



Full wwPDB EM Validation Report ⓘ

Mar 25, 2026 – 10:22 AM UTC

PDB ID : 8K4S / pdb_00008k4s
EMDB ID : EMD-36890
Title : CryoEM structure of Gq coupled MRGPRX4 with agonist DCA-3P
Authors : Yang, J.; Fan, J.P.; Lei, X.G.
Deposited on : 2023-07-20
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

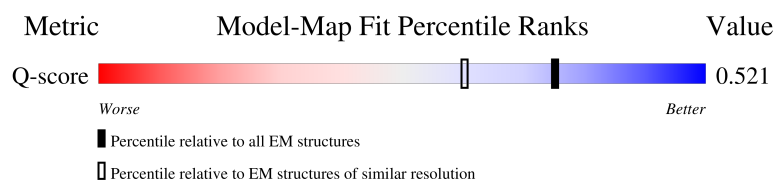
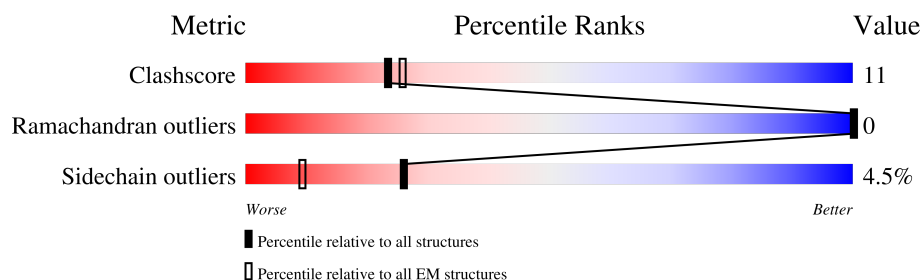
1 Overall quality at a glance

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	E	710	
2	A	246	
3	B	340	
4	C	80	

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Mol	Chain	Length	Quality of chain
5	D	254	68% 22% 9%

2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 8196 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called Soluble cytochrome b562,Mas-related G-protein coupled receptor member X4,Green fluorescent protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
1	E	255	1956	1304	314	322	16	0	0

There are 63 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
E	-115	ASP	-	expression tag	UNP P0ABE7
E	-114	TYR	-	expression tag	UNP P0ABE7
E	-113	LYS	-	expression tag	UNP P0ABE7
E	-112	ASP	-	expression tag	UNP P0ABE7
E	-111	ASP	-	expression tag	UNP P0ABE7
E	-110	ASP	-	expression tag	UNP P0ABE7
E	-109	ASP	-	expression tag	UNP P0ABE7
E	-108	LYS	-	expression tag	UNP P0ABE7
E	-107	GLU	-	expression tag	UNP P0ABE7
E	-106	PHE	-	expression tag	UNP P0ABE7
E	-99	TRP	MET	conflict	UNP P0ABE7
E	-4	ILE	HIS	conflict	UNP P0ABE7
E	0	LEU	ARG	conflict	UNP P0ABE7
E	323	LEU	-	linker	UNP Q96LA9
E	324	GLU	-	linker	UNP Q96LA9
E	325	LEU	-	linker	UNP Q96LA9
E	326	GLU	-	linker	UNP Q96LA9
E	327	VAL	-	linker	UNP Q96LA9
E	328	LEU	-	linker	UNP Q96LA9
E	329	PHE	-	linker	UNP Q96LA9
E	330	GLN	-	linker	UNP Q96LA9
E	331	GLY	-	linker	UNP Q96LA9
E	332	PRO	-	linker	UNP Q96LA9
E	361	ARG	SER	conflict	UNP P42212
E	370	ASN	TYR	conflict	UNP P42212
E	395	LEU	PHE	conflict	UNP P42212
E	396	THR	SER	conflict	UNP P42212

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Chain	Residue	Modelled	Actual	Comment	Reference
E	411	ARG	GLN	conflict	UNP P42212
E	430	SER	PHE	conflict	UNP P42212
E	436	THR	ASN	conflict	UNP P42212
E	476	PHE	TYR	conflict	UNP P42212
E	484	THR	MET	conflict	UNP P42212
E	494	ALA	VAL	conflict	UNP P42212
E	502	VAL	ILE	conflict	UNP P42212
E	537	VAL	ALA	conflict	UNP P42212
E	567	TRP	-	expression tag	UNP P42212
E	568	SER	-	expression tag	UNP P42212
E	569	HIS	-	expression tag	UNP P42212
E	570	PRO	-	expression tag	UNP P42212
E	571	GLN	-	expression tag	UNP P42212
E	572	PHE	-	expression tag	UNP P42212
E	573	GLU	-	expression tag	UNP P42212
E	574	LYS	-	expression tag	UNP P42212
E	575	GLY	-	expression tag	UNP P42212
E	576	GLY	-	expression tag	UNP P42212
E	577	GLY	-	expression tag	UNP P42212
E	578	SER	-	expression tag	UNP P42212
E	579	GLY	-	expression tag	UNP P42212
E	580	GLY	-	expression tag	UNP P42212
E	581	GLY	-	expression tag	UNP P42212
E	582	SER	-	expression tag	UNP P42212
E	583	GLY	-	expression tag	UNP P42212
E	584	GLY	-	expression tag	UNP P42212
E	585	SER	-	expression tag	UNP P42212
E	586	ALA	-	expression tag	UNP P42212
E	587	TRP	-	expression tag	UNP P42212
E	588	SER	-	expression tag	UNP P42212
E	589	HIS	-	expression tag	UNP P42212
E	590	PRO	-	expression tag	UNP P42212
E	591	GLN	-	expression tag	UNP P42212
E	592	PHE	-	expression tag	UNP P42212
E	593	GLU	-	expression tag	UNP P42212
E	594	LYS	-	expression tag	UNP P42212

- Molecule 2 is a protein called Gs-mini-Gq chimera.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	A	222	Total	C	N	O	S	0	0
			1673	1069	296	301	7		

- 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	338	Total	C	N	O	S	0	0
			2481	1544	440	477	20		

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	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	C	47	Total	C	N	O	S	0	0
			329	210	56	61	2		

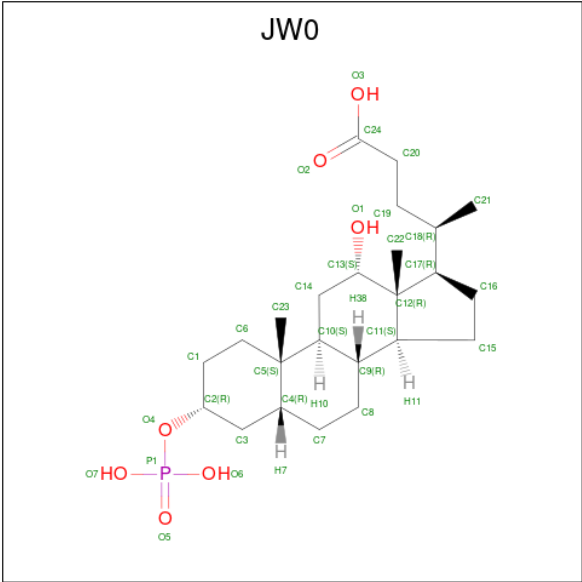
There are 9 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
C	72	GLY	-	expression tag	UNP P59768
C	73	SER	-	expression tag	UNP P59768
C	74	ALA	-	expression tag	UNP P59768
C	75	GLY	-	expression tag	UNP P59768
C	76	SER	-	expression tag	UNP P59768
C	77	ALA	-	expression tag	UNP P59768
C	78	GLY	-	expression tag	UNP P59768
C	79	SER	-	expression tag	UNP P59768
C	80	ALA	-	expression tag	UNP P59768

- Molecule 5 is a protein called scFv16.

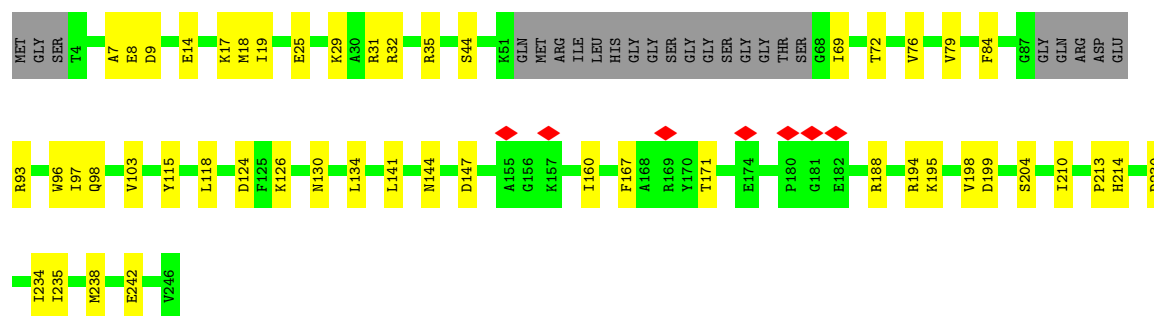
Mol	Chain	Residues	Atoms					AltConf	Trace
5	D	231	Total	C	N	O	S	0	0
			1725	1098	288	329	10		

- Molecule 6 is (4 {R})-4-[(3 {R},5 {R},8 {R},9 {S},10 {S},12 {S},13 {R},14 {S},17 {R})-10,13-dimethyl-12-oxidanyl-3-phosphonooxy-2,3,4,5,6,7,8,9,11,12,14,15,16,17-tetradecahydro-1 {H}-cyclopenta[a]phenanthren-17-yl]pentanoic acid (CCD ID: JW0) (formula: C₂₄H₄₁O₇P) (labeled as "Ligand of Interest" by depositor).



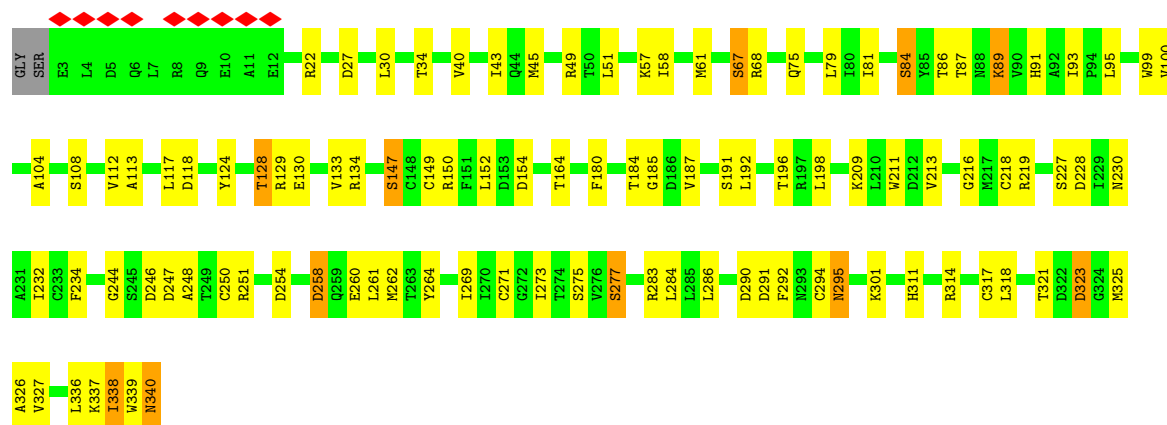
Mol	Chain	Residues	Atoms				AltConf
			Total	C	O	P	
6	E	1	32	24	7	1	0

Chain A: 

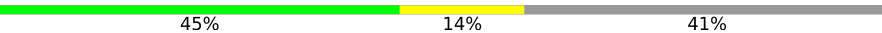


- Molecule 3: Guanine nucleotide-binding protein G(I)/G(S)/G(T) subunit beta-1

Chain B: 



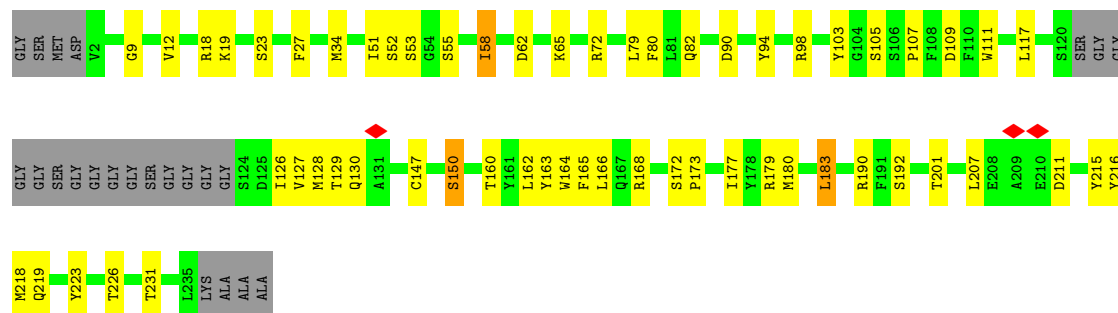
- Molecule 4: Guanine nucleotide-binding protein G(I)/G(S)/G(O) subunit gamma-2

Chain C: 



- Molecule 5: scFv16

Chain D: 



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	451859	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 ($e^-/\text{\AA}^2$)	60	Depositor
Minimum defocus (nm)	1100	Depositor
Maximum defocus (nm)	2200	Depositor
Magnification	Not provided	
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor
Maximum map value	7.418	Depositor
Minimum map value	-5.504	Depositor
Average map value	-0.001	Depositor
Map value standard deviation	0.138	Depositor
Recommended contour level	0.555	Depositor
Map size (Å)	266.24, 266.24, 266.24	wwPDB
Map dimensions	256, 256, 256	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.04, 1.04, 1.04	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: JW0

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	E	0.14	0/2003	0.38	0/2744
2	A	0.12	0/1702	0.28	0/2309
3	B	0.13	0/2528	0.31	0/3443
4	C	0.11	0/335	0.30	0/459
5	D	0.13	0/1769	0.34	0/2406
All	All	0.13	0/8337	0.33	0/11361

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	E	1956	0	1986	41	0
2	A	1673	0	1571	35	0
3	B	2481	0	2305	74	0
4	C	329	0	309	8	0
5	D	1725	0	1614	37	0
6	E	32	0	0	3	0
All	All	8196	0	7785	176	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 11.

All (176) 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:E:67:ASN:ND2	1:E:143:CYS:SG	2.44	0.88
3:B:104:ALA:HB3	3:B:113:ALA:HB3	1.69	0.74
3:B:283:ARG:HB3	4:C:51:LEU:HD21	1.72	0.72
2:A:98:GLN:OE1	3:B:314:ARG:NH1	2.22	0.72
1:E:95:ARG:HG2	6:E:601:JW0:P1	2.30	0.72
2:A:44:SER:O	2:A:144:ASN:ND2	2.22	0.71
5:D:190:ARG:NH2	5:D:211:ASP:OD2	2.26	0.68
5:D:165:PHE:HE2	5:D:218:MET:HG2	1.58	0.67
3:B:286:LEU:HB3	3:B:318:LEU:HD21	1.76	0.66
3:B:152:LEU:HD12	3:B:192:LEU:HD21	1.78	0.66
5:D:19:LYS:HE2	5:D:80:PHE:HB3	1.77	0.66
3:B:219:ARG:HG2	3:B:219:ARG:HH11	1.60	0.65
1:E:134:ARG:O	2:A:31:ARG:NH2	2.29	0.65
5:D:105:SER:O	5:D:179:ARG:NH2	2.30	0.64
2:A:195:LYS:HA	2:A:198:VAL:HG22	1.80	0.64
1:E:106:TYR:OH	1:E:229:GLY:O	2.12	0.63
1:E:131:ARG:NH2	2:A:242:GLU:OE2	2.31	0.62
3:B:277:SER:HB2	3:B:318:LEU:HD23	1.81	0.62
5:D:162:LEU:HB3	5:D:180:MET:HB2	1.81	0.62
5:D:52:SER:O	5:D:72:ARG:NH1	2.30	0.62
3:B:134:ARG:HH11	3:B:134:ARG:HG3	1.63	0.61
5:D:51:ILE:HG21	5:D:79:LEU:HD11	1.83	0.60
2:A:214:HIS:NE2	2:A:230:ASP:OD2	2.27	0.60
3:B:248:ALA:HB1	3:B:269:ILE:HG22	1.83	0.60
5:D:164:TRP:HD1	5:D:177:ILE:HD11	1.66	0.60
2:A:199:ASP:N	2:A:199:ASP:OD1	2.34	0.60
3:B:79:LEU:HB2	3:B:95:LEU:HD21	1.84	0.60
5:D:127:VAL:H	5:D:150:SER:HB3	1.66	0.60
1:E:113:LEU:HD21	1:E:268:ASN:HD21	1.66	0.59
3:B:51:LEU:HB2	3:B:336:LEU:HB2	1.85	0.59
2:A:141:LEU:HB3	2:A:213:PRO:HA	1.84	0.59
3:B:95:LEU:HD13	3:B:100:VAL:HG11	1.84	0.59
3:B:67:SER:HB3	3:B:321:THR:HB	1.85	0.58
1:E:76:LEU:HA	1:E:79:GLN:HB2	1.86	0.58
2:A:115:TYR:HA	2:A:118:LEU:HB2	1.86	0.58
5:D:207:LEU:H	5:D:207:LEU:HD12	1.68	0.57
3:B:130:GLU:HA	5:D:27:PHE:HB2	1.86	0.57
3:B:57:LYS:HE2	3:B:75:GLN:HG3	1.86	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:B:244:GLY:HA3	3:B:273:ILE:HG21	1.87	0.57
1:E:100:SER:OG	1:E:158:TRP:NE1	2.33	0.56
1:E:185:ILE:O	1:E:189:VAL:HG12	2.04	0.56
3:B:22:ARG:NE	3:B:258:ASP:O	2.34	0.56
3:B:49:ARG:HD2	3:B:87:THR:HG23	1.86	0.56
2:A:160:ILE:HG12	2:A:167:PHE:CE2	2.41	0.56
2:A:171:THR:HA	2:A:188:ARG:HH12	1.71	0.56
3:B:40:VAL:HG21	3:B:284:LEU:HD21	1.88	0.56
1:E:128:ILE:HD13	2:A:235:ILE:HD12	1.87	0.55
2:A:93:ARG:NH2	2:A:124:ASP:OD1	2.35	0.55
3:B:149:CYS:O	3:B:150:ARG:NH1	2.38	0.55
1:E:95:ARG:O	1:E:99:VAL:HG22	2.06	0.55
2:A:8:GLU:OE2	5:D:163:TYR:OH	2.21	0.55
3:B:230:ASN:ND2	3:B:246:ASP:OD1	2.27	0.55
1:E:155:MET:SD	1:E:155:MET:N	2.80	0.55
3:B:250:CYS:HB2	3:B:264:TYR:HB2	1.88	0.54
5:D:180:MET:HG2	5:D:180:MET:O	2.08	0.54
3:B:219:ARG:HG2	3:B:219:ARG:NH1	2.22	0.54
3:B:30:LEU:HD22	3:B:262:MET:HE1	1.89	0.54
5:D:62:ASP:O	5:D:65:LYS:NZ	2.41	0.54
1:E:131:ARG:HG3	2:A:235:ILE:HG23	1.90	0.53
3:B:323:ASP:OD1	3:B:323:ASP:N	2.40	0.53
1:E:41:GLY:O	1:E:45:ASN:ND2	2.42	0.53
1:E:135:PRO:HG2	1:E:138:LEU:HB2	1.90	0.53
3:B:311:HIS:CE1	3:B:337:LYS:HG3	2.44	0.53
3:B:152:LEU:HD21	3:B:213:VAL:HG11	1.91	0.53
1:E:132:CYS:HB3	2:A:32:ARG:HA	1.90	0.52
1:E:53:GLY:O	1:E:58:ARG:NH2	2.43	0.52
3:B:325:MET:HA	4:C:49:PRO:HG2	1.91	0.52
2:A:130:ASN:ND2	2:A:204:SER:OG	2.43	0.52
5:D:51:ILE:HD11	5:D:55:SER:HA	1.91	0.52
2:A:35:ARG:HG2	2:A:84:PHE:HE2	1.75	0.52
3:B:61:MET:HG3	3:B:317:CYS:HB2	1.90	0.52
2:A:25:GLU:O	2:A:29:LYS:HG3	2.10	0.51
3:B:196:THR:HG22	3:B:196:THR:O	2.10	0.51
5:D:164:TRP:HB2	5:D:177:ILE:HG13	1.91	0.51
2:A:14:GLU:HA	2:A:17:LYS:HE2	1.91	0.51
5:D:52:SER:OG	5:D:53:SER:N	2.44	0.51
3:B:283:ARG:HG2	4:C:51:LEU:HD11	1.93	0.51
5:D:166:LEU:HD23	5:D:168:ARG:HH21	1.76	0.50
3:B:128:THR:OG1	3:B:129:ARG:N	2.44	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:D:90:ASP:OD1	5:D:94:TYR:OH	2.28	0.50
3:B:271:CYS:SG	3:B:291:ASP:HB2	2.51	0.50
3:B:191:SER:HB2	3:B:232:ILE:HG23	1.93	0.50
1:E:95:ARG:HG2	6:E:601:JW0:O6	2.12	0.49
4:C:38:MET:O	4:C:42:GLU:HG2	2.13	0.49
5:D:9:GLY:HA2	5:D:117:LEU:HD12	1.93	0.49
5:D:219:GLN:HE21	5:D:226:THR:H	1.59	0.49
3:B:68:ARG:O	3:B:84:SER:OG	2.27	0.49
3:B:147:SER:OG	3:B:187:VAL:O	2.20	0.49
2:A:234:ILE:O	2:A:238:MET:HG3	2.12	0.48
1:E:155:MET:HA	1:E:158:TRP:HB2	1.94	0.48
3:B:129:ARG:O	3:B:130:GLU:HG2	2.12	0.48
3:B:112:VAL:HG23	3:B:124:TYR:HB2	1.95	0.48
3:B:294:CYS:SG	3:B:295:ASN:N	2.85	0.48
5:D:98:ARG:HE	5:D:109:ASP:HB2	1.78	0.48
1:E:239:ILE:HG21	6:E:601:JW0:C23	2.43	0.48
3:B:230:ASN:ND2	3:B:273:ILE:O	2.40	0.48
2:A:93:ARG:HA	2:A:96:TRP:NE1	2.29	0.48
3:B:180:PHE:HE1	3:B:216:GLY:HA2	1.77	0.48
3:B:275:SER:OG	3:B:318:LEU:HB2	2.14	0.48
3:B:326:ALA:HB1	3:B:338:ILE:HG23	1.95	0.48
5:D:130:GLN:HE22	5:D:216:TYR:HA	1.79	0.47
1:E:72:ASP:O	1:E:76:LEU:HD22	2.14	0.47
1:E:95:ARG:HA	1:E:98:LEU:HD12	1.97	0.47
5:D:19:LYS:HE3	5:D:82:GLN:HG2	1.97	0.47
3:B:271:CYS:HB2	3:B:290:ASP:HB2	1.97	0.47
3:B:81:ILE:HB	3:B:91:HIS:HB2	1.96	0.47
1:E:43:THR:O	1:E:47:VAL:HG12	2.15	0.46
3:B:251:ARG:HG2	3:B:260:GLU:HG3	1.98	0.46
2:A:97:ILE:HG12	2:A:134:LEU:HD11	1.97	0.46
3:B:84:SER:HB2	4:C:61:PHE:HE1	1.79	0.46
4:C:48:ASP:OD1	4:C:51:LEU:HB2	2.16	0.46
3:B:292:PHE:HA	3:B:314:ARG:HA	1.97	0.46
5:D:130:GLN:HG2	5:D:147:CYS:HB3	1.96	0.46
1:E:225:PHE:O	1:E:230:LEU:HB2	2.16	0.46
3:B:134:ARG:HG3	3:B:134:ARG:NH1	2.31	0.45
3:B:34:THR:O	3:B:301:LYS:NZ	2.50	0.45
5:D:12:VAL:HG22	5:D:18:ARG:HH21	1.82	0.45
5:D:130:GLN:OE1	5:D:231:THR:OG1	2.29	0.45
5:D:166:LEU:HD13	5:D:215:TYR:CZ	2.52	0.45
3:B:93:ILE:HD12	3:B:93:ILE:O	2.16	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:7:ALA:HB1	5:D:223:TYR:CE2	2.52	0.44
1:E:148:GLY:HA2	1:E:151:LEU:HD12	1.99	0.44
1:E:59:ASN:OD1	1:E:59:ASN:N	2.51	0.44
3:B:45:MET:HA	3:B:340:ASN:O	2.16	0.44
3:B:89:LYS:HB2	3:B:89:LYS:HE2	1.79	0.44
1:E:76:LEU:O	1:E:80:ILE:HG13	2.18	0.44
3:B:43:ILE:HG21	3:B:45:MET:HE3	1.98	0.44
3:B:58:ILE:HD13	3:B:336:LEU:HG	2.00	0.44
3:B:108:SER:OG	3:B:154:ASP:OD1	2.34	0.44
5:D:111:TRP:CE3	5:D:173:PRO:HG2	2.53	0.44
5:D:164:TRP:CD1	5:D:177:ILE:HD11	2.50	0.44
3:B:254:ASP:OD1	3:B:261:LEU:HD22	2.18	0.44
1:E:49:LEU:HD12	1:E:49:LEU:HA	1.89	0.43
3:B:86:THR:O	3:B:87:THR:OG1	2.33	0.43
3:B:211:TRP:CZ3	3:B:218:CYS:HB2	2.53	0.43
3:B:262:MET:HE3	3:B:262:MET:HB2	1.94	0.43
1:E:228:CYS:HB3	1:E:264:ASN:HB2	2.00	0.43
2:A:8:GLU:OE1	5:D:107:PRO:HG3	2.19	0.43
3:B:325:MET:HE2	3:B:325:MET:HB2	1.85	0.43
5:D:51:ILE:HD13	5:D:58:ILE:HD11	2.00	0.43
1:E:190:VAL:HA	1:E:193:VAL:HG12	1.99	0.43
2:A:69:ILE:HD12	3:B:99:TRP:CD1	2.54	0.42
3:B:57:LYS:HE2	3:B:57:LYS:HB2	1.87	0.42
2:A:194:ARG:O	2:A:198:VAL:HG13	2.20	0.42
1:E:102:MET:O	1:E:105:PRO:HD2	2.19	0.42
2:A:19:ILE:HG21	3:B:89:LYS:HD2	2.01	0.42
2:A:147:ASP:OD1	2:A:147:ASP:N	2.51	0.42
5:D:177:ILE:HG22	5:D:183:LEU:HD12	2.02	0.42
1:E:58:ARG:HB3	1:E:63:ILE:HG13	2.02	0.42
2:A:96:TRP:HB2	3:B:117:LEU:HD21	2.01	0.42
2:A:126:LYS:HB2	2:A:126:LYS:HE3	1.88	0.42
1:E:237:ALA:HA	1:E:240:TYR:CD2	2.55	0.42
2:A:160:ILE:HG12	2:A:167:PHE:HE2	1.84	0.42
3:B:327:VAL:HG13	3:B:339:TRP:HB2	2.01	0.42
1:E:53:GLY:HA2	1:E:58:ARG:HH21	1.85	0.42
3:B:180:PHE:CE1	3:B:216:GLY:HA2	2.54	0.42
1:E:68:LEU:HD11	1:E:268:ASN:ND2	2.35	0.41
1:E:270:ILE:HA	1:E:274:PHE:CD2	2.55	0.41
4:C:33:ALA:HA	4:C:36:ASP:OD2	2.20	0.41
2:A:18:MET:HE2	2:A:18:MET:HB3	1.84	0.41
5:D:34:MET:HE3	5:D:34:MET:HB3	1.91	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:69:ILE:HD11	3:B:117:LEU:HD13	2.03	0.41
3:B:227:SER:HB3	3:B:246:ASP:HB2	2.03	0.41
4:C:22:GLU:HA	4:C:25:ILE:HD11	2.02	0.41
1:E:231:PRO:HA	1:E:234:ILE:HG12	2.02	0.41
3:B:209:LYS:HD3	3:B:211:TRP:CZ2	2.56	0.41
1:E:94:ILE:HD12	1:E:95:ARG:N	2.34	0.41
3:B:27:ASP:OD1	3:B:27:ASP:N	2.53	0.41
3:B:68:ARG:HD3	5:D:103:TYR:CZ	2.56	0.41
5:D:128:MET:HE3	5:D:128:MET:HB3	1.76	0.41
3:B:247:ASP:OD1	3:B:247:ASP:N	2.54	0.41
1:E:113:LEU:HA	1:E:113:LEU:HD23	1.86	0.40
2:A:76:VAL:O	2:A:79:VAL:HG12	2.21	0.40
1:E:106:TYR:CD1	1:E:106:TYR:C	2.99	0.40
1:E:223:LEU:O	1:E:227:LEU:N	2.50	0.40
3:B:164:THR:HG22	3:B:185:GLY:C	2.46	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	E	251/710 (35%)	231 (92%)	20 (8%)	0	100	100
2	A	216/246 (88%)	206 (95%)	10 (5%)	0	100	100
3	B	336/340 (99%)	325 (97%)	11 (3%)	0	100	100
4	C	45/80 (56%)	43 (96%)	2 (4%)	0	100	100
5	D	227/254 (89%)	214 (94%)	13 (6%)	0	100	100
All	All	1075/1630 (66%)	1019 (95%)	56 (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	E	212/621 (34%)	207 (98%)	5 (2%)	43	75
2	A	160/213 (75%)	156 (98%)	4 (2%)	42	74
3	B	248/282 (88%)	231 (93%)	17 (7%)	14	41
4	C	30/61 (49%)	29 (97%)	1 (3%)	33	67
5	D	180/203 (89%)	170 (94%)	10 (6%)	19	50
All	All	830/1380 (60%)	793 (96%)	37 (4%)	26	58

All (37) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	E	42	LEU
1	E	52	LEU
1	E	62	SER
1	E	103	THR
1	E	214	LEU
2	A	9	ASP
2	A	72	THR
2	A	103	VAL
2	A	210	ILE
3	B	67	SER
3	B	84	SER
3	B	89	LYS
3	B	118	ASP
3	B	128	THR
3	B	133	VAL
3	B	147	SER
3	B	184	THR
3	B	198	LEU
3	B	228	ASP
3	B	234	PHE
3	B	258	ASP
3	B	277	SER
3	B	295	ASN

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Mol	Chain	Res	Type
3	B	323	ASP
3	B	338	ILE
3	B	340	ASN
4	C	37	LEU
5	D	23	SER
5	D	58	ILE
5	D	126	ILE
5	D	129	THR
5	D	150	SER
5	D	160	THR
5	D	172	SER
5	D	183	LEU
5	D	192	SER
5	D	201	THR

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

Mol	Chain	Res	Type
1	E	243	HIS
1	E	268	ASN
2	A	80	ASN
2	A	82	HIS
2	A	119	GLN
3	B	75	GLN
3	B	239	ASN
5	D	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

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	JW0	E	601	-	35,35,35	2.23	11 (31%)	56,56,56	2.42	20 (35%)

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	JW0	E	601	-	-	9/14/76/76	0/4/4/4

All (11) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	E	601	JW0	P1-O4	6.17	1.70	1.59
6	E	601	JW0	O1-C13	-4.75	1.35	1.43
6	E	601	JW0	C12-C17	-4.73	1.47	1.55
6	E	601	JW0	C14-C10	-4.60	1.46	1.53
6	E	601	JW0	C6-C5	-3.80	1.47	1.54
6	E	601	JW0	C16-C15	2.82	1.61	1.54
6	E	601	JW0	C12-C11	-2.44	1.51	1.55
6	E	601	JW0	C5-C4	-2.32	1.51	1.55
6	E	601	JW0	C6-C1	2.28	1.57	1.53
6	E	601	JW0	C5-C10	2.18	1.59	1.56
6	E	601	JW0	C9-C10	-2.09	1.49	1.53

All (20) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	E	601	JW0	C12-C17-C18	-8.54	109.14	119.48
6	E	601	JW0	C12-C11-C9	-5.67	108.59	114.69

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	E	601	JW0	C14-C10-C5	-4.86	108.77	113.70
6	E	601	JW0	C11-C9-C10	-4.30	103.47	109.09
6	E	601	JW0	C11-C12-C13	3.80	110.89	107.42
6	E	601	JW0	C22-C12-C11	-3.65	105.48	111.20
6	E	601	JW0	C22-C12-C13	3.65	112.71	109.06
6	E	601	JW0	C15-C11-C12	-3.41	100.24	103.54
6	E	601	JW0	C17-C12-C13	-3.40	114.61	117.67
6	E	601	JW0	C21-C18-C17	-3.32	107.90	112.88
6	E	601	JW0	C16-C17-C12	-3.29	100.35	103.54
6	E	601	JW0	C10-C5-C4	3.23	113.00	108.51
6	E	601	JW0	C15-C11-C9	-2.81	114.62	119.10
6	E	601	JW0	C17-C12-C11	2.72	102.84	100.11
6	E	601	JW0	C23-C5-C10	-2.59	107.70	111.18
6	E	601	JW0	C16-C15-C11	-2.39	100.47	105.14
6	E	601	JW0	C20-C19-C18	-2.26	110.24	114.46
6	E	601	JW0	O1-C13-C12	-2.21	107.30	111.02
6	E	601	JW0	O3-C24-C20	2.18	120.88	114.00
6	E	601	JW0	C4-C3-C2	2.05	115.72	111.65

There are no chirality outliers.

All (9) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
6	E	601	JW0	C1-C2-O4-P1
6	E	601	JW0	C12-C17-C18-C21
6	E	601	JW0	C16-C17-C18-C21
6	E	601	JW0	C12-C17-C18-C19
6	E	601	JW0	C16-C17-C18-C19
6	E	601	JW0	C21-C18-C19-C20
6	E	601	JW0	C19-C20-C24-O3
6	E	601	JW0	C18-C19-C20-C24
6	E	601	JW0	C19-C20-C24-O2

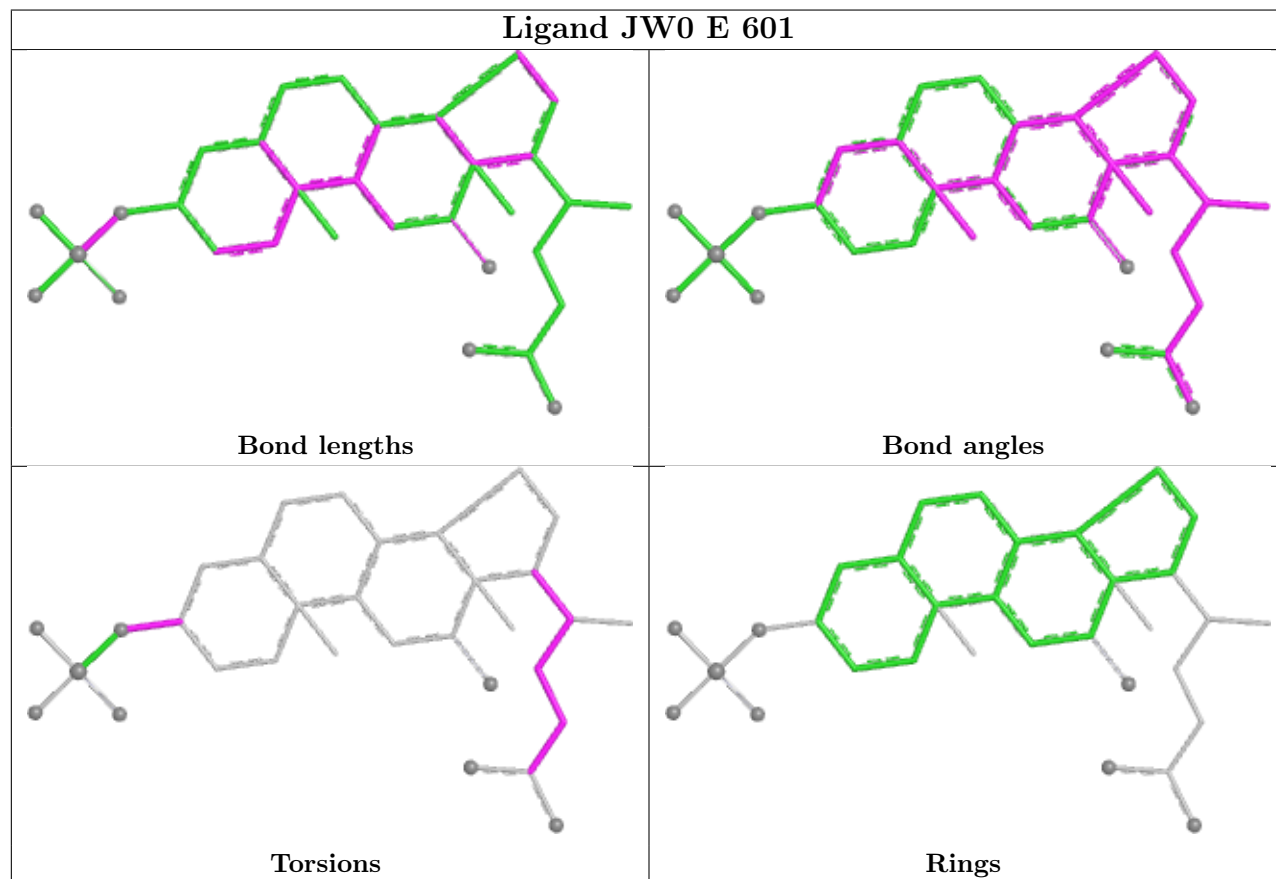
There are no ring outliers.

1 monomer is involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	E	601	JW0	3	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 [i](#)

There are no chain breaks in this entry.

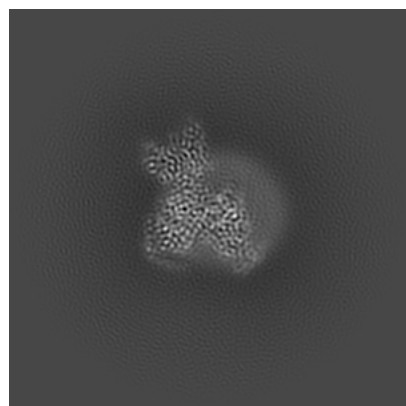
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-36890. These allow visual inspection of the internal detail of the map and identification of artifacts.

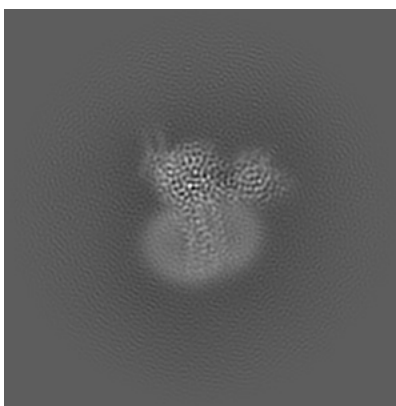
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

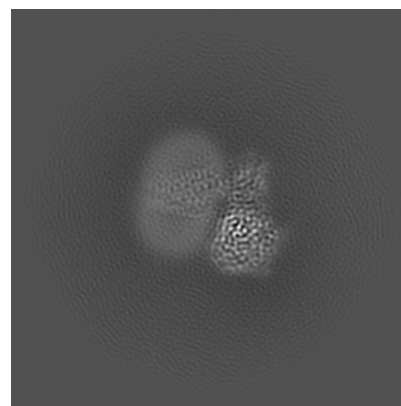
6.1.1 Primary map



X

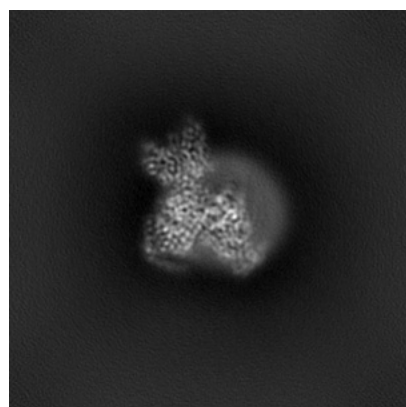


Y

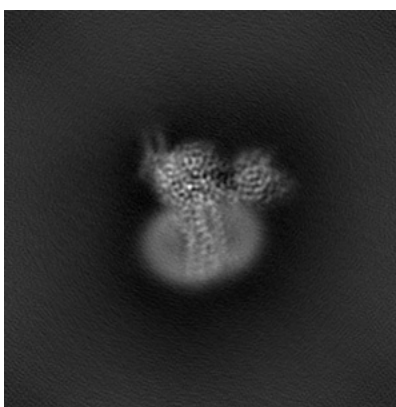


Z

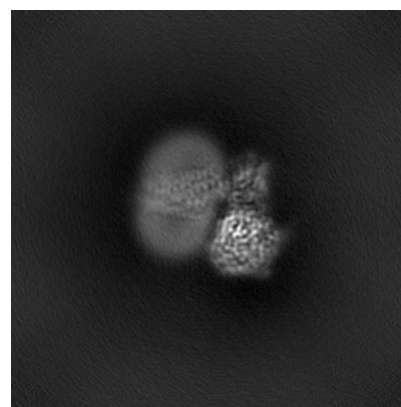
6.1.2 Raw map



X



Y

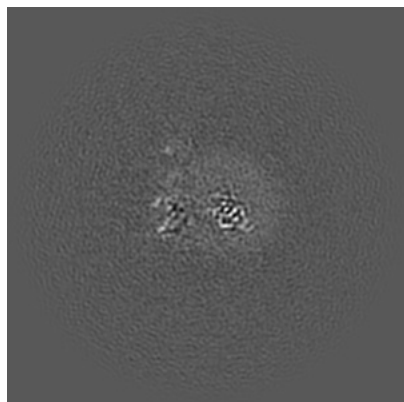


Z

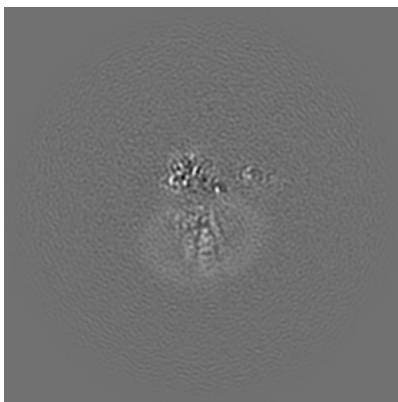
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

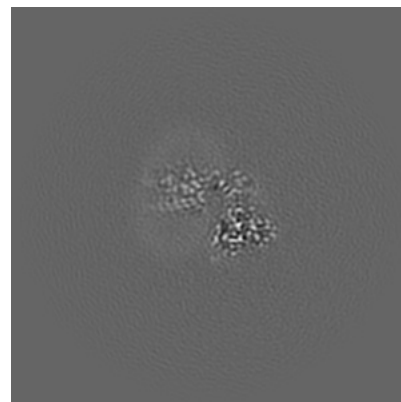
6.2.1 Primary map



X Index: 128

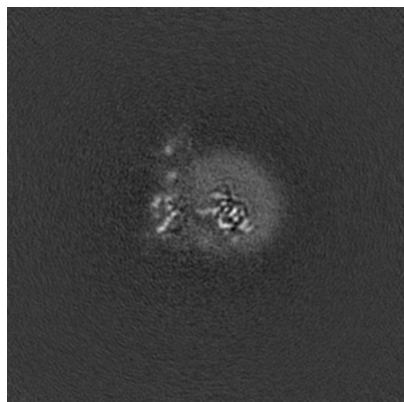


Y Index: 128

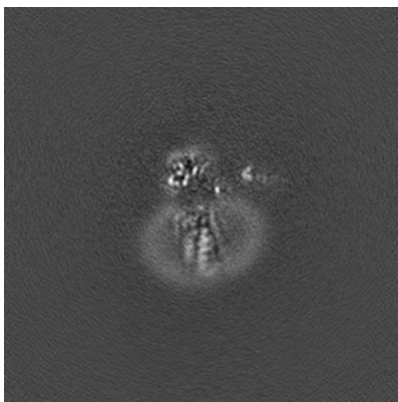


Z Index: 128

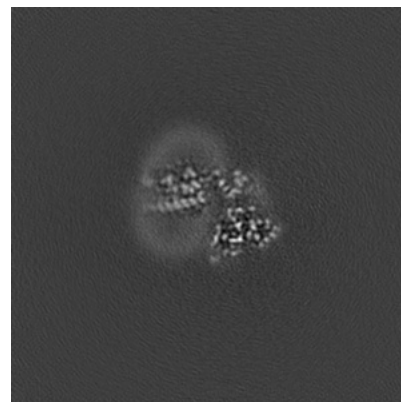
6.2.2 Raw map



X Index: 128



Y Index: 128

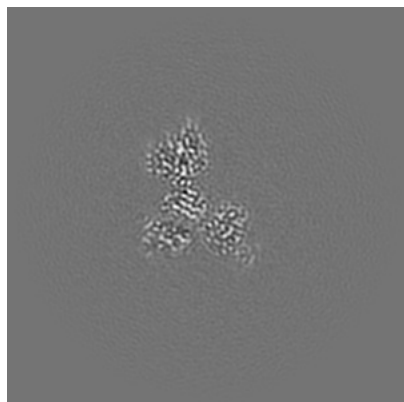


Z Index: 128

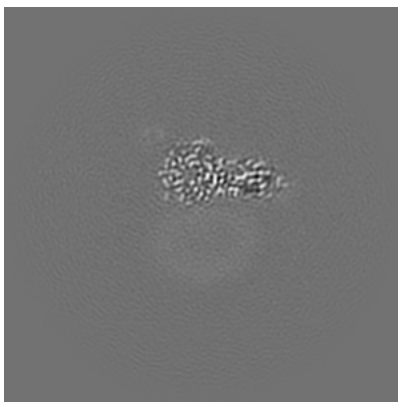
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

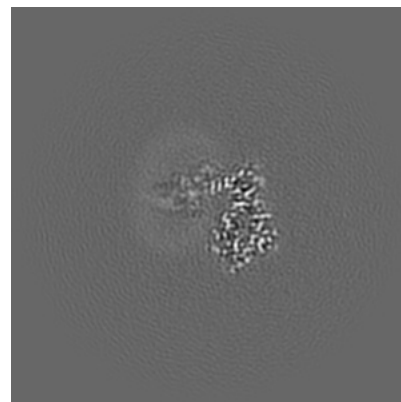
6.3.1 Primary map



X Index: 146

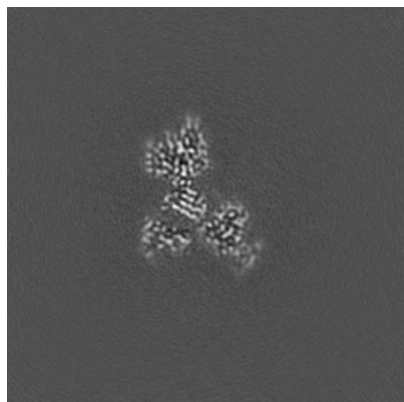


Y Index: 113

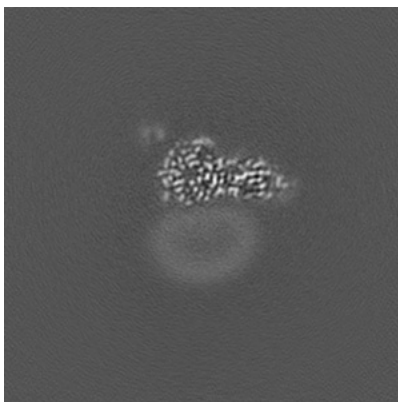


Z Index: 116

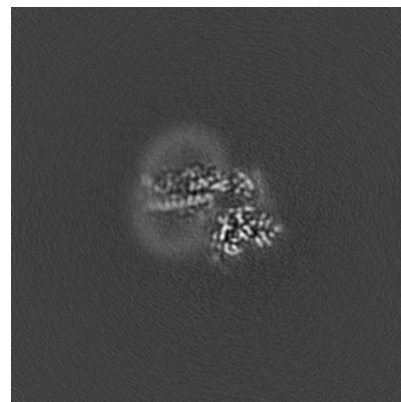
6.3.2 Raw map



X Index: 146



Y Index: 113

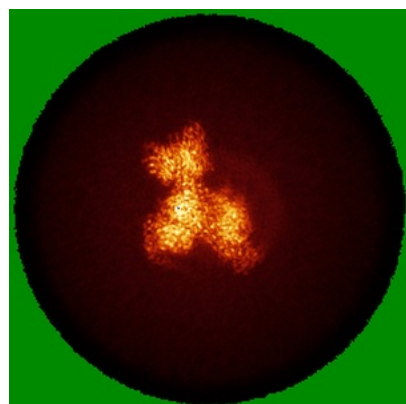


Z Index: 126

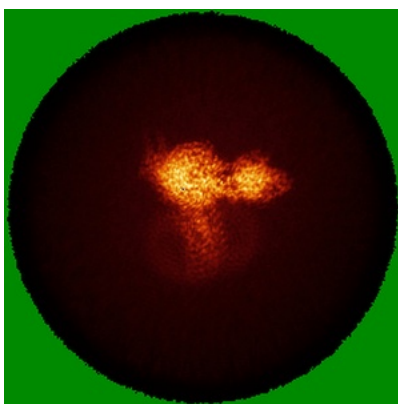
The images above show the largest variance slices of the map in three orthogonal directions.

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

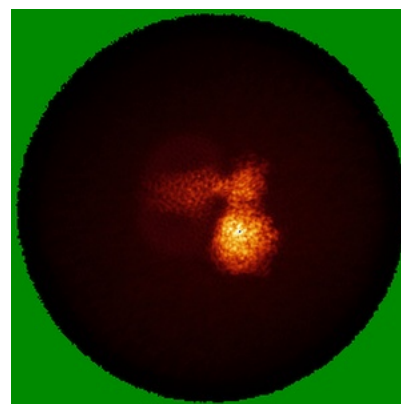
6.4.1 Primary map



X

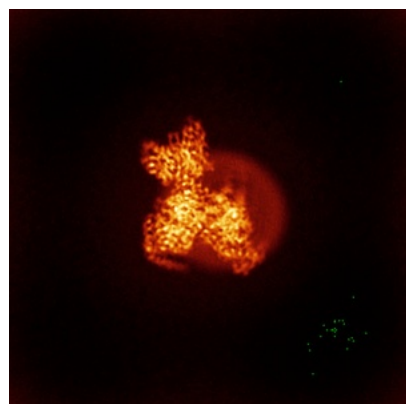


Y

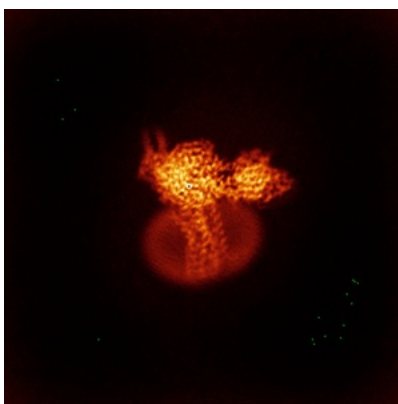


Z

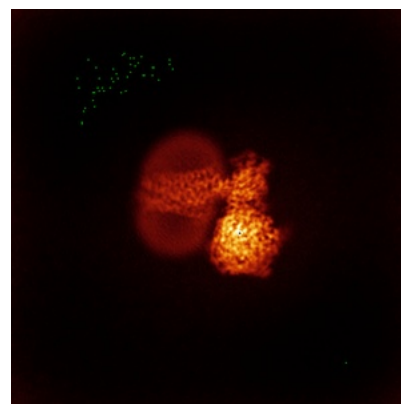
6.4.2 Raw map



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](#)

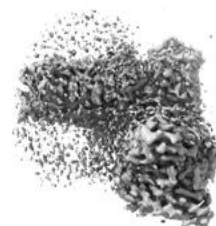
6.5.1 Primary map



X



Y



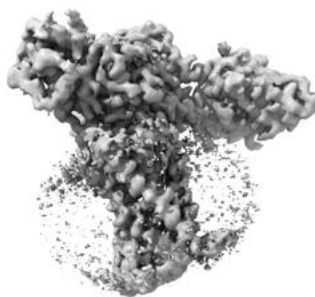
Z

The images above show the 3D surface view of the map at the recommended contour level 0.555. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

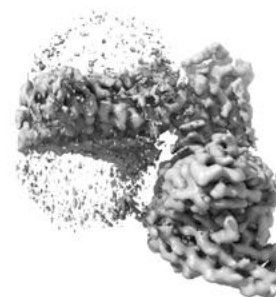
6.5.2 Raw map



X



Y



Z

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.

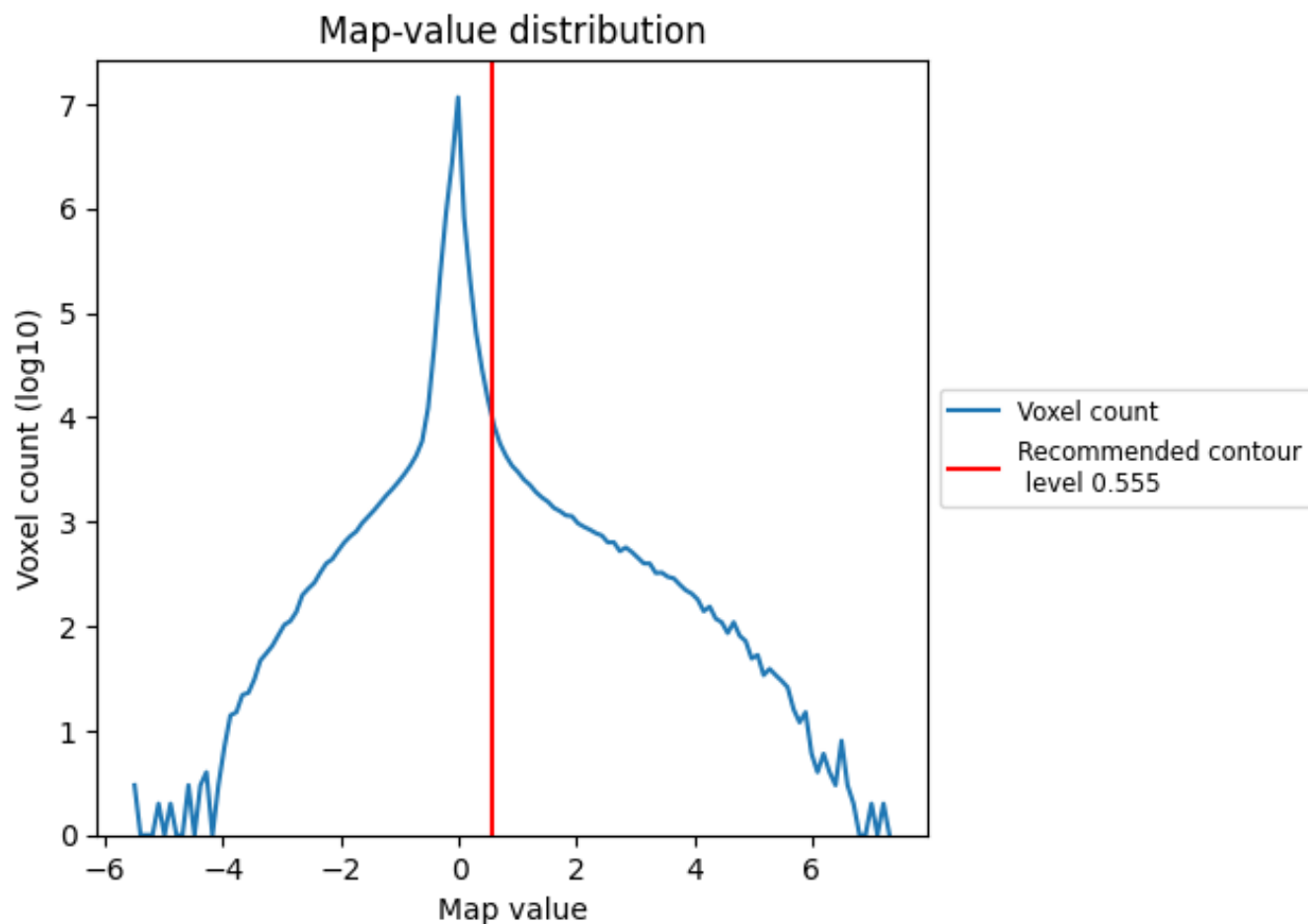
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

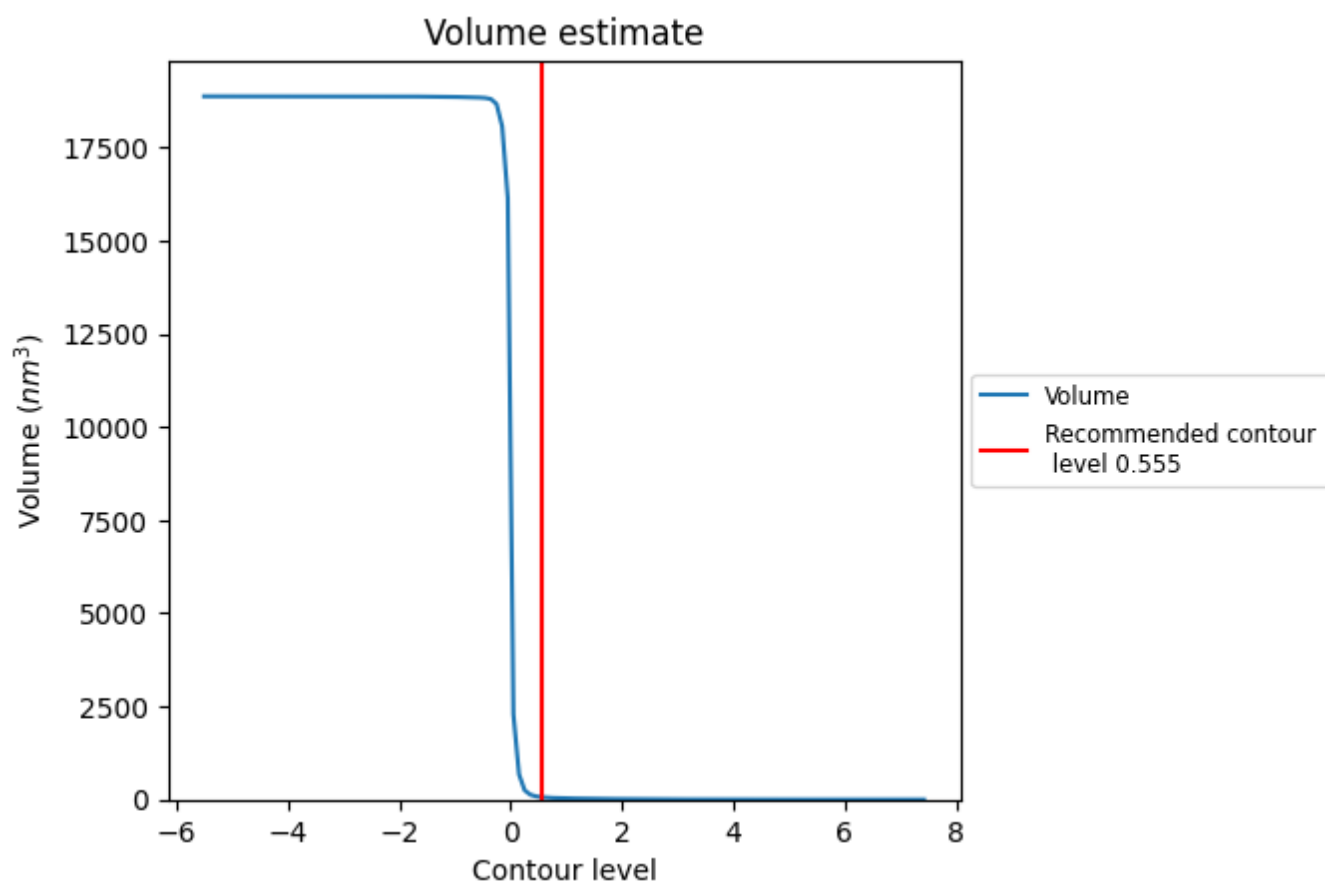
This section contains the results of statistical analysis of the map.

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.

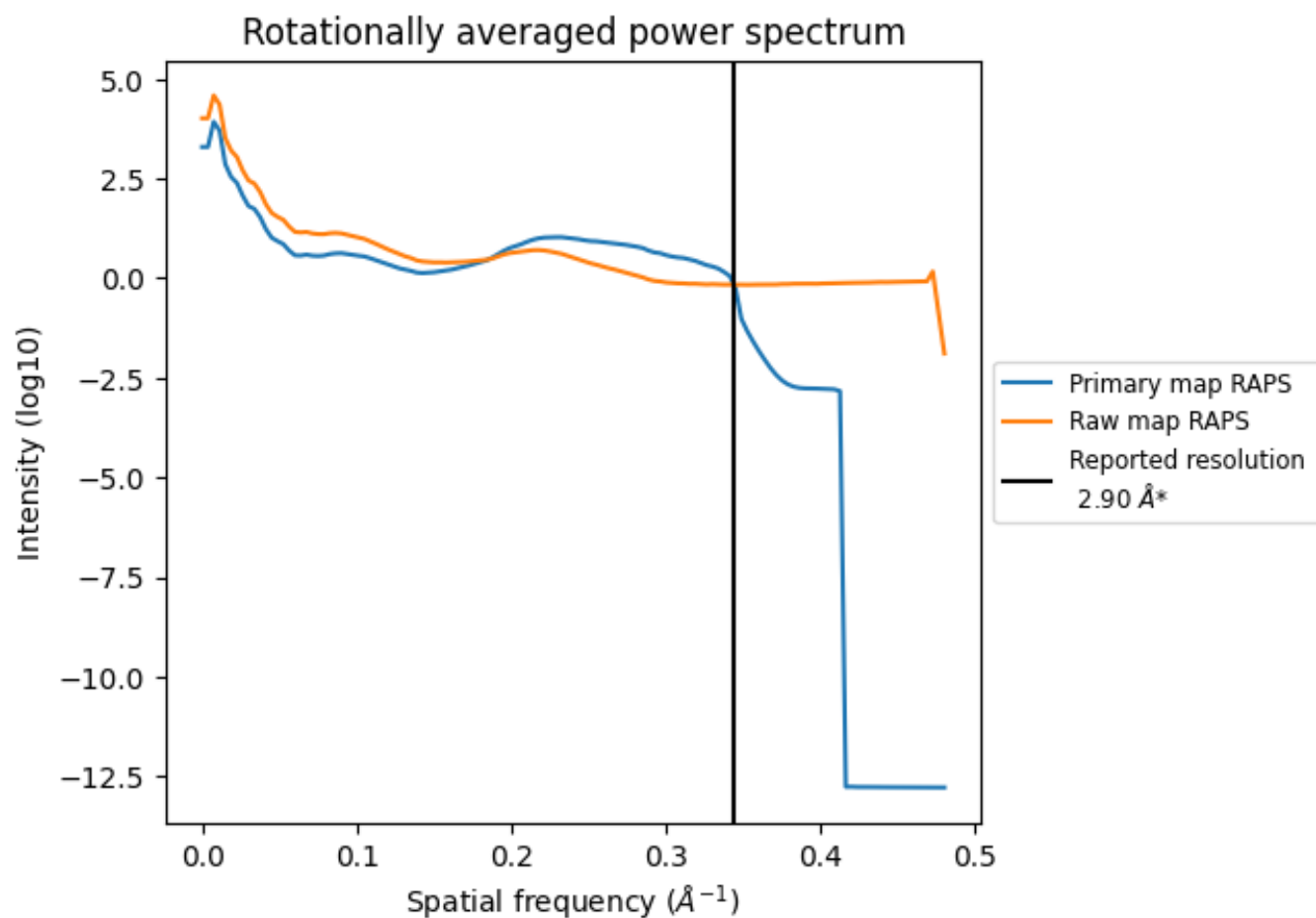
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 64 nm³; this corresponds to an approximate mass of 58 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 ⓘ

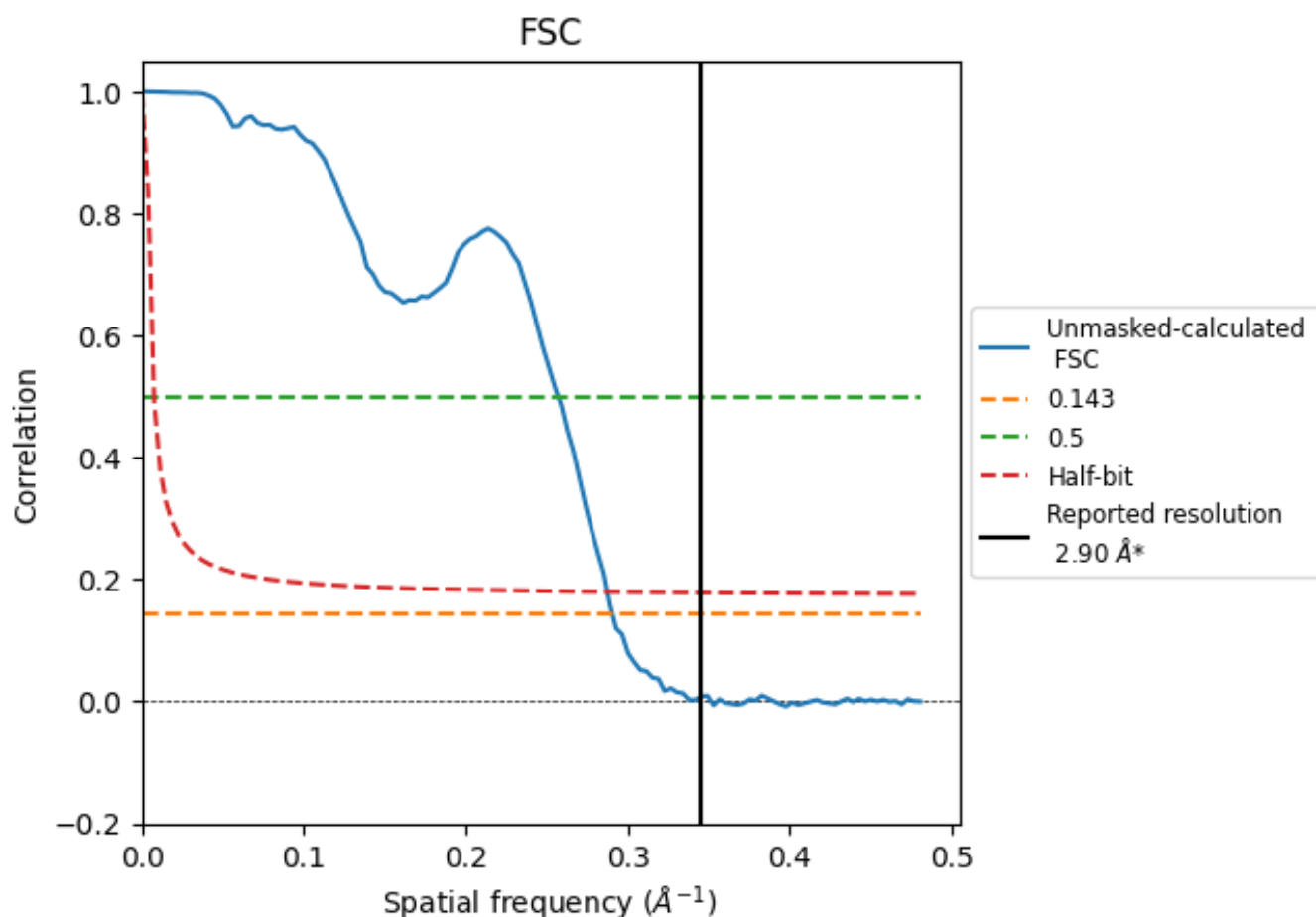


*Reported resolution corresponds to spatial frequency of $0.345 \text{ \AA}^{-1}$

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](#)

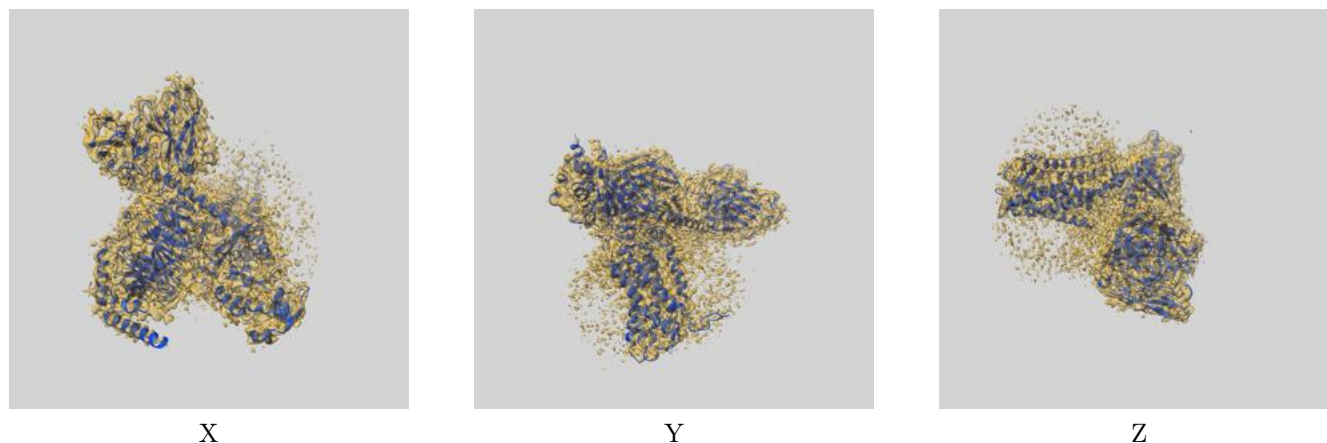
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	2.90	-	-
Author-provided FSC curve	-	-	-
Unmasked-calculated*	3.44	3.89	3.48

*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 3.44 differs from the reported value 2.9 by more than 10 %

9 Map-model fit [i](#)

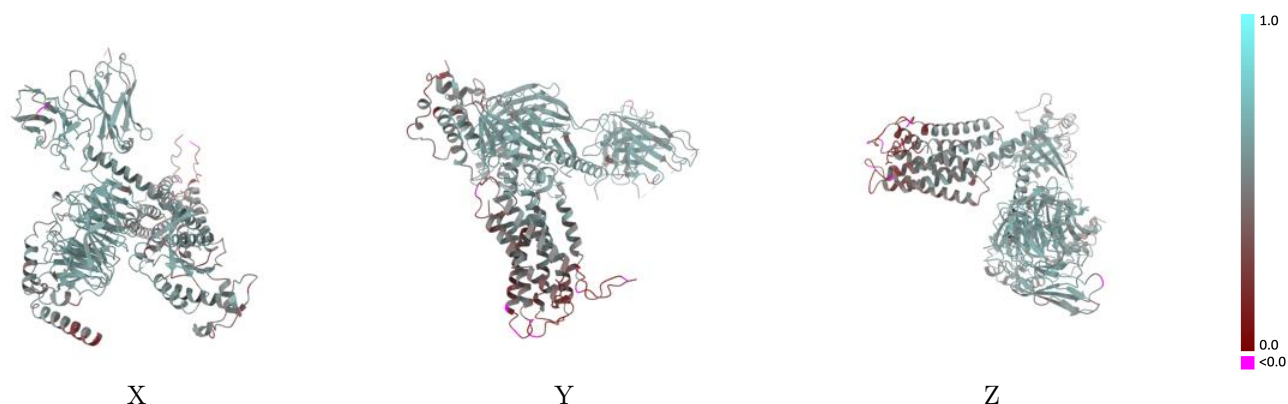
This section contains information regarding the fit between EMDB map EMD-36890 and PDB model 8K4S. Per-residue inclusion information can be found in section [3](#) on page [8](#).

9.1 Map-model overlay [i](#)



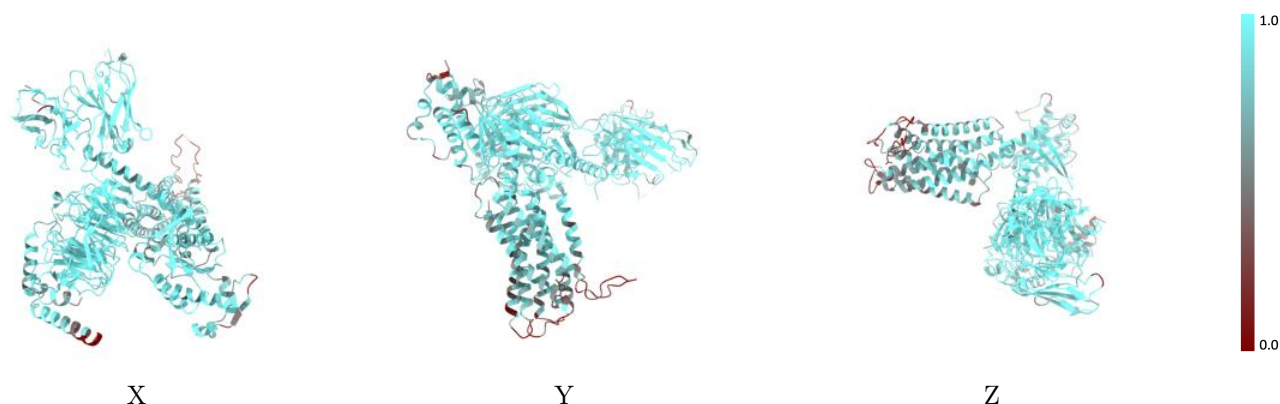
The images above show the 3D surface view of the map at the recommended contour level 0.555 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



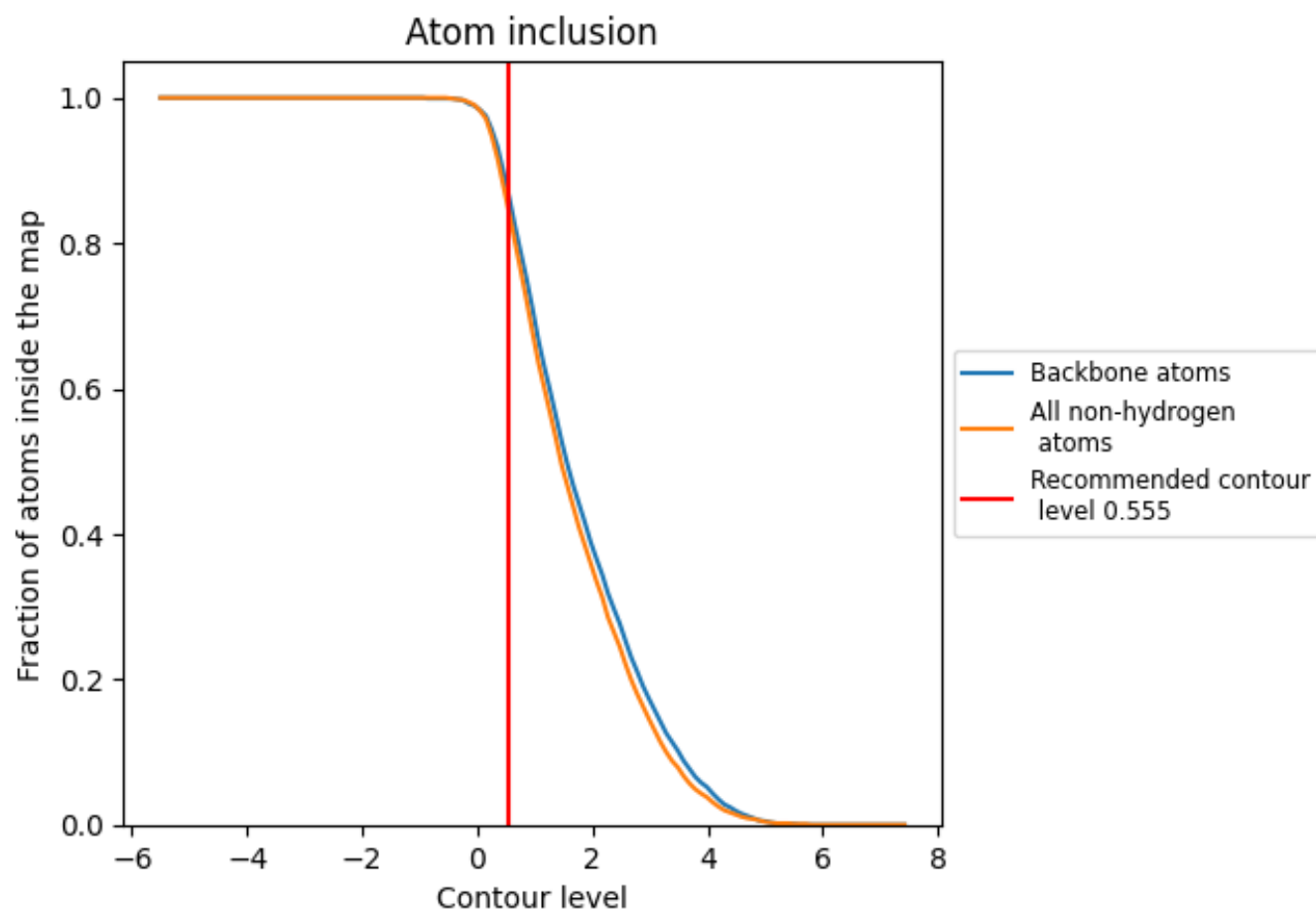
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.555).

9.4 Atom inclusion [i](#)



At the recommended contour level, 86% 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 (0.555) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.8400	0.5210
A	0.8680	0.5380
B	0.9260	0.5830
C	0.8040	0.5080
D	0.9060	0.5650
E	0.6580	0.3950

