Full wwPDB EM Validation Report ⓘ

Sep 28, 2022 – 02:42 AM JST

PDB ID	:	7YU6
EMDB ID	:	EMD-34100
Title	:	Human Lysophosphatidic Acid Receptor 1-Gi complex bound to ONO-0740556, state2
Authors	:	Akasaka, H.; Shihoya, W.; Nureki, O.
Deposited on	:	2022-08-16
Resolution	:	3.50 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:

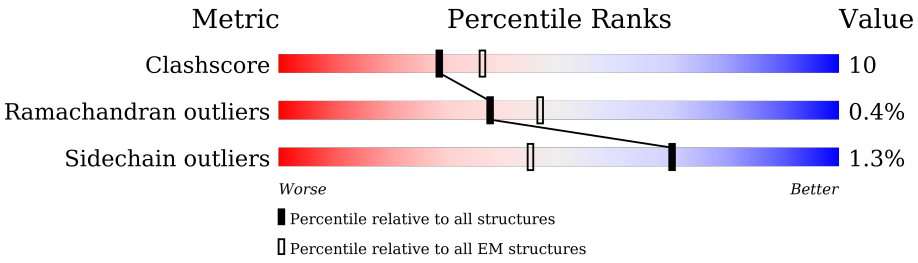
EMDB validation analysis	:	0.0.1.dev43
Mogul	:	1.8.5 (274361), CSD as541be (2020)
MolProbity	:	4.02b-467
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ	:	1.9.9
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.31.2

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
ELECTRON MICROSCOPY

The reported resolution of this entry is 3.50 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	158937	4297
Ramachandran outliers	154571	4023
Sidechain outliers	154315	3826

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 <=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	B	351	11% 74% 21%
2	A	354	12% 51% 12% 37%
3	G	68	28% 63% 16% 21%
4	R	379	32% 52% 23% 23%
5	S	260	15% 72% 18% 11%

2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 8787 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
1	B	338	2597	1602	467	507	21	0	0

There are 12 discrepancies between the modelled and reference sequences:

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

- Molecule 2 is a protein called Guanine nucleotide-binding protein G(i) subunit alpha-1.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
2	A	222	1780	1131	296	340	13	0	0

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
3	G	54	413	260	71	79	3	0	0

There is a discrepancy between the modelled and reference sequences:

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

- Molecule 4 is a protein called Lysophosphatidic acid receptor 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	R	290	Total	C	N	O	S	0	0
			2223	1468	356	376	23		

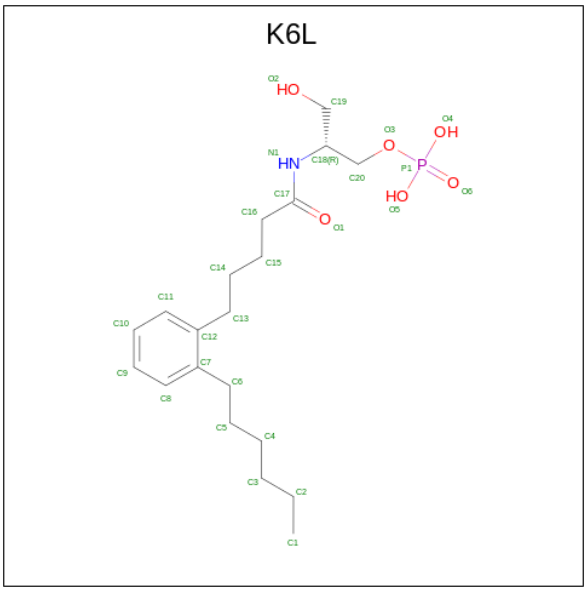
There are 16 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
R	-8	ASP	-	expression tag	UNP Q92633
R	-7	TYR	-	expression tag	UNP Q92633
R	-6	LYS	-	expression tag	UNP Q92633
R	-5	ASP	-	expression tag	UNP Q92633
R	-4	ASP	-	expression tag	UNP Q92633
R	-3	ASP	-	expression tag	UNP Q92633
R	-2	ASP	-	expression tag	UNP Q92633
R	-1	ALA	-	expression tag	UNP Q92633
R	0	MET	-	expression tag	UNP Q92633
R	1	GLY	-	expression tag	UNP Q92633
R	365	GLU	-	expression tag	UNP Q92633
R	366	ASN	-	expression tag	UNP Q92633
R	367	LEU	-	expression tag	UNP Q92633
R	368	TYR	-	expression tag	UNP Q92633
R	369	PHE	-	expression tag	UNP Q92633
R	370	GLN	-	expression tag	UNP Q92633

- Molecule 5 is a protein called scFv16.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	S	232	Total	C	N	O	S	0	0
			1746	1114	294	328	10		

- Molecule 6 is [(2 {R})-2-[5-(2-hexylphenyl)pentanoylamino]-3-oxidanyl-propyl] dihydrogen phosphate (three-letter code: K6L) (formula: $C_{20}H_{34}NO_6P$) (labeled as "Ligand of Interest" by depositor).

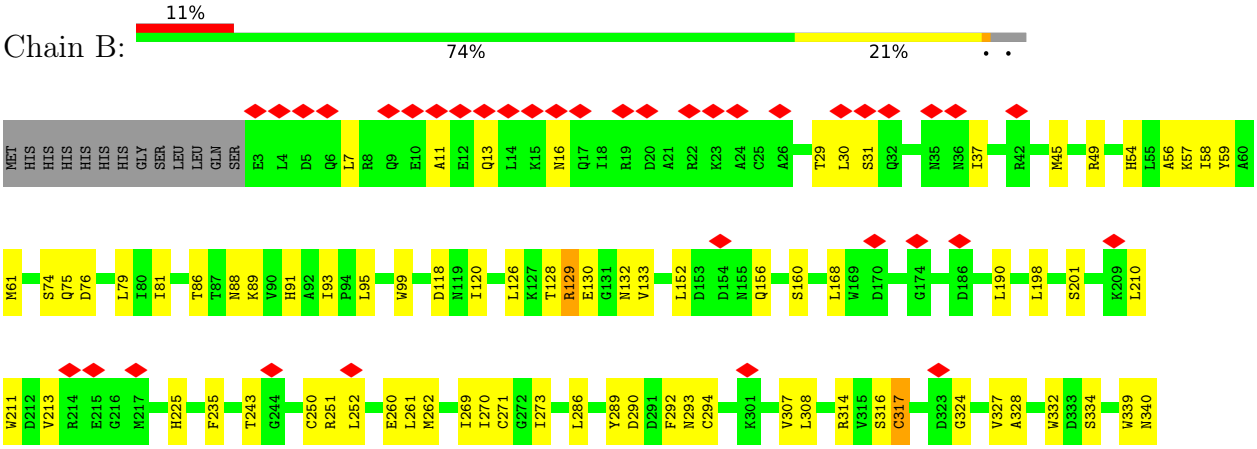


Mol	Chain	Residues	Atoms					AltConf
6	R	1	Total	C	N	O	P	0
			28	20	1	6	1	

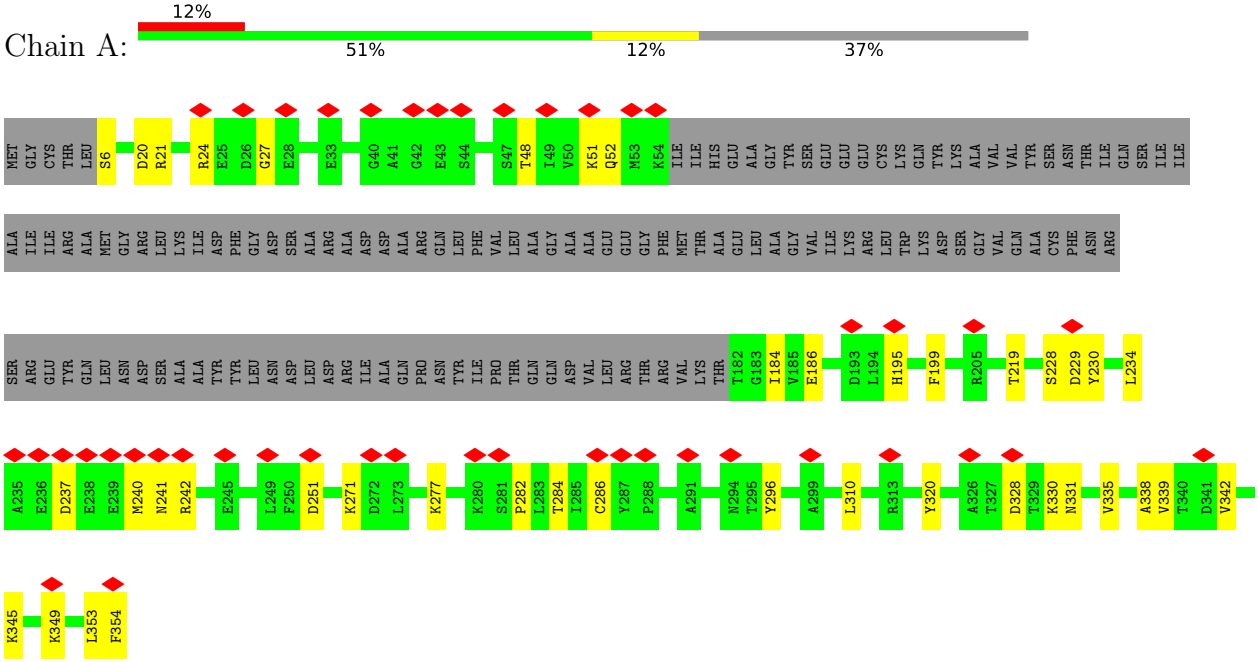
3 Residue-property plots (i)

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion in map density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red diamond above a residue indicates a poor fit to the EM map for this residue (all-atom inclusion < 40%). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

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

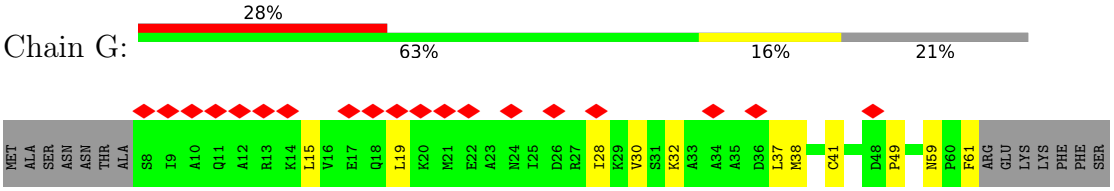


• Molecule 2: Guanine nucleotide-binding protein G(i) subunit alpha-1



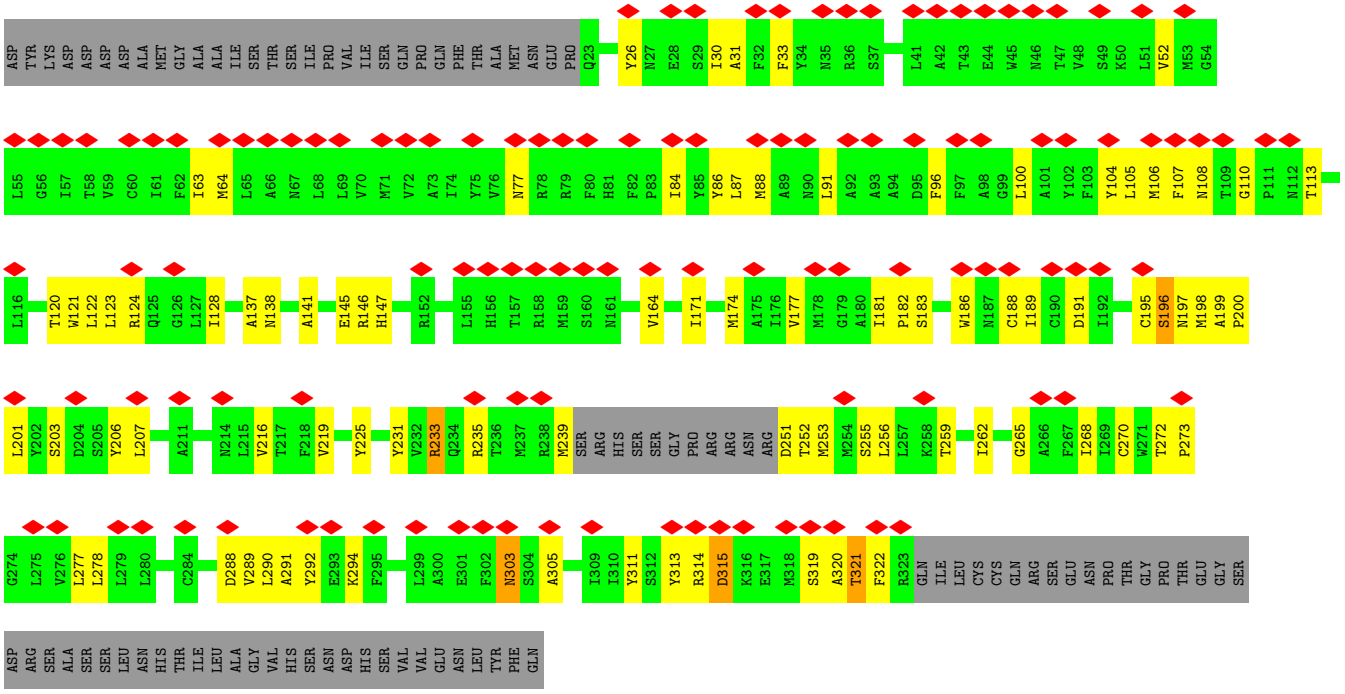
• Molecule 3: Guanine nucleotide-binding protein G(I)/G(S)/G(O) subunit gamma-2

Chain G:



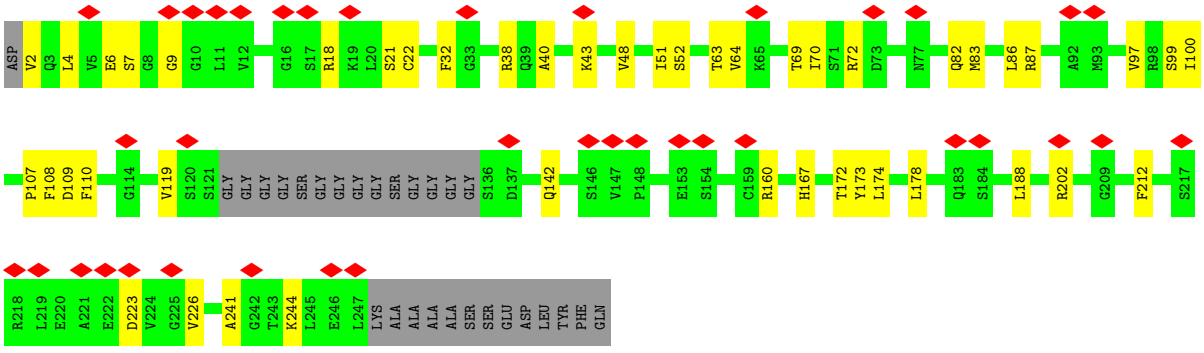
• Molecule 4: Lysophosphatidic acid receptor 1

Chain R:



• Molecule 5: scFv16

Chain S:



4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	127465	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 ($e^-/Å^2$)	50	Depositor
Minimum defocus (nm)	500	Depositor
Maximum defocus (nm)	2500	Depositor
Magnification	Not provided	
Image detector	GATAN K3 (6k x 4k)	Depositor
Maximum map value	8.556	Depositor
Minimum map value	-6.039	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.444	Depositor
Recommended contour level	1.4	Depositor
Map size (Å)	169.7184, 126.69119, 160.1568	wwPDB
Map dimensions	142, 106, 134	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.1952, 1.1952, 1.1952	Depositor

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: K6L

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	B	0.83	0/2644	0.90	0/3584
2	A	0.77	0/1810	0.85	0/2428
3	G	0.61	0/419	0.86	0/566
4	R	0.72	0/2277	0.86	0/3112
5	S	0.72	0/1790	0.82	0/2432
All	All	0.76	0/8940	0.86	0/12122

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

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	B	2597	0	2501	57	0
2	A	1780	0	1757	29	0
3	G	413	0	423	14	0
4	R	2223	0	2174	71	0
5	S	1746	0	1667	30	0
6	R	28	0	0	2	0
All	All	8787	0	8522	180	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 10.

All (180) 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)
2:A:6:SER:HB3	5:S:167:HIS:CD2	2.19	0.78
1:B:89:LYS:HD2	2:A:20:ASP:OD1	1.86	0.75
4:R:26:TYR:HB3	4:R:189:ILE:HG21	1.72	0.71
1:B:59:TYR:HE2	1:B:75:GLN:HG2	1.54	0.70
1:B:59:TYR:HE2	1:B:75:GLN:CG	2.04	0.69
4:R:26:TYR:HB3	4:R:189:ILE:CG2	2.23	0.68
4:R:105:LEU:HD12	4:R:128:ILE:HG13	1.75	0.68
4:R:289:VAL:C	4:R:291:ALA:H	1.96	0.67
1:B:79:LEU:HB3	1:B:93:ILE:HB	1.78	0.66
5:S:9:GLY:O	5:S:18:ARG:NH2	2.29	0.66
2:A:229:ASP:HB3	2:A:242:ARG:HB2	1.78	0.66
4:R:104:TYR:O	4:R:108:ASN:ND2	2.28	0.65
1:B:271:CYS:HB3	1:B:290:ASP:HB2	1.79	0.64
4:R:87:LEU:HD12	4:R:145:GLU:OE1	1.98	0.64
1:B:314:ARG:HD2	1:B:332:TRP:CZ2	2.32	0.63
4:R:265:GLY:HA2	4:R:268:ILE:HG22	1.81	0.63
2:A:21:ARG:O	2:A:21:ARG:HG2	2.00	0.62
5:S:142:GLN:NE2	5:S:241:ALA:O	2.25	0.61
1:B:160:SER:HB3	1:B:190:LEU:HD23	1.82	0.61
5:S:109:ASP:OD1	5:S:110:PHE:N	2.34	0.61
2:A:6:SER:HB3	5:S:167:HIS:NE2	2.15	0.60
4:R:121:TRP:CZ3	4:R:201:LEU:HB2	2.37	0.59
1:B:37:ILE:HD11	3:G:38:MET:HG3	1.85	0.59
1:B:324:GLY:O	3:G:49:PRO:HB2	2.01	0.58
5:S:202:ARG:NH2	5:S:223:ASP:OD2	2.37	0.58
1:B:314:ARG:HD2	1:B:332:TRP:CE2	2.37	0.58
5:S:63:THR:HG23	5:S:64:VAL:HG13	1.86	0.58
2:A:271:LYS:HB2	2:A:296:TYR:OH	2.03	0.57
4:R:121:TRP:HZ3	4:R:201:LEU:HB2	1.69	0.57
1:B:59:TYR:HE2	1:B:75:GLN:CD	2.09	0.56
1:B:286:LEU:HD22	1:B:327:VAL:HG11	1.88	0.56
4:R:84:ILE:O	4:R:88:MET:HG2	2.05	0.56
5:S:178:LEU:HB2	5:S:188:LEU:HD11	1.87	0.56
4:R:33:PHE:CD2	4:R:201:LEU:HD21	2.40	0.56
4:R:110:GLY:O	4:R:113:THR:HG22	2.06	0.56
1:B:59:TYR:CE2	1:B:75:GLN:HG2	2.38	0.56
2:A:230:TYR:O	2:A:241:ASN:ND2	2.39	0.55
4:R:289:VAL:C	4:R:291:ALA:N	2.61	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:R:233:ARG:HG3	4:R:253:MET:CE	2.38	0.54
2:A:328:ASP:HB3	2:A:330:LYS:HG3	1.89	0.53
4:R:141:ALA:HB2	4:R:171:ILE:HD11	1.90	0.53
4:R:188:CYS:HB2	4:R:191:ASP:O	2.08	0.53
1:B:261:LEU:HD21	3:G:30:VAL:HG23	1.92	0.52
3:G:28:ILE:HD11	3:G:32:LYS:HD3	1.90	0.52
5:S:6:GLU:HA	5:S:22:CYS:HA	1.92	0.52
1:B:235:PHE:CE2	3:G:37:LEU:CD2	2.93	0.52
1:B:290:ASP:C	1:B:292:PHE:H	2.14	0.51
1:B:225:HIS:NE2	1:B:243:THR:OG1	2.41	0.51
1:B:61:MET:HG3	1:B:317:CYS:HB2	1.93	0.51
4:R:272:THR:N	4:R:273:PRO:HD2	2.26	0.51
4:R:91:LEU:HD13	4:R:138:ASN:CB	2.41	0.51
4:R:121:TRP:CZ3	4:R:201:LEU:HD23	2.46	0.51
4:R:198:MET:SD	4:R:277:LEU:HD21	2.51	0.51
1:B:75:GLN:HA	1:B:75:GLN:OE1	2.12	0.50
4:R:33:PHE:CG	4:R:201:LEU:HD21	2.47	0.50
2:A:234:LEU:HB2	2:A:237:ASP:OD1	2.12	0.50
1:B:168:LEU:HD22	1:B:213:VAL:HG12	1.94	0.50
2:A:338:ALA:O	2:A:342:VAL:HG23	2.11	0.49
4:R:320:ALA:C	4:R:322:PHE:N	2.63	0.49
5:S:4:LEU:HD12	5:S:110:PHE:HD2	1.75	0.49
1:B:293:ASN:HD22	1:B:307:VAL:HG13	1.78	0.49
2:A:24:ARG:O	2:A:27:GLY:N	2.45	0.49
4:R:262:ILE:HD11	4:R:313:TYR:CE1	2.47	0.49
5:S:32:PHE:CD1	5:S:100:ILE:HB	2.48	0.49
1:B:54:HIS:CD2	1:B:58:ILE:HD11	2.47	0.49
4:R:77:ASN:OD1	4:R:321:THR:HG21	2.12	0.49
2:A:186:GLU:HG2	2:A:199:PHE:CD1	2.48	0.49
1:B:29:THR:HG22	1:B:31:SER:H	1.78	0.48
1:B:49:ARG:NH1	3:G:61:PHE:HA	2.29	0.48
4:R:106:MET:O	4:R:107:PHE:HB2	2.13	0.48
4:R:88:MET:HE1	4:R:311:TYR:HD2	1.79	0.48
4:R:320:ALA:O	4:R:322:PHE:N	2.47	0.48
4:R:146:ARG:NH1	4:R:225:TYR:OH	2.46	0.48
4:R:196:SER:OG	4:R:197:ASN:N	2.47	0.47
5:S:52:SER:O	5:S:72:ARG:NH1	2.47	0.47
4:R:137:ALA:HB3	4:R:171:ILE:HG23	1.95	0.47
4:R:122:LEU:HD22	4:R:183:SER:HA	1.96	0.47
5:S:172:THR:O	5:S:174:LEU:N	2.43	0.47
2:A:6:SER:CB	5:S:167:HIS:CD2	2.95	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:R:181:ILE:N	4:R:182:PRO:HD2	2.29	0.47
1:B:316:SER:OG	1:B:332:TRP:CD1	2.67	0.47
1:B:235:PHE:CE2	3:G:37:LEU:HD23	2.49	0.47
5:S:2:VAL:O	5:S:2:VAL:HG22	2.14	0.47
1:B:59:TYR:CE2	1:B:75:GLN:CD	2.89	0.46
1:B:126:LEU:HA	1:B:133:VAL:HG22	1.97	0.46
4:R:33:PHE:CZ	4:R:201:LEU:HD11	2.49	0.46
5:S:83:MET:HB3	5:S:86:LEU:HD21	1.98	0.46
1:B:30:LEU:HB3	1:B:262:MET:HE2	1.98	0.46
1:B:269:ILE:HG21	1:B:289:TYR:CE2	2.50	0.46
4:R:52:VAL:HG11	4:R:294:LYS:HD3	1.98	0.46
1:B:251:ARG:NH1	1:B:260:GLU:OE2	2.43	0.46
2:A:186:GLU:HG2	2:A:199:PHE:HD1	1.81	0.46
1:B:129:ARG:NH1	5:S:2:VAL:HG11	2.31	0.46
4:R:91:LEU:HD13	4:R:138:ASN:HB2	1.98	0.46
1:B:49:ARG:HH11	3:G:61:PHE:HD1	1.63	0.46
4:R:100:LEU:HA	4:R:100:LEU:HD23	1.84	0.46
1:B:7:LEU:O	1:B:11:ALA:N	2.42	0.45
1:B:308:LEU:HD23	1:B:339:TRP:CD2	2.52	0.45
4:R:270:CYS:HB3	4:R:303:ASN:HB2	1.98	0.45
4:R:30:ILE:HG13	4:R:31:ALA:N	2.32	0.45
1:B:81:ILE:HD13	1:B:91:HIS:HB2	1.99	0.45
4:R:121:TRP:CH2	4:R:200:PRO:HD2	2.53	0.45
4:R:146:ARG:O	4:R:147:HIS:C	2.55	0.45
1:B:235:PHE:HZ	3:G:41:CYS:SG	2.40	0.44
1:B:250:CYS:SG	1:B:273:ILE:HD13	2.57	0.44
4:R:177:VAL:O	4:R:181:ILE:HG12	2.18	0.44
4:R:290:LEU:H	4:R:290:LEU:HD12	1.82	0.44
1:B:235:PHE:CZ	3:G:37:LEU:HD22	2.53	0.44
4:R:196:SER:HB3	4:R:199:ALA:O	2.18	0.44
1:B:76:ASP:N	1:B:76:ASP:OD1	2.48	0.44
4:R:63:ILE:HG12	4:R:305:ALA:HA	1.98	0.44
2:A:228:SER:O	2:A:277:LYS:NZ	2.36	0.44
4:R:207:LEU:HD12	4:R:278:LEU:HD22	2.00	0.44
1:B:86:THR:OG1	1:B:88:ASN:OD1	2.30	0.43
1:B:198:LEU:HB3	1:B:210:LEU:HD11	1.98	0.43
2:A:237:ASP:HB2	2:A:240:MET:HE1	2.00	0.43
2:A:282:PRO:HB2	2:A:284:THR:HG22	1.99	0.43
4:R:64:MET:HG2	4:R:96:PHE:CE1	2.53	0.43
1:B:79:LEU:HB2	1:B:95:LEU:HD21	1.98	0.43
5:S:87:ARG:O	5:S:119:VAL:HG21	2.18	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:R:278:LEU:HD11	6:R:401:K6L:C5	2.48	0.43
4:R:320:ALA:C	4:R:322:PHE:H	2.22	0.43
5:S:51:ILE:HG13	5:S:70:ILE:HD13	2.00	0.43
1:B:56:ALA:O	1:B:334:SER:OG	2.33	0.43
1:B:61:MET:CE	1:B:328:ALA:HB3	2.49	0.43
2:A:320:TYR:CD2	4:R:239:MET:HE2	2.54	0.43
4:R:233:ARG:HG3	4:R:253:MET:HE1	1.99	0.43
2:A:345:LYS:O	2:A:349:LYS:HG2	2.19	0.43
4:R:231:TYR:CE1	4:R:235:ARG:HD2	2.54	0.43
1:B:132:ASN:O	1:B:133:VAL:C	2.56	0.43
2:A:354:PHE:HE1	4:R:252:THR:HA	1.84	0.43
5:S:99:SER:HB2	5:S:107:PRO:HB3	2.01	0.43
1:B:57:LYS:HB2	1:B:332:TRP:HA	2.01	0.43
4:R:64:MET:HA	4:R:96:PHE:HD1	1.83	0.43
5:S:69:THR:HB	5:S:82:GLN:HB3	2.01	0.43
1:B:13:GLN:OE1	1:B:16:ASN:ND2	2.52	0.43
1:B:45:MET:HE2	1:B:308:LEU:HD21	2.00	0.43
4:R:91:LEU:HD13	4:R:138:ASN:HB3	2.01	0.42
2:A:331:ASN:O	2:A:335:VAL:HG23	2.19	0.42
4:R:189:ILE:HD13	4:R:201:LEU:HD12	2.01	0.42
4:R:216:VAL:HA	4:R:219:VAL:HG22	2.00	0.42
4:R:186:TRP:HD1	4:R:206:TYR:HB2	1.84	0.42
2:A:230:TYR:O	2:A:286:CYS:HB3	2.19	0.42
2:A:251:ASP:HB2	2:A:310:LEU:HD12	2.01	0.42
5:S:7:SER:OG	5:S:21:SER:OG	2.27	0.42
3:G:37:LEU:HD23	3:G:37:LEU:HA	1.85	0.42
5:S:38:ARG:HD3	5:S:48:VAL:HG11	2.01	0.42
5:S:174:LEU:HD13	5:S:212:PHE:CG	2.55	0.42
1:B:118:ASP:OD2	1:B:120:ILE:HD12	2.19	0.42
1:B:340:ASN:ND2	3:G:59:ASN:OD1	2.53	0.42
2:A:219:THR:HG21	2:A:339:VAL:HG13	2.02	0.42
4:R:174:MET:HA	4:R:177:VAL:HG12	2.02	0.42
5:S:97:VAL:HG11	5:S:108:PHE:CD2	2.55	0.42
5:S:174:LEU:HD13	5:S:212:PHE:CD1	2.55	0.42
4:R:86:TYR:HB2	4:R:164:VAL:HG21	2.01	0.42
4:R:233:ARG:HG3	4:R:253:MET:HE2	2.01	0.42
4:R:255:SER:OG	4:R:314:ARG:NH1	2.53	0.42
2:A:353:LEU:HG	4:R:256:LEU:HD11	2.02	0.41
4:R:315:ASP:OD1	4:R:315:ASP:N	2.53	0.41
1:B:152:LEU:HB2	1:B:156:GLN:HB2	2.02	0.41
1:B:308:LEU:HD23	1:B:339:TRP:CG	2.56	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:237:ASP:HB2	2:A:240:MET:CE	2.50	0.41
2:A:320:TYR:CD2	4:R:239:MET:CE	3.03	0.41
5:S:160:ARG:NH1	5:S:160:ARG:HB3	2.35	0.41
4:R:195:CYS:HB2	4:R:203:SER:HA	2.03	0.41
5:S:51:ILE:HG22	5:S:52:SER:O	2.21	0.41
1:B:99:TRP:CD1	2:A:184:ILE:HD13	2.56	0.41
4:R:251:ASP:OD2	4:R:253:MET:HB2	2.20	0.41
4:R:259:THR:OG1	4:R:314:ARG:NE	2.54	0.41
4:R:138:ASN:OD1	4:R:171:ILE:HD13	2.21	0.41
5:S:226:VAL:HA	5:S:244:LYS:HA	2.03	0.41
1:B:252:LEU:HD21	3:G:37:LEU:HD13	2.03	0.40
1:B:74:SER:HB3	1:B:76:ASP:OD1	2.22	0.40
3:G:15:LEU:O	3:G:19:LEU:HD12	2.22	0.40
4:R:120:THR:O	4:R:123:LEU:HB3	2.21	0.40
4:R:124:ARG:NH2	6:R:401:K6L:O6	2.55	0.40
4:R:319:SER:O	4:R:322:PHE:HB2	2.21	0.40
1:B:201:SER:OG	1:B:211:TRP:NE1	2.49	0.40
2:A:48:THR:HG22	2:A:52:GLN:NE2	2.35	0.40
5:S:40:ALA:HB3	5:S:43:LYS:HB2	2.04	0.40

There are no symmetry-related clashes.

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

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	B	336/351 (96%)	317 (94%)	19 (6%)	0	100	100
2	A	218/354 (62%)	208 (95%)	10 (5%)	0	100	100
3	G	52/68 (76%)	52 (100%)	0	0	100	100
4	R	286/379 (76%)	271 (95%)	12 (4%)	3 (1%)	15	54
5	S	228/260 (88%)	220 (96%)	7 (3%)	1 (0%)	34	72

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
All	All	1120/1412 (79%)	1068 (95%)	48 (4%)	4 (0%)	38 72

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
5	S	173	TYR
4	R	196	SER
4	R	288	ASP
4	R	321	THR

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	B	280/293 (96%)	274 (98%)	6 (2%)	53 79
2	A	194/305 (64%)	192 (99%)	2 (1%)	76 88
3	G	44/56 (79%)	44 (100%)	0	100 100
4	R	229/333 (69%)	225 (98%)	4 (2%)	60 82
5	S	184/209 (88%)	184 (100%)	0	100 100
All	All	931/1196 (78%)	919 (99%)	12 (1%)	70 86

All (12) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	128	THR
1	B	129	ARG
1	B	130	GLU
1	B	270	ILE
1	B	294	CYS
1	B	317	CYS
2	A	51	LYS
2	A	195	HIS
4	R	233	ARG
4	R	292	TYR

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Mol	Chain	Res	Type
4	R	303	ASN
4	R	315	ASP

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (7) such sidechains are listed below:

Mol	Chain	Res	Type
1	B	340	ASN
2	A	269	ASN
2	A	346	ASN
4	R	90	ASN
4	R	214	ASN
4	R	303	ASN
5	S	231	GLN

5.3.3 RNA

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates

There are no monosaccharides 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	K6L	R	401	-	28,28,28	0.34	0	33,35,35	1.02	1 (3%)

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	K6L	R	401	-	-	7/25/25/25	0/1/1/1

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
6	R	401	K6L	C20-C18-N1	-3.29	103.11	109.58

There are no chirality outliers.

All (7) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
6	R	401	K6L	N1-C18-C20-O3
6	R	401	K6L	C15-C16-C17-O1
6	R	401	K6L	C15-C16-C17-N1
6	R	401	K6L	C19-C18-C20-O3
6	R	401	K6L	C11-C12-C13-C14
6	R	401	K6L	C7-C12-C13-C14
6	R	401	K6L	C19-C18-N1-C17

There are no ring outliers.

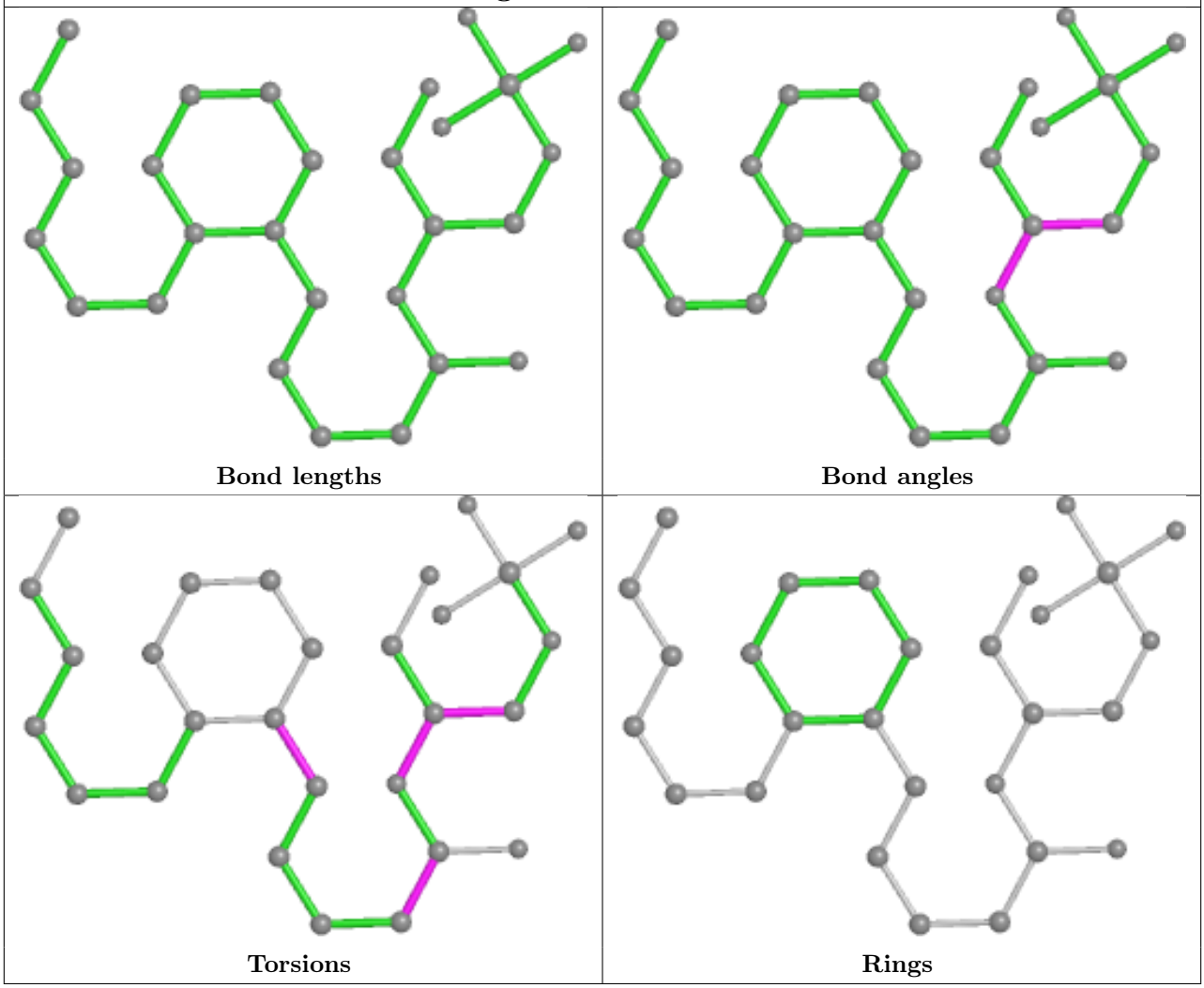
1 monomer is involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	R	401	K6L	2	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 then 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.

Ligand K6L R 401



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.

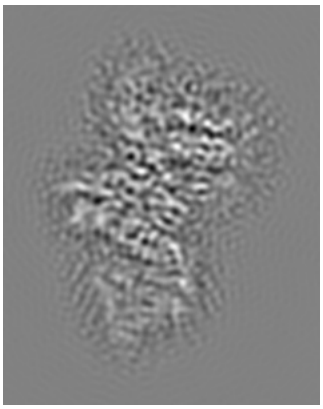
6 Map visualisation

This section contains visualisations of the EMDB entry EMD-34100. These allow visual inspection of the internal detail of the map and identification of artifacts.

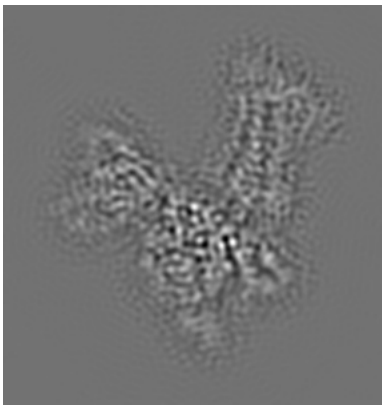
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections

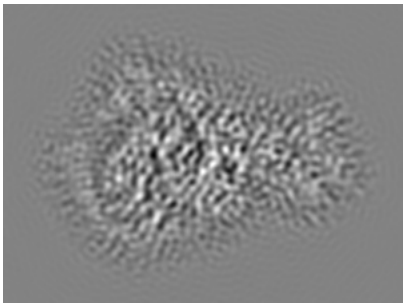
6.1.1 Primary map



X

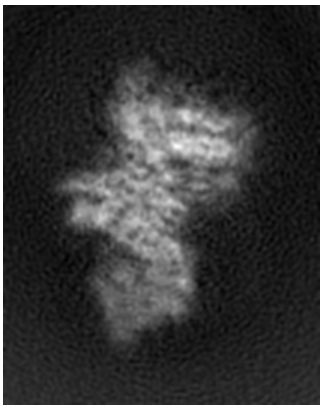


Y

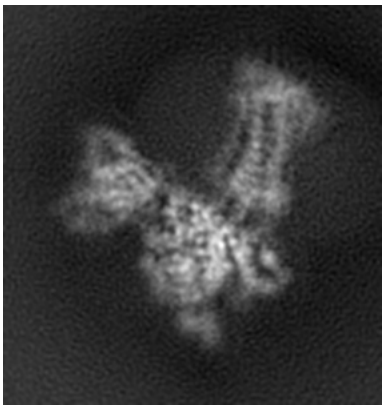


Z

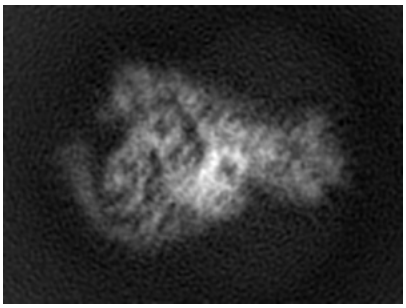
6.1.2 Raw map



X



Y

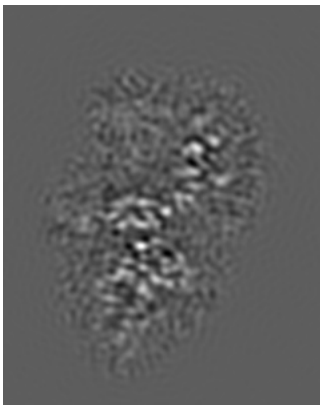


Z

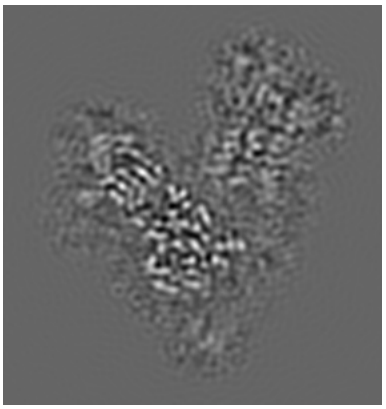
The images above show the map projected in three orthogonal directions.

6.2 Central slices (i)

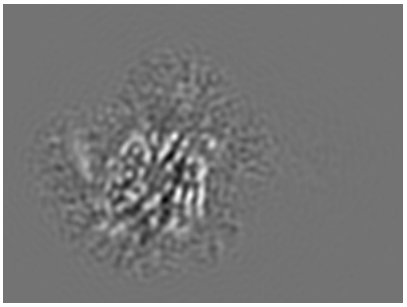
6.2.1 Primary map



X Index: 71

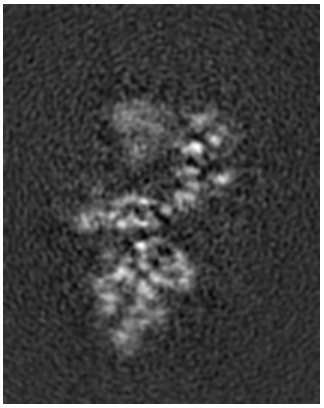


Y Index: 53

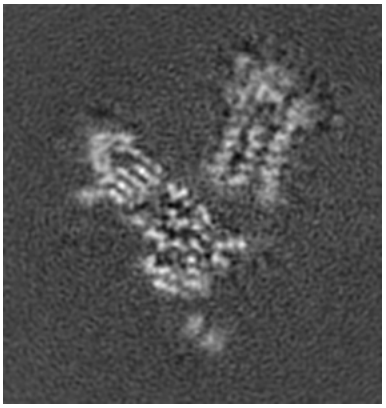


Z Index: 67

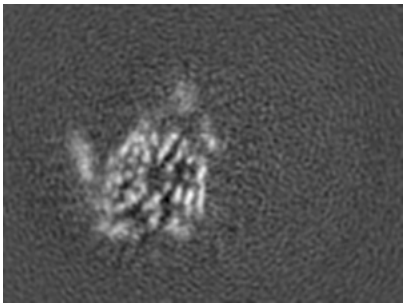
6.2.2 Raw map



X Index: 71



Y Index: 53

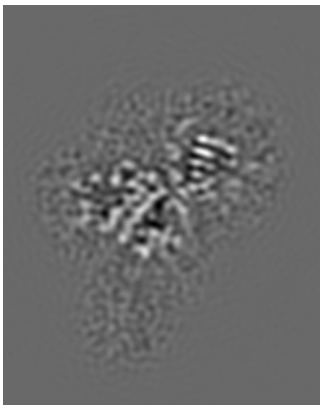


Z Index: 67

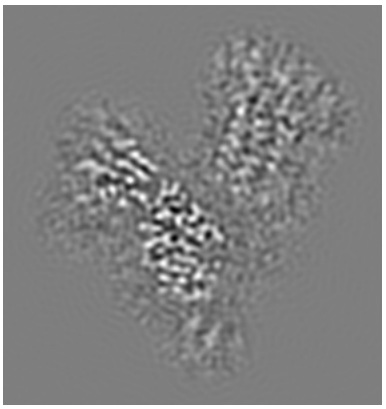
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

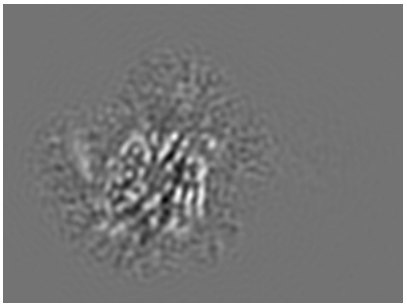
6.3.1 Primary map



X Index: 59

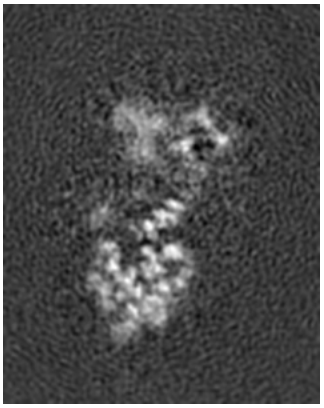


Y Index: 50

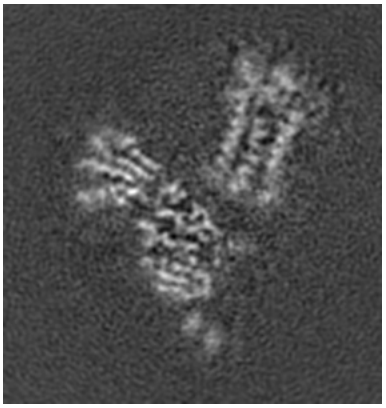


Z Index: 67

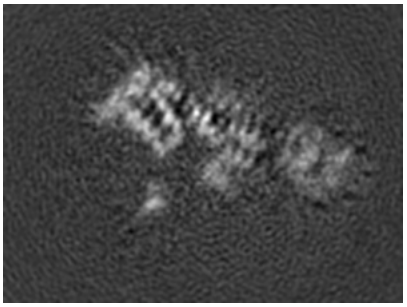
6.3.2 Raw map



X Index: 74



Y Index: 51

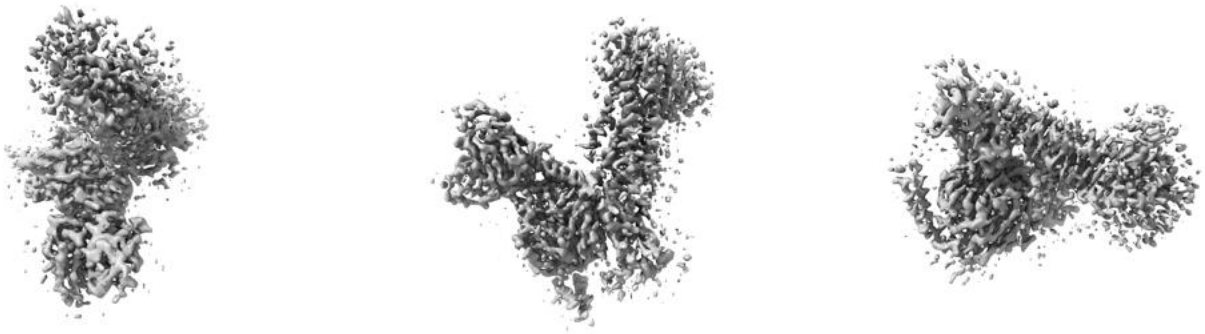


Z Index: 85

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

6.4 Orthogonal surface views (i)

6.4.1 Primary map



X Y Z

The images above show the 3D surface view of the map at the recommended contour level 1.4. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

6.4.2 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.

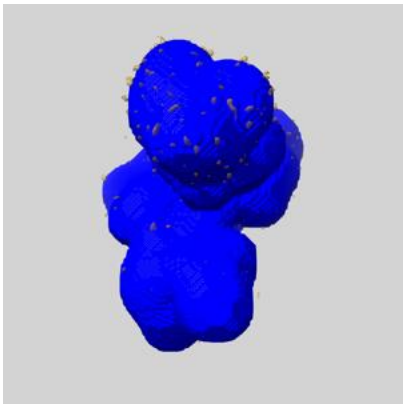
6.5 Mask visualisation (i)

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

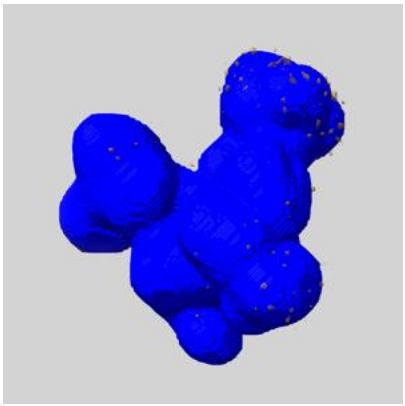
A mask typically either:

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

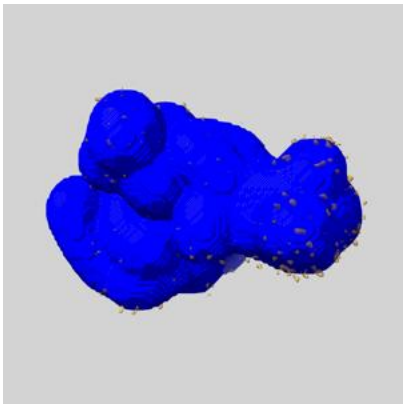
6.5.1 emd_34100_msk_1.map (i)



X



Y

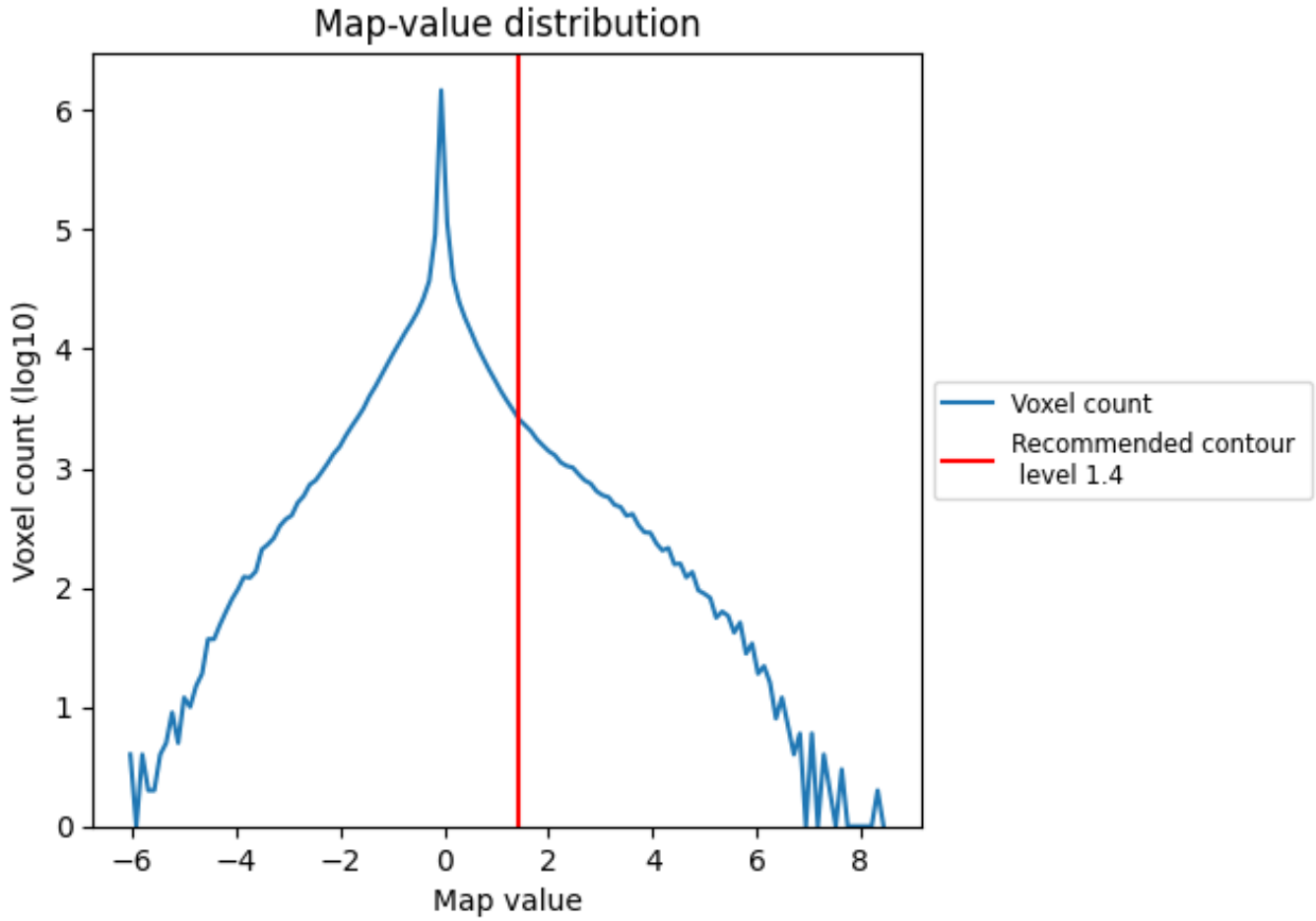


Z

7 Map analysis

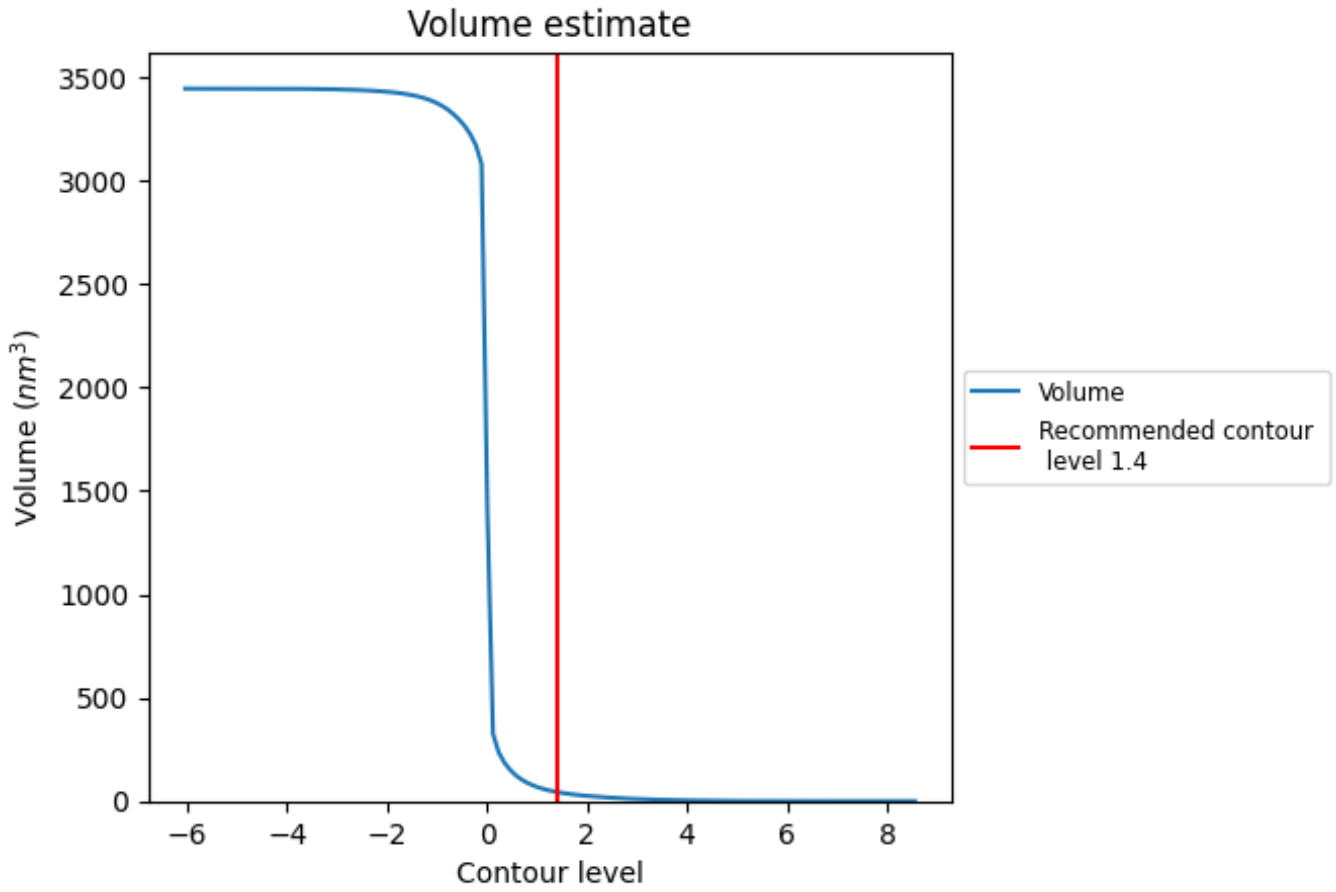
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution



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



The volume at the recommended contour level is 44 nm^3; this corresponds to an approximate mass of 40 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.

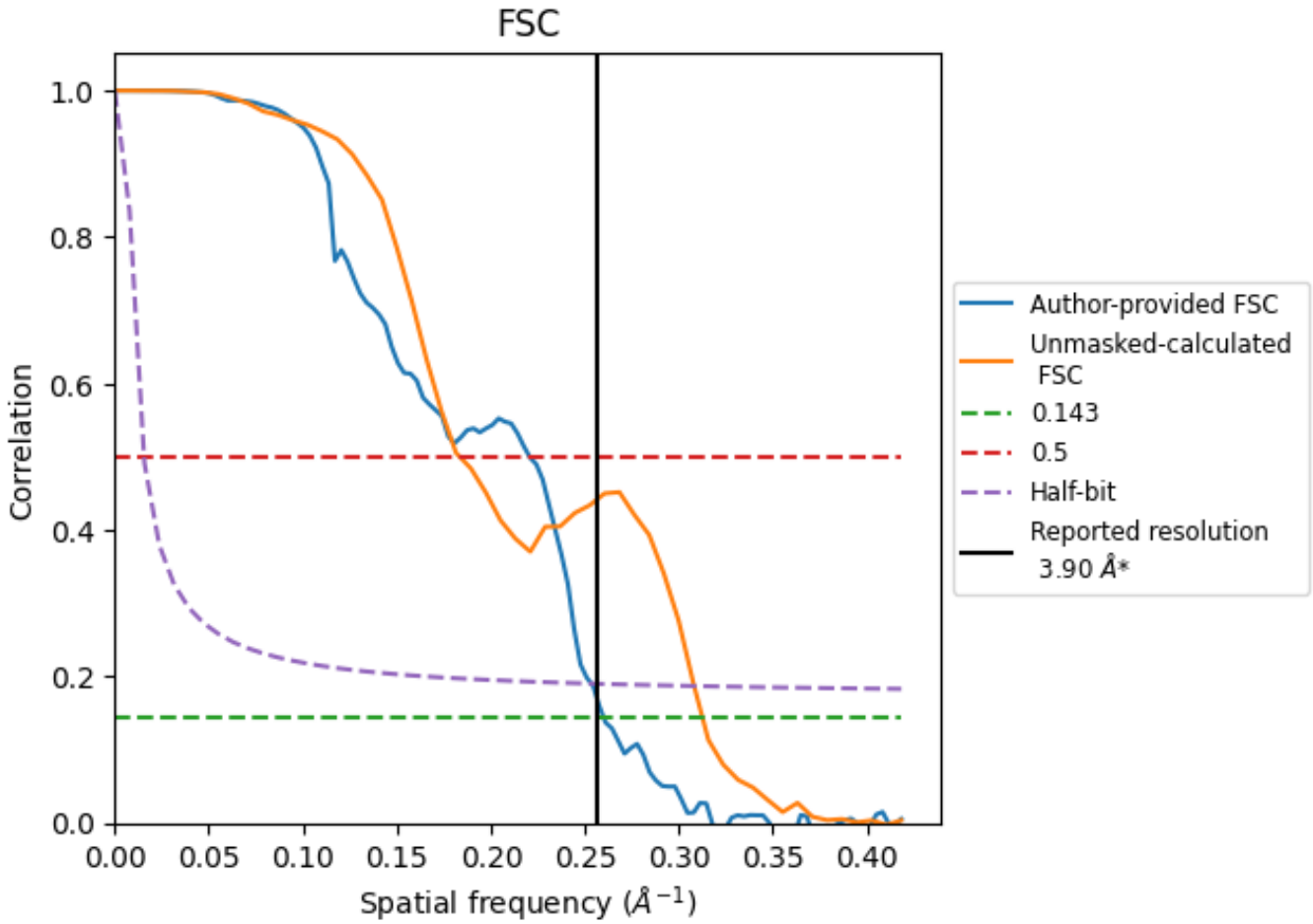
7.3 Rotationally averaged power spectrum

This section was not generated. The rotationally averaged power spectrum is only generated for cubic maps.

8 Fourier-Shell correlation

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



*Reported resolution corresponds to spatial frequency of 0.256 Å^{-1}

8.2 Resolution estimates (i)

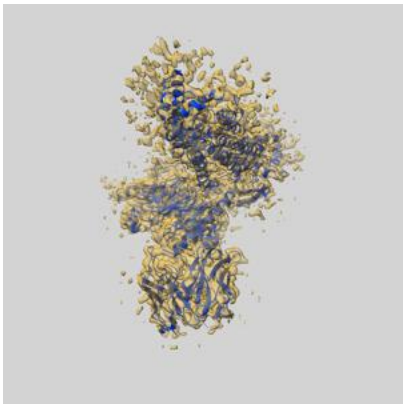
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.90	-	-
Author-provided FSC curve	3.84	4.53	3.92
Unmasked-calculated*	3.20	5.45	3.25

*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 3.20 differs from the reported value 3.9 by more than 10 %

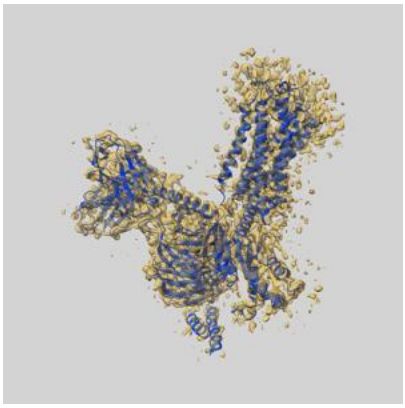
9 Map-model fit

This section contains information regarding the fit between EMDB map EMD-34100 and PDB model 7YU6. Per-residue inclusion information can be found in section 3 on page 6.

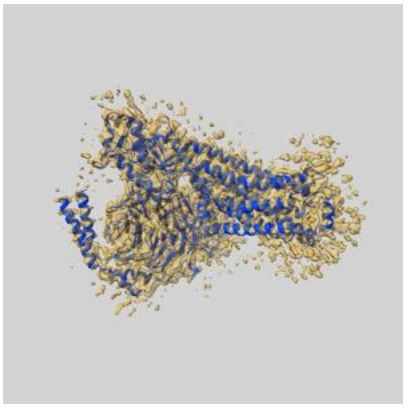
9.1 Map-model overlay



X



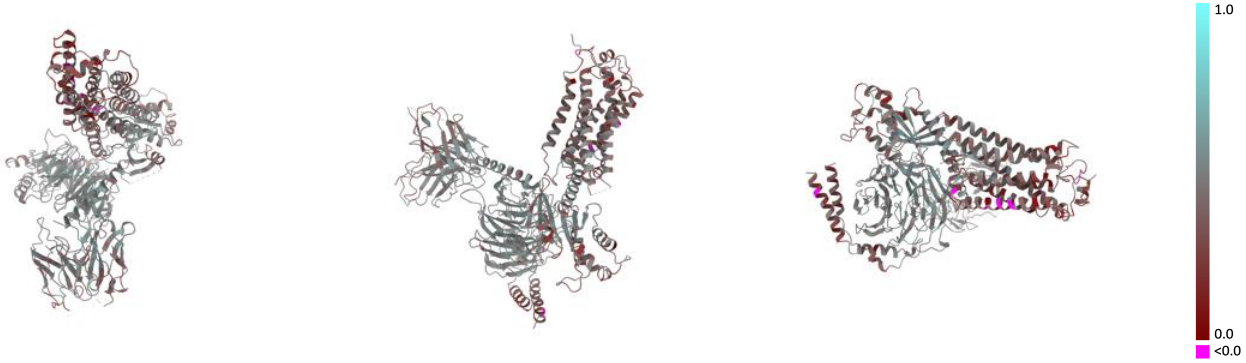
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 1.4 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.

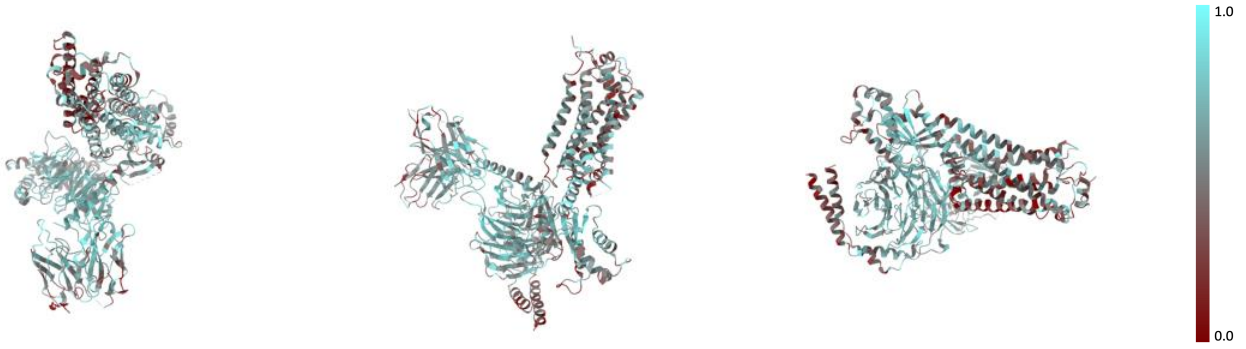
9.2 Q-score mapped to coordinate model (i)



X Y Z

The images above show the model with each residue coloured according 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.

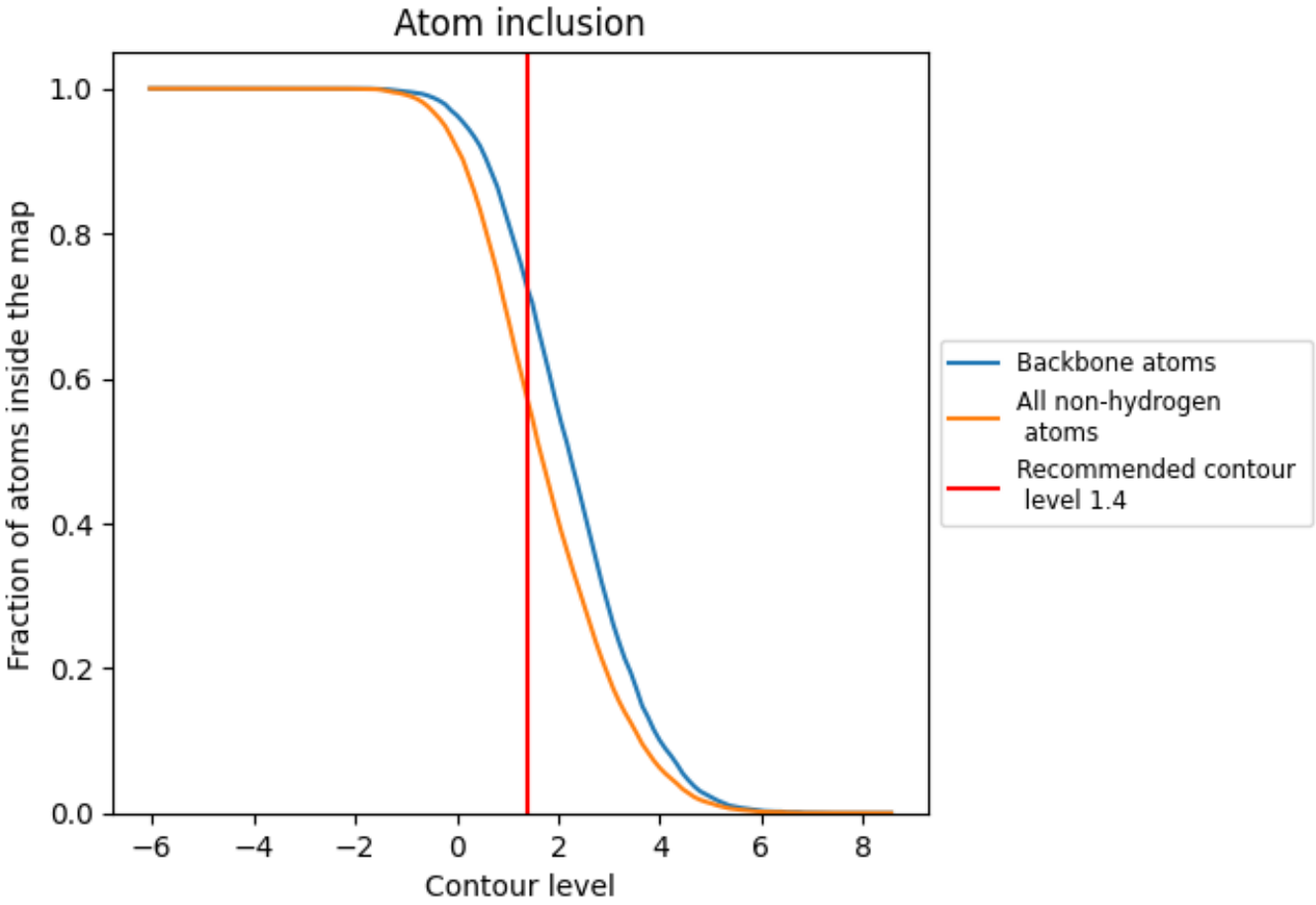
9.3 Atom inclusion mapped to coordinate model (i)



X Y Z

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 (1.4).

9.4 Atom inclusion (i)



At the recommended contour level, 72% of all backbone atoms, 57% 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 (1.4) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.5687	0.4260
A	0.5849	0.4360
B	0.6480	0.4710
G	0.5221	0.3940
R	0.4545	0.3540
S	0.5932	0.4480