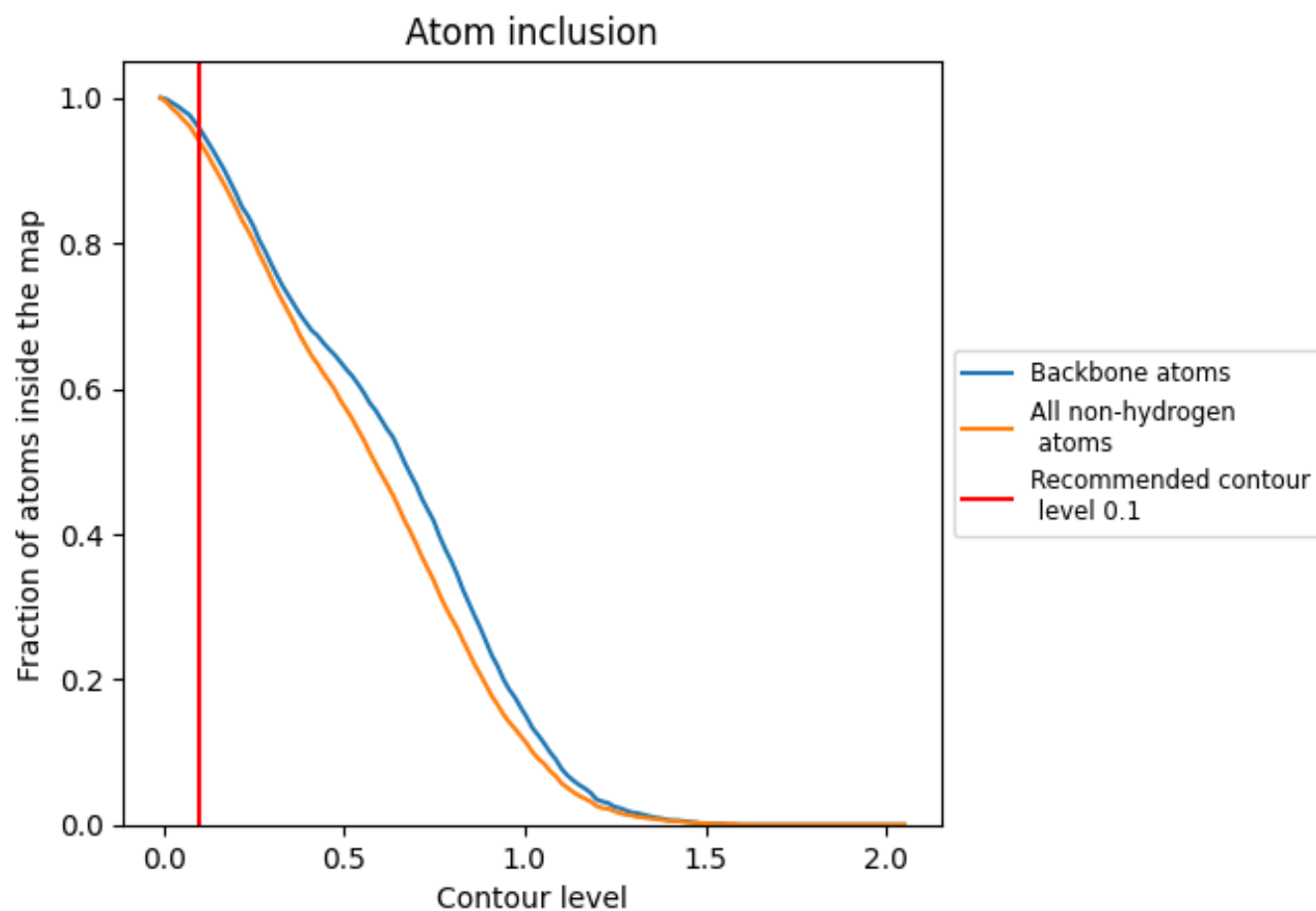
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.1).

9.4 Atom inclusion [i](#)



At the recommended contour level, 96% of all backbone atoms, 94% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary ⓘ

The table lists the average atom inclusion at the recommended contour level (0.1) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.9400	0.5670
A	0.9430	0.5840
B	0.9620	0.6060
G	0.8830	0.5390
R	0.8900	0.4730
S	0.9740	0.6050

