Full wwPDB EM Validation Report (i)

Sep 28, 2022 – 02:36 AM JST

PDB ID	:	7YU7
EMDB ID	:	EMD-34101
Title	:	Human Lysophosphatidic Acid Receptor 1-Gi complex bound to ONO-0740556, state3
Authors	:	Akasaka, H.; Shihoya, W.; Nureki, O.
Deposited on	:	2022-08-16
Resolution	:	3.80 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 (i) 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 (1)) were used in the production of this report:

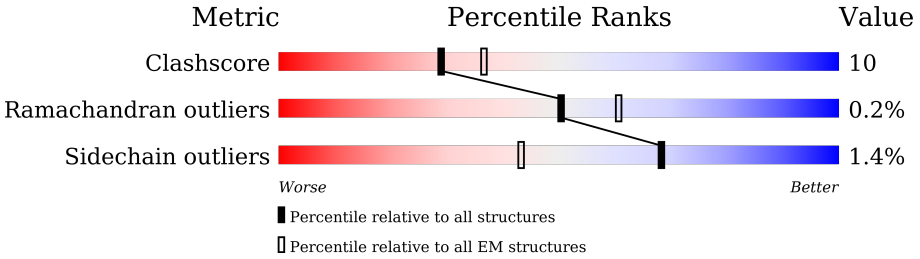
EMDB validation analysis	:	0.0.1.dev43
Mogul	:	1.8.5 (274361), CSD as541be (2020)
MolProbity	:	4.02b-467
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ	:	1.9.9
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (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 3.80 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	A	354	45%; 49%, 14%, •, 37%
2	R	379	70%; 56%, 19%, •, 23%
3	B	351	48%; 72%, 25%, •
4	G	68	53%; 60%, 19%, 21%
5	S	260	47%; 73%, 17%, 11%

2 Entry composition (i)

There are 6 unique types of molecules in this entry. The entry contains 8769 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) subunit alpha-1.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
1	A	222	1762	1122	287	340	13	0	0

- Molecule 2 is a protein called Lysophosphatidic acid receptor 1.

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

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 3 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		
3	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 4 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		
4	G	54	413	260	71	79	3	0	0

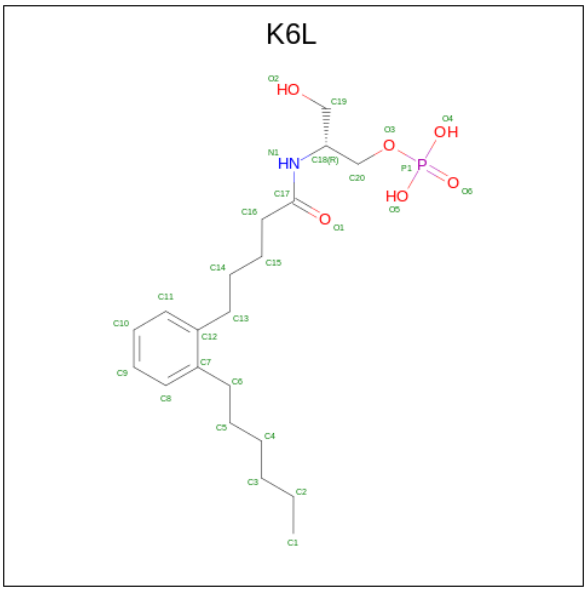
There is a discrepancy between the modelled and reference sequences:

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

- Molecule 5 is a protein called scFv16.

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

- 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).



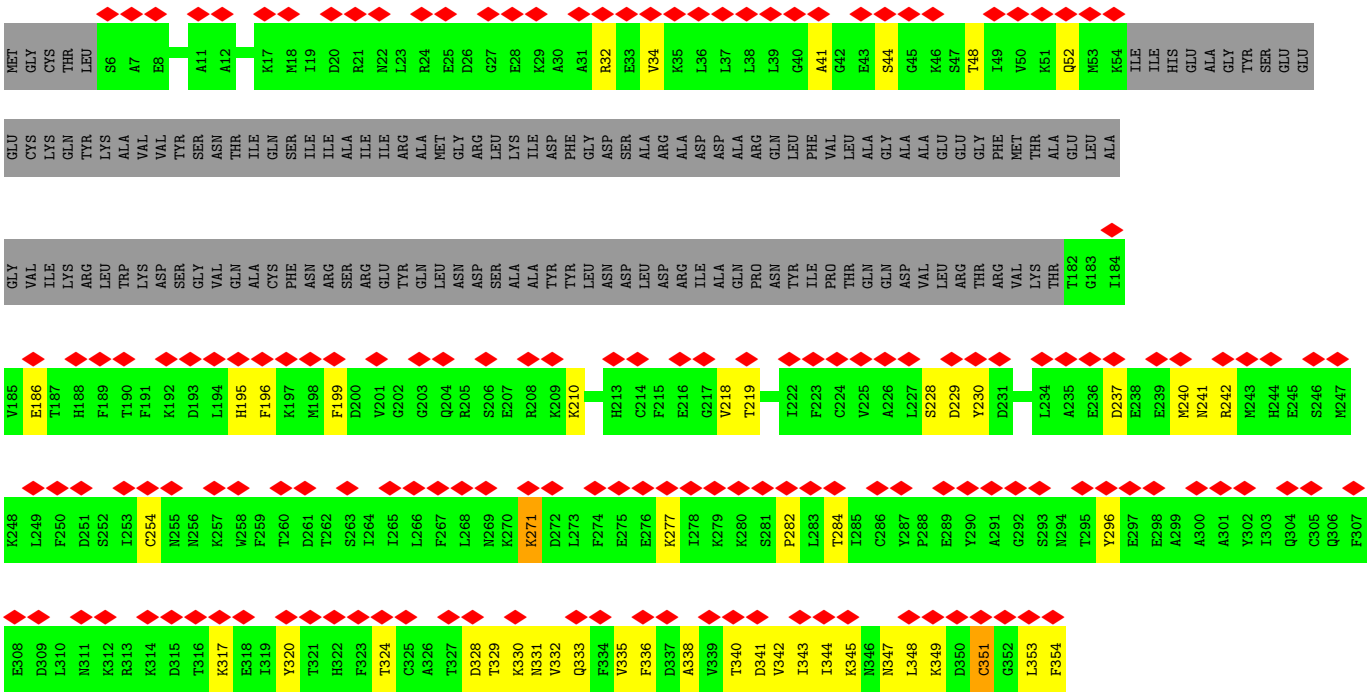
Mol	Chain	Residues	Atoms					AltConf
			Total	C	N	O	P	
6	R	1	28	20	1	6	1	0

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.

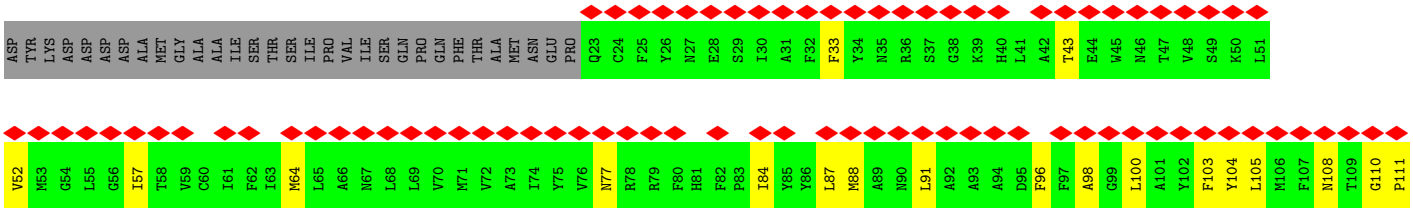
• Molecule 1: Guanine nucleotide-binding protein G(i) subunit alpha-1

Chain A:



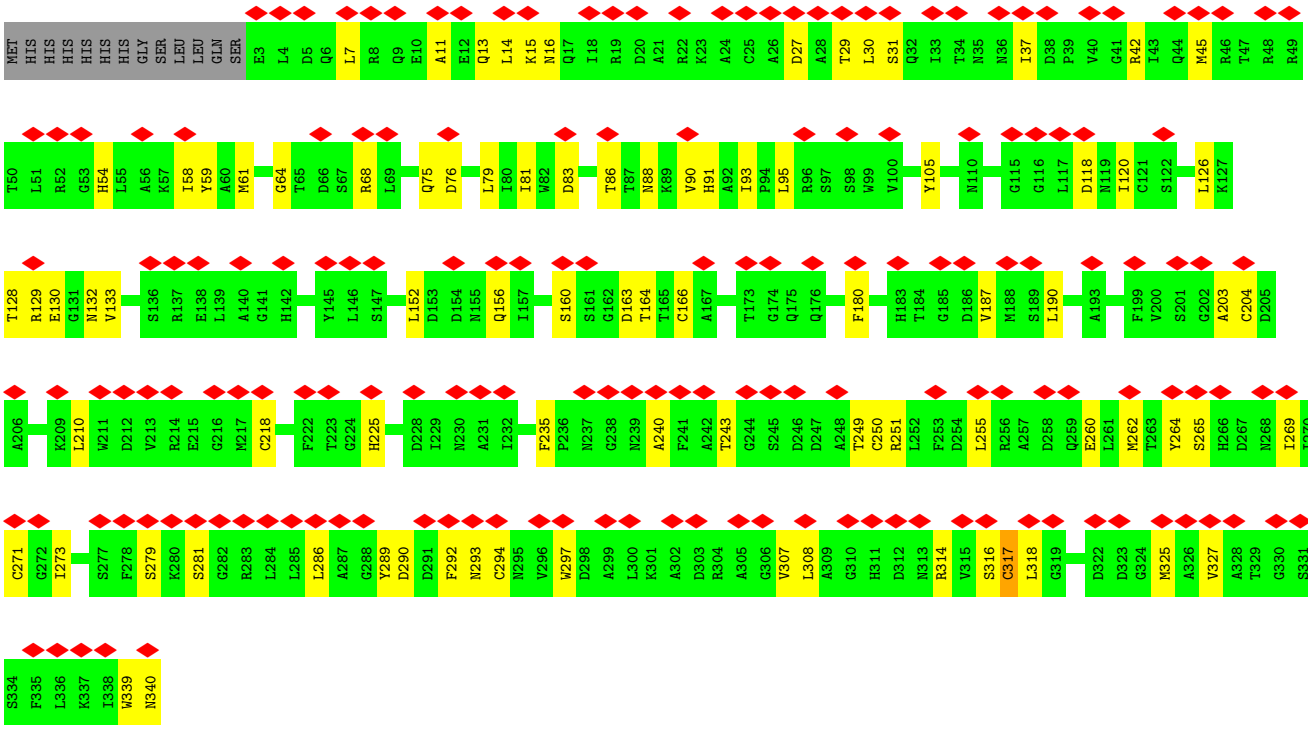
• Molecule 2: Lysophosphatidic acid receptor 1

Chain R:



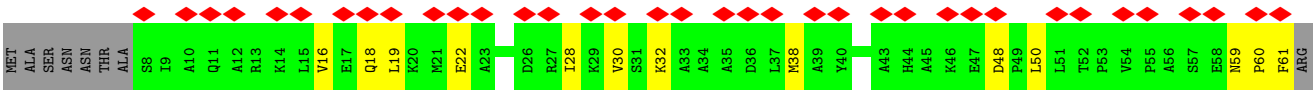
- Molecule 3: Guanine nucleotide-binding protein G(I)/G(S)/G(T) subunit beta-1

Chain B:



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

Chain G:



GLU LYS LYS PHE PHE SER

- Molecule 5: scFv16

Chain S:

ASP V2 Q3 L4 V5 E6 S7 G8 G9 G10 L11 V12 Q13 R18 K19 L20 S21 C22 S23 A24 F32 G33 M34 H35 W36 V37 R38 Q39 A40 P41 E42 L45 E46 W47 V48 S52 S55 A61 D62 T63 V64 R67 F68 T69 R72 D73 D74 T78 L79 F80 L81

Q82 M83 L86 R87 S88 E89 D90 T91 A92 M93 C96 V97 R98 S99 I100 Y101 Y102 Y103 S106 P107 F108 D109 F110 Q113 G114 T115 T116 L117 T118 V119 S120 S121 GLY GLY GLY GLY SER GLY GLY GLY GLY SER GLY GLY GLY GLY S136 Q142 A143 T144 S145 S146 V147 P148 V149

T150 P151 G152 E153 S154 V155 S156 I157 S158 C159 R160 S161 S162 L165 L166 H167 G170 N171 L174 Y175 W176 F177 L178 Q179 R180 P181 G182 Q183 S184 P185 Q186 L187 L188 I189 Y190 R191 M192 S193 G198 V199 P200 D201 R202 F203 S204 G205 S206 G207 S208 A211 F212 T213 L214 T215 T216

S217 R218 L219 E220 A221 E222 D223 V224 G225 V226 Y227 M230 Q231 H232 L233 E234 Y235 P236 L237 T238 F239 G240 A241 G242 T243 K244 L245 E246 L247 LYS ALA ALA ALA ALA SER SER GLU ASP LEU TYR PHE GLN

4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	55709	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	8.880	Depositor
Minimum map value	-6.865	Depositor
Average map value	0.001	Depositor
Map value standard deviation	0.462	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 (i)

5.1 Standard geometry (i)

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	A	0.81	0/1792	1.01	0/2407
2	R	0.75	0/2277	0.84	0/3112
3	B	0.75	0/2644	0.81	0/3584
4	G	0.63	0/419	0.71	0/566
5	S	0.68	0/1790	0.68	0/2432
All	All	0.74	0/8922	0.83	0/12101

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	A	1762	0	1724	41	0
2	R	2223	0	2174	65	0
3	B	2597	0	2501	58	0
4	G	413	0	423	14	0
5	S	1746	0	1667	26	0
6	R	28	0	0	1	0
All	All	8769	0	8489	177	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 (177) 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:219:THR:HA	2:R:155:LEU:HD22	1.50	0.94
1:A:353:LEU:HD22	2:R:146:ARG:HD3	1.63	0.81
2:R:121:TRP:HZ3	2:R:201:LEU:HB2	1.50	0.75
1:A:351:CYS:SG	1:A:353:LEU:HB3	2.30	0.71
2:R:121:TRP:CZ3	2:R:201:LEU:HB2	2.26	0.70
3:B:281:SER:HB3	4:G:48:ASP:OD2	1.92	0.69
5:S:142:GLN:NE2	5:S:241:ALA:O	2.25	0.67
1:A:328:ASP:HB3	1:A:330:LYS:HG3	1.76	0.67
3:B:225:HIS:HE2	3:B:243:THR:HG1	1.38	0.66
2:R:104:TYR:O	2:R:108:ASN:ND2	2.29	0.65
2:R:87:LEU:HD12	2:R:145:GLU:OE1	1.95	0.64
3:B:271:CYS:HB3	3:B:290:ASP:HB2	1.79	0.63
5:S:202:ARG:NH2	5:S:223:ASP:OD2	2.31	0.63
5:S:9:GLY:O	5:S:18:ARG:NH2	2.32	0.63
3:B:314:ARG:HD2	3:B:332:TRP:CZ2	2.33	0.62
3:B:79:LEU:HB3	3:B:93:ILE:HB	1.82	0.61
3:B:340:ASN:HD22	4:G:61:PHE:HB2	1.65	0.61
3:B:286:LEU:HD22	3:B:327:VAL:HG11	1.83	0.60
1:A:344:ILE:HD12	2:R:150:VAL:O	2.02	0.59
3:B:314:ARG:HD2	3:B:332:TRP:CE2	2.38	0.59
3:B:293:ASN:HD22	3:B:307:VAL:HG13	1.69	0.58
5:S:109:ASP:OD1	5:S:110:PHE:N	2.37	0.57
1:A:353:LEU:HD22	2:R:146:ARG:CD	2.32	0.57
2:R:110:GLY:O	2:R:113:THR:HG22	2.04	0.57
1:A:348:LEU:HG	1:A:354:PHE:HB2	1.86	0.57
1:A:348:LEU:HG	1:A:353:LEU:O	2.05	0.57
5:S:178:LEU:HB2	5:S:188:LEU:HD11	1.86	0.57
2:R:105:LEU:HD12	2:R:128:ILE:HG13	1.87	0.56
3:B:160:SER:HB3	3:B:190:LEU:HD23	1.88	0.56
5:S:63:THR:HG23	5:S:64:VAL:HG13	1.87	0.56
4:G:28:ILE:HD11	4:G:32:LYS:HD3	1.88	0.56
2:R:84:ILE:O	2:R:88:MET:HG2	2.05	0.55
1:A:219:THR:HG23	2:R:155:LEU:HD13	1.88	0.55
2:R:91:LEU:HD13	2:R:138:ASN:CB	2.36	0.55
2:R:265:GLY:HA2	2:R:268:ILE:HG22	1.89	0.55
1:A:345:LYS:O	1:A:349:LYS:HG2	2.07	0.55
2:R:320:ALA:C	2:R:322:PHE:N	2.58	0.54
2:R:33:PHE:CD2	2:R:201:LEU:HD21	2.43	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:B:29:THR:HG22	3:B:31:SER:H	1.73	0.54
1:A:343:ILE:HG23	2:R:154:GLN:O	2.08	0.53
5:S:6:GLU:HA	5:S:22:CYS:HA	1.90	0.53
2:R:188:CYS:HB2	2:R:191:ASP:O	2.09	0.53
1:A:34:VAL:HB	1:A:196:PHE:HD1	1.74	0.53
3:B:45:MET:HE2	3:B:308:LEU:HD21	1.90	0.53
2:R:320:ALA:O	2:R:322:PHE:N	2.42	0.53
1:A:338:ALA:O	1:A:342:VAL:HG23	2.08	0.52
1:A:48:THR:HG22	1:A:52:GLN:NE2	2.24	0.52
1:A:186:GLU:HG2	1:A:199:PHE:CD1	2.45	0.52
3:B:81:ILE:HD13	3:B:91:HIS:HB2	1.91	0.52
2:R:52:VAL:HG11	2:R:294:LYS:HD3	1.91	0.51
1:A:186:GLU:HG2	1:A:199:PHE:HD1	1.76	0.51
3:B:61:MET:HG3	3:B:317:CYS:HB2	1.92	0.51
3:B:316:SER:OG	3:B:332:TRP:CD1	2.64	0.51
2:R:141:ALA:HB2	2:R:171:ILE:HD11	1.93	0.51
1:A:320:TYR:HB3	2:R:239:MET:HE3	1.93	0.50
3:B:325:MET:HG2	4:G:60:PRO:HD2	1.93	0.50
2:R:33:PHE:CZ	2:R:201:LEU:HD11	2.46	0.50
1:A:282:PRO:HB2	1:A:284:THR:HG22	1.94	0.50
3:B:15:LYS:HG3	4:G:19:LEU:CD2	2.41	0.49
5:S:32:PHE:CD1	5:S:100:ILE:HB	2.48	0.49
2:R:320:ALA:C	2:R:322:PHE:H	2.15	0.49
2:R:91:LEU:HD13	2:R:138:ASN:HB2	1.95	0.49
5:S:52:SER:O	5:S:72:ARG:NH1	2.45	0.48
2:R:88:MET:HE1	2:R:311:TYR:HD2	1.78	0.48
1:A:229:ASP:HB3	1:A:242:ARG:HB2	1.96	0.48
1:A:324:THR:HA	1:A:331:ASN:HD21	1.78	0.48
1:A:336:PHE:O	1:A:340:THR:HG23	2.14	0.48
3:B:340:ASN:ND2	4:G:59:ASN:OD1	2.46	0.48
1:A:271:LYS:HB2	1:A:296:TYR:OH	2.13	0.48
3:B:68:ARG:HD3	5:S:103:TYR:CZ	2.49	0.48
2:R:137:ALA:HB3	2:R:171:ILE:HG23	1.95	0.48
2:R:207:LEU:HD12	2:R:278:LEU:HD22	1.96	0.48
2:R:33:PHE:CG	2:R:201:LEU:HD21	2.48	0.48
2:R:216:VAL:HA	2:R:219:VAL:HG22	1.96	0.48
2:R:141:ALA:CB	2:R:171:ILE:HD11	2.44	0.47
2:R:91:LEU:HD13	2:R:138:ASN:HB3	1.95	0.47
2:R:122:LEU:HD22	2:R:183:SER:HA	1.96	0.47
3:B:249:THR:HG22	3:B:265:SER:HB3	1.96	0.47
1:A:353:LEU:O	1:A:353:LEU:HG	2.14	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:B:132:ASN:O	3:B:133:VAL:C	2.51	0.47
3:B:281:SER:CB	4:G:48:ASP:OD2	2.62	0.47
1:A:344:ILE:CD1	2:R:150:VAL:O	2.63	0.47
2:R:105:LEU:HA	2:R:124:ARG:HD2	1.95	0.47
2:R:186:TRP:HD1	2:R:206:TYR:HB2	1.79	0.47
5:S:12:VAL:HG21	5:S:18:ARG:HG3	1.95	0.47
3:B:218:CYS:HB3	4:G:18:GLN:HE22	1.80	0.47
2:R:272:THR:N	2:R:273:PRO:HD2	2.30	0.47
3:B:225:HIS:CD2	3:B:243:THR:HG1	2.32	0.47
3:B:294:CYS:SG	3:B:318:LEU:HD11	2.55	0.46
3:B:279:SER:OG	4:G:50:LEU:HD12	2.15	0.46
2:R:177:VAL:O	2:R:181:ILE:HG12	2.15	0.46
2:R:189:ILE:HD13	2:R:201:LEU:HD12	1.96	0.46
5:S:4:LEU:HD12	5:S:110:PHE:HD2	1.79	0.46
3:B:7:LEU:O	3:B:11:ALA:N	2.44	0.46
2:R:77:ASN:OD1	2:R:321:THR:HG21	2.16	0.46
1:A:347:ASN:HB3	2:R:149:THR:HG22	1.98	0.46
3:B:27:ASP:H	4:G:30:VAL:HG12	1.81	0.46
1:A:347:ASN:ND2	2:R:149:THR:O	2.49	0.45
3:B:54:HIS:CD2	3:B:58:ILE:HD11	2.51	0.45
1:A:240:MET:SD	1:A:240:MET:N	2.90	0.45
5:S:61:ALA:HB3	5:S:64:VAL:HG22	1.98	0.45
1:A:351:CYS:HA	2:R:84:ILE:HG21	1.99	0.45
5:S:187:LEU:HD21	5:S:190:TYR:HB3	1.98	0.45
3:B:90:VAL:HG13	5:S:102:TYR:HB2	1.99	0.45
3:B:64:GLY:HA2	3:B:105:TYR:CD2	2.52	0.45
5:S:38:ARG:HD3	5:S:48:VAL:HG11	1.98	0.45
5:S:83:MET:HB3	5:S:86:LEU:HD21	1.99	0.44
5:S:160:ARG:NH1	5:S:160:ARG:HB3	2.33	0.44
3:B:79:LEU:HB2	3:B:95:LEU:HD21	1.99	0.44
2:R:270:CYS:HB3	2:R:303:ASN:HB2	2.00	0.44
3:B:59:TYR:HE2	3:B:75:GLN:CD	2.21	0.44
1:A:329:THR:O	1:A:332:VAL:HG12	2.18	0.44
1:A:254:CYS:O	1:A:317:LYS:NZ	2.38	0.43
2:R:138:ASN:OD1	2:R:171:ILE:HD13	2.18	0.43
3:B:187:VAL:HA	3:B:203:ALA:HA	1.99	0.43
2:R:43:THR:O	2:R:111:PRO:HB3	2.18	0.43
3:B:13:GLN:OE1	3:B:16:ASN:ND2	2.51	0.43
3:B:75:GLN:HA	3:B:75:GLN:OE1	2.19	0.43
3:B:118:ASP:OD2	3:B:120:ILE:HD12	2.17	0.43
3:B:290:ASP:C	3:B:292:PHE:H	2.22	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:B:42:ARG:HD2	3:B:42:ARG:HA	1.83	0.43
3:B:269:ILE:HG21	3:B:289:TYR:CE2	2.53	0.43
5:S:69:THR:HB	5:S:82:GLN:HB3	1.99	0.43
5:S:226:VAL:HA	5:S:244:LYS:HA	2.00	0.43
3:B:76:ASP:N	3:B:76:ASP:OD1	2.51	0.43
3:B:14:LEU:CD2	4:G:16:VAL:O	2.66	0.43
2:R:121:TRP:HZ3	2:R:201:LEU:CB	2.25	0.43
1:A:32:ARG:HA	2:R:154:GLN:HG2	1.99	0.43
1:A:210:LYS:HE2	3:B:204:CYS:SG	2.59	0.43
1:A:348:LEU:HD12	1:A:348:LEU:HA	1.51	0.43
5:S:87:ARG:O	5:S:119:VAL:HG21	2.19	0.43
1:A:348:LEU:HD23	1:A:354:PHE:CD1	2.54	0.42
2:R:121:TRP:CZ3	2:R:201:LEU:HD23	2.54	0.42
5:S:192:MET:O	5:S:193:SER:OG	2.31	0.42
2:R:57:ILE:HG13	2:R:103:PHE:HE1	1.84	0.42
3:B:166:CYS:HB2	3:B:180:PHE:HB2	2.00	0.42
3:B:308:LEU:HD23	3:B:339:TRP:CD2	2.55	0.42
5:S:178:LEU:HD13	5:S:227:TYR:CZ	2.54	0.42
1:A:41:ALA:N	1:A:44:SER:OG	2.51	0.42
3:B:152:LEU:HB2	3:B:156:GLN:HB2	2.01	0.42
4:G:19:LEU:H	4:G:19:LEU:HD12	1.85	0.42
3:B:251:ARG:NH1	3:B:260:GLU:OE2	2.41	0.42
1:A:331:ASN:O	1:A:335:VAL:HG23	2.19	0.42
2:R:154:GLN:HB2	2:R:157:THR:OG1	2.19	0.42
3:B:30:LEU:HB3	3:B:262:MET:HE2	2.01	0.42
3:B:250:CYS:SG	3:B:273:ILE:HD13	2.60	0.42
2:R:64:MET:HA	2:R:96:PHE:HD1	1.83	0.41
2:R:100:LEU:HD23	2:R:100:LEU:HA	1.87	0.41
3:B:37:ILE:HD11	4:G:38:MET:HG3	2.02	0.41
5:S:97:VAL:HG11	5:S:108:PHE:CD2	2.55	0.41
2:R:278:LEU:HD11	6:R:401:K6L:C5	2.50	0.41
1:A:343:ILE:CG2	2:R:154:GLN:O	2.68	0.41
2:R:52:VAL:HG21	2:R:294:LYS:CG	2.50	0.41
2:R:196:SER:OG	2:R:197:ASN:N	2.54	0.41
3:B:163:ASP:O	3:B:164:THR:OG1	2.32	0.41
5:S:7:SER:OG	5:S:21:SER:OG	2.28	0.41
3:B:264:TYR:HB3	3:B:297:TRP:CD2	2.55	0.41
5:S:32:PHE:CE1	5:S:100:ILE:HB	2.55	0.41
2:R:214:ASN:HD22	2:R:275:LEU:HD21	1.85	0.41
3:B:83:ASP:OD2	3:B:86:THR:OG1	2.39	0.41
3:B:235:PHE:HB2	3:B:240:ALA:HB3	2.03	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:R:166:VAL:O	2:R:169:VAL:HG22	2.20	0.41
1:A:230:TYR:O	1:A:241:ASN:ND2	2.52	0.41
2:R:172:TRP:O	2:R:176:ILE:HG12	2.21	0.41
2:R:255:SER:OG	2:R:314:ARG:NH1	2.53	0.41
4:G:19:LEU:HA	4:G:22:GLU:HB2	2.02	0.41
2:R:121:TRP:CH2	2:R:200:PRO:HD2	2.56	0.41
2:R:195:CYS:HB2	2:R:203:SER:HA	2.02	0.41
3:B:86:THR:OG1	3:B:88:ASN:OD1	2.35	0.40
3:B:210:LEU:HD22	3:B:255:LEU:HD22	2.02	0.40
3:B:308:LEU:HD23	3:B:339:TRP:CG	2.56	0.40
1:A:341:ASP:O	1:A:345:LYS:HB2	2.22	0.40
1:A:228:SER:O	1:A:277:LYS:NZ	2.37	0.40
2:R:98:ALA:HA	2:R:131:SER:HB2	2.04	0.40
1:A:237:ASP:HB2	1:A:240:MET:HE1	2.03	0.40
2:R:188:CYS:SG	2:R:201:LEU:HA	2.62	0.40
3:B:126:LEU:HD23	3:B:133:VAL:HG22	2.03	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	A	218/354 (62%)	206 (94%)	12 (6%)	0	100 100
2	R	286/379 (76%)	269 (94%)	15 (5%)	2 (1%)	22 60
3	B	336/351 (96%)	316 (94%)	20 (6%)	0	100 100
4	G	52/68 (76%)	52 (100%)	0	0	100 100
5	S	228/260 (88%)	220 (96%)	8 (4%)	0	100 100
All	All	1120/1412 (79%)	1063 (95%)	55 (5%)	2 (0%)	50 79

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	R	321	THR
2	R	196	SER

5.3.2 Protein sidechains (i)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	191/305 (63%)	186 (97%)	5 (3%)	46	69
2	R	229/333 (69%)	225 (98%)	4 (2%)	60	78
3	B	280/293 (96%)	276 (99%)	4 (1%)	67	81
4	G	44/56 (79%)	44 (100%)	0	100	100
5	S	184/209 (88%)	184 (100%)	0	100	100
All	All	928/1196 (78%)	915 (99%)	13 (1%)	68	81

All (13) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	195	HIS
1	A	218	VAL
1	A	271	LYS
1	A	333	GLN
1	A	351	CYS
2	R	114	ARG
2	R	196	SER
2	R	303	ASN
2	R	315	ASP
3	B	128	THR
3	B	129	ARG
3	B	130	GLU
3	B	317	CYS

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

Mol	Chain	Res	Type
1	A	269	ASN
1	A	333	GLN
2	R	90	ASN
2	R	156	HIS
2	R	214	ASN
2	R	303	ASN
3	B	293	ASN
3	B	340	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 monosaccharides in this entry.

5.6 Ligand geometry (i)

1 ligand is modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
6	K6L	R	401	-	28,28,28	0.42	0	33,35,35	0.84	0

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	-	-	6/25/25/25	0/1/1/1

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (6) torsion outliers are listed below:

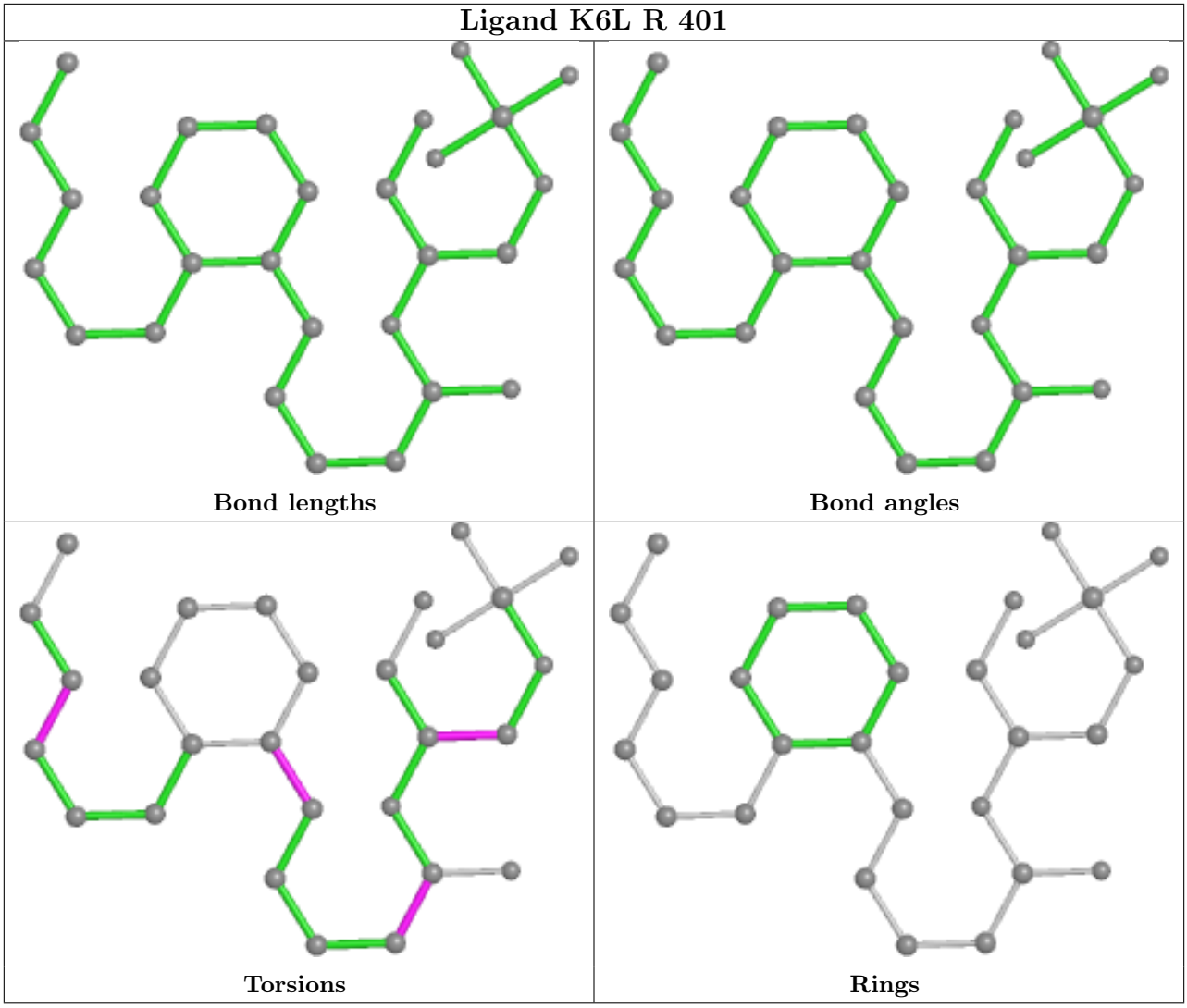
Mol	Chain	Res	Type	Atoms
6	R	401	K6L	C15-C16-C17-O1
6	R	401	K6L	C15-C16-C17-N1
6	R	401	K6L	C19-C18-C20-O3
6	R	401	K6L	C11-C12-C13-C14
6	R	401	K6L	C7-C12-C13-C14
6	R	401	K6L	C2-C3-C4-C5

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	R	401	K6L	1	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less 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.



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.

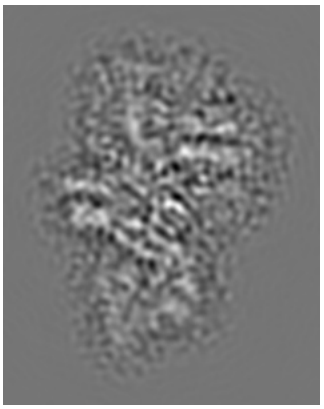
6 Map visualisation (i)

This section contains visualisations of the EMDB entry EMD-34101. These allow visual inspection of the internal detail of the map and identification of artifacts.

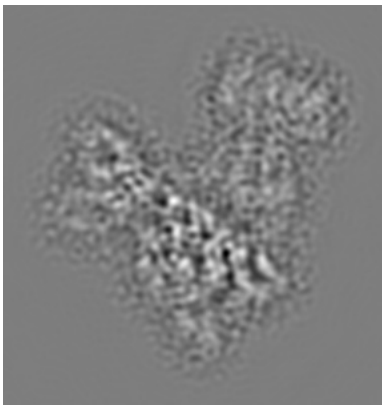
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections (i)

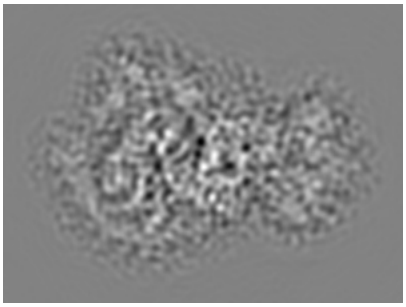
6.1.1 Primary map



X

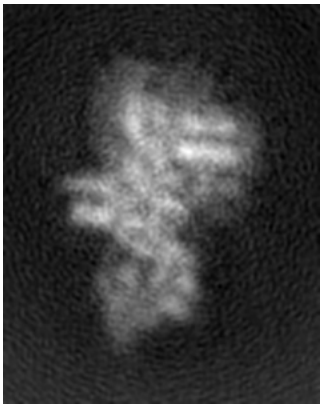


Y

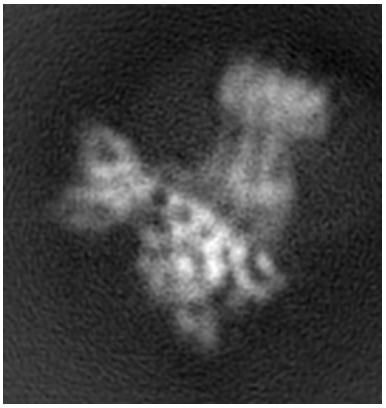


Z

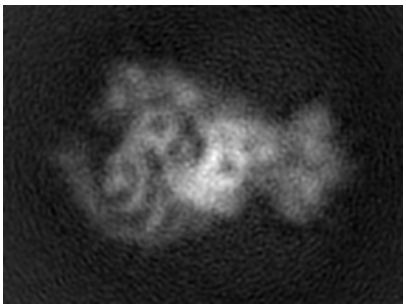
6.1.2 Raw map



X



Y

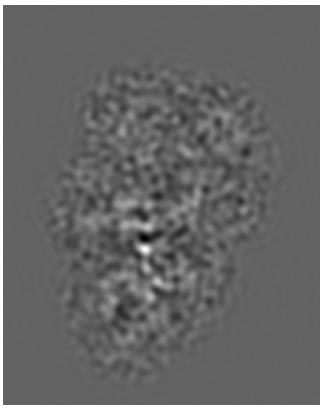


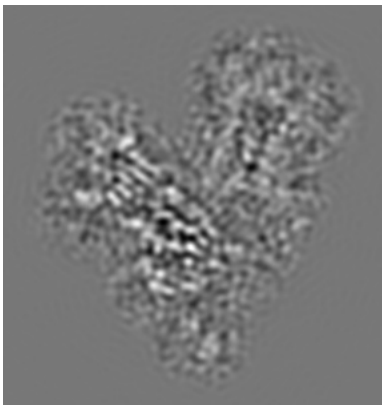
Z

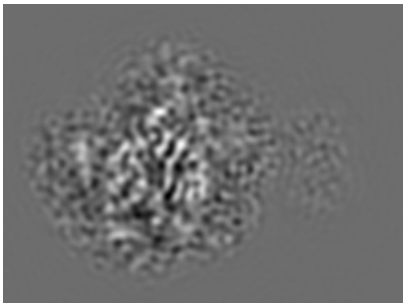
The images above show the map projected in three orthogonal directions.

6.2 Central slices (i)

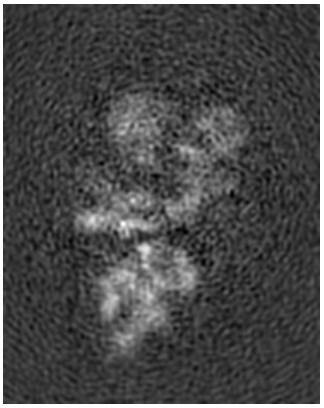
6.2.1 Primary map

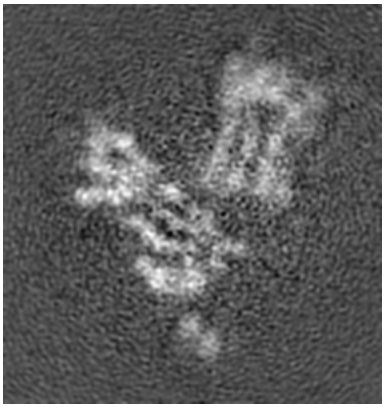

X Index: 71

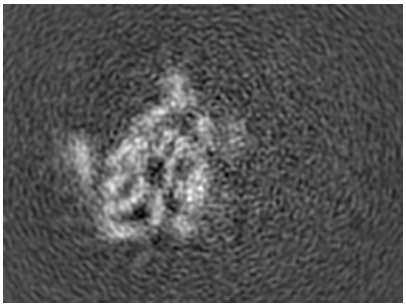

Y Index: 53


Z Index: 67

6.2.2 Raw map


X Index: 71

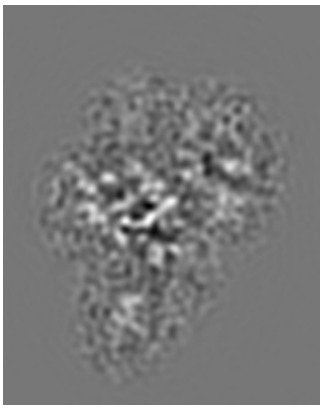

Y Index: 53

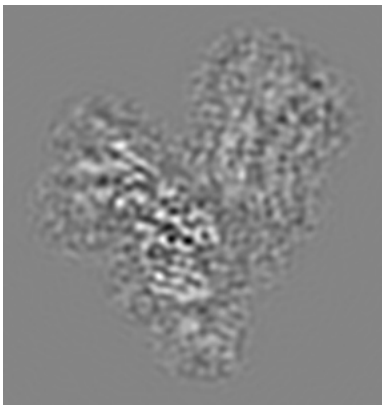

Z Index: 67

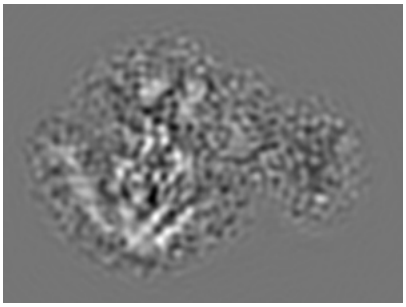
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

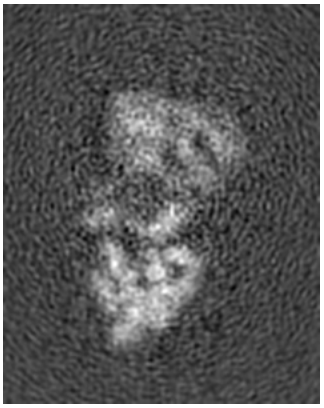
6.3.1 Primary map

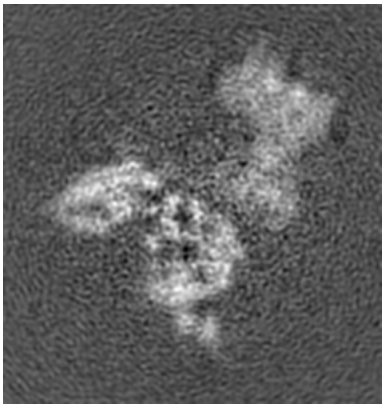

X Index: 62

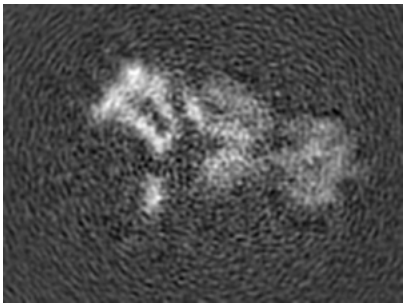

Y Index: 51


Z Index: 73

6.3.2 Raw map


X Index: 74


Y Index: 43


Z Index: 83

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.

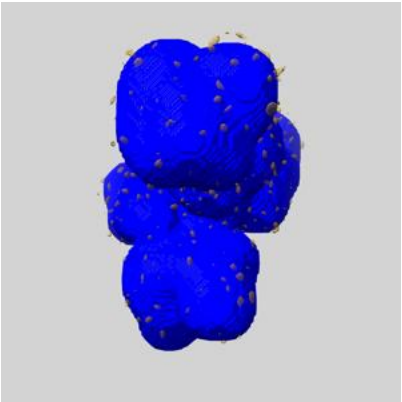
6.5 Mask visualisation (i)

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

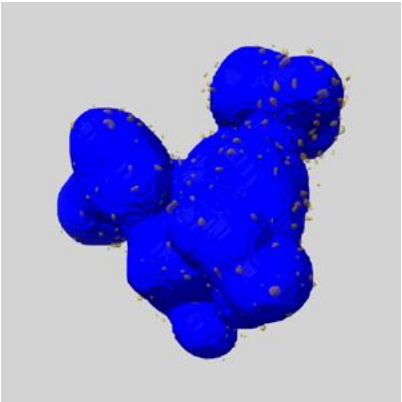
A mask typically either:

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

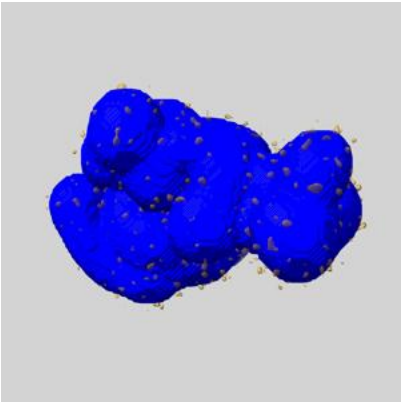
6.5.1 emd_34101_msk_1.map (i)



X



Y

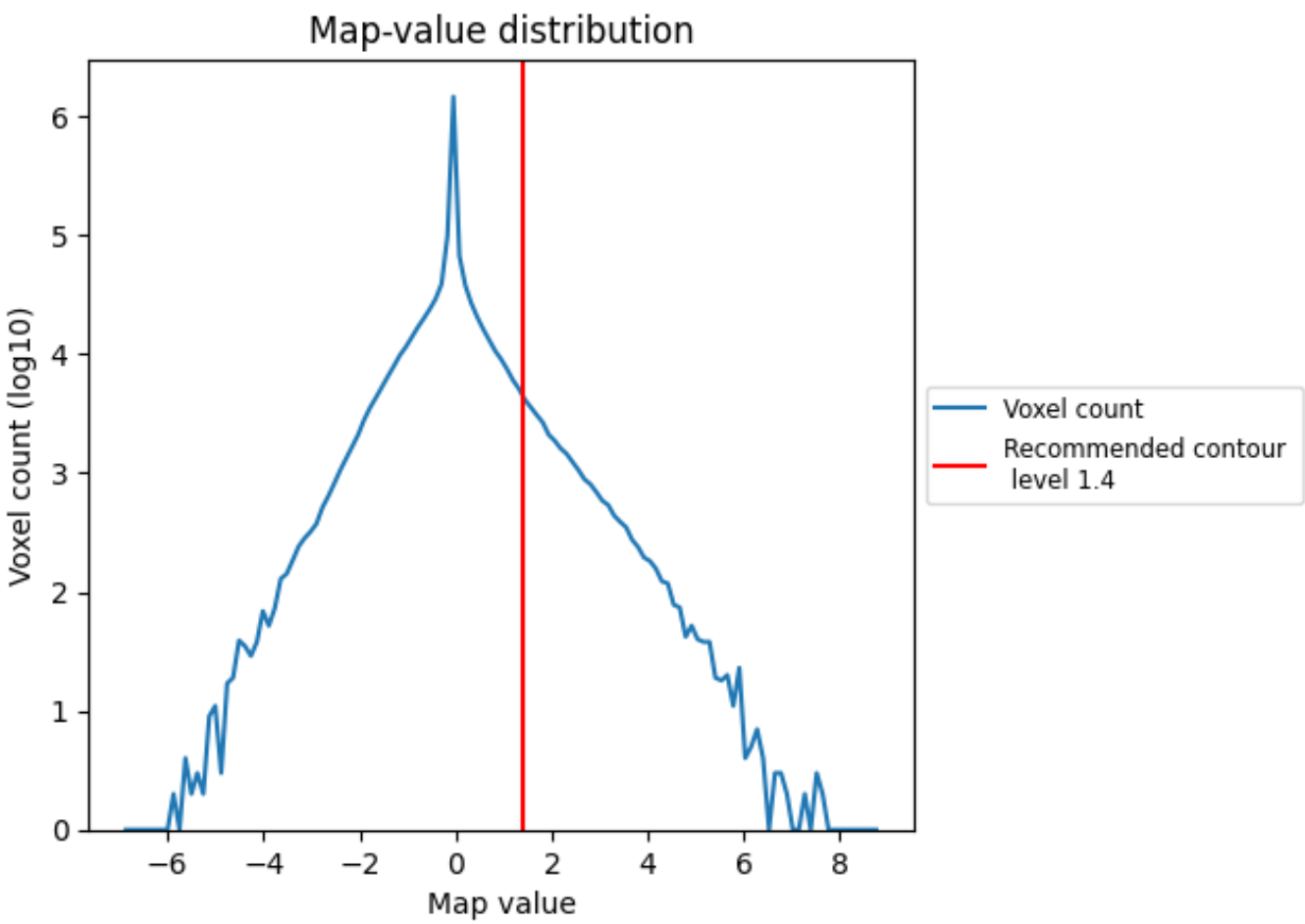


Z

7 Map analysis (i)

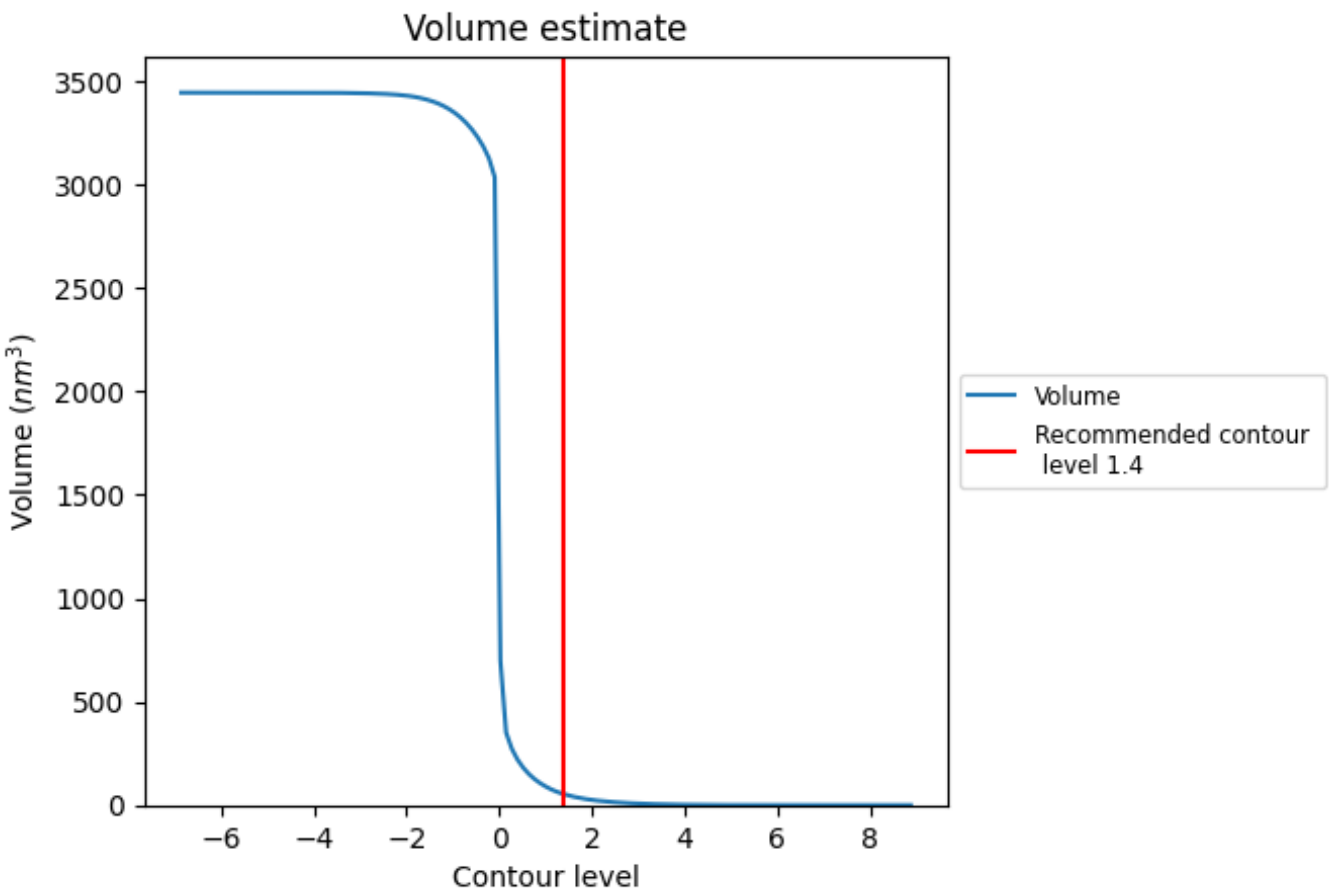
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution (i)



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

7.2 Volume estimate (i)



The volume at the recommended contour level is 53 nm^3; this corresponds to an approximate mass of 48 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.

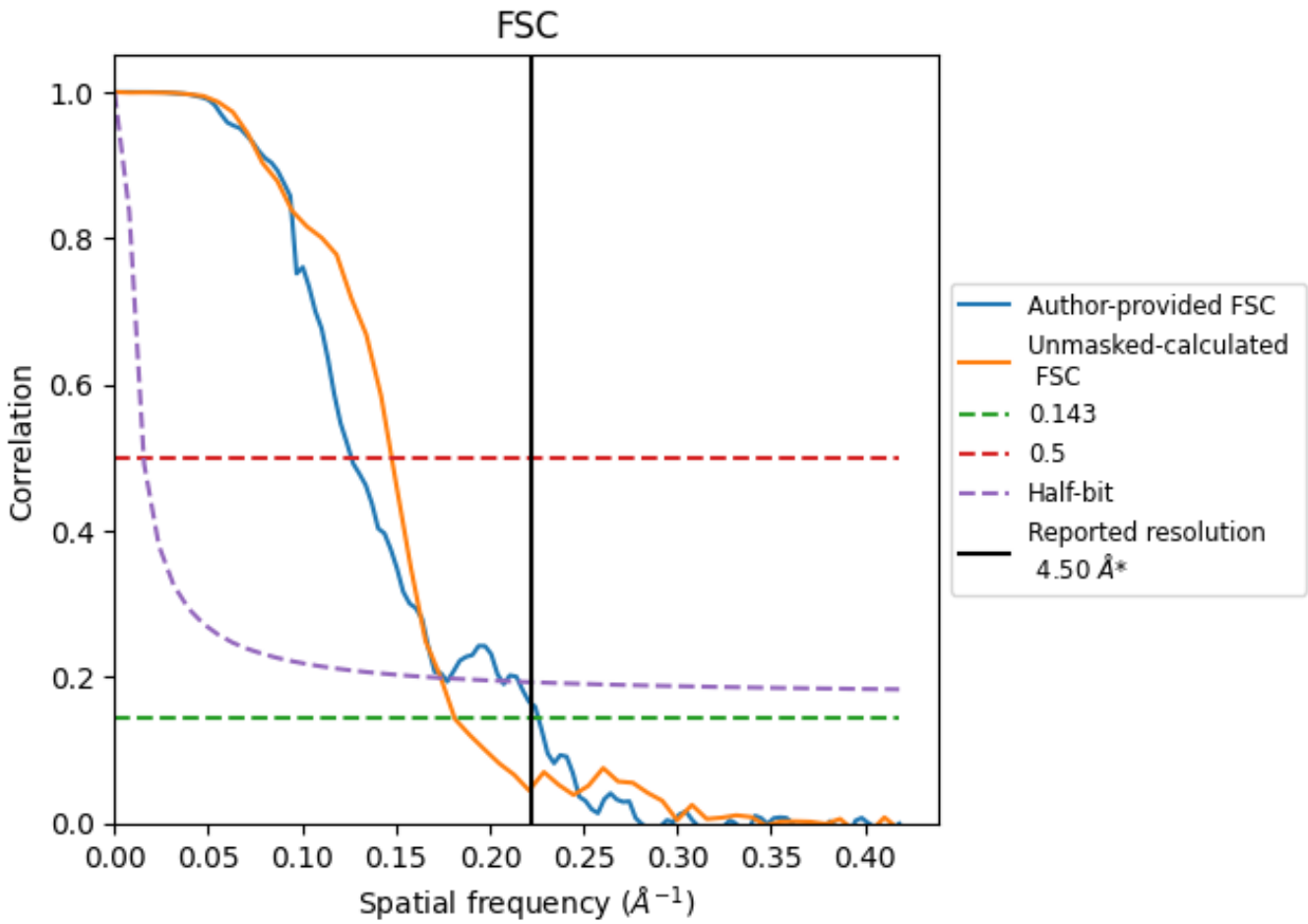
7.3 Rotationally averaged power spectrum (i)

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

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 0.222 Å^{-1}

8.2 Resolution estimates (i)

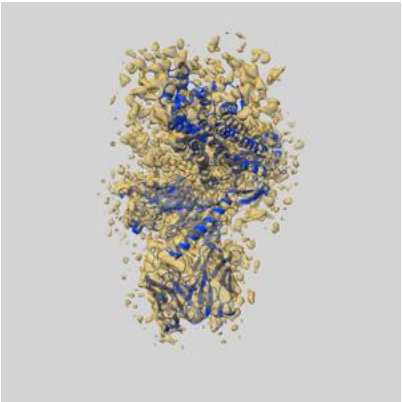
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	4.50	-	-
Author-provided FSC curve	4.42	7.92	4.59
Unmasked-calculated*	5.51	6.77	5.75

*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 5.51 differs from the reported value 4.5 by more than 10 %

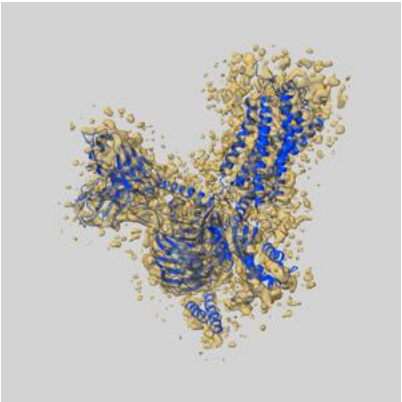
9 Map-model fit (i)

This section contains information regarding the fit between EMDB map EMD-34101 and PDB model 7YU7. Per-residue inclusion information can be found in section 3 on page 6.

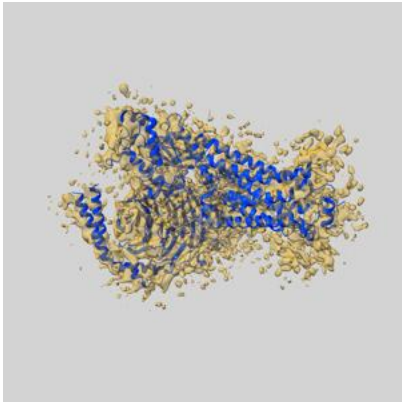
9.1 Map-model overlay (i)



X



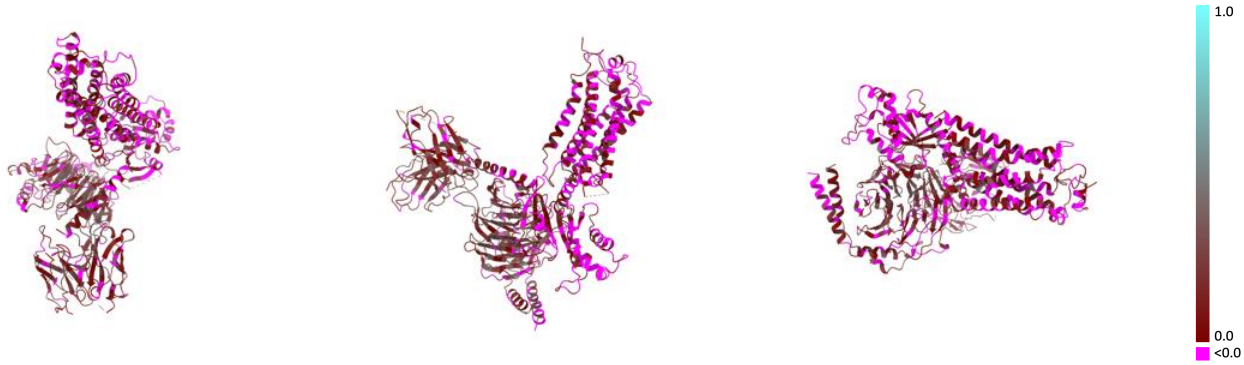
Y



Z

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

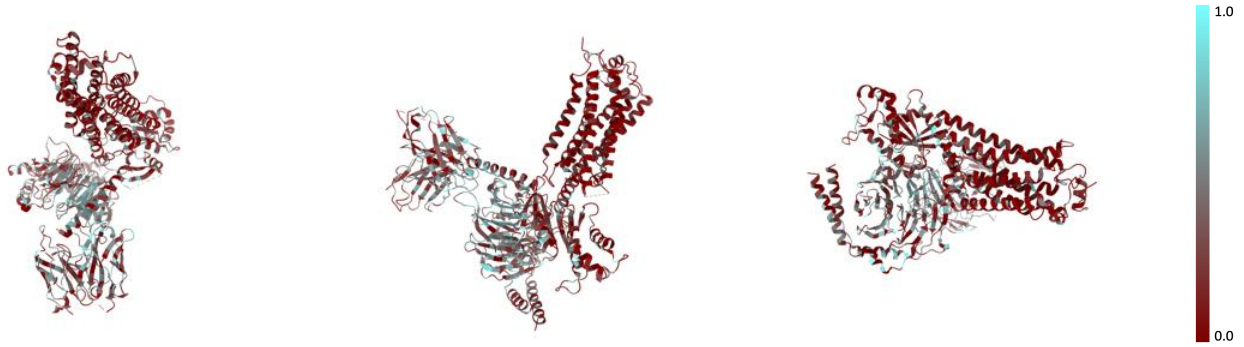
9.2 Q-score mapped to coordinate model (i)



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.

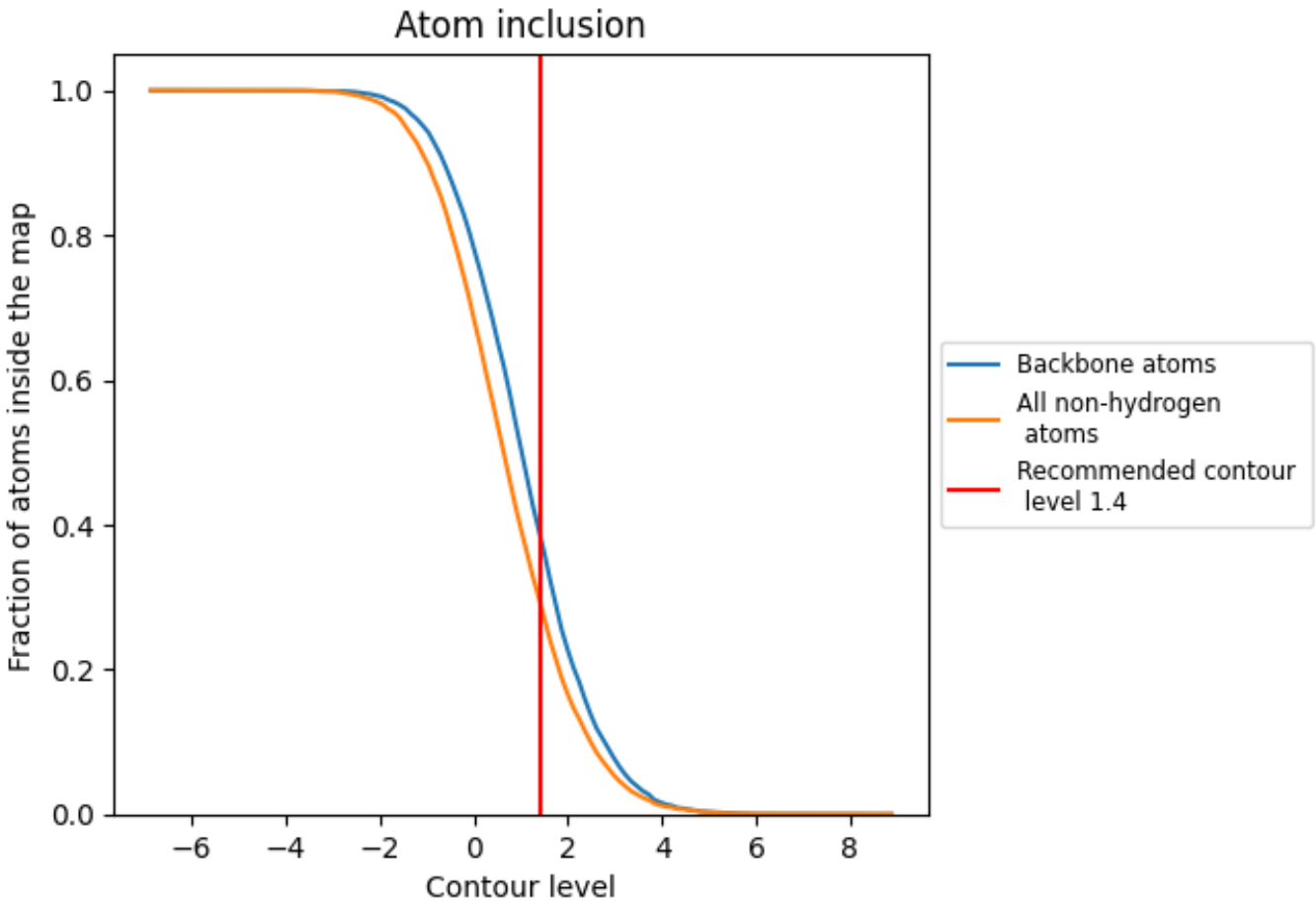
9.3 Atom inclusion mapped to coordinate model (i)



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, 39% of all backbone atoms, 29% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary (i)

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	0.2944	0.0980
A	0.2620	0.0260
B	0.4009	0.1600
G	0.3015	0.0820
R	0.1253	0.0270
S	0.3869	0.1740