



Full wwPDB EM Validation Report ⓘ

Mar 5, 2026 – 08:13 PM UTC

PDB ID : 9DQJ / pdb_00009dqj
EMDB ID : EMD-47114
Title : CryoEM structure of Gq-coupled MRGPRD with a new agonist EP-3945
Authors : Cao, C.; Wang, C.; Liu, Y.; Fay, J.F.; Roth, B.L.
Deposited on : 2024-09-24
Resolution : 2.90 Å(reported)

This is a Full wwPDB EM Validation Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/EMValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

EMDB validation analysis : 0.0.1.dev132
Mogul : 2022.3.0, CSD as543be (2022)
MolProbity : 4-5-2 with Phenix2.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
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

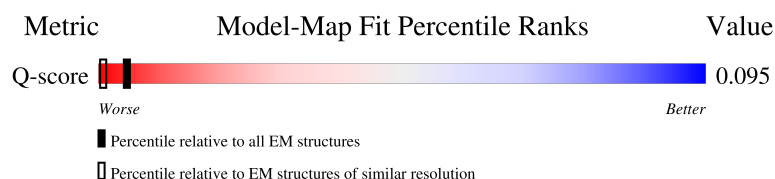
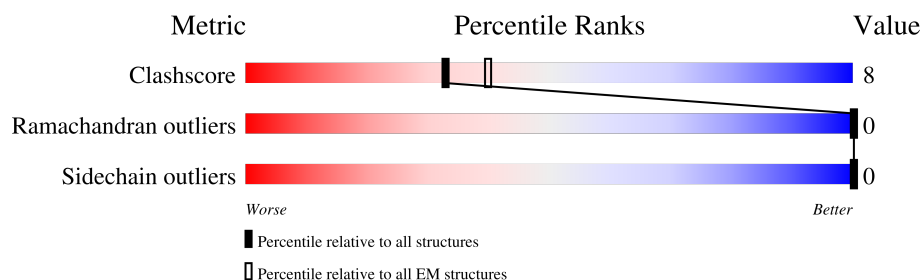
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 2.90 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	13054 (2.40 - 3.40)

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	322	25% 65% 14% 22%
2	B	246	25% 69% 17% 14%
3	C	345	25% 77% 21% .
4	D	71	23% 63% 8% 28%

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Mol	Chain	Length	Quality of chain
5	E	257	

2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 8043 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 Mas-related G-protein coupled receptor member D.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	252	Total	C	N	O	S	0	0
			1827	1214	296	301	16		

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	0	GLY	-	expression tag	UNP Q8TDS7
A	1	PRO	-	expression tag	UNP Q8TDS7

- Molecule 2 is a protein called 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
2	B	212	Total	C	N	O	S	0	0
			1649	1050	289	303	7		

There are 43 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	3	SER	CYS	engineered mutation	UNP P04899
B	31	ARG	ALA	engineered mutation	UNP P04899
B	33	THR	GLU	engineered mutation	UNP P04899
B	34	LEU	VAL	engineered mutation	UNP P04899
B	35	ARG	LYS	engineered mutation	UNP P04899
B	42	ASP	GLY	engineered mutation	UNP P04899
B	43	ASN	GLU	engineered mutation	UNP P04899
B	54	ARG	LYS	engineered mutation	UNP P04899
B	56	LEU	ILE	engineered mutation	UNP P04899
B	58	GLY	-	linker	UNP P04899
B	59	GLY	-	linker	UNP P04899
B	60	SER	-	linker	UNP P04899
B	61	GLY	-	linker	UNP P04899
B	62	GLY	-	linker	UNP P04899

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Chain	Residue	Modelled	Actual	Comment	Reference
B	63	SER	-	linker	UNP P04899
B	64	GLY	-	linker	UNP P04899
B	65	GLY	-	linker	UNP P04899
B	111	ASP	ALA	engineered mutation	UNP Q5JWF2
B	114	ASP	SER	engineered mutation	UNP Q5JWF2
B	?	-	ASN	deletion	UNP Q5JWF2
B	?	-	MET	deletion	UNP Q5JWF2
B	?	-	VAL	deletion	UNP Q5JWF2
B	?	-	ILE	deletion	UNP Q5JWF2
B	?	-	ARG	deletion	UNP Q5JWF2
B	?	-	GLU	deletion	UNP Q5JWF2
B	?	-	ASP	deletion	UNP Q5JWF2
B	?	-	ASN	deletion	UNP Q5JWF2
B	?	-	GLN	deletion	UNP Q5JWF2
B	?	-	THR	deletion	UNP Q5JWF2
B	124	ASP	LEU	engineered mutation	UNP Q5JWF2
B	195	LYS	ASP	engineered mutation	UNP Q5JWF2
B	198	VAL	LEU	engineered mutation	UNP Q5JWF2
B	199	ASP	ARG	engineered mutation	UNP Q5JWF2
B	210	ILE	TYR	engineered mutation	UNP Q5JWF2
B	224	ALA	ILE	engineered mutation	UNP Q5JWF2
B	227	ILE	VAL	engineered mutation	UNP Q5JWF2
B	232	LYS	ARG	engineered mutation	UNP Q5JWF2
B	236	LEU	GLN	engineered mutation	UNP Q5JWF2
B	237	GLN	ARG	engineered mutation	UNP Q5JWF2
B	239	ASN	HIS	engineered mutation	UNP Q5JWF2
B	242	GLU	GLN	engineered mutation	UNP Q5JWF2
B	244	ASN	GLU	engineered mutation	UNP Q5JWF2
B	246	VAL	LEU	engineered mutation	UNP Q5JWF2

- 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	C	338	Total	C	N	O	S	0	0
			2471	1536	438	478	19		

There are 6 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
C	-4	GLY	-	expression tag	UNP P62873
C	-3	PRO	-	expression tag	UNP P62873

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Chain	Residue	Modelled	Actual	Comment	Reference
C	-2	GLY	-	expression tag	UNP P62873
C	-1	SER	-	expression tag	UNP P62873
C	0	SER	-	expression tag	UNP P62873
C	1	GLY	-	expression tag	UNP P62873

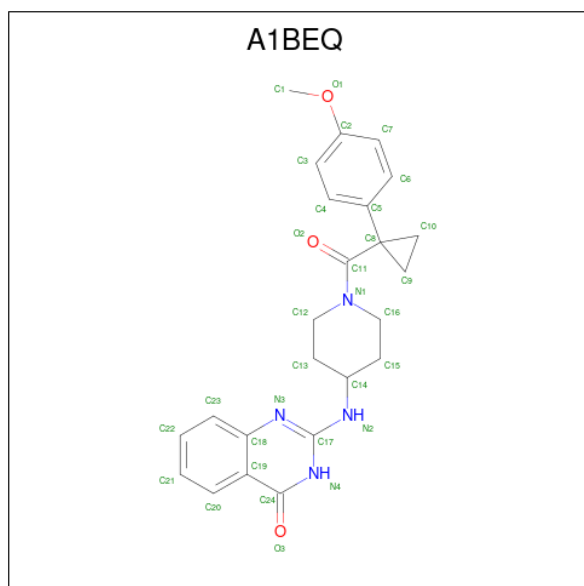
- Molecule 4 is a protein called Guanine nucleotide-binding protein G(I)/G(S)/G(O) subunit gamma-2.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	D	51	Total	C	N	O	S	0	0
			353	222	60	69	2		

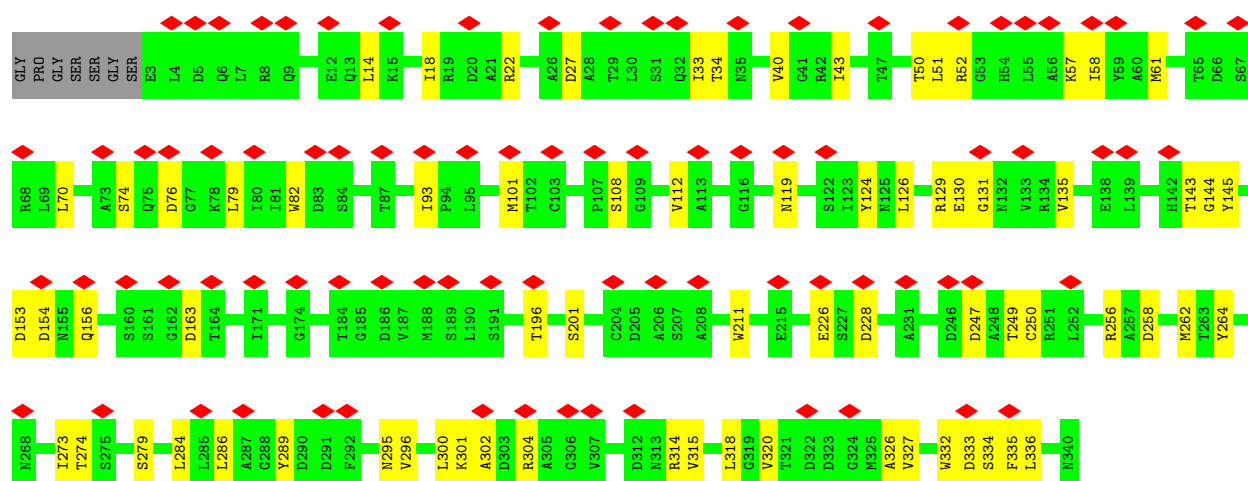
- Molecule 5 is a protein called scFv16.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	E	230	Total	C	N	O	S	0	0
			1712	1091	287	325	9		

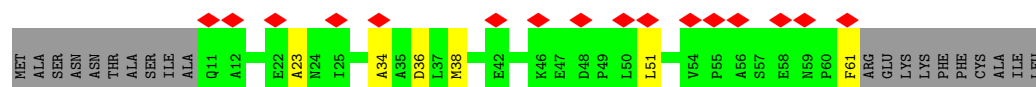
- Molecule 6 is 2-({1-[1-(4-methoxyphenyl)cyclopropane-1-carbonyl]piperidin-4-yl}amino)quinazolin-4(3H)-one (CCD ID: A1BEQ) (formula: C₂₄H₂₆N₄O₃) (labeled as "Ligand of Interest" by depositor).



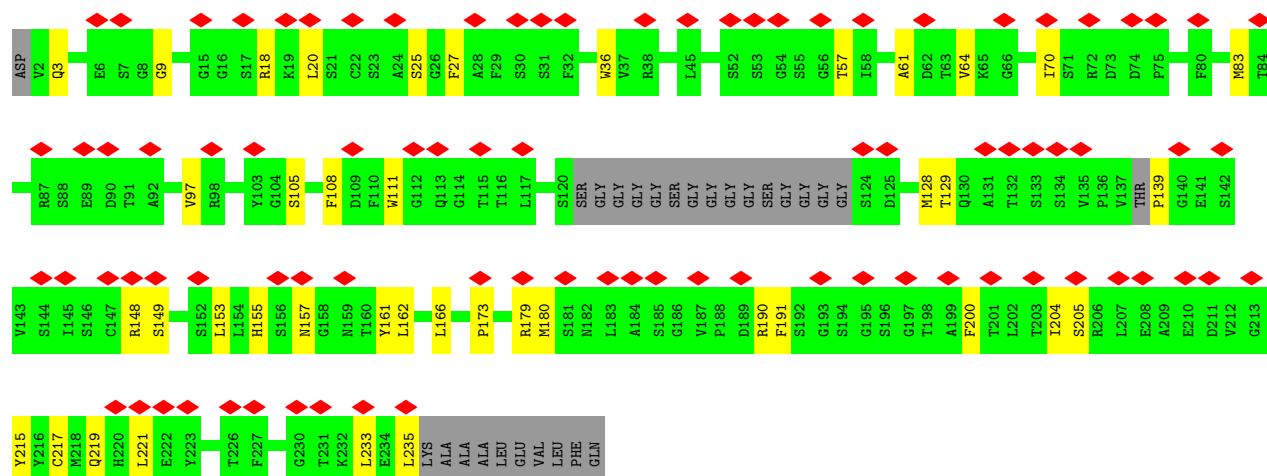
Mol	Chain	Residues	Atoms				AltConf
6	A	1	Total	C	N	O	0
			31	24	4	3	



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



- Molecule 5: scFv16



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	318286	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TALOS ARCTICA	Depositor
Voltage (kV)	200	Depositor
Electron dose ($e^-/\text{\AA}^2$)	56.9	Depositor
Minimum defocus (nm)	200	Depositor
Maximum defocus (nm)	3000	Depositor
Magnification	Not provided	
Image detector	GATAN K3 (6k x 4k)	Depositor
Maximum map value	1.635	Depositor
Minimum map value	-0.024	Depositor
Average map value	0.001	Depositor
Map value standard deviation	0.022	Depositor
Recommended contour level	0.1	Depositor
Map size (Å)	253.44, 253.44, 253.44	wwPDB
Map dimensions	288, 288, 288	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	0.88, 0.88, 0.88	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: A1BEQ

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	0.31	0/1875	0.45	1/2574 (0.0%)
2	B	0.36	0/1677	0.44	0/2267
3	C	0.37	0/2516	0.44	0/3427
4	D	0.27	0/359	0.32	0/492
5	E	0.37	0/1755	0.40	0/2384
All	All	0.35	0/8182	0.43	1/11144 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	79	MET	CB-CG-SD	-5.33	96.72	112.70

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	1827	0	1698	27	0
2	B	1649	0	1580	28	0
3	C	2471	0	2295	53	0
4	D	353	0	317	6	0
5	E	1712	0	1606	29	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
6	A	31	0	0	1	0
All	All	8043	0	7496	131	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 8.

All (131) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:22:ARG:NH1	3:C:258:ASP:O	2.07	0.87
3:C:295:ASN:OD1	3:C:304:ARG:NH1	2.16	0.78
3:C:33:ILE:HG22	4:D:38:MET:HE1	1.69	0.75
5:E:128:MET:HE3	5:E:219:GLN:HB3	1.72	0.71
1:A:74:LEU:HD22	1:A:108:ALA:HB2	1.73	0.70
2:B:170:TYR:O	2:B:188:ARG:NH1	2.25	0.69
1:A:38:CYS:HA	1:A:76:LEU:HD22	1.77	0.66
3:C:101:MET:HE1	3:C:145:TYR:CD2	2.31	0.65
2:B:83:MET:HE2	2:B:107:ILE:HD12	1.80	0.64
2:B:14:GLU:OE2	5:E:57:THR:OG1	2.16	0.63
3:C:43:ILE:HD11	3:C:296:VAL:HG21	1.81	0.62
1:A:91:VAL:O	1:A:95:ASP:N	2.23	0.61
5:E:111:TRP:CE3	5:E:173:PRO:HG2	2.35	0.61
3:C:130:GLU:HA	5:E:27:PHE:HB2	1.83	0.60
3:C:34:THR:HG21	3:C:300:LEU:HB3	1.84	0.60
3:C:74:SER:OG	3:C:76:ASP:OD1	2.16	0.60
3:C:256:ARG:NH1	4:D:36:ASP:OD2	2.30	0.60
5:E:162:LEU:HB3	5:E:180:MET:HB3	1.84	0.59
3:C:58:ILE:HD13	3:C:336:LEU:HD23	1.84	0.59
2:B:234:ILE:O	2:B:238:MET:HG3	2.05	0.57
3:C:274:THR:OG1	3:C:315:VAL:O	2.20	0.57
1:A:233:CYS:HB3	1:A:268:SER:HB2	1.86	0.57
2:B:95:LYS:NZ	3:C:228:ASP:OD1	2.37	0.57
2:B:15:ARG:HH21	2:B:15:ARG:HG3	1.70	0.57
3:C:279:SER:HB2	3:C:284:LEU:HB2	1.86	0.56
5:E:105:SER:O	5:E:179:ARG:NH2	2.38	0.56
5:E:128:MET:HE1	5:E:153:LEU:HD11	1.88	0.56
2:B:243:TYR:O	2:B:245:LEU:N	2.38	0.56
3:C:50:THR:HG23	3:C:52:ARG:NH1	2.20	0.56
3:C:34:THR:O	3:C:301:LYS:NZ	2.38	0.56
5:E:166:LEU:HD13	5:E:215:TYR:CZ	2.41	0.55
2:B:147:ASP:OD1	2:B:148:LEU:N	2.40	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:201:SER:HB3	3:C:211:TRP:HE1	1.70	0.55
1:A:153:CYS:O	1:A:157:ASN:ND2	2.40	0.54
5:E:20:LEU:HG	5:E:83:MET:HE2	1.90	0.54
5:E:128:MET:CE	5:E:219:GLN:HB3	2.36	0.54
1:A:233:CYS:HA	1:A:264:SER:OG	2.07	0.54
1:A:131:ILE:HG12	2:B:235:ILE:HD13	1.90	0.54
2:B:144:ASN:OD1	2:B:145:LYS:N	2.40	0.53
3:C:61:MET:HE2	3:C:70:LEU:HD13	1.89	0.53
2:B:76:VAL:HG11	2:B:228:PHE:HB2	1.90	0.53
3:C:320:VAL:HG22	3:C:327:VAL:HG22	1.91	0.53
5:E:162:LEU:HD11	5:E:217:CYS:HB2	1.90	0.53
1:A:201:LEU:HD22	1:A:223:VAL:HG21	1.91	0.52
5:E:162:LEU:HD22	5:E:200:PHE:CG	2.45	0.52
3:C:108:SER:OG	3:C:154:ASP:OD1	2.25	0.52
3:C:101:MET:HE1	3:C:145:TYR:HD2	1.72	0.52
1:A:218:ARG:NH1	2:B:244:ASN:O	2.42	0.52
5:E:191:PHE:CE1	5:E:204:ILE:HD12	2.44	0.52
3:C:196:THR:HG22	3:C:196:THR:O	2.10	0.51
3:C:52:ARG:HG3	3:C:335:PHE:HE1	1.76	0.51
3:C:286:LEU:HD13	3:C:296:VAL:HG22	1.93	0.51
2:B:5:VAL:O	2:B:10:LYS:NZ	2.43	0.50
3:C:51:LEU:HD12	3:C:336:LEU:HD11	1.93	0.50
2:B:86:VAL:HG21	2:B:96:TRP:CZ2	2.46	0.50
5:E:215:TYR:CE2	5:E:233:LEU:HD22	2.47	0.50
1:A:81:SER:CB	1:A:101:MET:HE1	2.42	0.49
1:A:251:PRO:HD2	1:A:252:GLU:H	1.77	0.49
5:E:129:THR:HG23	5:E:148:ARG:HB2	1.95	0.49
3:C:112:VAL:HG13	3:C:126:LEU:HD11	1.95	0.49
2:B:241:ARG:HH11	2:B:241:ARG:HG3	1.78	0.48
5:E:153:LEU:HA	5:E:221:LEU:HD22	1.94	0.48
3:C:40:VAL:HG11	4:D:51:LEU:HD11	1.96	0.48
5:E:139:PRO:HG3	5:E:235:LEU:HD22	1.95	0.47
1:A:105:MET:HE3	1:A:106:TYR:CE1	2.50	0.47
3:C:57:LYS:HB3	3:C:332:TRP:CD1	2.49	0.47
3:C:284:LEU:HD13	3:C:296:VAL:HG11	1.95	0.47
2:B:8:GLU:HG3	5:E:161:TYR:CE2	2.49	0.47
1:A:85:LEU:HD22	1:A:98:HIS:HB2	1.97	0.46
3:C:247:ASP:HB2	3:C:249:THR:HG22	1.96	0.46
1:A:38:CYS:CB	1:A:80:ALA:HB2	2.46	0.46
5:E:155:HIS:HB3	5:E:157:ASN:OD1	2.15	0.46
3:C:314:ARG:HD3	3:C:332:TRP:CZ3	2.51	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:14:LEU:HD23	3:C:14:LEU:HA	1.82	0.46
3:C:124:TYR:CE1	3:C:135:VAL:HG22	2.50	0.46
3:C:273:ILE:HG12	3:C:289:TYR:CE2	2.51	0.46
3:C:27:ASP:OD1	3:C:27:ASP:N	2.48	0.46
3:C:286:LEU:HB3	3:C:318:LEU:HD21	1.96	0.46
1:A:102:LYS:NZ	1:A:103:ARG:HH12	2.14	0.45
2:B:93:ARG:HA	2:B:96:TRP:CE2	2.50	0.45
2:B:44:SER:HB2	2:B:109:VAL:HG12	1.98	0.45
2:B:195:LYS:HA	2:B:198:VAL:HG12	1.98	0.45
1:A:183:ALA:HB2	6:A:401:A1BEQ:O1	2.17	0.45
2:B:111:ASP:OD2	2:B:145:LYS:HD2	2.17	0.45
3:C:153:ASP:OD1	3:C:156:GLN:N	2.48	0.45
3:C:119:ASN:ND2	3:C:143:THR:O	2.50	0.45
5:E:3:GLN:HB3	5:E:25:SER:HG	1.82	0.45
5:E:9:GLY:O	5:E:18:ARG:NH2	2.50	0.45
5:E:97:VAL:HG11	5:E:108:PHE:CD1	2.52	0.45
3:C:52:ARG:HG3	3:C:335:PHE:CE1	2.52	0.45
1:A:217:THR:HA	1:A:220:PHE:HD2	1.82	0.44
3:C:226:GLU:N	3:C:247:ASP:OD2	2.50	0.44
5:E:166:LEU:HD13	5:E:215:TYR:CE1	2.51	0.44
5:E:36:TRP:HD1	5:E:70:ILE:HD12	1.82	0.44
1:A:201:LEU:HD21	1:A:219:LEU:HD21	1.99	0.44
3:C:262:MET:SD	3:C:302:ALA:HB2	2.58	0.44
1:A:159:LEU:HG	1:A:178:VAL:HG21	1.99	0.44
3:C:333:ASP:O	3:C:334:SER:OG	2.28	0.44
1:A:198:SER:HB3	1:A:223:VAL:HG13	2.01	0.43
3:C:250:CYS:HB2	3:C:264:TYR:HB2	2.00	0.43
1:A:65:ILE:HD11	1:A:276:TYR:HB3	2.00	0.43
3:C:262:MET:HE1	3:C:300:LEU:O	2.18	0.43
1:A:233:CYS:CB	1:A:268:SER:HB2	2.49	0.43
1:A:85:LEU:CD2	1:A:98:HIS:HB2	2.48	0.43
2:B:172:THR:HA	2:B:173:PRO:HD3	1.85	0.43
3:C:79:LEU:HB2	3:C:93:ILE:HB	2.01	0.43
3:C:326:ALA:HB2	4:D:61:PHE:CE2	2.54	0.42
5:E:179:ARG:C	5:E:180:MET:HG3	2.45	0.42
5:E:179:ARG:O	5:E:180:MET:HG3	2.19	0.42
3:C:18:ILE:HD11	4:D:23:ALA:HA	2.00	0.42
3:C:34:THR:O	3:C:34:THR:HG22	2.19	0.42
5:E:190:ARG:HB2	5:E:205:SER:O	2.20	0.42
1:A:191:THR:HB	1:A:192:PRO:HD3	2.02	0.42
3:C:112:VAL:HG23	3:C:124:TYR:HB2	2.02	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:63:ILE:O	1:A:67:ASN:ND2	2.39	0.41
3:C:51:LEU:HB3	3:C:82:TRP:CZ3	2.55	0.41
2:B:183:ASP:HB3	2:B:186:VAL:HG12	2.02	0.41
2:B:231:CYS:O	2:B:235:ILE:HD12	2.20	0.41
2:B:110:VAL:CG1	2:B:143:LEU:HD13	2.51	0.41
3:C:144:GLY:H	3:C:163:ASP:HB3	1.85	0.41
5:E:128:MET:HE1	5:E:149:SER:HB2	2.01	0.41
1:A:83:LEU:HD21	1:A:262:ARG:NE	2.35	0.41
3:C:33:ILE:HD12	4:D:34:ALA:HB3	2.02	0.41
3:C:129:ARG:C	3:C:131:GLY:H	2.29	0.41
2:B:118:LEU:HD12	2:B:118:LEU:HA	1.88	0.41
1:A:239:ILE:O	1:A:243:VAL:HG23	2.21	0.41
2:B:15:ARG:HG3	2:B:15:ARG:NH2	2.35	0.41
3:C:51:LEU:HD12	3:C:336:LEU:CD1	2.51	0.41
2:B:38:LEU:O	2:B:39:LEU:HD23	2.21	0.40
2:B:222:GLU:O	2:B:226:ARG:HG3	2.22	0.40
5:E:61:ALA:HB3	5:E:64:VAL:HG22	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	248/322 (77%)	234 (94%)	14 (6%)	0	100	100
2	B	204/246 (83%)	192 (94%)	12 (6%)	0	100	100
3	C	336/345 (97%)	319 (95%)	17 (5%)	0	100	100
4	D	49/71 (69%)	48 (98%)	1 (2%)	0	100	100
5	E	224/257 (87%)	212 (95%)	12 (5%)	0	100	100
All	All	1061/1241 (86%)	1005 (95%)	56 (5%)	0	100	100

There are no Ramachandran outliers to report.

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	172/289 (60%)	172 (100%)	0	100	100
2	B	168/213 (79%)	168 (100%)	0	100	100
3	C	246/285 (86%)	246 (100%)	0	100	100
4	D	31/58 (53%)	31 (100%)	0	100	100
5	E	178/207 (86%)	178 (100%)	0	100	100
All	All	795/1052 (76%)	795 (100%)	0	100	100

There are no protein residues with a non-rotameric sidechain to report.

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (6) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	182	GLN
2	B	209	HIS
3	C	230	ASN
5	E	82	GLN
5	E	167	GLN
5	E	182	ASN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

1 ligand is modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
6	A1BEQ	A	401	-	34,35,35	0.61	0	48,51,51	0.62	1 (2%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
6	A1BEQ	A	401	-	-	7/22/36/36	0/5/5/5

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	A	401	A1BEQ	O2-C11-C8	-2.00	118.28	121.57

There are no chirality outliers.

All (7) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
6	A	401	A1BEQ	O2-C11-N1-C16
6	A	401	A1BEQ	C8-C11-N1-C16
6	A	401	A1BEQ	C4-C5-C8-C11
6	A	401	A1BEQ	C6-C5-C8-C11
6	A	401	A1BEQ	C4-C5-C8-C9

Continued on next page...

Continued from previous page...

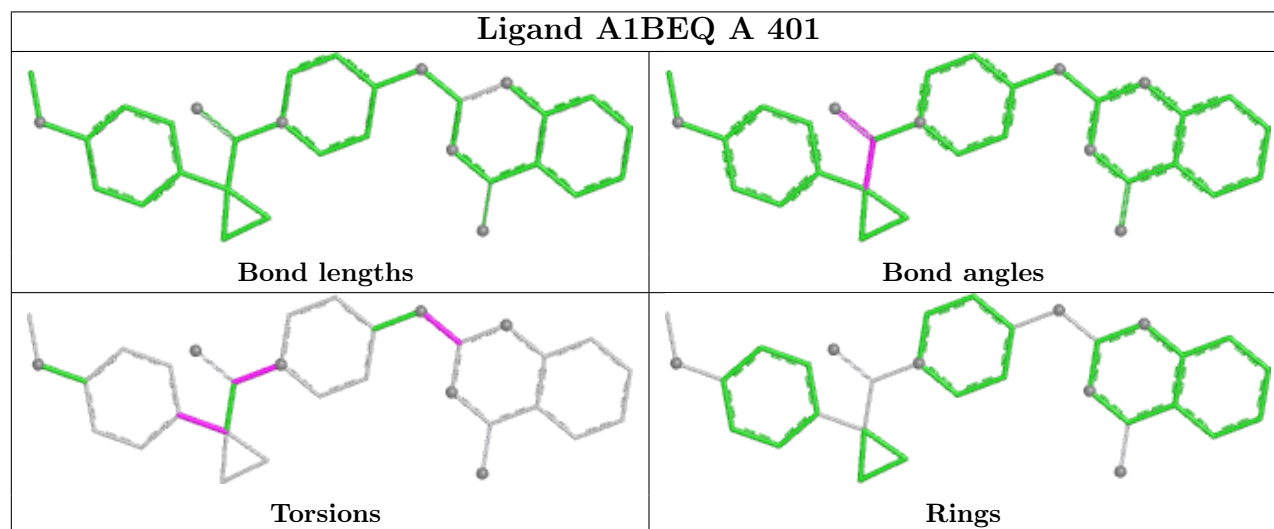
Mol	Chain	Res	Type	Atoms
6	A	401	A1BEQ	C6-C5-C8-C9
6	A	401	A1BEQ	N3-C17-N2-C14

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	A	401	A1BEQ	1	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.



5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

There are no chain breaks in this entry.

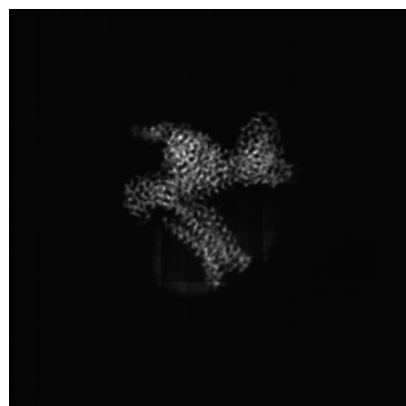
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-47114. These allow visual inspection of the internal detail of the map and identification of artifacts.

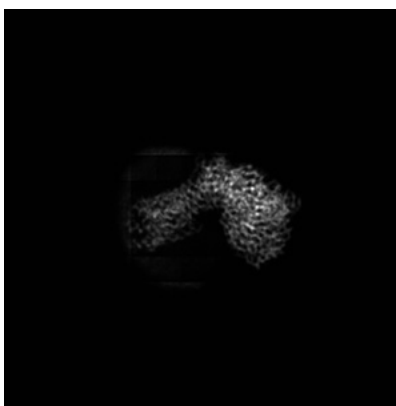
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

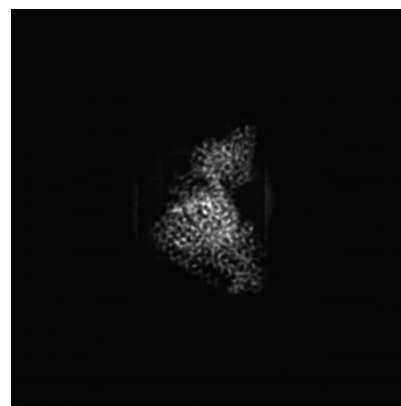
6.1.1 Primary map



X

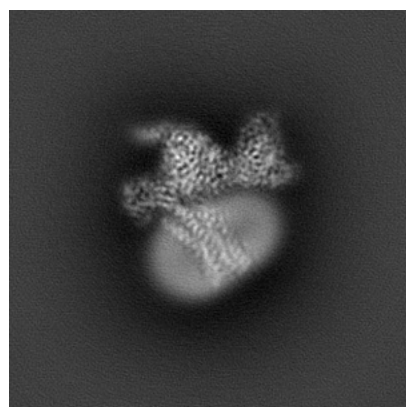


Y

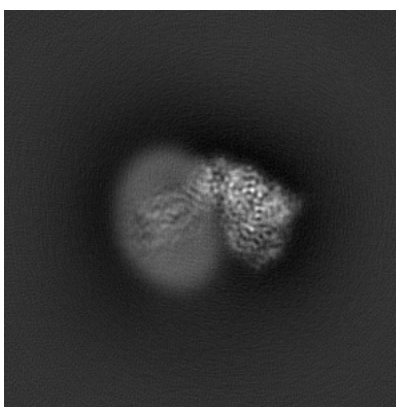


Z

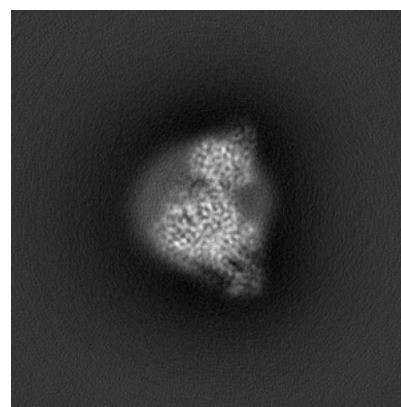
6.1.2 Raw map



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: 144

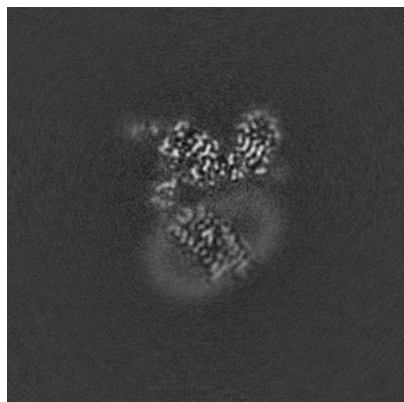


Y Index: 144

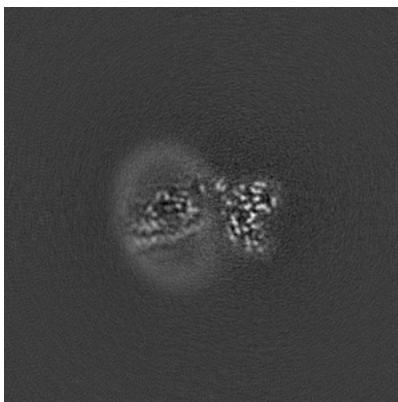


Z Index: 144

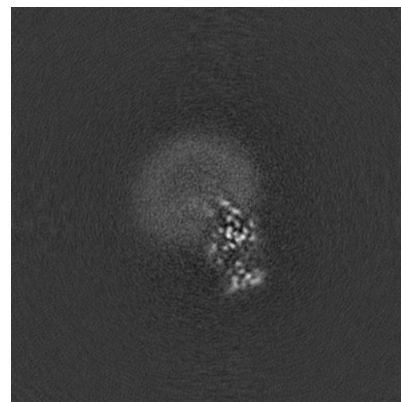
6.2.2 Raw map



X Index: 144



Y Index: 144



Z Index: 144

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

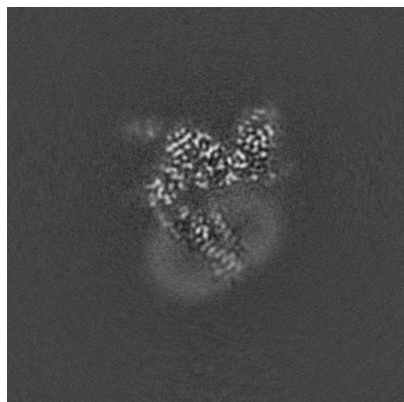


Y Index: 125

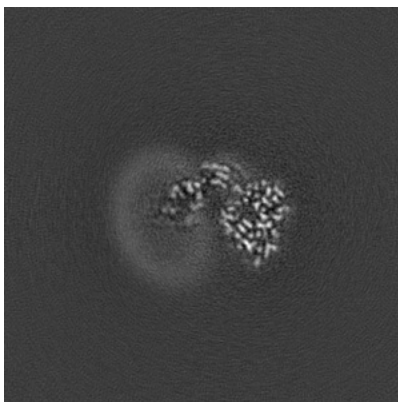


Z Index: 178

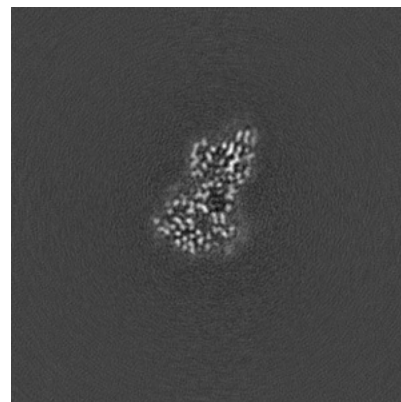
6.3.2 Raw map



X Index: 149



Y Index: 130

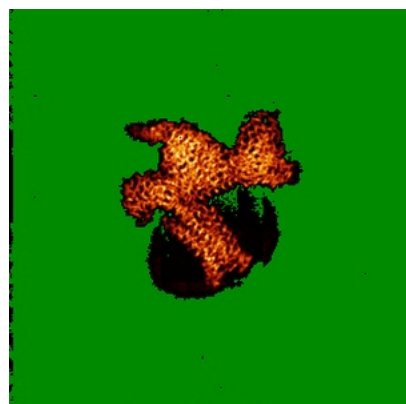


Z Index: 178

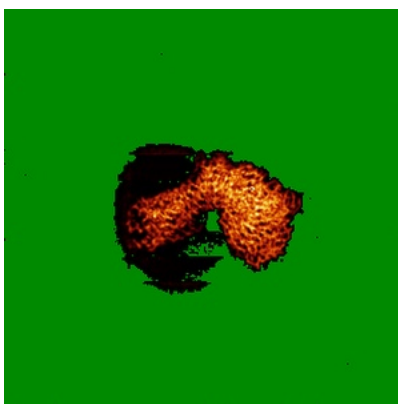
The images above show the largest variance slices of the map in three orthogonal directions.

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

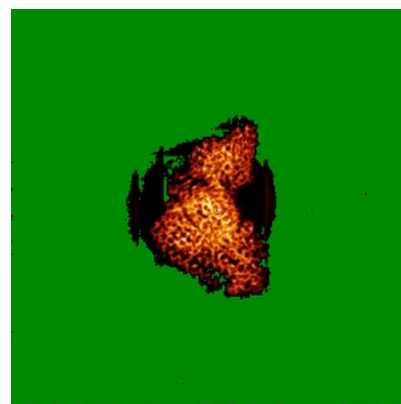
6.4.1 Primary map



X

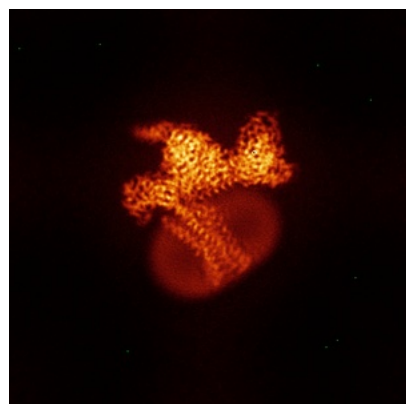


Y

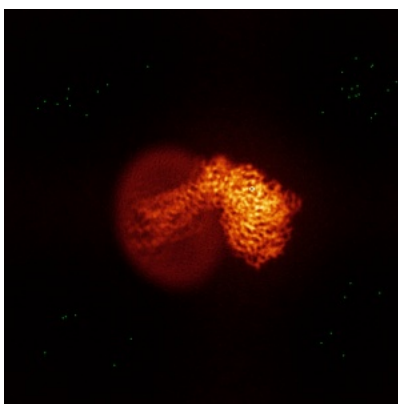


Z

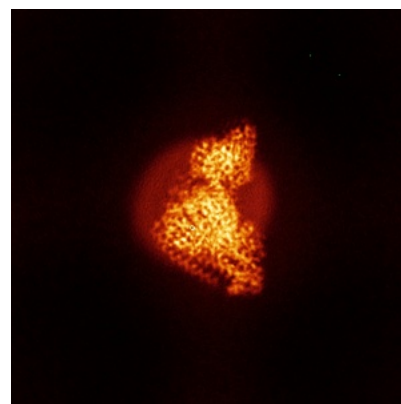
6.4.2 Raw map



X



Y

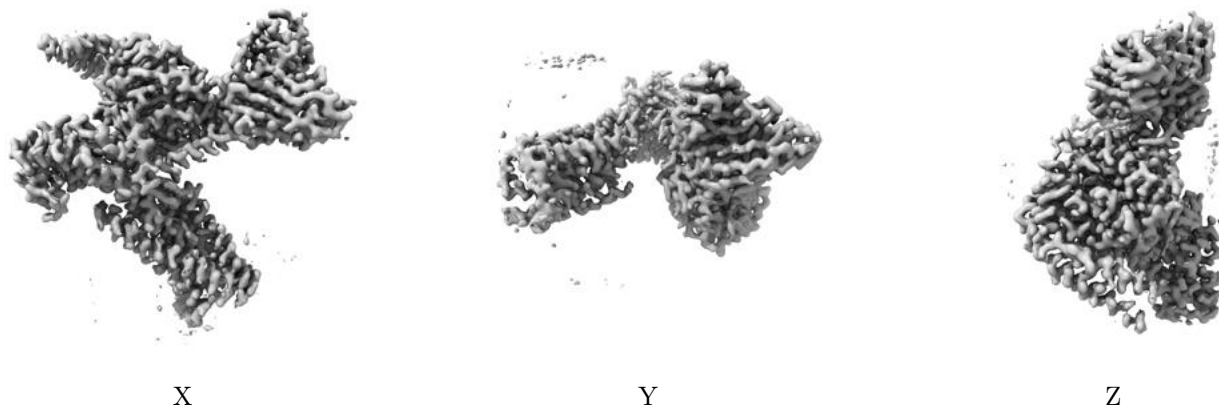


Z

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.

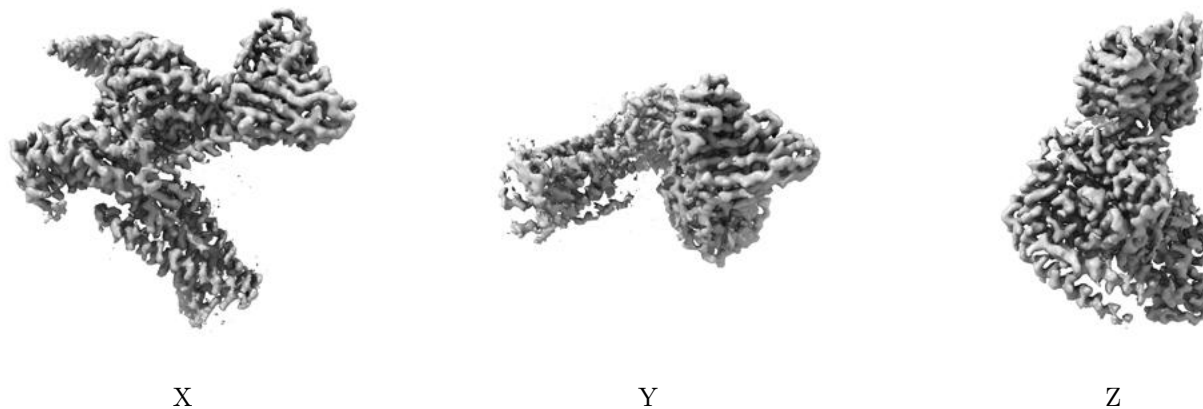
6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.1. 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.

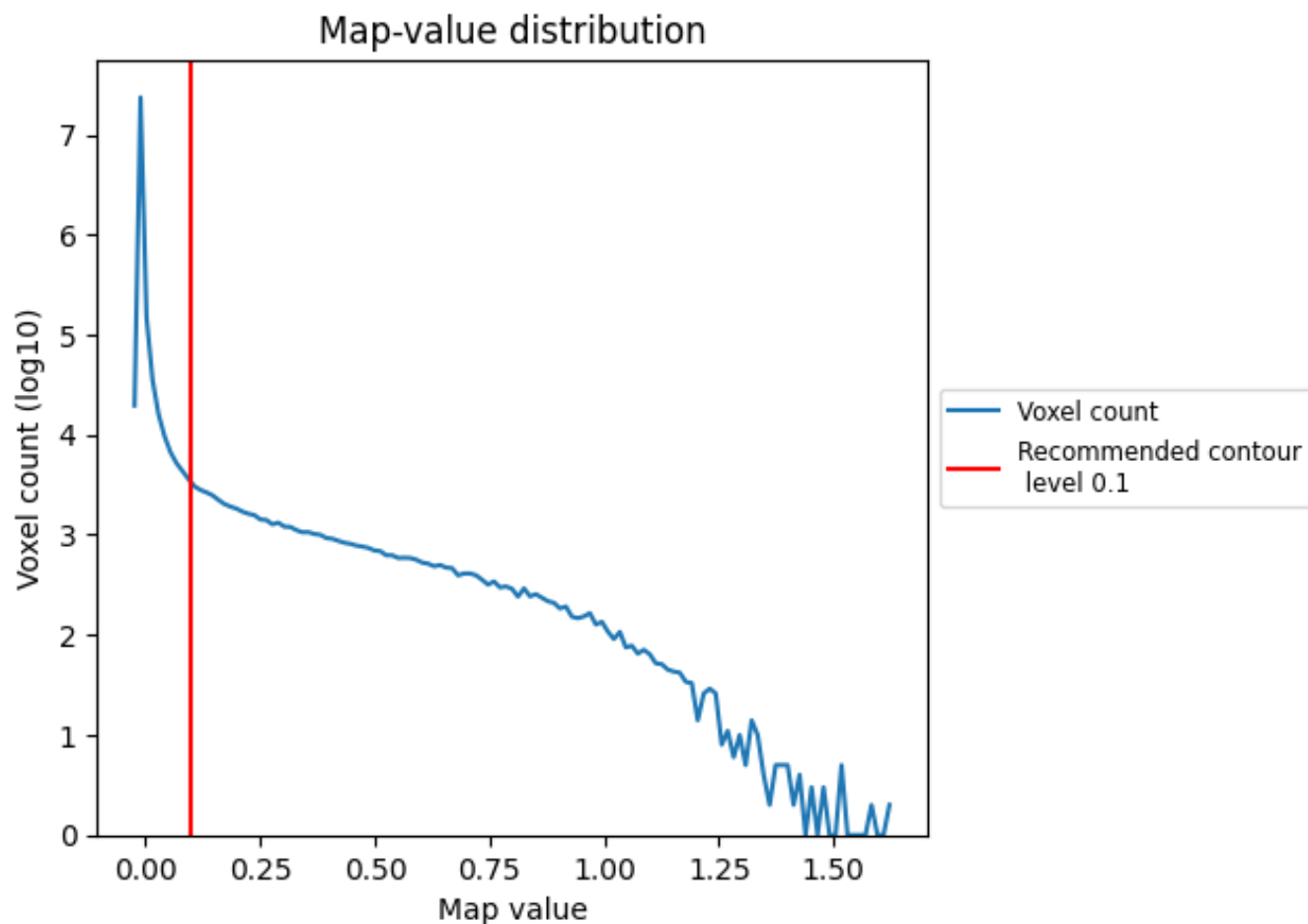
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

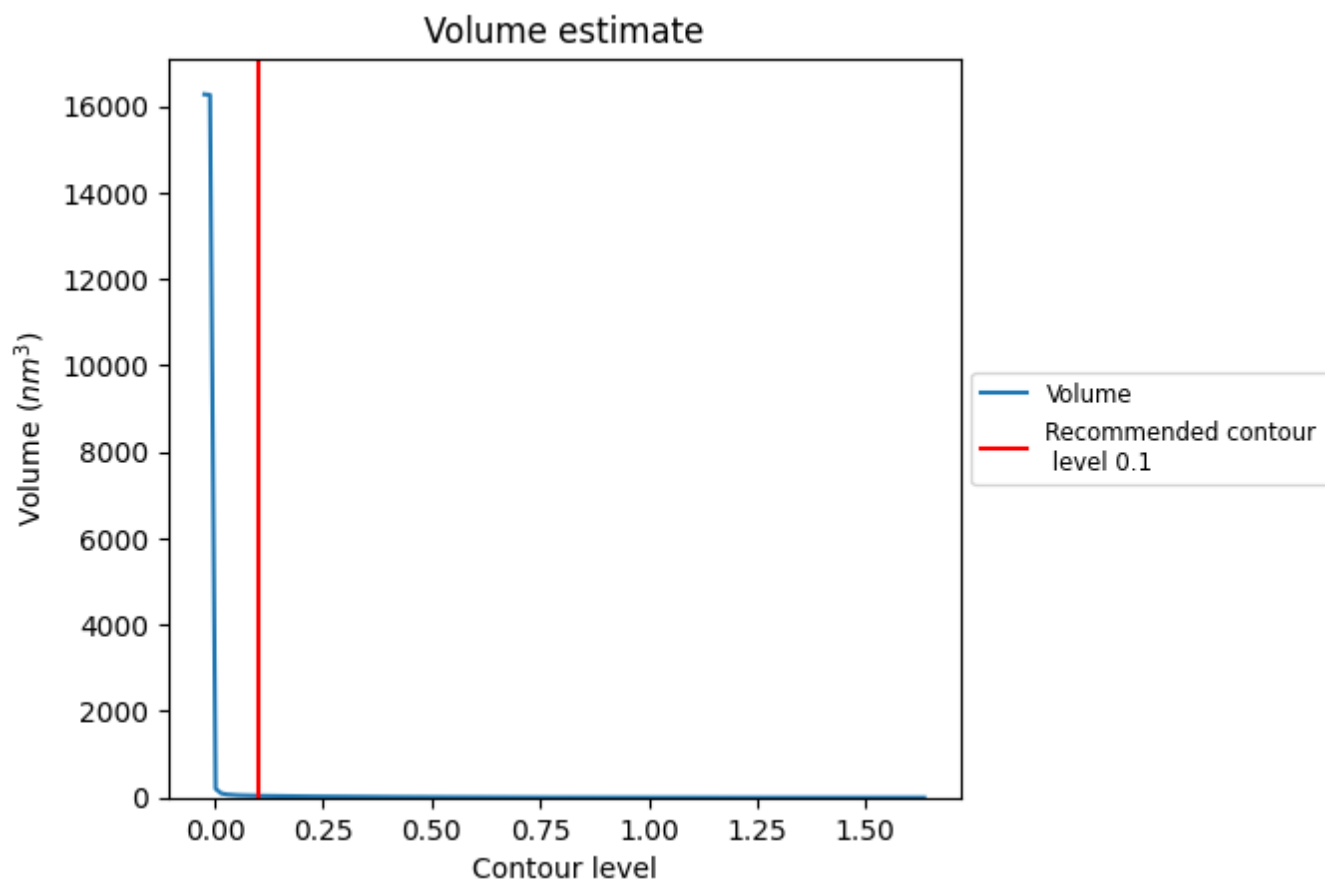
This section contains the results of statistical analysis of the map.

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.

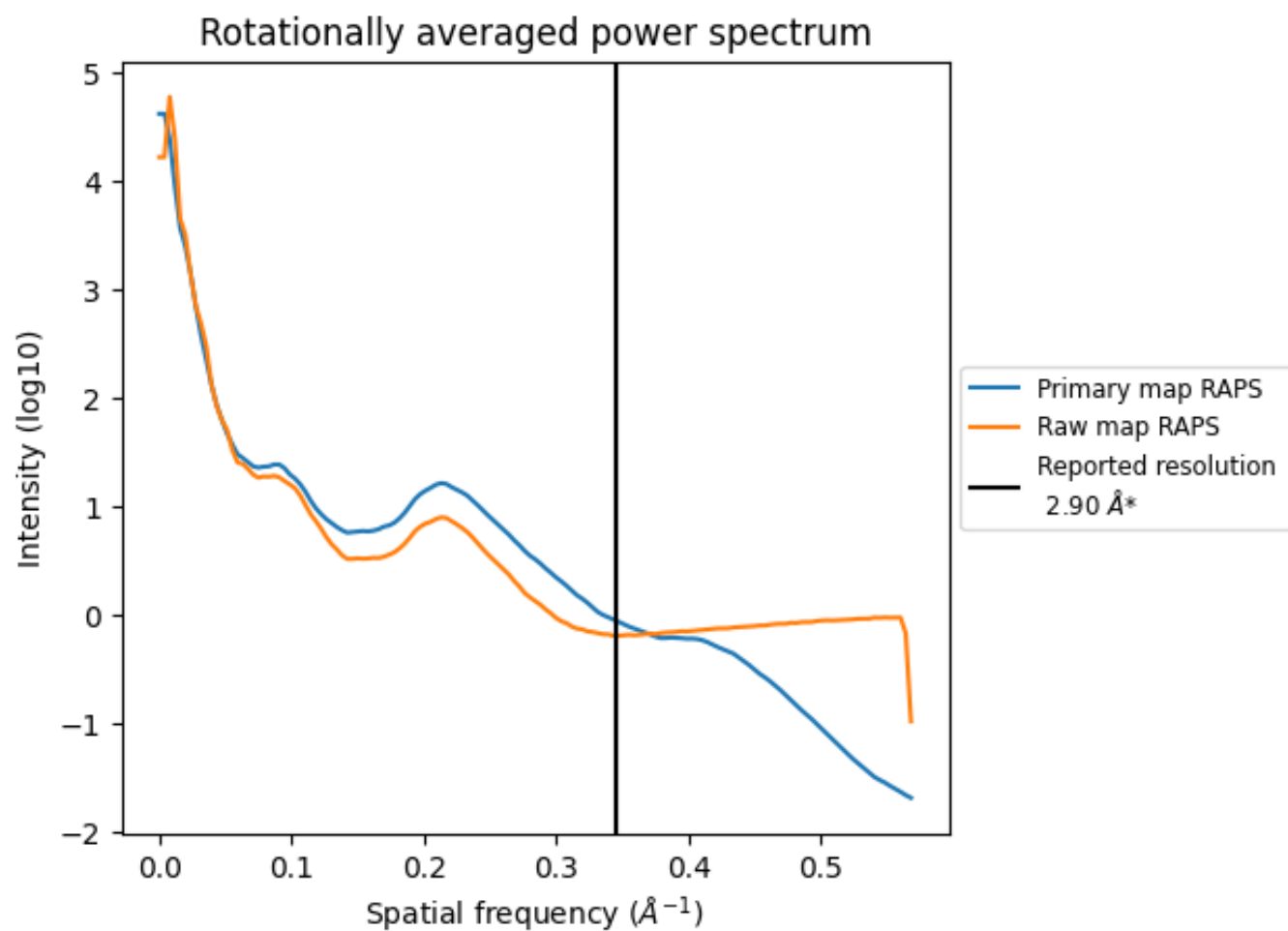
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 42 nm^3 ; this corresponds to an approximate mass of 38 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 ⓘ

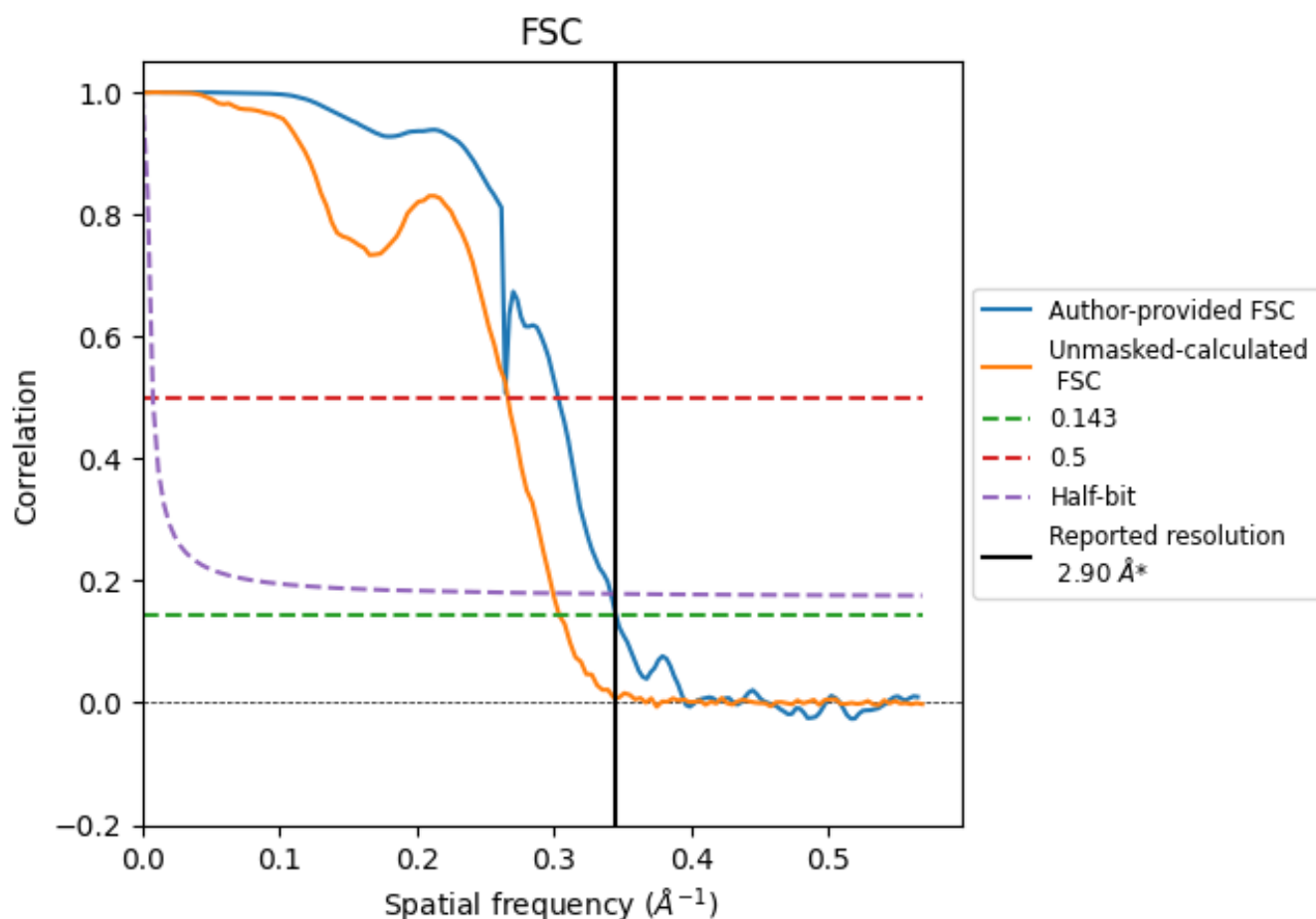


*Reported resolution corresponds to spatial frequency of $0.345 \text{ \AA}^{-1}$

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 $0.345 \text{ \AA}^{-1}$

8.2 Resolution estimates [i](#)

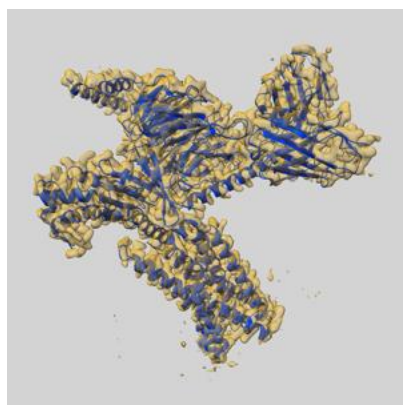
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	2.90	-	-
Author-provided FSC curve	2.90	3.30	2.93
Unmasked-calculated*	3.29	3.76	3.34

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 3.29 differs from the reported value 2.9 by more than 10 %

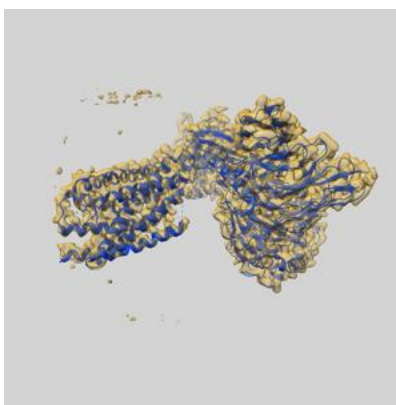
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-47114 and PDB model 9DQJ. Per-residue inclusion information can be found in section 3 on page 7.

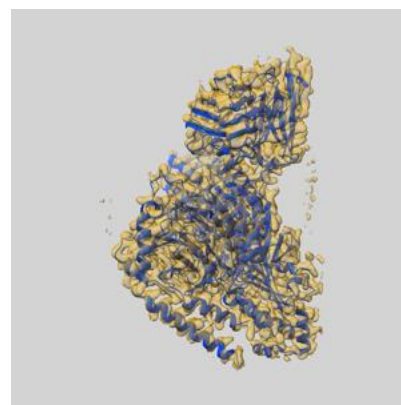
9.1 Map-model overlay [i](#)



X



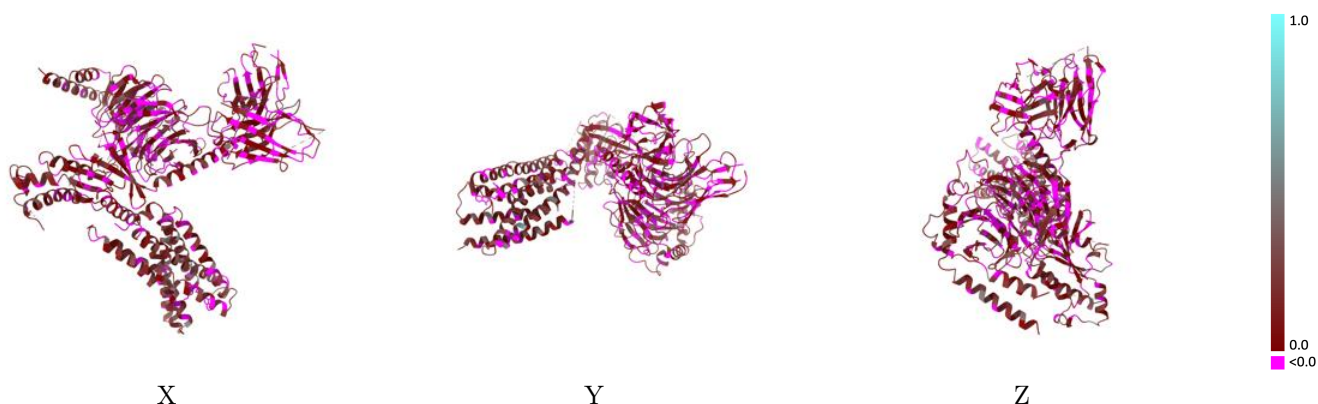
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.1 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](#)

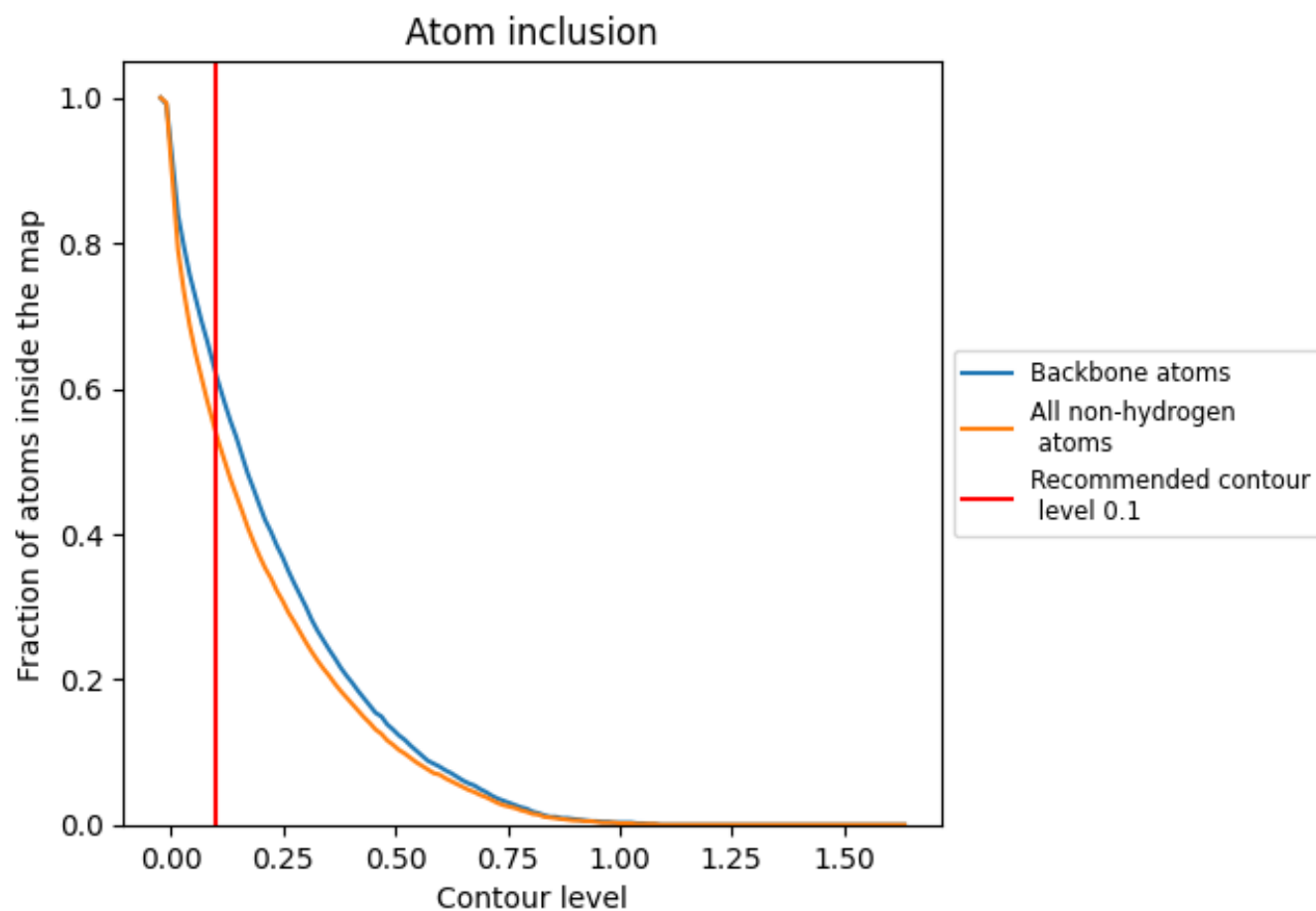


The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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

This section was not generated.

9.4 Atom inclusion [i](#)



At the recommended contour level, 62% of all backbone atoms, 54% 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	0.5380	0.0950
A	0.5670	0.1430
B	0.5250	0.0940
C	0.5530	0.0820
D	0.5230	0.0910
E	0.5010	0.0620

