



Full wwPDB EM Validation Report ⓘ

Nov 4, 2024 – 05:11 PM JST

PDB ID : 8KH5
EMDB ID : EMD-37237
Title : Cryo-EM structure of the GPR174-Gs complex bound to endogenous lysoPS
Authors : Nie, Y.; Qiu, Z.; Zheng, S.; Chen, S.
Deposited on : 2023-08-21
Resolution : 2.83 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.dev113
Mogul : 1.8.5 (274361), CSD as541be (2020)
MolProbity : 4.02b-467
buster-report : 1.1.7 (2018)
Percentile statistics : 20231227.v01 (using entries in the PDB archive December 27th 2023)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.39

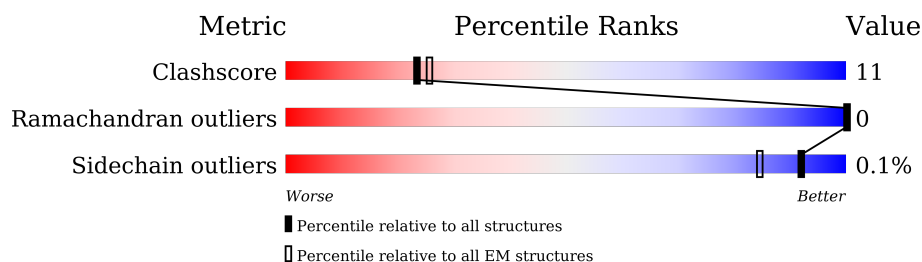
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 2.83 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	EM structures (#Entries)
Clashscore	210492	15764
Ramachandran outliers	207382	16835
Sidechain outliers	206894	16415

The table below summarises the geometric issues observed across the polymeric chains and their fit to the map. The red, orange, yellow and green segments of the bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. 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	340	
2	B	248	
3	C	357	
4	E	160	
5	D	71	

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
7	LPS	A	402	X	-	-	-

2 Entry composition

There are 7 unique types of molecules in this entry. The entry contains 7838 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 Probable G-protein coupled receptor 174.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	281	Total	C	N	O	S	0	0
			2214	1489	348	355	22		

There are 18 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-7	ASP	-	expression tag	UNP Q9BXC1
A	-6	TYR	-	expression tag	UNP Q9BXC1
A	-5	LYS	-	expression tag	UNP Q9BXC1
A	-4	ASP	-	expression tag	UNP Q9BXC1
A	-3	ASP	-	expression tag	UNP Q9BXC1
A	-2	ASP	-	expression tag	UNP Q9BXC1
A	-1	ASP	-	expression tag	UNP Q9BXC1
A	0	LYS	-	expression tag	UNP Q9BXC1
A	1	ALA	-	expression tag	UNP Q9BXC1
A	324	GLU	THR	conflict	UNP Q9BXC1
A	325	LEU	ALA	conflict	UNP Q9BXC1
A	326	GLU	SER	conflict	UNP Q9BXC1
A	327	VAL	THR	conflict	UNP Q9BXC1
A	328	LEU	MET	conflict	UNP Q9BXC1
A	329	PHE	-	expression tag	UNP Q9BXC1
A	330	GLN	-	expression tag	UNP Q9BXC1
A	331	GLY	-	expression tag	UNP Q9BXC1
A	332	PRO	-	expression tag	UNP Q9BXC1

- Molecule 2 is a protein called Guanine nucleotide-binding protein G(s) subunit alpha isoforms short.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	B	228	Total	C	N	O	S	0	0
			1778	1130	325	316	7		

There are 24 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	49	ASP	GLY	engineered mutation	UNP P63092
B	50	ASN	GLU	engineered mutation	UNP P63092
B	196	GLY	-	linker	UNP P63092
B	197	GLY	-	linker	UNP P63092
B	198	SER	-	linker	UNP P63092
B	199	GLY	-	linker	UNP P63092
B	200	GLY	-	linker	UNP P63092
B	201	SER	-	linker	UNP P63092
B	202	GLY	-	linker	UNP P63092
B	203	GLY	-	linker	UNP P63092
B	249	ASP	ALA	engineered mutation	UNP P63092
B	252	ASP	SER	engineered mutation	UNP P63092
B	?	-	ASN	deletion	UNP P63092
B	?	-	MET	deletion	UNP P63092
B	?	-	VAL	deletion	UNP P63092
B	?	-	ILE	deletion	UNP P63092
B	?	-	ARG	deletion	UNP P63092
B	?	-	GLU	deletion	UNP P63092
B	?	-	ASP	deletion	UNP P63092
B	?	-	ASN	deletion	UNP P63092
B	?	-	GLN	deletion	UNP P63092
B	?	-	THR	deletion	UNP P63092
B	372	ALA	ILE	conflict	UNP P63092
B	375	ILE	VAL	conflict	UNP P63092

- 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	2	0
			2467	1532	440	474	21		

There are 19 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
C	-16	HIS	-	expression tag	UNP P62873
C	-15	HIS	-	expression tag	UNP P62873
C	-14	HIS	-	expression tag	UNP P62873
C	-13	HIS	-	expression tag	UNP P62873
C	-12	HIS	-	expression tag	UNP P62873
C	-11	HIS	-	expression tag	UNP P62873
C	-10	LEU	-	expression tag	UNP P62873
C	-9	GLU	-	expression tag	UNP P62873

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Chain	Residue	Modelled	Actual	Comment	Reference
C	-8	VAL	-	expression tag	UNP P62873
C	-7	LEU	-	expression tag	UNP P62873
C	-6	PHE	-	expression tag	UNP P62873
C	-5	GLN	-	expression tag	UNP P62873
C	-4	GLY	-	expression tag	UNP P62873
C	-3	PRO	-	expression tag	UNP P62873
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
C	145	ARG	TYR	engineered mutation	UNP P62873

- Molecule 4 is a protein called Nanobody 35.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	E	128	Total	C	N	O	S	0	0
			946	588	164	188	6		

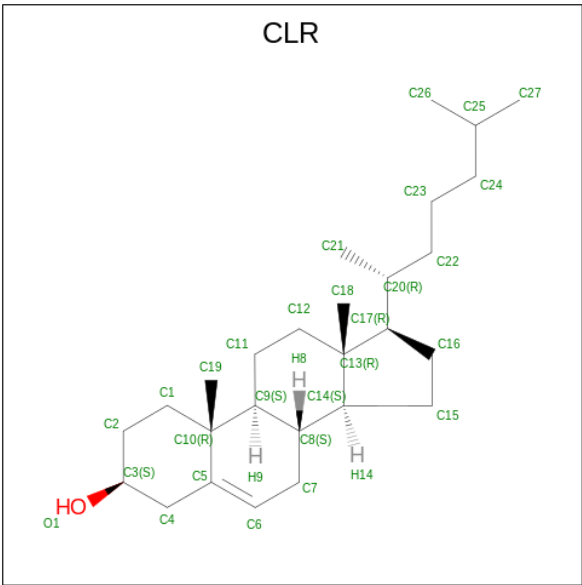
- Molecule 5 is a protein called Guanine nucleotide-binding protein G(I)/G(S)/G(O) subunit gamma-2.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	D	55	Total	C	N	O	S	0	0
			345	220	61	63	1		

There is a discrepancy between the modelled and reference sequences:

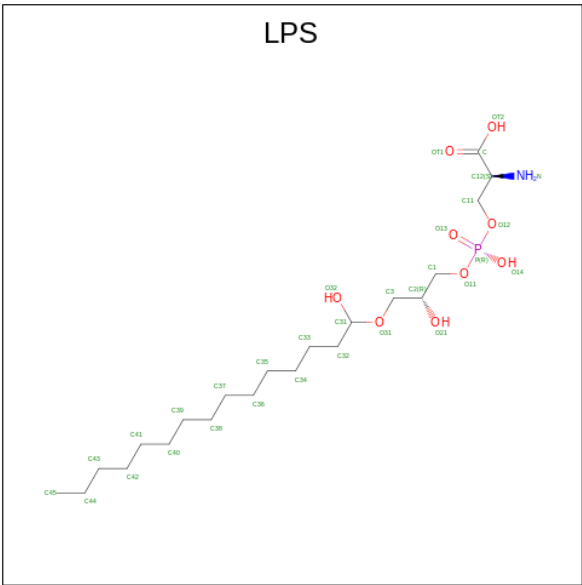
Chain	Residue	Modelled	Actual	Comment	Reference
D	68	SER	CYS	engineered mutation	UNP P59768

- Molecule 6 is CHOLESTEROL (three-letter code: CLR) (formula: C₂₇H₄₆O).

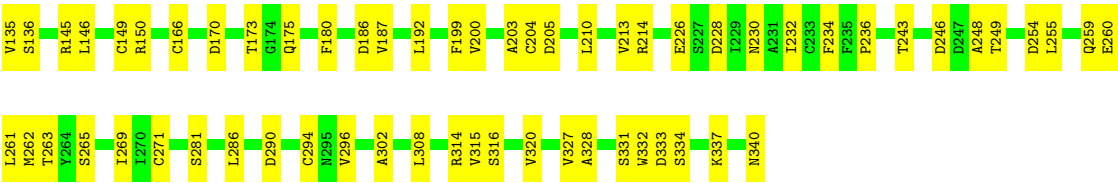


Mol	Chain	Residues	Atoms			AltConf
6	A	1	Total	C	O	0
			28	27	1	
6	A	1	Total	C	O	0
			28	27	1	

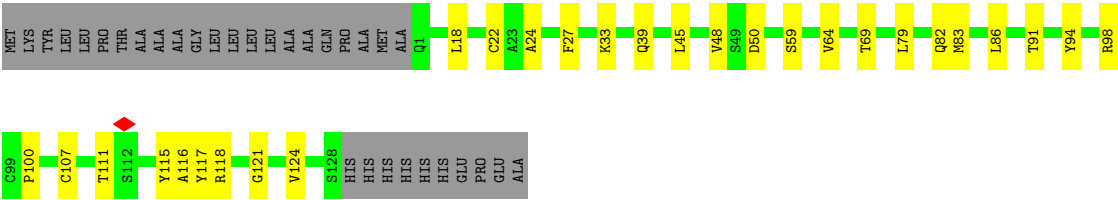
- Molecule 7 is O-{HYDROXY[(((2R)-2-HYDROXY-3-{[(1S)-1-HYDROXYPENTADECYL]OXY}PROPYL)OXY]PHOSPHORYL)}-L-SERINE (three-letter code: LPS) (formula: C₂₁H₄₄NO₉P).



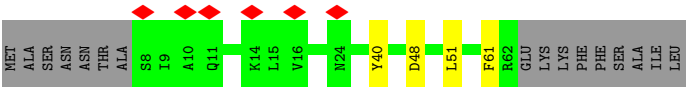
Mol	Chain	Residues	Atoms					AltConf
7	A	1	Total	C	N	O	P	0
			32	21	1	9	1	



• Molecule 4: Nanobody 35



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



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	807893	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 ($e^-/\text{\AA}^2$)	50	Depositor
Minimum defocus (nm)	1390	Depositor
Maximum defocus (nm)	2780	Depositor
Magnification	64000	Depositor
Image detector	GATAN K3 BIOQUANTUM (6k x 4k)	Depositor
Maximum map value	4.554	Depositor
Minimum map value	-2.976	Depositor
Average map value	0.002	Depositor
Map value standard deviation	0.126	Depositor
Recommended contour level	0.38	Depositor
Map size (Å)	194.40001, 194.40001, 194.40001	wwPDB
Map dimensions	180, 180, 180	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.08, 1.08, 1.08	Depositor

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: CLR, LPS

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	0.60	1/2276 (0.0%)	0.63	1/3106 (0.0%)
2	B	0.27	0/1814	0.49	0/2457
3	C	0.34	0/2518	0.55	1/3428 (0.0%)
4	E	0.29	0/966	0.51	0/1313
5	D	0.24	0/351	0.39	0/488
All	All	0.41	1/7925 (0.0%)	0.55	2/10792 (0.0%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	1

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	123	PRO	C-O	9.11	1.41	1.23

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	C	146	LEU	CB-CG-CD2	-5.22	102.12	111.00
1	A	126	PHE	O-C-N	-5.11	114.52	122.70

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	126	PHE	Mainchain

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	2214	0	2222	74	0
2	B	1778	0	1680	28	0
3	C	2467	0	2304	58	0
4	E	946	0	881	19	0
5	D	345	0	285	5	0
6	A	56	0	92	13	0
7	A	32	0	40	4	0
All	All	7838	0	7504	166	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 (166) 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:A:111:CYS:SG	6:A:403:CLR:H151	2.04	0.97
3:C:271:CYS:HB2	3:C:290:ASP:HB2	1.59	0.84
4:E:94:TYR:O	4:E:121:GLY:HA2	1.86	0.75
1:A:238:VAL:HG21	1:A:291:ILE:HD13	1.70	0.72
1:A:242:CYS:CB	1:A:284:ASN:HB2	2.19	0.71
3:C:210:LEU:HD22	3:C:255:LEU:HD22	1.73	0.70
2:B:228:ARG:NH1	3:C:186:ASP:OD1	2.25	0.69
1:A:142:TRP:CD1	6:A:401:CLR:H183	2.28	0.69
3:C:320:VAL:HG22	3:C:327:VAL:HG22	1.74	0.69
1:A:135:LEU:HD11	6:A:401:CLR:H11	1.76	0.68
3:C:213:VAL:HG23	3:C:214:ARG:HD2	1.76	0.68
1:A:242:CYS:SG	1:A:284:ASN:HB2	2.32	0.68
3:C:149:CYS:O	3:C:150:ARG:NH1	2.25	0.68
3:C:145:ARG:HH22	3:C:186:ASP:HB3	1.59	0.67
4:E:50:ASP:OD1	4:E:59:SER:OG	2.10	0.66
3:C:49:ARG:NH1	5:D:61:PHE:O	2.30	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:254:ASP:HB2	3:C:261:LEU:HD11	1.80	0.64
1:A:133:TYR:O	1:A:137:ILE:HG13	1.97	0.64
3:C:286:LEU:HD22	3:C:327:VAL:HG11	1.80	0.64
1:A:242:CYS:HB3	1:A:284:ASN:HB2	1.78	0.63
4:E:83:MET:HE2	4:E:86:LEU:HD11	1.79	0.63
1:A:19:TYR:HE1	1:A:170:VAL:HG11	1.63	0.63
1:A:15:THR:HA	1:A:18:ARG:HD3	1.79	0.62
1:A:145:ILE:HG13	7:A:402:LPS:H452	1.79	0.62
3:C:101:MET:CE	3:C:145:ARG:HD2	2.29	0.62
1:A:69:VAL:HA	1:A:72:LEU:HD13	1.81	0.61
1:A:246:TYR:HA	1:A:277:ALA:HB1	1.82	0.61
1:A:238:VAL:HG21	1:A:291:ILE:CD1	2.31	0.60
2:B:386:MET:O	2:B:390:GLN:HG3	2.01	0.60
1:A:44:PHE:HZ	1:A:293:TYR:HE1	1.49	0.60
2:B:214:VAL:HG21	2:B:376:PHE:HB2	1.83	0.60
1:A:198:LEU:HD11	1:A:240:LEU:HD13	1.82	0.60
1:A:78:TYR:OH	1:A:171:ASP:OD2	2.20	0.59
2:B:239:ASN:HA	2:B:285:ILE:HD11	1.84	0.58
1:A:75:ARG:NH2	1:A:94:CYS:O	2.37	0.58
1:A:209:VAL:HG13	1:A:229:LEU:HD11	1.83	0.58
2:B:237:CYS:SG	3:C:75:GLN:NE2	2.76	0.57
1:A:107:TYR:CE1	6:A:403:CLR:H161	2.39	0.57
1:A:156:ARG:HH22	1:A:257:LYS:HD3	1.69	0.57
3:C:101:MET:HE2	3:C:145:ARG:HD2	1.86	0.57
1:A:115:ARG:HB3	2:B:394:LEU:HD21	1.85	0.57
4:E:115:TYR:HD2	4:E:118:ARG:HB2	1.69	0.57
3:C:249:THR:HG22	3:C:265:SER:HB3	1.86	0.57
1:A:43:VAL:HG13	1:A:302:ARG:HD2	1.87	0.56
1:A:152:PHE:HD1	7:A:402:LPS:H321	1.70	0.56
2:B:227:GLN:NE2	3:C:119:ASN:HD21	2.03	0.56
4:E:91:THR:HA	4:E:124:VAL:O	2.06	0.56
1:A:115:ARG:HG2	2:B:394:LEU:HD11	1.88	0.56
1:A:146:CYS:O	1:A:150:VAL:HG23	2.06	0.55
3:C:145:ARG:HH22	3:C:186:ASP:CB	2.19	0.55
3:C:226:GLU:O	4:E:98:ARG:NH2	2.40	0.55
1:A:136:TYR:N	1:A:136:TYR:CD1	2.70	0.54
3:C:248:ALA:HB1	3:C:269:ILE:HG22	1.90	0.54
3:C:145:ARG:NH2	3:C:186:ASP:HB3	2.21	0.54
2:B:229:ASP:HB2	4:E:111:THR:HG23	1.89	0.54
1:A:118:TRP:HD1	1:A:126:PHE:HD1	1.54	0.54
3:C:294:CYS:HB2	3:C:308:LEU:HB2	1.89	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:84:TRP:NE1	1:A:91:CYS:HB2	2.24	0.53
2:B:45:LEU:HD23	2:B:223:ASP:HB2	1.91	0.53
3:C:124:TYR:CE2	3:C:135:VAL:HG22	2.43	0.53
1:A:131:GLN:O	1:A:131:GLN:HG3	2.09	0.53
3:C:22:ARG:O	3:C:259:GLN:NE2	2.42	0.52
1:A:289:PRO:HA	1:A:293:TYR:HD2	1.73	0.52
3:C:81:ILE:HB	3:C:91:HIS:HB2	1.92	0.52
3:C:93:ILE:HG12	3:C:133:VAL:HG21	1.92	0.52
4:E:39:GLN:HB2	4:E:45:LEU:HD13	1.92	0.51
1:A:152:PHE:CD1	7:A:402:LPS:H321	2.45	0.51
1:A:188:ILE:O	1:A:192:ILE:HG22	2.10	0.51
1:A:74:LEU:HD23	1:A:84:TRP:HH2	1.76	0.51
3:C:228:ASP:OD1	4:E:117:TYR:OH	2.28	0.51
3:C:260:GLU:OE2	3:C:263:THR:OG1	2.29	0.51
2:B:43:LEU:HB2	2:B:221:MET:HG3	1.93	0.51
1:A:33:GLY:O	1:A:37:ASN:ND2	2.44	0.51
1:A:44:PHE:HZ	1:A:293:TYR:CE1	2.28	0.51
1:A:128:ASP:O	1:A:131:GLN:HG2	2.10	0.50
1:A:25:THR:HG21	1:A:279:CYS:HB3	1.92	0.50
1:A:296:THR:HG22	1:A:298:GLU:H	1.75	0.50
3:C:61:MET:HE3	3:C:328:ALA:HB3	1.92	0.50
1:A:221:ASP:OD2	2:B:385:ARG:NH2	2.39	0.50
3:C:232:ILE:HG13	3:C:243:THR:HG22	1.94	0.50
1:A:19:TYR:O	1:A:20:PHE:C	2.44	0.49
1:A:44:PHE:HE1	2:B:393:LEU:HD12	1.76	0.49
3:C:236:PRO:HB2	5:D:40:TYR:CE1	2.48	0.49
1:A:74:LEU:HD22	1:A:94:CYS:SG	2.52	0.49
2:B:237:CYS:HA	3:C:59:TYR:OH	2.13	0.49
1:A:29:ILE:HG23	1:A:286:CYS:HB3	1.93	0.48
1:A:107:TYR:CD1	6:A:403:CLR:H161	2.48	0.48
3:C:262:MET:SD	3:C:302:ALA:HB2	2.53	0.48
3:C:101:MET:HE1	3:C:145:ARG:HD2	1.95	0.48
2:B:240:ASP:OD2	3:C:57:LYS:NZ	2.47	0.48
3:C:192:LEU:HD23	3:C:199:PHE:HB3	1.96	0.48
3:C:333:ASP:O	3:C:334:SER:OG	2.32	0.48
6:A:403:CLR:H221	6:A:403:CLR:H162	1.40	0.47
3:C:230:ASN:ND2	3:C:246:ASP:OD1	2.35	0.47
3:C:57:LYS:NZ	3:C:75:GLN:HG3	2.29	0.47
1:A:19:TYR:CD1	1:A:79:TYR:CD1	3.01	0.47
1:A:112:ILE:HG23	2:B:394:LEU:HD23	1.97	0.47
3:C:170:ASP:HB3	3:C:173:THR:HG22	1.97	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:84:TRP:CE2	1:A:91:CYS:HB2	2.50	0.47
1:A:234:THR:O	1:A:238:VAL:HG23	2.15	0.47
5:D:48:ASP:HB3	5:D:51:LEU:HB3	1.97	0.47
1:A:256:VAL:HG13	1:A:267:ARG:HG2	1.97	0.47
1:A:100:VAL:HA	1:A:149:CYS:SG	2.55	0.46
1:A:156:ARG:HG2	1:A:156:ARG:O	2.16	0.46
2:B:46:LEU:HD11	2:B:235:ILE:HD11	1.97	0.46
1:A:151:LEU:HD21	1:A:185:MET:SD	2.56	0.46
1:A:296:THR:HG21	2:B:393:LEU:HD22	1.98	0.46
6:A:401:CLR:H222	6:A:401:CLR:H162	1.54	0.46
3:C:204:CYS:O	4:E:117:TYR:OH	2.32	0.46
4:E:22:CYS:HB3	4:E:79:LEU:HB3	1.98	0.46
7:A:402:LPS:H341	7:A:402:LPS:H371	1.59	0.45
3:C:58:ILE:O	3:C:316:SER:OG	2.19	0.45
1:A:111:CYS:HG	6:A:403:CLR:H151	1.78	0.45
1:A:115:ARG:NH2	1:A:134:ASP:OD1	2.49	0.45
1:A:44:PHE:CZ	1:A:293:TYR:CE1	3.06	0.44
1:A:289:PRO:HA	1:A:293:TYR:CD2	2.52	0.44
2:B:211:LYS:HG2	2:B:220:HIS:HB3	1.99	0.44
1:A:200:ILE:HD13	6:A:403:CLR:H183	1.99	0.44
2:B:32:LYS:HE3	2:B:32:LYS:HB2	1.69	0.44
3:C:200:VAL:HG22	3:C:234:PHE:CE2	2.53	0.44
1:A:192:ILE:HG23	1:A:193:GLY:N	2.32	0.43
2:B:44:LEU:HD23	2:B:244:ILE:HG12	1.99	0.43
3:C:57:LYS:HB2	3:C:57:LYS:HE2	1.86	0.43
3:C:47:THR:HG23	3:C:337:LYS:HB3	2.00	0.43
3:C:286:LEU:HG	3:C:296:VAL:HG22	2.00	0.43
4:E:18:LEU:HD23	4:E:18:LEU:HA	1.90	0.43
4:E:24:ALA:HB1	4:E:27:PHE:CZ	2.54	0.43
4:E:33:LYS:HD2	4:E:107:CYS:SG	2.59	0.43
3:C:75:GLN:O	3:C:98:SER:OG	2.37	0.42
1:A:25:THR:HG22	1:A:29:ILE:HD12	2.01	0.42
1:A:139:ILE:O	1:A:139:ILE:HG22	2.19	0.42
1:A:177:VAL:HG13	1:A:182:SER:HB3	2.00	0.42
1:A:18:ARG:HG2	1:A:275:SER:OG	2.20	0.42
1:A:167:LYS:HA	1:A:171:ASP:HB2	2.01	0.42
3:C:340:ASN:HD21	5:D:61:PHE:HB2	1.84	0.42
3:C:173:THR:HG23	3:C:175:GLN:H	1.85	0.42
2:B:236:GLN:HG2	2:B:281:TRP:CD1	2.55	0.42
1:A:25:THR:HG21	1:A:279:CYS:CB	2.49	0.42
3:C:281:SER:OG	5:D:48:ASP:OD2	2.33	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:34:LEU:O	1:A:38:ILE:HG12	2.20	0.42
2:B:266:LEU:HD23	2:B:266:LEU:HA	1.91	0.42
2:B:346:LEU:HA	2:B:349:SER:HB3	2.02	0.42
3:C:294:CYS:SG	3:C:315:VAL:HG11	2.60	0.42
1:A:55:VAL:HG23	1:A:59:ILE:HG13	2.01	0.41
3:C:150:ARG:HA	3:C:150:ARG:HD3	1.88	0.41
1:A:235:CYS:O	1:A:236:ALA:C	2.55	0.41
2:B:234:TRP:HB2	3:C:117:LEU:HD21	2.00	0.41
4:E:69:THR:HB	4:E:82:GLN:HB3	2.02	0.41
4:E:48:VAL:HG13	4:E:64:VAL:HG21	2.03	0.41
2:B:232:ARG:HD3	4:E:100:PRO:HG3	2.03	0.41
6:A:401:CLR:H8	6:A:401:CLR:H182	1.74	0.41
1:A:60:ASN:OD1	6:A:401:CLR:H191	2.21	0.41
6:A:401:CLR:H22	6:A:401:CLR:H192	1.88	0.41
1:A:60:ASN:HB3	1:A:108:PHE:CE2	2.55	0.41
1:A:75:ARG:HH22	1:A:95:PHE:HA	1.85	0.41
3:C:205:ASP:HA	4:E:116:ALA:HB1	2.02	0.41
3:C:125:ASN:HB2	3:C:136:SER:HB2	2.02	0.41
2:B:334:VAL:O	2:B:338:LYS:HG3	2.21	0.40
3:C:166:CYS:HB2	3:C:180:PHE:HB2	2.01	0.40
3:C:187:VAL:HA	3:C:203:ALA:HA	2.02	0.40
4:E:27:PHE:CE2	4:E:98:ARG:HD3	2.56	0.40
2:B:227:GLN:HE21	3:C:119:ASN:HD21	1.65	0.40
3:C:314:ARG:C	3:C:331:SER:HG	2.24	0.40
1:A:105:SER:O	1:A:109:LEU:HG	2.21	0.40
1:A:142:TRP:NE1	6:A:401:CLR:H183	2.37	0.40
3:C:57:LYS:HD2	3:C:332:TRP:CD2	2.57	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	277/340 (82%)	265 (96%)	12 (4%)	0	100	100
2	B	224/248 (90%)	222 (99%)	2 (1%)	0	100	100
3	C	338/357 (95%)	326 (96%)	12 (4%)	0	100	100
4	E	126/160 (79%)	123 (98%)	3 (2%)	0	100	100
5	D	53/71 (75%)	53 (100%)	0	0	100	100
All	All	1018/1176 (87%)	989 (97%)	29 (3%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	233/308 (76%)	232 (100%)	1 (0%)	89	95
2	B	174/219 (80%)	174 (100%)	0	100	100
3	C	248/297 (84%)	248 (100%)	0	100	100
4	E	99/129 (77%)	99 (100%)	0	100	100
5	D	23/58 (40%)	23 (100%)	0	100	100
All	All	777/1011 (77%)	776 (100%)	1 (0%)	92	98

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

Mol	Chain	Res	Type
1	A	145	ILE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (5) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	82	HIS
3	C	44	GLN
3	C	75	GLN
3	C	119	ASN

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Mol	Chain	Res	Type
4	E	31	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](#)

3 ligands are 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	CLR	A	401	-	31,31,31	1.22	5 (16%)	48,48,48	1.79	14 (29%)
7	LPS	A	402	-	30,31,31	1.58	2 (6%)	32,37,37	1.60	4 (12%)
6	CLR	A	403	-	31,31,31	0.99	1 (3%)	48,48,48	1.46	10 (20%)

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	CLR	A	401	-	-	5/10/68/68	0/4/4/4

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
7	LPS	A	402	-	1/1/5/5	16/35/35/35	-
6	CLR	A	403	-	-	7/10/68/68	0/4/4/4

All (8) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	A	402	LPS	O32-C31	-7.39	1.18	1.39
6	A	403	CLR	C13-C14	-2.61	1.50	1.55
6	A	401	CLR	C13-C14	-2.61	1.50	1.55
6	A	401	CLR	C20-C17	-2.30	1.50	1.54
6	A	401	CLR	C18-C13	-2.23	1.50	1.54
7	A	402	LPS	O31-C3	-2.17	1.39	1.43
6	A	401	CLR	C10-C9	-2.14	1.52	1.56
6	A	401	CLR	C13-C17	-2.04	1.51	1.55

All (28) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	A	402	LPS	O32-C31-C32	5.81	119.89	109.12
7	A	402	LPS	O12-C11-C12	-3.82	104.72	108.06
7	A	402	LPS	O31-C31-C32	3.52	120.40	109.49
6	A	401	CLR	C3-C4-C5	-3.49	106.11	112.03
6	A	403	CLR	C4-C5-C10	3.42	120.96	116.42
6	A	401	CLR	C8-C7-C6	-3.32	107.96	112.73
6	A	403	CLR	C2-C3-C4	-3.15	105.99	110.31
6	A	401	CLR	C13-C14-C8	-3.14	109.73	114.38
6	A	403	CLR	C8-C7-C6	-3.08	108.31	112.73
6	A	401	CLR	C15-C14-C8	-3.02	114.11	119.08
6	A	401	CLR	C16-C17-C20	-2.98	107.54	112.15
6	A	401	CLR	C4-C5-C6	-2.91	116.41	120.61
6	A	403	CLR	C17-C13-C14	2.68	103.25	100.07
6	A	403	CLR	C18-C13-C14	-2.59	106.89	111.71
6	A	403	CLR	C4-C5-C6	-2.56	116.92	120.61
6	A	401	CLR	C11-C12-C13	-2.55	108.41	112.78
6	A	403	CLR	C11-C12-C13	-2.53	108.44	112.78
6	A	401	CLR	C7-C8-C14	-2.45	107.36	110.91
6	A	401	CLR	C7-C8-C9	2.42	112.65	109.71
6	A	401	CLR	C18-C13-C14	-2.41	107.21	111.71
6	A	403	CLR	C3-C4-C5	-2.37	108.01	112.03
6	A	403	CLR	C7-C6-C5	-2.36	120.70	125.06
6	A	403	CLR	C13-C14-C8	-2.30	110.98	114.38
6	A	401	CLR	C2-C3-C4	-2.23	107.25	110.31

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	A	402	LPS	OT2-C-C12	2.18	120.80	113.38
6	A	401	CLR	C9-C10-C5	2.17	113.05	109.65
6	A	401	CLR	C13-C17-C20	-2.14	116.14	119.49
6	A	401	CLR	C12-C13-C17	2.13	119.76	116.57

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
7	A	402	LPS	C31

All (28) torsion outliers are listed below:

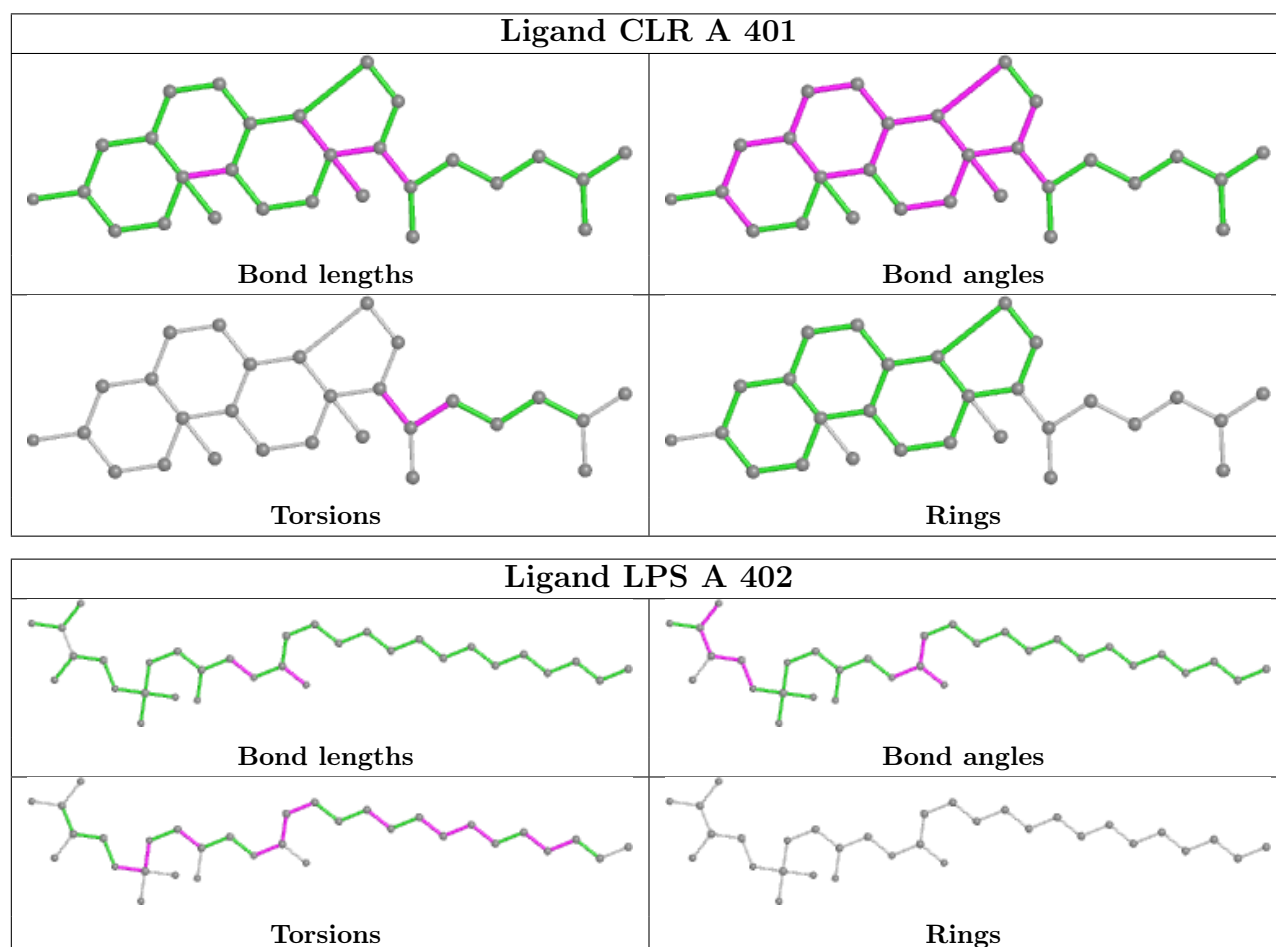
Mol	Chain	Res	Type	Atoms
7	A	402	LPS	C1-O11-P-O14
7	A	402	LPS	O11-C1-C2-O21
7	A	402	LPS	O32-C31-C32-C33
6	A	403	CLR	C13-C17-C20-C22
6	A	403	CLR	C13-C17-C20-C21
7	A	402	LPS	C34-C35-C36-C37
6	A	401	CLR	C13-C17-C20-C22
7	A	402	LPS	O11-C1-C2-C3
6	A	403	CLR	C17-C20-C22-C23
6	A	401	CLR	C13-C17-C20-C21
6	A	403	CLR	C16-C17-C20-C21
7	A	402	LPS	C1-O11-P-O12
6	A	403	CLR	C21-C20-C22-C23
7	A	402	LPS	C40-C41-C42-C43
6	A	403	CLR	C16-C17-C20-C22
6	A	401	CLR	C16-C17-C20-C21
6	A	401	CLR	C16-C17-C20-C22
7	A	402	LPS	C41-C42-C43-C44
7	A	402	LPS	C1-O11-P-O13
7	A	402	LPS	C32-C31-O31-C3
7	A	402	LPS	C36-C37-C38-C39
7	A	402	LPS	C38-C39-C40-C41
6	A	403	CLR	C22-C23-C24-C25
7	A	402	LPS	C31-C32-C33-C34
7	A	402	LPS	O31-C31-C32-C33
6	A	401	CLR	C21-C20-C22-C23
7	A	402	LPS	C11-O12-P-O13
7	A	402	LPS	C37-C38-C39-C40

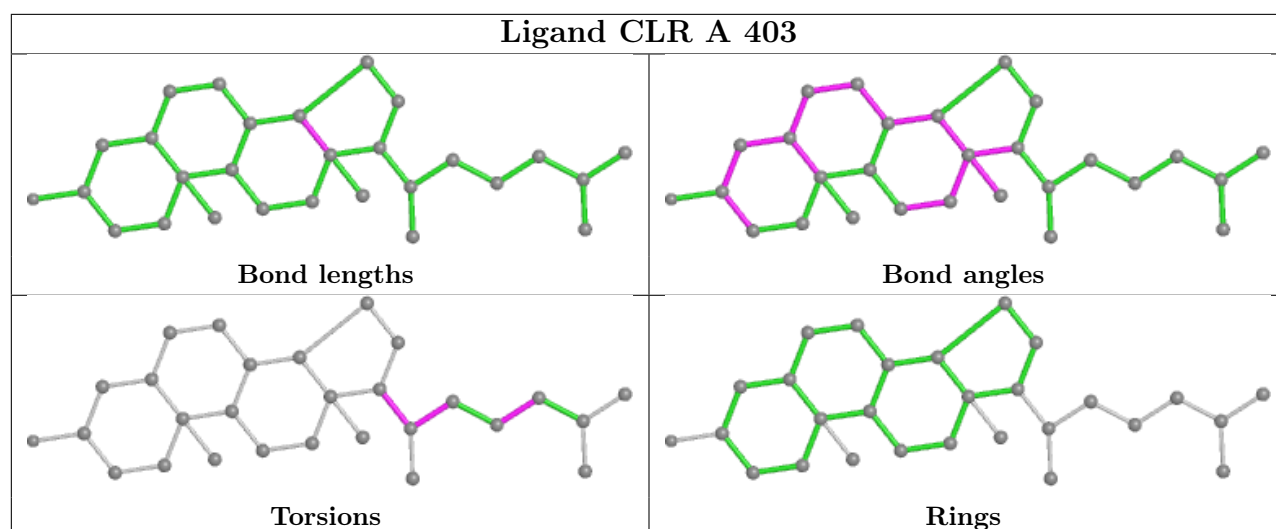
There are no ring outliers.

3 monomers are involved in 17 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	A	401	CLR	7	0
7	A	402	LPS	4	0
6	A	403	CLR	6	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.

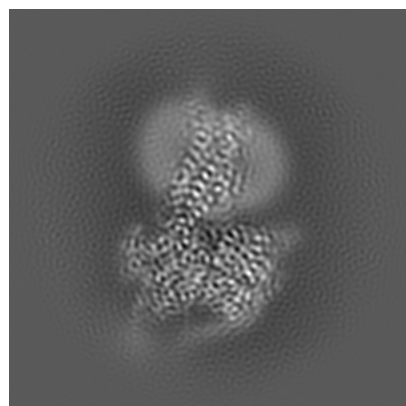
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-37237. These allow visual inspection of the internal detail of the map and identification of artifacts.

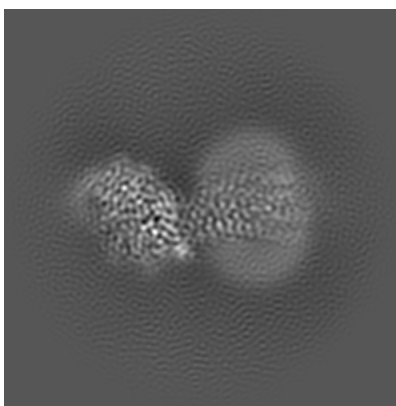
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

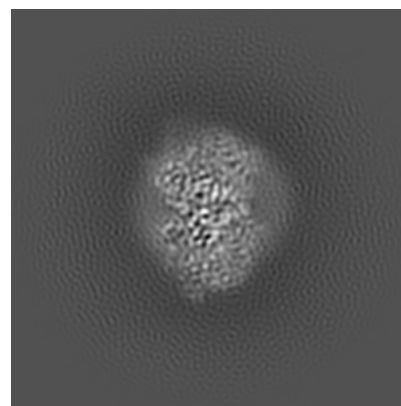
6.1.1 Primary map



X

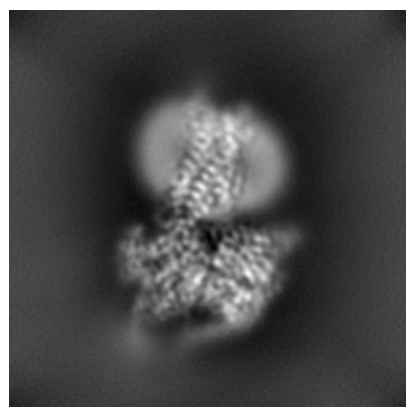


Y

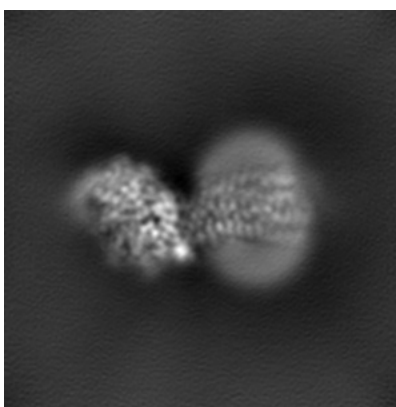


Z

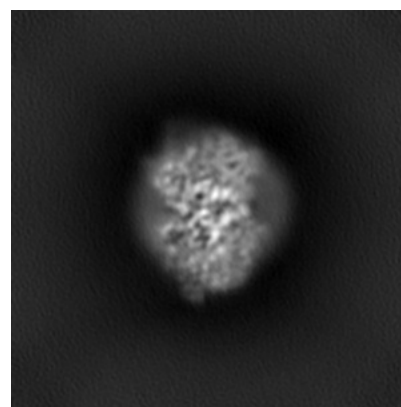
6.1.2 Raw map



X



Y

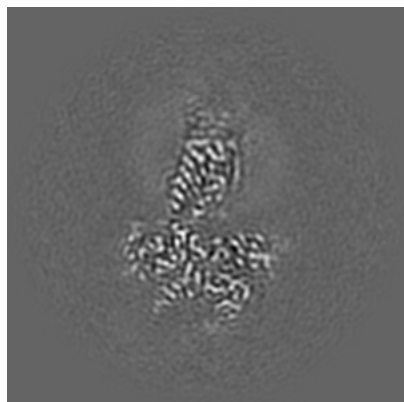


Z

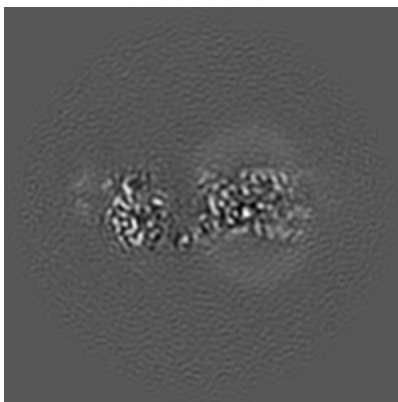
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

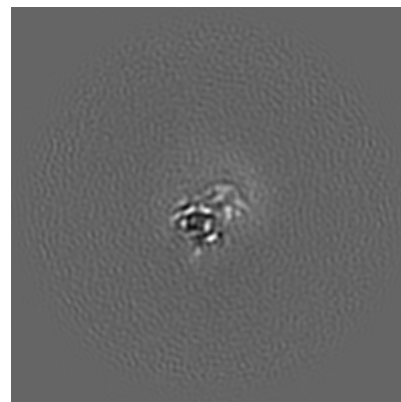
6.2.1 Primary map



X Index: 90

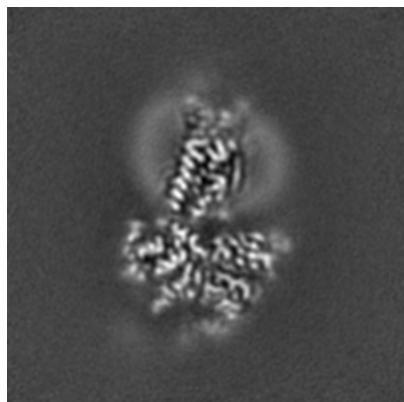


Y Index: 90

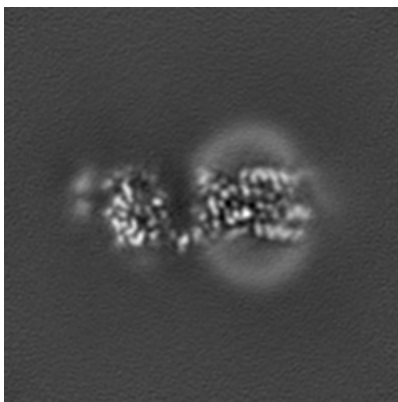


Z Index: 90

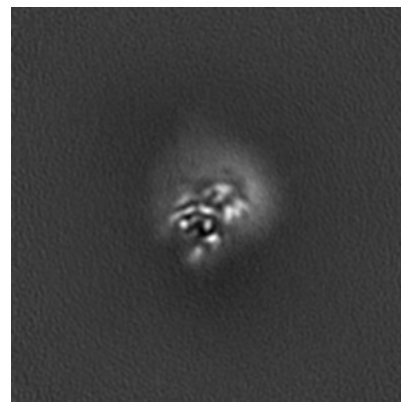
6.2.2 Raw map



X Index: 90



Y Index: 90

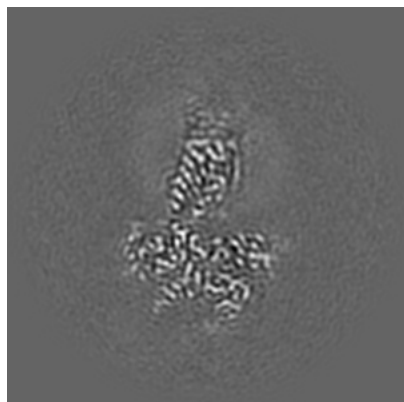


Z Index: 90

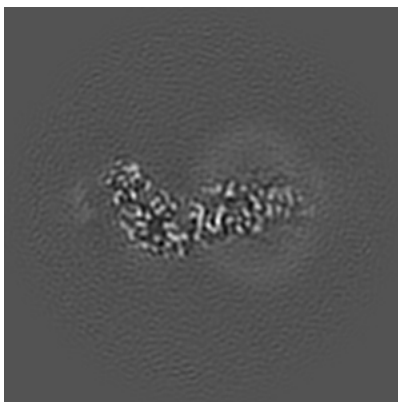
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

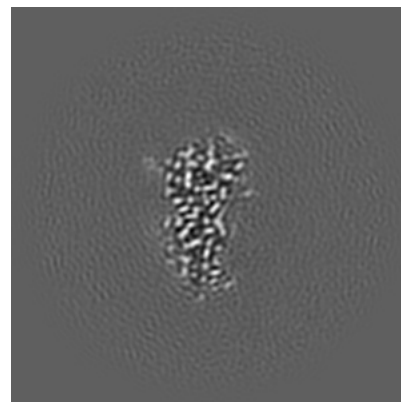
6.3.1 Primary map



X Index: 90

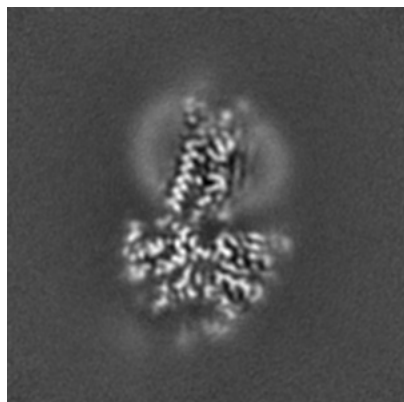


Y Index: 84

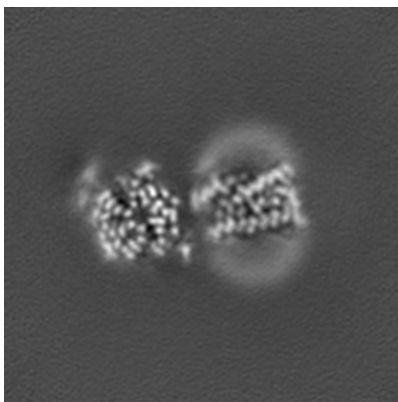


Z Index: 68

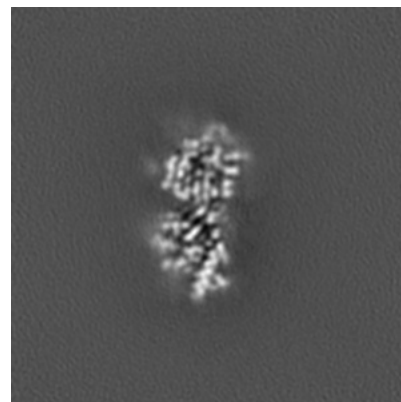
6.3.2 Raw map



X Index: 91



Y Index: 98

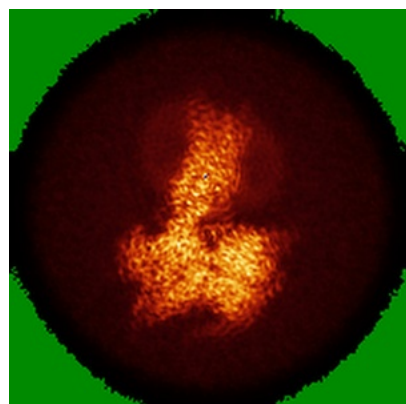


Z Index: 71

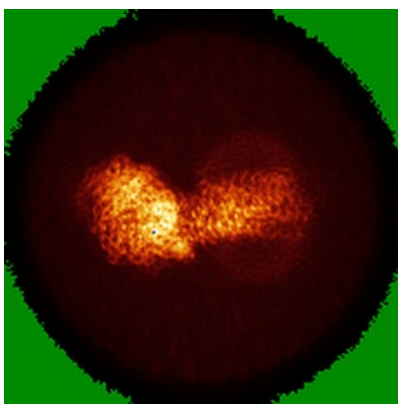
The images above show the largest variance slices of the map in three orthogonal directions.

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

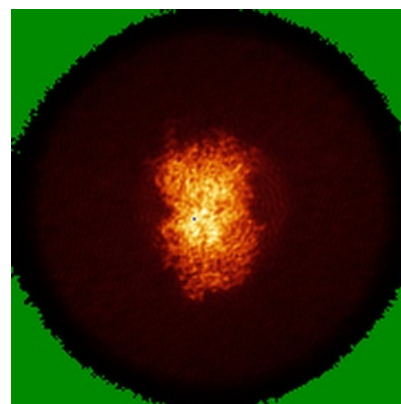
6.4.1 Primary map



X

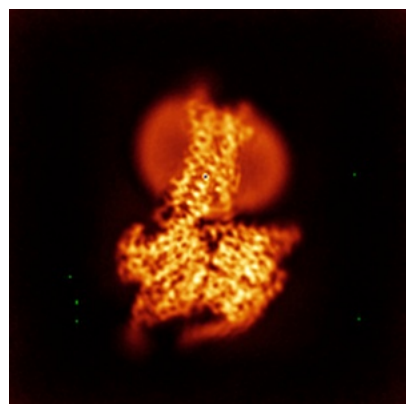


Y

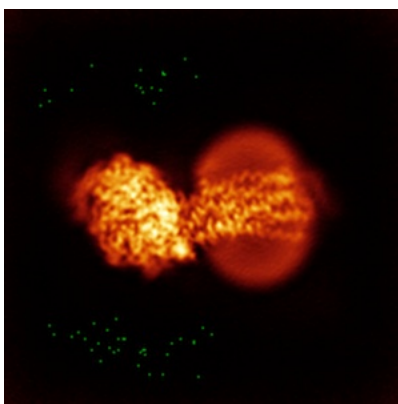


Z

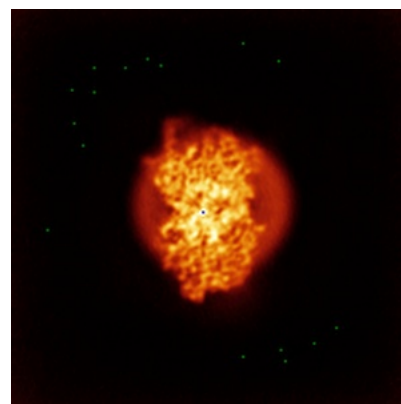
6.4.2 Raw map



X



Y

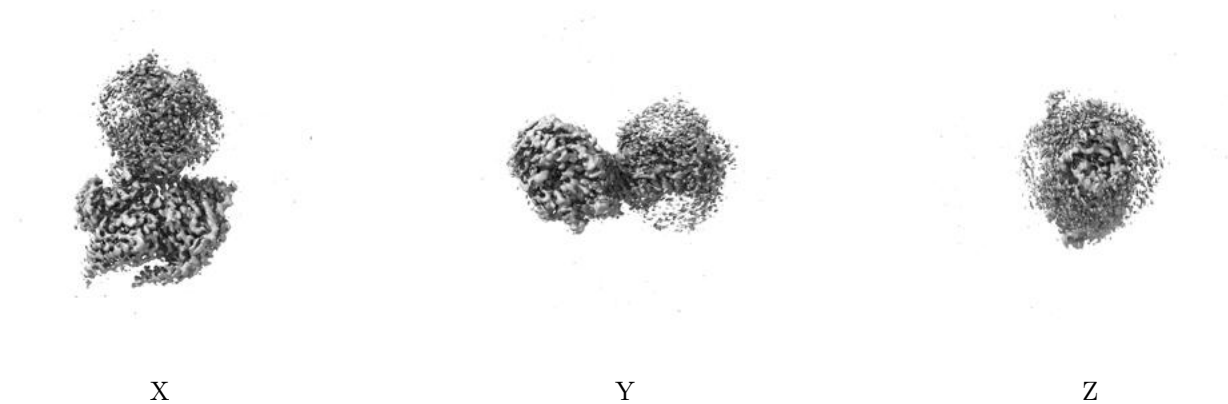


Z

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.

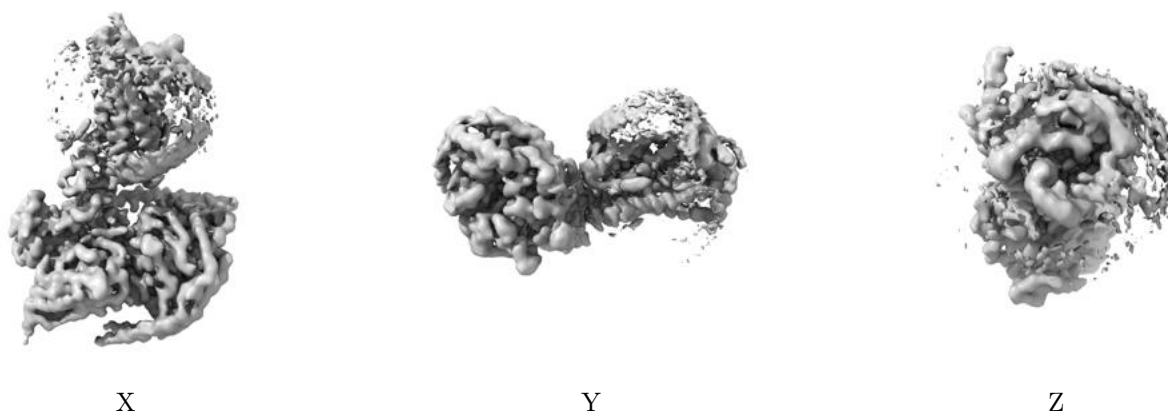
6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.38. 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.

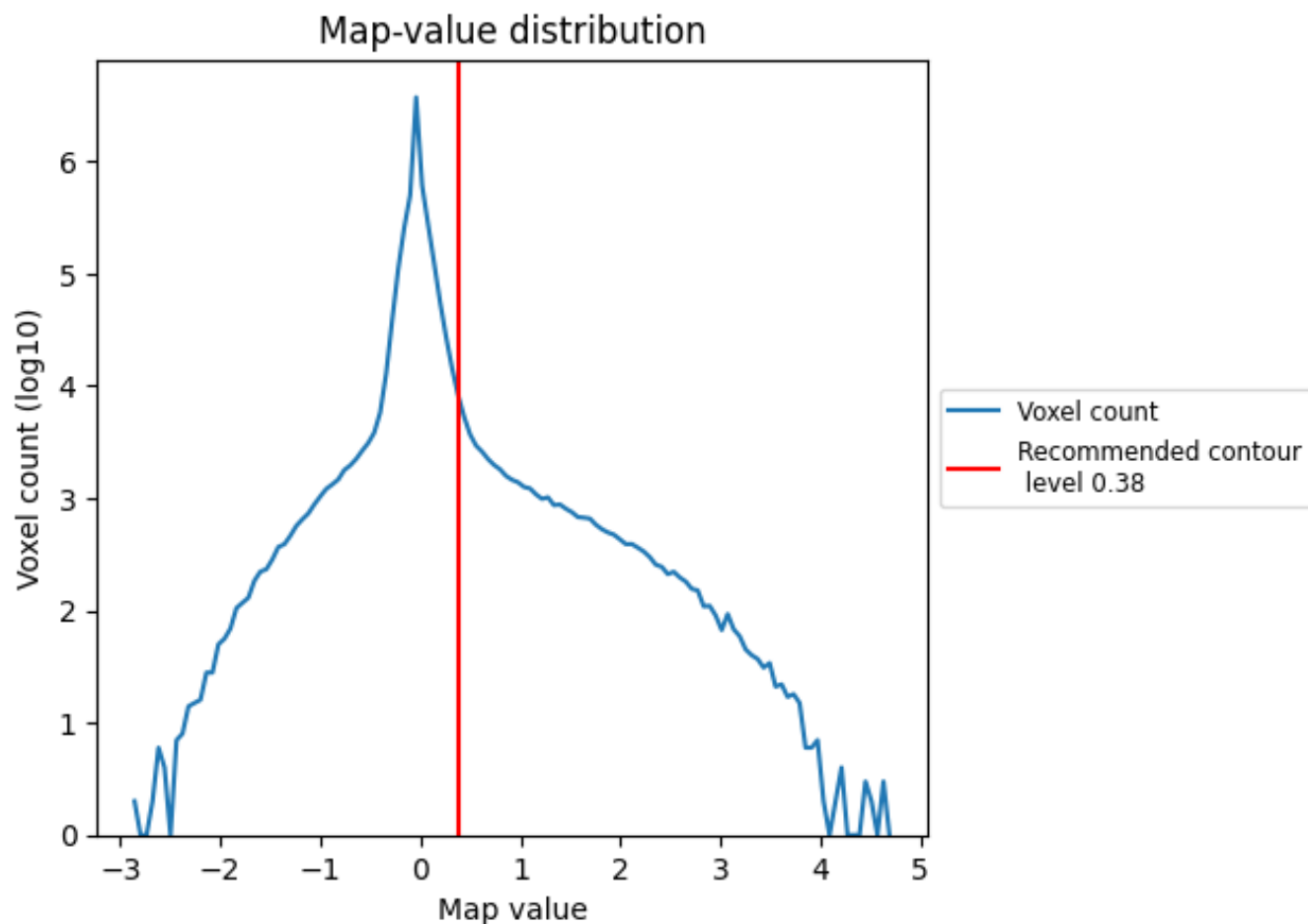
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

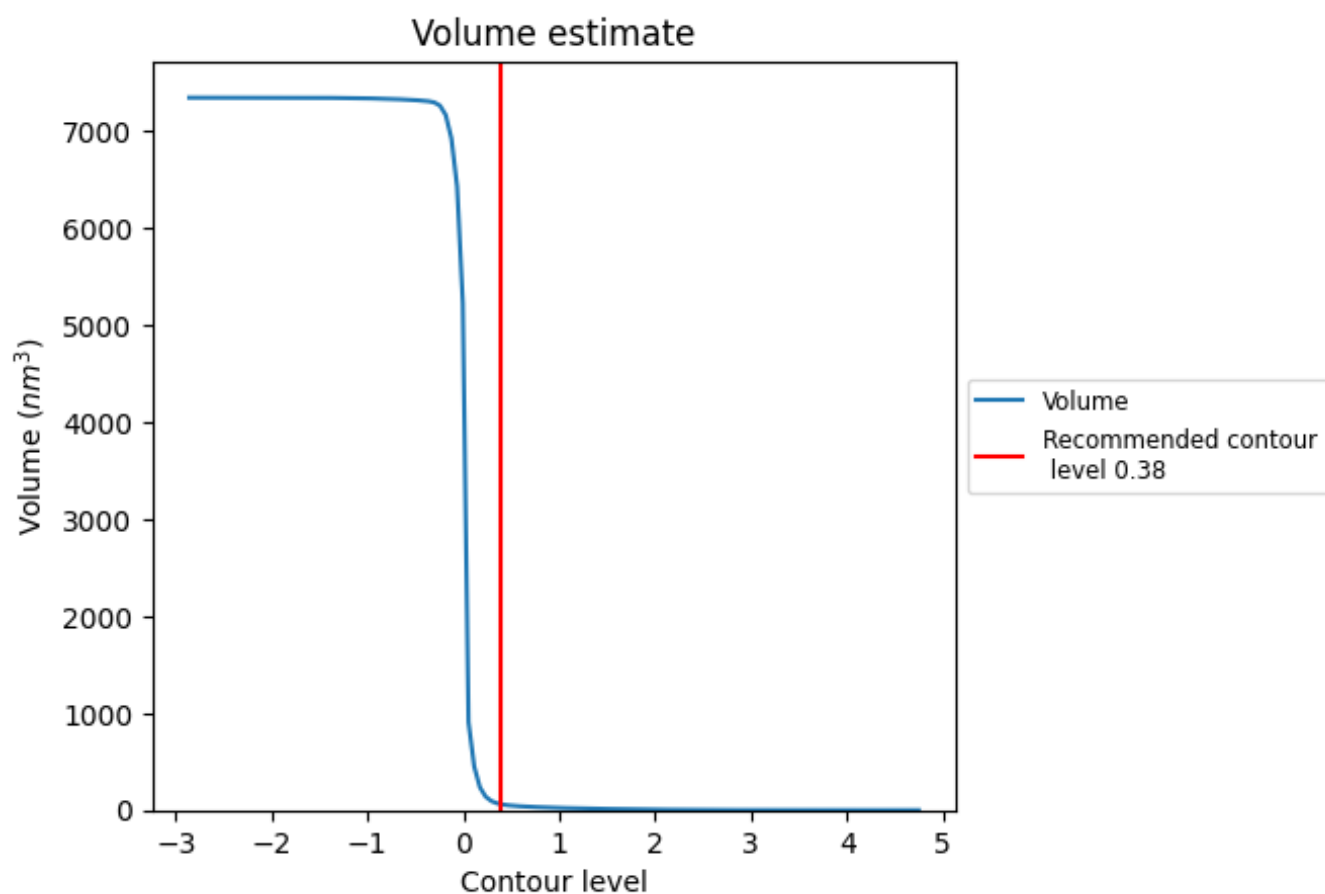
This section contains the results of statistical analysis of the map.

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.

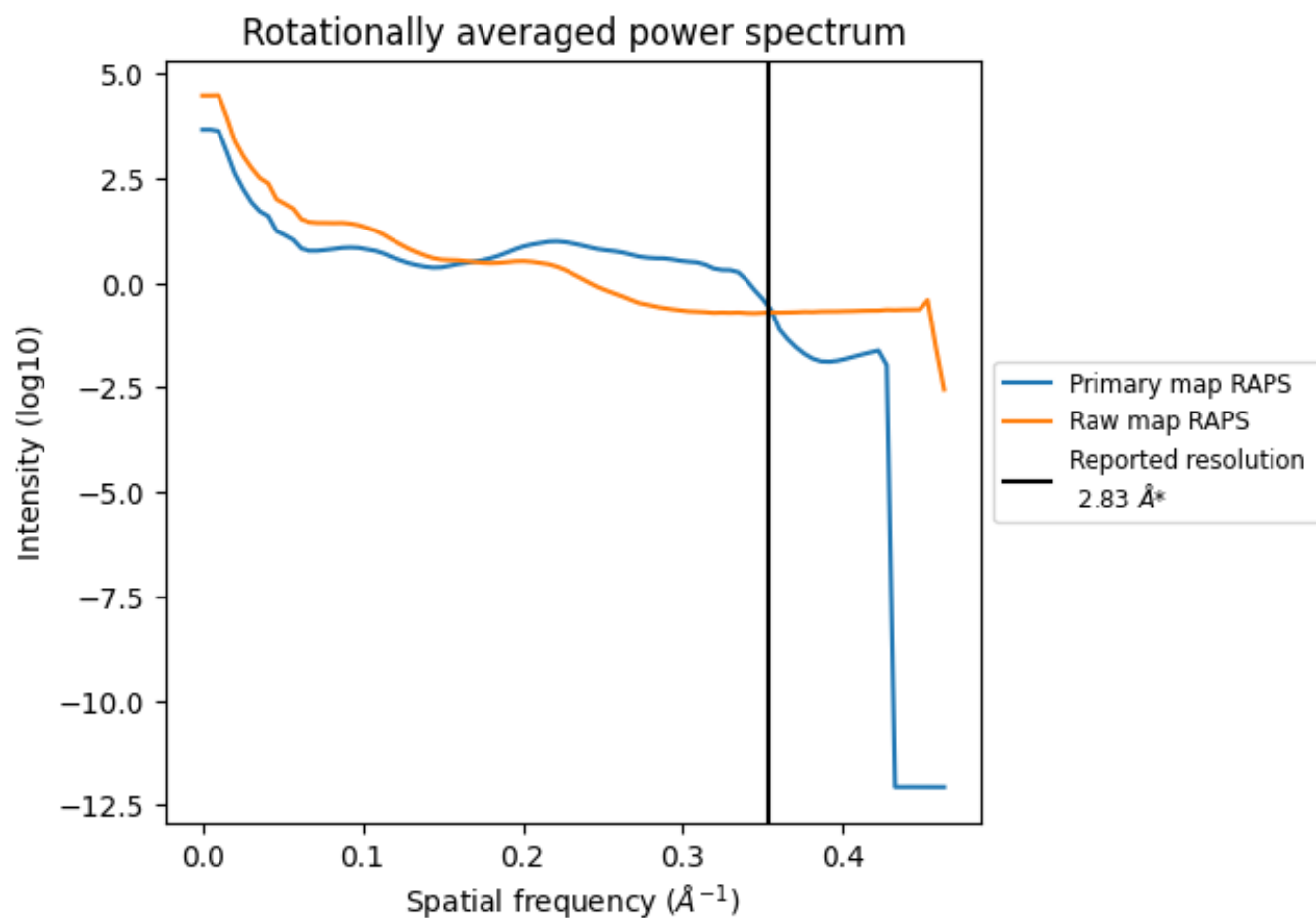
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 65 nm^3 ; 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 ⓘ

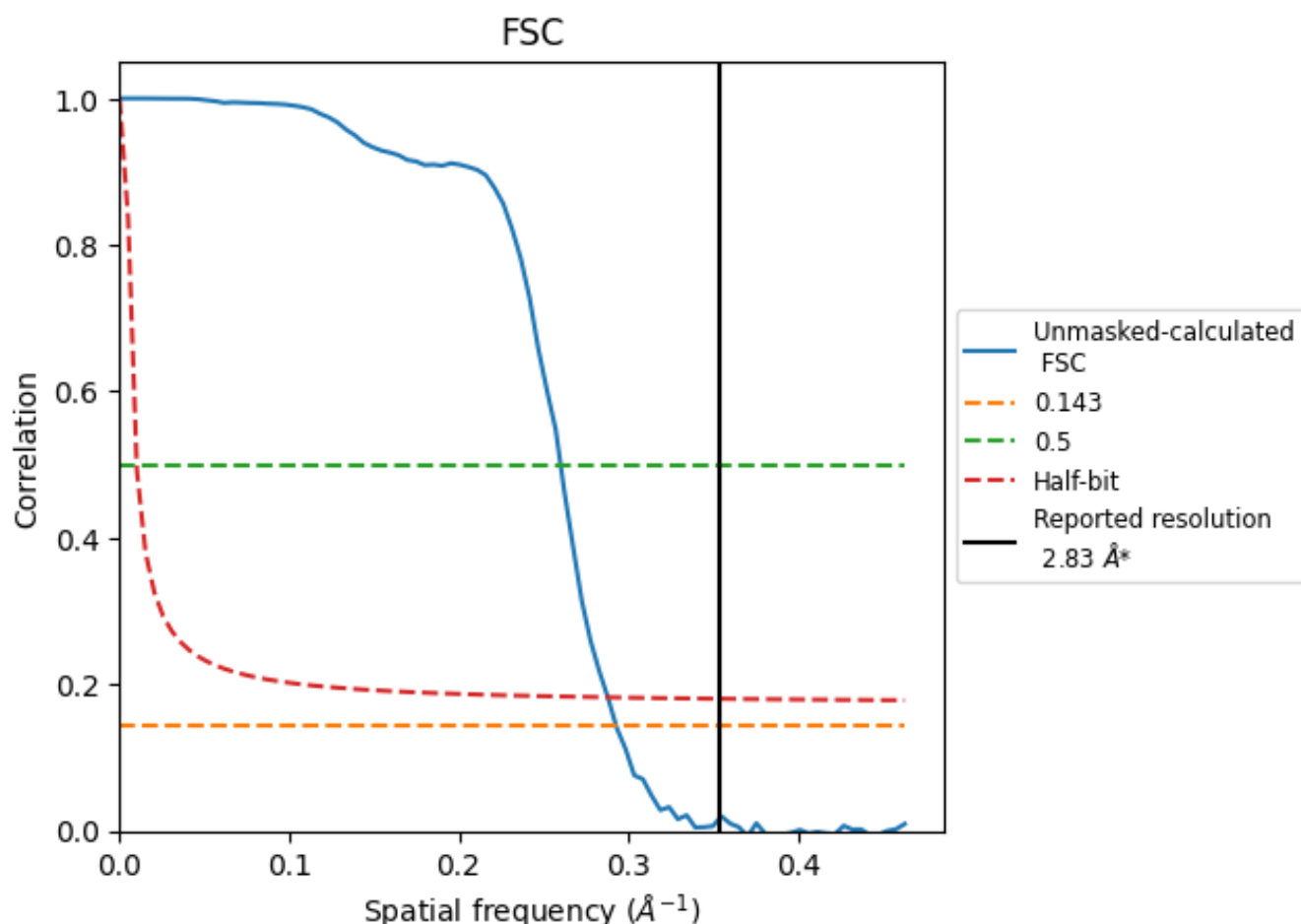


*Reported resolution corresponds to spatial frequency of 0.353 Å⁻¹

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 0.353 \AA^{-1}

8.2 Resolution estimates [i](#)

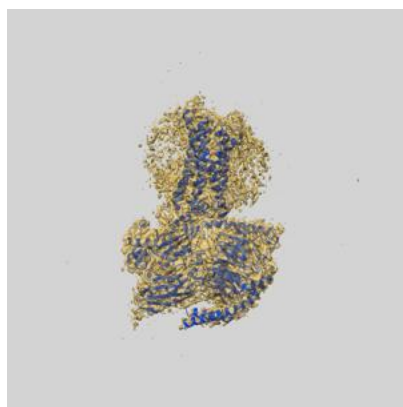
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	2.83	-	-
Author-provided FSC curve	-	-	-
Unmasked-calculated*	3.42	3.84	3.47

*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 3.42 differs from the reported value 2.83 by more than 10 %

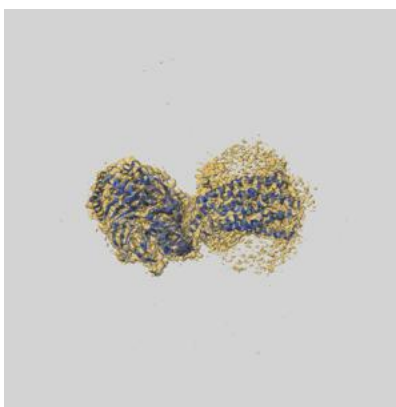
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-37237 and PDB model 8KH5. Per-residue inclusion information can be found in section [3](#) on page [8](#).

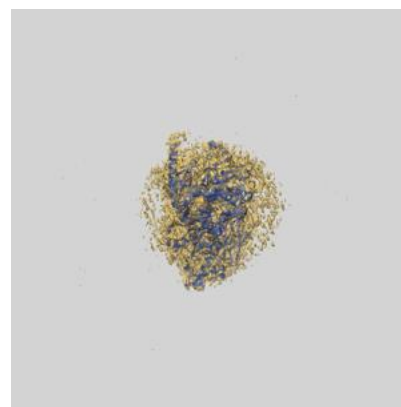
9.1 Map-model overlay [i](#)



X



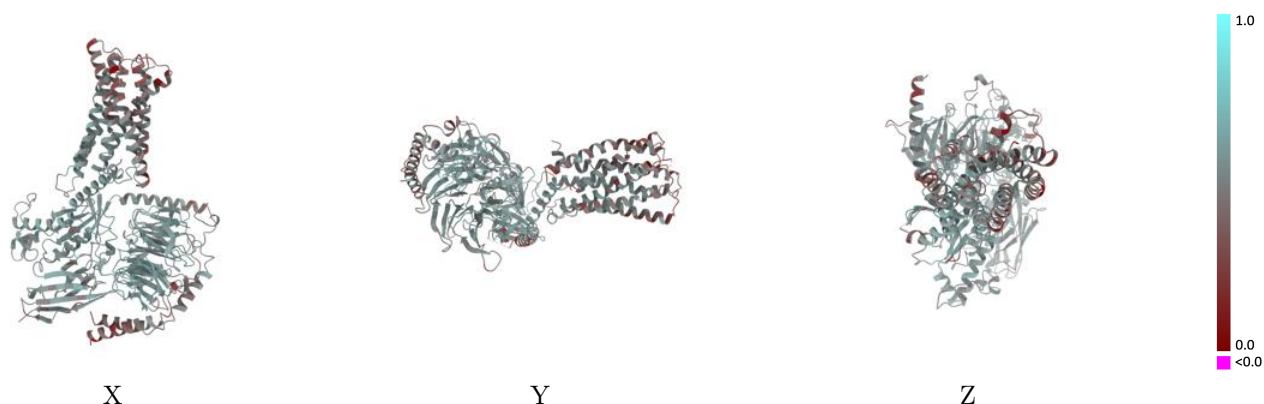
Y



Z

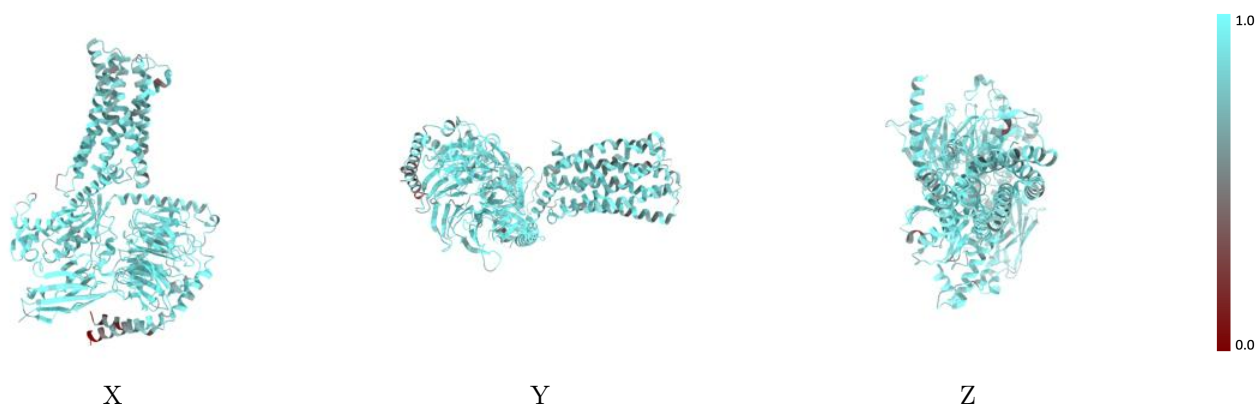
The images above show the 3D surface view of the map at the recommended contour level 0.38 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



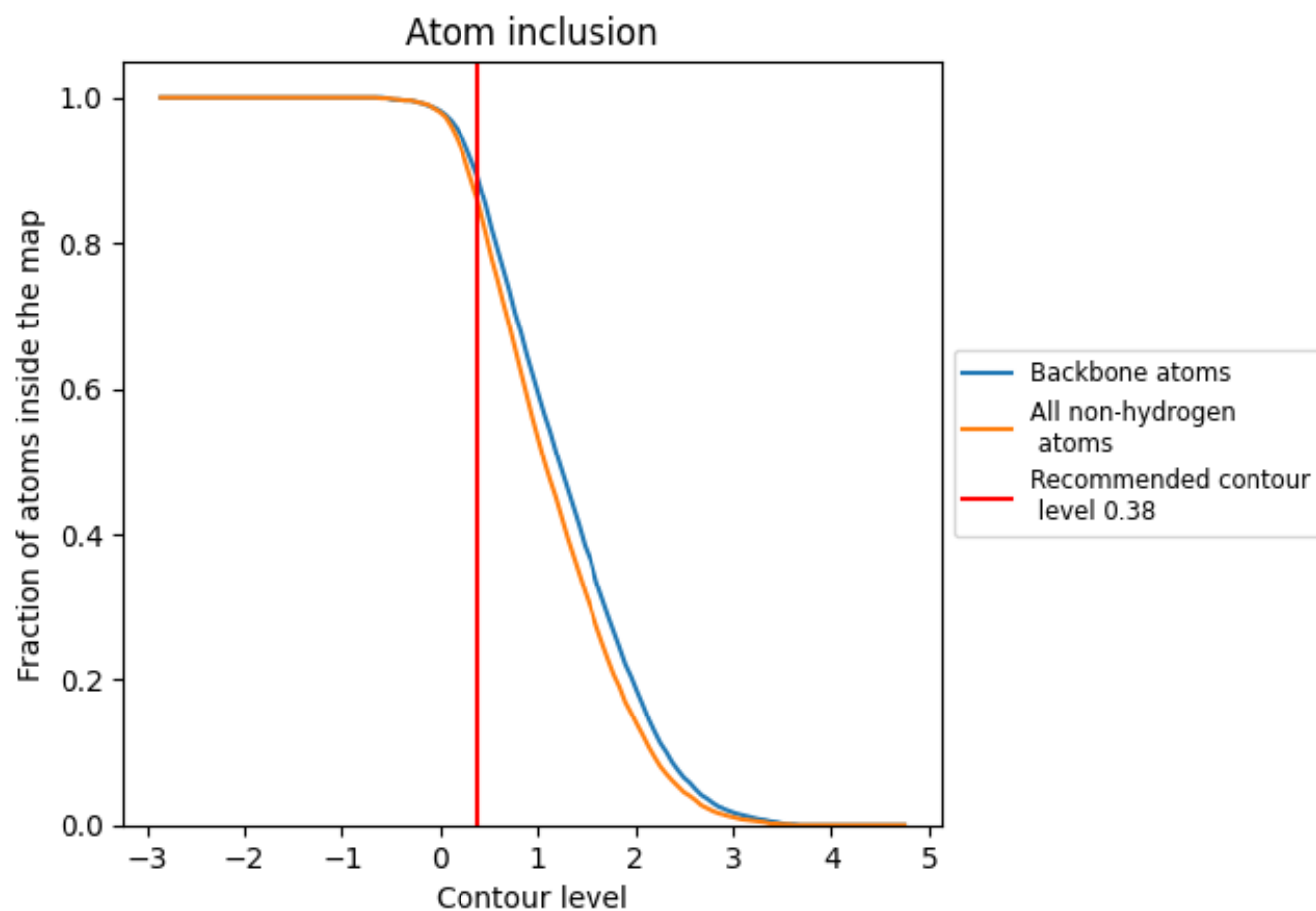
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.38).

9.4 Atom inclusion [i](#)



At the recommended contour level, 89% of all backbone atoms, 86% 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 (0.38) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	<div></div> 0.8610	<div></div> 0.5140
A	<div></div> 0.8150	<div></div> 0.4680
B	<div></div> 0.8850	<div></div> 0.5400
C	<div></div> 0.8890	<div></div> 0.5390
D	<div></div> 0.7570	<div></div> 0.4650
E	<div></div> 0.8920	<div></div> 0.5260

