



Full wwPDB EM Validation Report ⓘ

Apr 5, 2026 – 10:10 PM UTC

PDB ID : 9PPW / pdb_00009ppw
EMDB ID : EMD-71776
Title : CryoEM structure of delta opioid receptor bound to G proteins and Naltrindole
Authors : Fay, J.F.; Che, T.
Deposited on : 2025-07-22
Resolution : 3.32 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

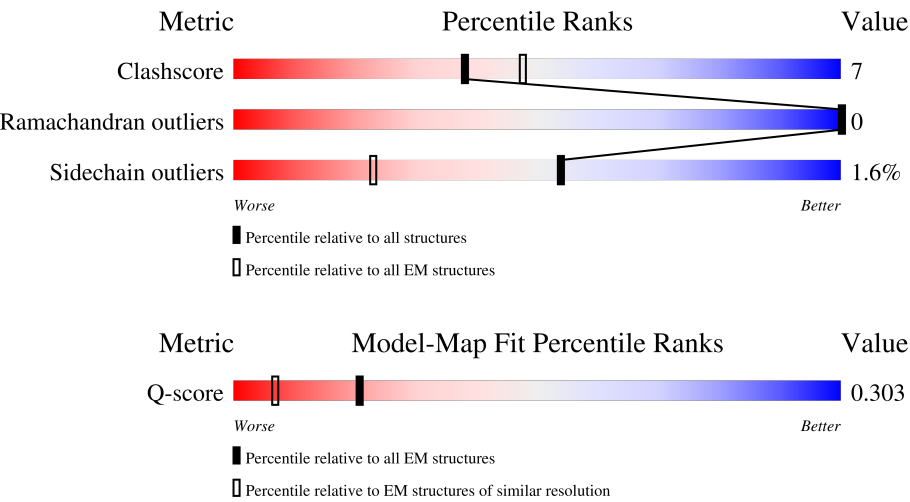
EMDB validation analysis : 0.0.1.dev132
Mogul : 2022.3.0, CSD as543be (2022)
MolProbity : 4-5-2 with Phenix2.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data in the EMDB archive up until May 2025)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

1 Overall quality at a glance i

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

The reported resolution of this entry is 3.32 Å.

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



Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
Q-score	-	25397	14518 (2.82 - 3.82)

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	303	
2	B	354	
3	C	340	
4	D	71	

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Mol	Chain	Length	Quality of chain
5	E	251	<div><div></div><div>84%</div><div>73%</div><div>19%</div><div>8%</div></div>

2 Entry composition [i](#)

There are 6 unique types of molecules in this entry. The entry contains 7820 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 Delta-type opioid receptor.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	279	Total	C	N	O	S	0	0
			1844	1205	310	315	14		

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	36	GLY	-	expression tag	UNP P41143
A	37	SER	-	expression tag	UNP P41143

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

Mol	Chain	Residues	Atoms					AltConf	Trace
2	B	200	Total	C	N	O	S	0	0
			1505	972	251	271	11		

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	47	ASN	SER	engineered mutation	UNP P63096
B	203	ALA	GLY	engineered mutation	UNP P63096
B	245	ALA	GLU	engineered mutation	UNP P63096
B	326	SER	ALA	engineered mutation	UNP P63096

- 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	335	Total	C	N	O	S	0	0
			2423	1518	431	455	19		

There is a discrepancy between the modelled and reference sequences:

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

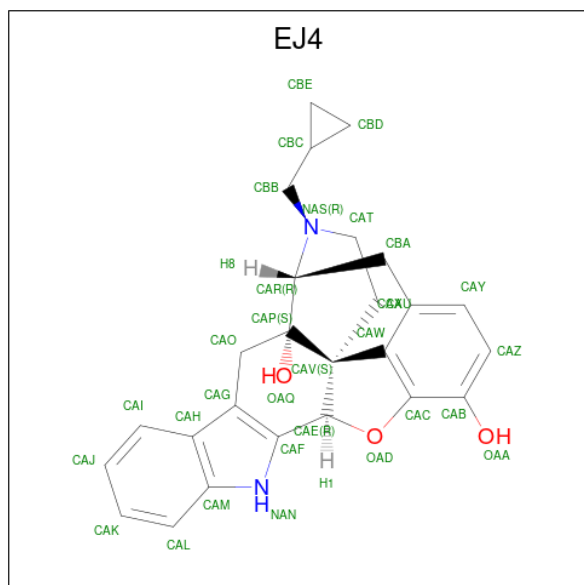
- Molecule 4 is a protein called Guanine nucleotide-binding protein G(I)/G(S)/G(O) subunit gamma-2.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	D	52	Total	C	N	O	S	0	0
			340	215	62	61	2		

- Molecule 5 is a protein called ScFv16 protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	E	232	Total	C	N	O	S	0	0
			1677	1081	284	303	9		

- Molecule 6 is (4bS,8R,8aS,14bR)-7-(cyclopropylmethyl)-5,6,7,8,14,14b-hexahydro-4,8-methano[1]benzofuro[2,3-a]pyrido[4,3-b]carbazole-1,8a(9H)-diol (CCD ID: EJ4) (formula: C₂₆H₂₆N₂O₃).



Mol	Chain	Residues	Atoms				AltConf
6	A	1	Total	C	N	O	0
			31	26	2	3	

G230	P169	S121	A61
T231	G170	GLY	D62
K232	Q171	GLY	T63
L233	S172	GLY	V64
E234	P173	SER	K65
L235	Q174	GLY	G66
LYS	L175	GLY	R67
ALA	L176	GLY	F68
ALA	I177	GLY	T69
ALA	Y178	SER	I70
	R179	GLY	S71
	M180	GLY	R72
	S181	S124	D73
	N182	D125	D74
	L183	I126	P75
	A184	V127	K76
	S185	M128	N77
	G186	T129	T78
	V187	Q130	L79
	P188	A131	F80
	D189	T132	L81
	R190	S133	Q82
	F191	S134	K83
	S192	V135	T84
	G193	P136	S85
	S194	V137	L86
	G195	T138	R87
	S196	P139	S88
	G197	G140	E89
	T198	E141	D90
	A199	S142	T91
	F200	V143	A92
	T201	S144	K93
	L202	I145	Y94
	T203	S146	Y95
	I204	C147	C96
	S205	R148	V97
	R206	S149	R98
	L207	S150	S99
	E208	K151	I100
	A209	S152	Y101
	E210	L153	Y102
	D211	L154	Y103
	V212	H155	G104
	G213	S156	S105
	V214	S157	S106
	Y215	G158	P107
	Y216	M159	F108
	C217	T160	A49
	M218	Y161	F110
	Q219	L162	W111
	H220	V163	G112
	L221	Y164	Q113
	E222	F165	G114
	Y223	L166	T115
	P224	Q167	L117
	L225	R168	L118
	T226		V119
	A229		S120

4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	850265	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TALOS ARCTICA	Depositor
Voltage (kV)	200	Depositor
Electron dose ($e^-/\text{\AA}^2$)	64.6	Depositor
Minimum defocus (nm)	200	Depositor
Maximum defocus (nm)	2500	Depositor
Magnification	Not provided	
Image detector	GATAN K3 (6k x 4k)	Depositor
Maximum map value	2.159	Depositor
Minimum map value	-0.030	Depositor
Average map value	0.001	Depositor
Map value standard deviation	0.021	Depositor
Recommended contour level	0.5	Depositor
Map size (\AA)	253.44, 253.44, 253.44	wwPDB
Map dimensions	288, 288, 288	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (\AA)	0.88, 0.88, 0.88	Depositor

5 Model quality [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: EJ4

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	0.16	0/1882	0.32	0/2599
2	B	0.16	0/1533	0.31	0/2075
3	C	0.20	0/2468	0.43	0/3361
4	D	0.14	0/346	0.23	0/477
5	E	0.19	0/1721	0.34	0/2349
All	All	0.18	0/7950	0.36	0/10861

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	1844	0	1592	22	0
2	B	1505	0	1398	16	0
3	C	2423	0	2216	39	0
4	D	340	0	288	5	0
5	E	1677	0	1524	34	0
6	A	31	0	26	4	0
All	All	7820	0	7044	110	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 7.

All (110) 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)
5:E:181:SER:O	5:E:182:ASN:ND2	2.20	0.74
3:C:271:CYS:HB2	3:C:290:ASP:HB2	1.70	0.73
5:E:143:VAL:HG12	5:E:207:LEU:HD11	1.74	0.70
3:C:30:LEU:HD13	4:D:34:ALA:HB1	1.72	0.69
1:A:114:TRP:H	1:A:196:VAL:HB	1.58	0.67
1:A:300:LEU:HD11	6:A:401:EJ4:H3	1.76	0.66
1:A:122:LYS:HG2	1:A:187:ALA:HB3	1.78	0.66
1:A:284:TRP:CE3	6:A:401:EJ4:H4	2.32	0.65
4:D:18:GLN:O	4:D:22:GLU:HG3	2.00	0.62
1:A:90:ASN:OD1	1:A:173:TRP:NE1	2.34	0.60
2:B:268:LEU:HD12	2:B:323:PHE:HE1	1.67	0.59
3:C:286:LEU:HD22	3:C:327:VAL:HG11	1.85	0.58
5:E:94:TYR:O	5:E:114:GLY:HA2	2.04	0.58
5:E:153:LEU:HA	5:E:221:LEU:HD22	1.85	0.57
5:E:12:VAL:HG21	5:E:86:LEU:HD13	1.85	0.56
3:C:250:CYS:HB2	3:C:264:TYR:HB2	1.89	0.55
1:A:277:ILE:HG21	6:A:401:EJ4:H19	1.88	0.55
3:C:158:VAL:HG22	3:C:168:LEU:HD13	1.89	0.55
5:E:68:PHE:CZ	5:E:83:MET:HG2	2.42	0.55
3:C:295:ASN:OD1	3:C:304:ARG:NH1	2.41	0.54
2:B:8:GLU:OE2	5:E:163:TYR:OH	2.22	0.54
3:C:96:ARG:O	3:C:98:SER:N	2.40	0.54
2:B:182:THR:OG1	2:B:183:GLY:N	2.38	0.54
1:A:273:CYS:CB	1:A:310:ASN:HB2	2.38	0.53
3:C:331:SER:OG	3:C:333:ASP:OD1	2.25	0.53
3:C:323:ASP:OD1	3:C:323:ASP:N	2.40	0.52
3:C:149:CYS:O	3:C:150:ARG:NH1	2.43	0.52
3:C:257:ALA:HB1	4:D:30:VAL:HG22	1.92	0.52
5:E:178:TYR:O	5:E:182:ASN:HB2	2.09	0.52
3:C:290:ASP:HA	3:C:314:ARG:HG3	1.91	0.51
3:C:161:SER:OG	3:C:162:GLY:N	2.43	0.51
1:A:261:ARG:O	1:A:265:VAL:HG12	2.10	0.50
3:C:75:GLN:HE22	3:C:99:TRP:HA	1.77	0.50
5:E:142:SER:HA	5:E:204:ILE:O	2.11	0.50
3:C:245:SER:OG	3:C:247:ASP:OD1	2.27	0.50
2:B:197:LYS:HB2	2:B:199:PHE:HE2	1.75	0.50
3:C:49:ARG:NH1	3:C:85:TYR:O	2.45	0.49
3:C:22:ARG:NE	3:C:258:ASP:O	2.45	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:152:LEU:HD12	3:C:168:LEU:HD11	1.94	0.49
3:C:311:HIS:CG	3:C:331:SER:HG	2.29	0.49
3:C:340:ASN:ND2	4:D:59:ASN:HD21	2.11	0.49
2:B:9:ASP:O	2:B:13:VAL:HG23	2.13	0.49
3:C:286:LEU:HG	3:C:296:VAL:HG22	1.95	0.49
2:B:184:ILE:HD11	3:C:117:LEU:HD13	1.94	0.49
1:A:218:PHE:HD1	1:A:278:HIS:HD1	1.60	0.48
1:A:258:ARG:NH1	2:B:354:PHE:O	2.46	0.48
3:C:168:LEU:O	3:C:177:THR:N	2.47	0.48
1:A:273:CYS:HB2	1:A:310:ASN:HB2	1.95	0.48
1:A:277:ILE:HD13	1:A:303:CYS:HB3	1.95	0.47
2:B:227:LEU:HD21	2:B:268:LEU:HD13	1.95	0.47
5:E:214:VAL:HG12	5:E:230:GLY:HA3	1.96	0.47
5:E:18:ARG:HA	5:E:18:ARG:HD3	1.75	0.47
1:A:67:ASN:O	1:A:71:MET:HG2	2.16	0.46
3:C:128:THR:HG22	3:C:130:GLU:N	2.30	0.46
3:C:112:VAL:HG23	3:C:124:TYR:HB2	1.98	0.46
5:E:153:LEU:HD12	5:E:200:PHE:CE2	2.50	0.46
1:A:90:ASN:CG	1:A:173:TRP:HE1	2.23	0.46
3:C:81:ILE:HB	3:C:91:HIS:HB2	1.98	0.46
5:E:218:MET:HE3	5:E:220:HIS:HB2	1.98	0.46
3:C:274:THR:HG21	3:C:314:ARG:HD3	1.98	0.45
3:C:123:ILE:O	3:C:136:SER:N	2.47	0.45
5:E:128:MET:HE1	5:E:149:SER:HB3	1.98	0.45
1:A:226:ILE:HD13	1:A:270:PHE:CD2	2.51	0.45
5:E:219:GLN:NE2	5:E:224:PRO:O	2.50	0.45
5:E:91:THR:OG1	5:E:118:THR:HA	2.16	0.45
2:B:254:CYS:O	2:B:317:LYS:NZ	2.49	0.45
5:E:36:TRP:HD1	5:E:70:ILE:HD12	1.81	0.44
5:E:106:SER:O	5:E:106:SER:OG	2.23	0.44
1:A:284:TRP:CZ3	6:A:401:EJ4:H4	2.51	0.44
3:C:128:THR:HG22	3:C:130:GLU:H	1.83	0.44
2:B:250:PHE:HE2	2:B:266:LEU:HD13	1.83	0.44
2:B:264:ILE:HD12	2:B:317:LYS:HD3	2.00	0.44
3:C:274:THR:OG1	3:C:315:VAL:O	2.24	0.44
1:A:136:ILE:HG12	1:A:270:PHE:HZ	1.83	0.44
5:E:39:GLN:HB2	5:E:45:LEU:HD23	1.99	0.44
3:C:289:TYR:CE1	3:C:295:ASN:HB2	2.53	0.44
3:C:283:ARG:NE	3:C:298:ASP:OD2	2.42	0.43
5:E:162:LEU:HD22	5:E:200:PHE:CD2	2.53	0.43
1:A:253:ASP:C	1:A:255:SER:H	2.27	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:E:147:CYS:HB2	5:E:164:TRP:CH2	2.53	0.43
5:E:219:GLN:HG3	5:E:220:HIS:H	1.83	0.43
3:C:191:SER:HB2	3:C:232:ILE:HG23	2.00	0.43
1:A:200:LEU:HD23	1:A:200:LEU:HA	1.88	0.42
5:E:100:ILE:HG23	5:E:105:SER:OG	2.18	0.42
5:E:166:LEU:HB2	5:E:176:LEU:HD11	1.99	0.42
5:E:162:LEU:HD22	5:E:200:PHE:CG	2.55	0.42
2:B:223:PHE:HZ	2:B:249:LEU:HB3	1.85	0.42
5:E:83:MET:HE3	5:E:83:MET:HB2	1.81	0.42
5:E:111:TRP:HE1	5:E:165:PHE:HE2	1.67	0.42
4:D:29:LYS:HE3	4:D:29:LYS:HB3	1.75	0.42
5:E:108:PHE:HE1	5:E:220:HIS:HD2	1.67	0.42
5:E:177:ILE:HG23	5:E:182:ASN:H	1.85	0.42
2:B:318:GLU:HG2	2:B:320:TYR:CZ	2.55	0.41
5:E:68:PHE:CE2	5:E:83:MET:HG2	2.55	0.41
2:B:197:LYS:HB2	2:B:199:PHE:CE2	2.54	0.41
3:C:26:ALA:O	3:C:28:ALA:N	2.52	0.41
2:B:192:LYS:HD2	2:B:336:PHE:CE2	2.54	0.41
5:E:65:LYS:HE2	5:E:65:LYS:HB2	1.92	0.41
5:E:220:HIS:HA	5:E:225:LEU:HD22	2.02	0.41
1:A:168:ILE:HD12	1:A:168:ILE:HA	1.89	0.41
5:E:106:SER:HB2	5:E:178:TYR:CE2	2.56	0.41
3:C:45:MET:HE2	3:C:308:LEU:HD21	2.03	0.41
3:C:145:TYR:OH	3:C:188:MET:HE1	2.20	0.41
1:A:145:ASP:OD1	1:A:160:ARG:NE	2.46	0.41
1:A:226:ILE:HA	1:A:226:ILE:HD12	1.79	0.40
3:C:225:HIS:NE2	3:C:251:ARG:HB2	2.36	0.40
3:C:326:ALA:HB1	3:C:338:ILE:HG23	2.02	0.40
5:E:97:VAL:HG11	5:E:108:PHE:CD2	2.56	0.40
2:B:18:MET:HE2	2:B:18:MET:HB3	1.84	0.40
3:C:78:LYS:HD3	3:C:78:LYS:HA	1.78	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	275/303 (91%)	261 (95%)	14 (5%)	0	100	100
2	B	192/354 (54%)	184 (96%)	8 (4%)	0	100	100
3	C	329/340 (97%)	316 (96%)	13 (4%)	0	100	100
4	D	50/71 (70%)	49 (98%)	1 (2%)	0	100	100
5	E	228/251 (91%)	220 (96%)	8 (4%)	0	100	100
All	All	1074/1319 (81%)	1030 (96%)	44 (4%)	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	139/259 (54%)	133 (96%)	6 (4%)	26	54
2	B	146/305 (48%)	146 (100%)	0	100	100
3	C	229/282 (81%)	226 (99%)	3 (1%)	61	73
4	D	24/58 (41%)	24 (100%)	0	100	100
5	E	157/201 (78%)	155 (99%)	2 (1%)	61	73
All	All	695/1105 (63%)	684 (98%)	11 (2%)	54	71

All (11) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	111	MET
1	A	127	ILE
1	A	186	MET
1	A	236	MET
1	A	243	VAL
1	A	300	LEU
3	C	49	ARG

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Mol	Chain	Res	Type
3	C	234	PHE
3	C	317	CYS
5	E	147	CYS
5	E	203	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (9) such sidechains are listed below:

Mol	Chain	Res	Type
2	B	322	HIS
2	B	346	ASN
3	C	75	GLN
3	C	119	ASN
4	D	59	ASN
5	E	130	GLN
5	E	167	GLN
5	E	182	ASN
5	E	219	GLN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

1 ligand is modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the

expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
6	EJ4	A	401	-	37,38,38	4.53	16 (43%)	57,63,63	2.05	14 (24%)

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	EJ4	A	401	-	-	3/4/60/60	0/1/8/8

All (16) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	A	401	EJ4	CBB-NAS	-15.72	1.18	1.47
6	A	401	EJ4	CAU-CAV	-14.34	1.35	1.54
6	A	401	EJ4	OAD-CAC	11.16	1.54	1.38
6	A	401	EJ4	CBA-CAX	5.32	1.61	1.51
6	A	401	EJ4	CAZ-CAB	4.33	1.47	1.39
6	A	401	EJ4	CAZ-CAY	4.21	1.45	1.38
6	A	401	EJ4	CAX-CAW	4.06	1.45	1.39
6	A	401	EJ4	CAU-CAT	4.00	1.63	1.52
6	A	401	EJ4	CAR-NAS	-3.09	1.44	1.48
6	A	401	EJ4	CAP-CAV	-2.62	1.50	1.53
6	A	401	EJ4	CAO-CAP	2.58	1.57	1.53
6	A	401	EJ4	CAH-CAM	-2.50	1.38	1.41
6	A	401	EJ4	OAD-CAE	-2.42	1.42	1.46
6	A	401	EJ4	OAA-CAB	2.24	1.40	1.36
6	A	401	EJ4	CAC-CAW	2.19	1.41	1.38
6	A	401	EJ4	CAB-CAC	2.04	1.44	1.40

All (14) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	A	401	EJ4	OAD-CAC-CAW	-6.04	105.82	112.80
6	A	401	EJ4	CBA-CAR-NAS	-6.03	109.19	115.63
6	A	401	EJ4	OAD-CAC-CAB	5.37	135.52	126.14
6	A	401	EJ4	CAV-CAP-CAR	4.01	111.54	106.44
6	A	401	EJ4	CAT-CAU-CAV	3.96	115.86	111.62
6	A	401	EJ4	CAV-CAW-CAC	3.24	112.18	109.23

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	A	401	EJ4	CBC-CBB-NAS	-3.08	108.02	113.42
6	A	401	EJ4	CAP-CAR-NAS	-2.96	102.61	105.41
6	A	401	EJ4	CAW-CAV-CAE	2.79	101.10	98.46
6	A	401	EJ4	CBA-CAR-CAP	2.70	117.92	113.50
6	A	401	EJ4	CAP-CAV-CAE	-2.32	116.33	118.08
6	A	401	EJ4	CAO-CAP-CAV	2.21	113.44	111.30
6	A	401	EJ4	CAL-CAM-CAH	-2.18	120.08	122.19
6	A	401	EJ4	CAU-CAV-CAE	-2.03	109.80	111.97

There are no chirality outliers.

All (3) torsion outliers are listed below:

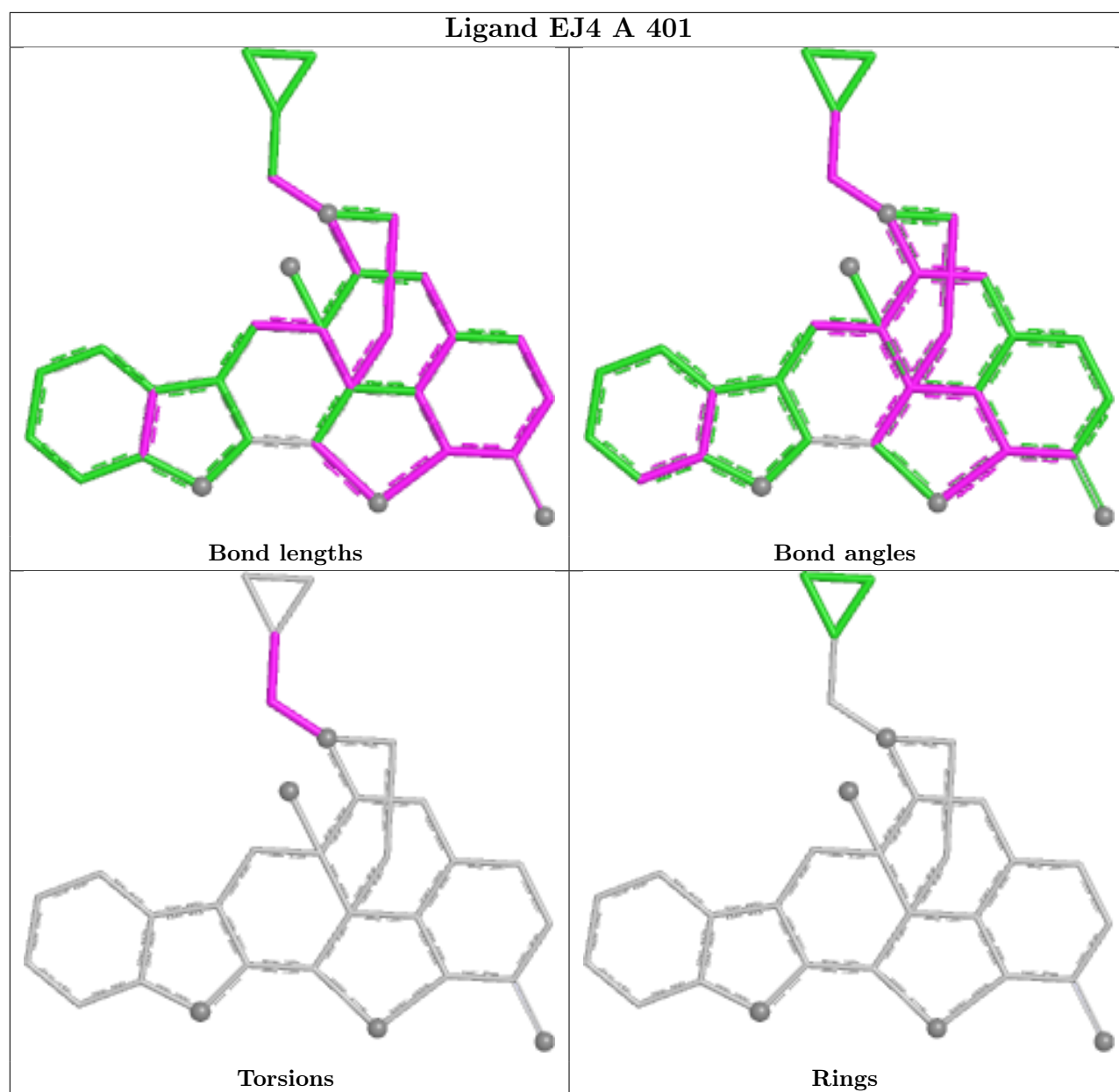
Mol	Chain	Res	Type	Atoms
6	A	401	EJ4	CBC-CBB-NAS-CAT
6	A	401	EJ4	NAS-CBB-CBC-CBD
6	A	401	EJ4	CBC-CBB-NAS-CAR

There are no ring outliers.

1 monomer is involved in 4 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	A	401	EJ4	4	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.

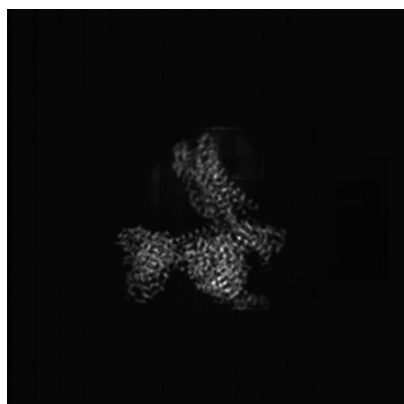
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-71776. These allow visual inspection of the internal detail of the map and identification of artifacts.

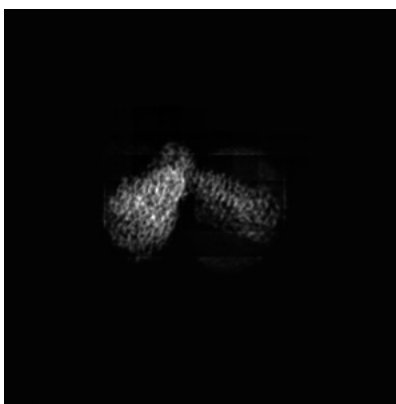
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

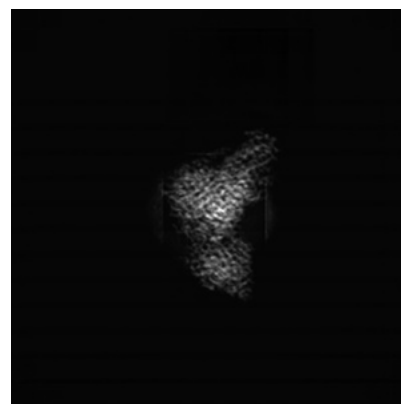
6.1.1 Primary map



X

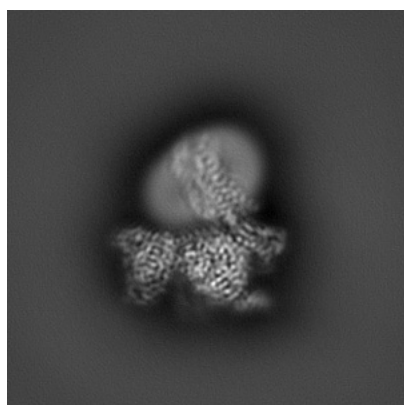


Y

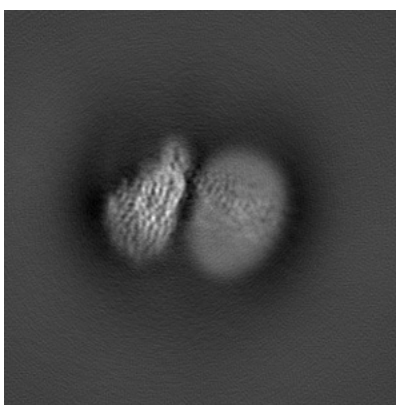


Z

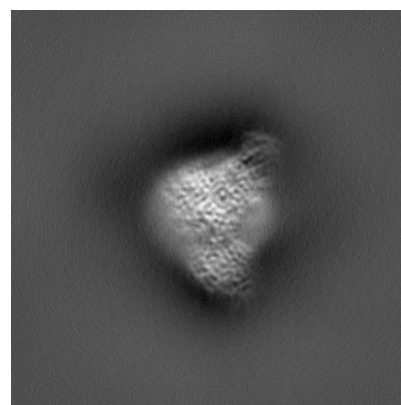
6.1.2 Raw map



X



Y



Z

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

6.2 Central slices [i](#)

6.2.1 Primary map



X Index: 144

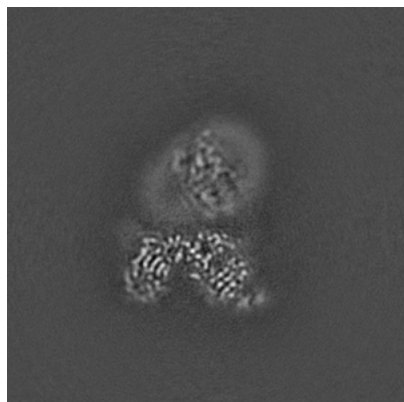


Y Index: 144

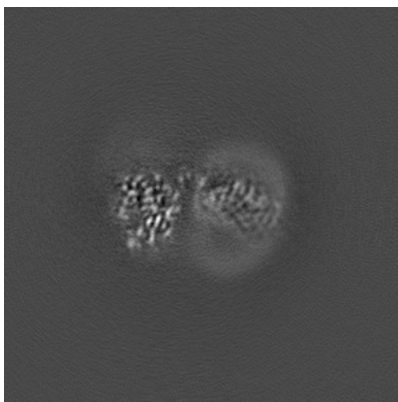


Z Index: 144

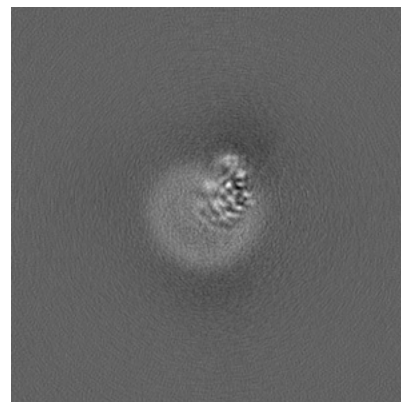
6.2.2 Raw map



X Index: 144



Y Index: 144



Z Index: 144

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

6.3 Largest variance slices [i](#)

6.3.1 Primary map



X Index: 151

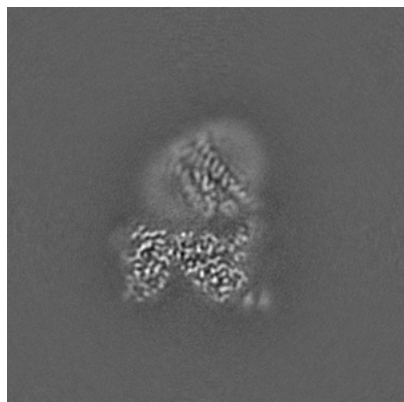


Y Index: 153

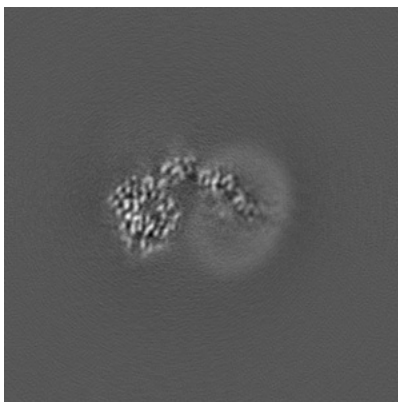


Z Index: 111

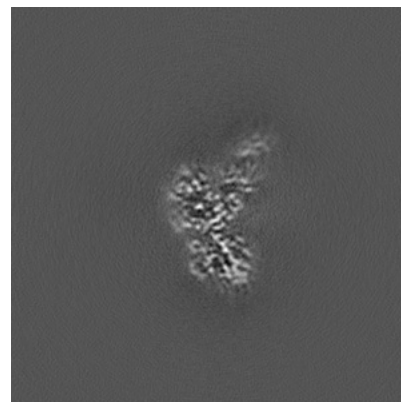
6.3.2 Raw map



X Index: 151



Y Index: 153

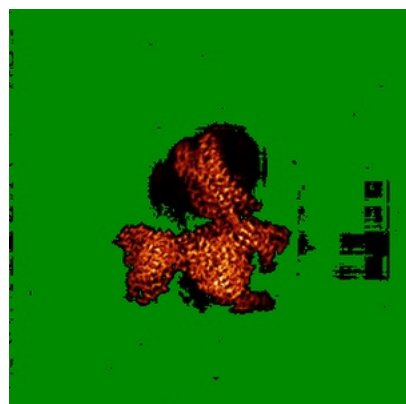


Z Index: 111

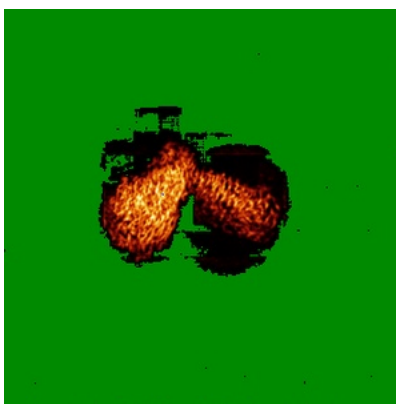
The images above show the largest variance slices of the map in three orthogonal directions.

6.4 Orthogonal standard-deviation projections (False-color) ⓘ

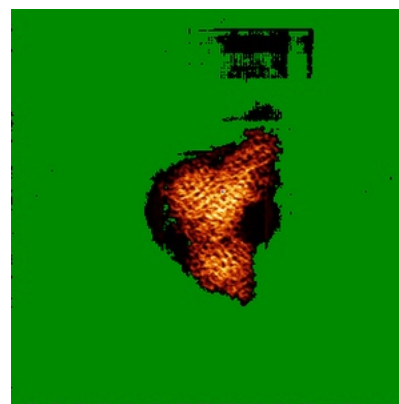
6.4.1 Primary map



X

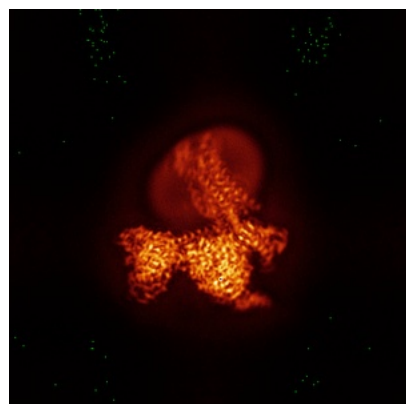


Y

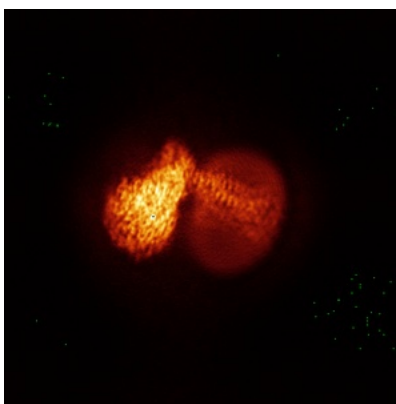


Z

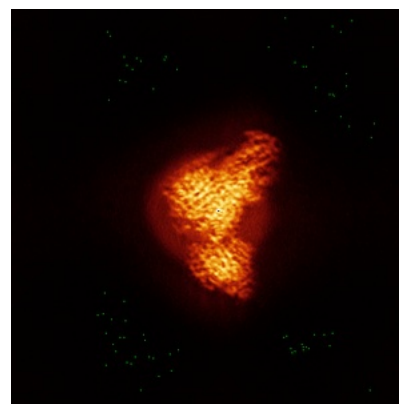
6.4.2 Raw map



X



Y

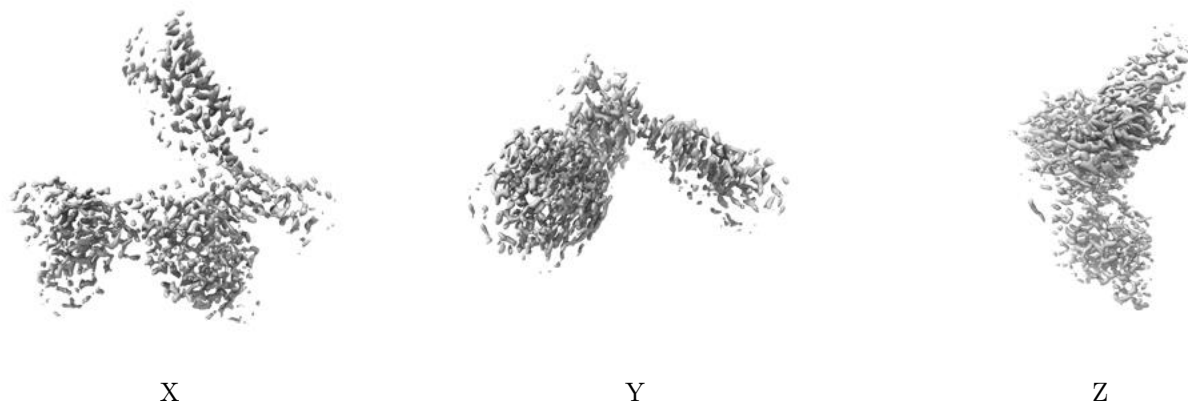


Z

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.

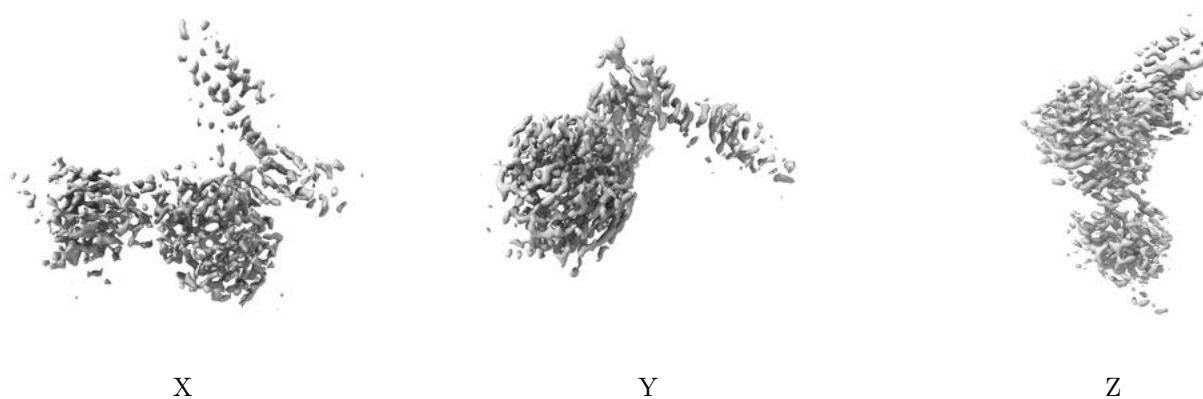
6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.5. 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.

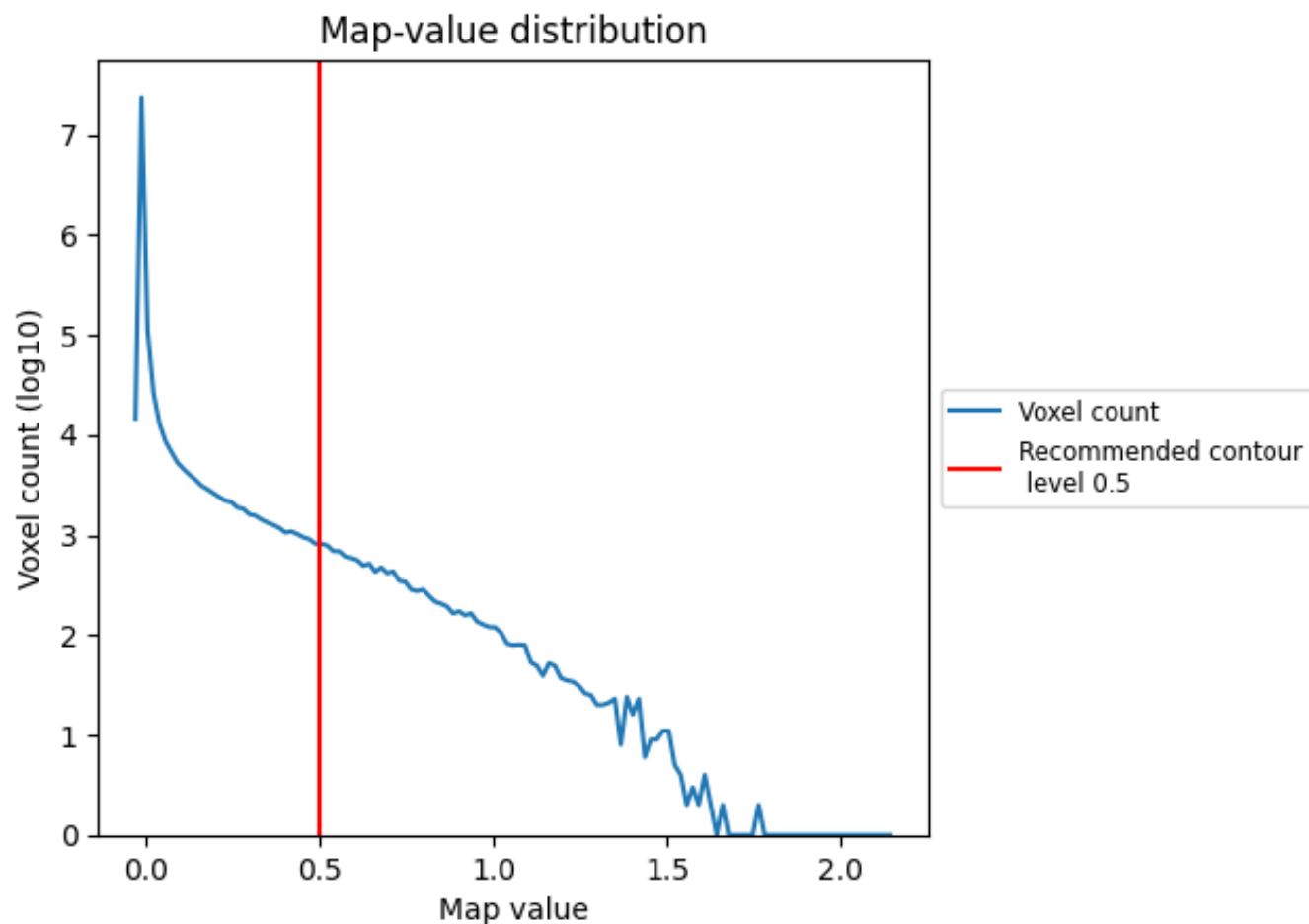
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

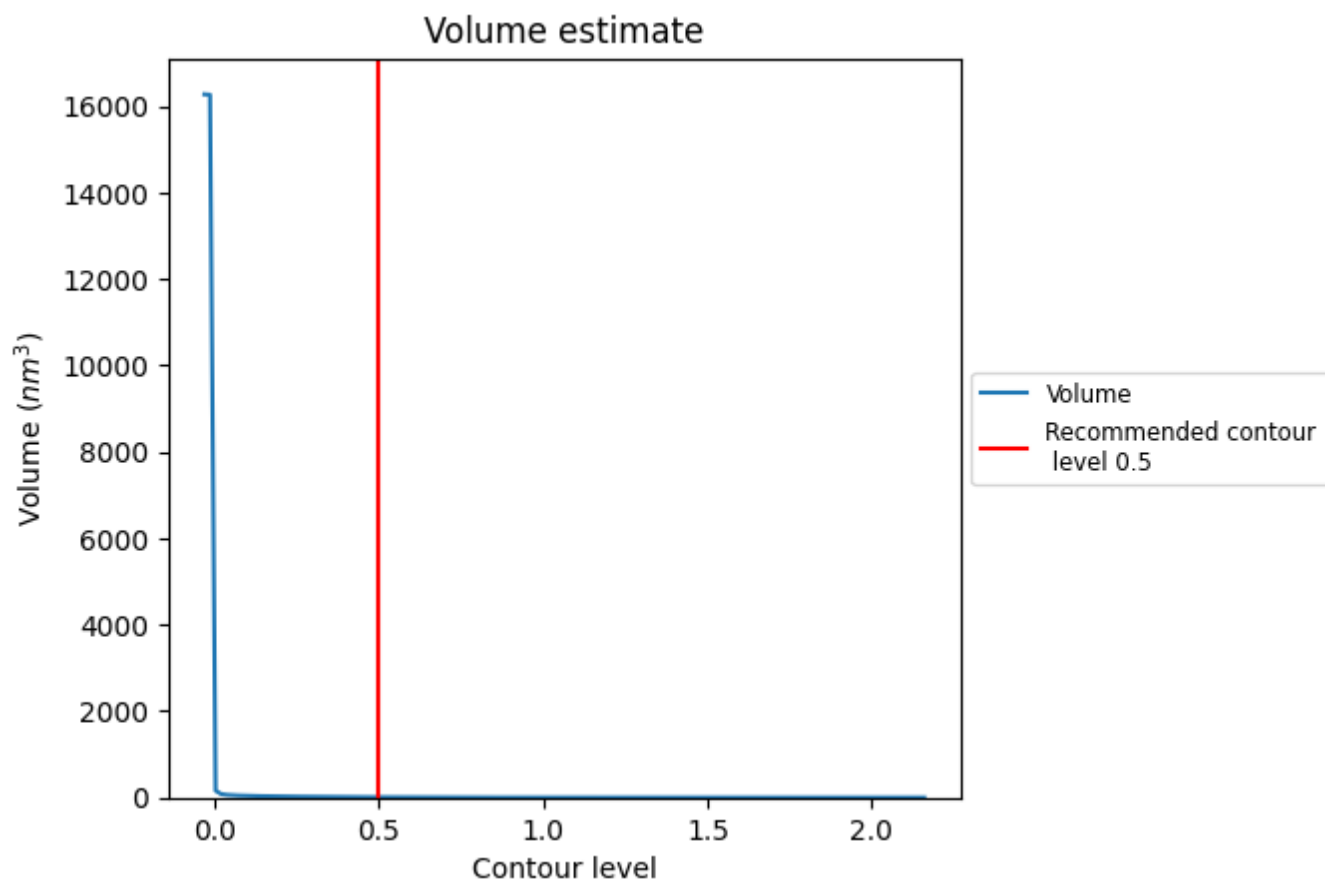
This section contains the results of statistical analysis of the map.

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.

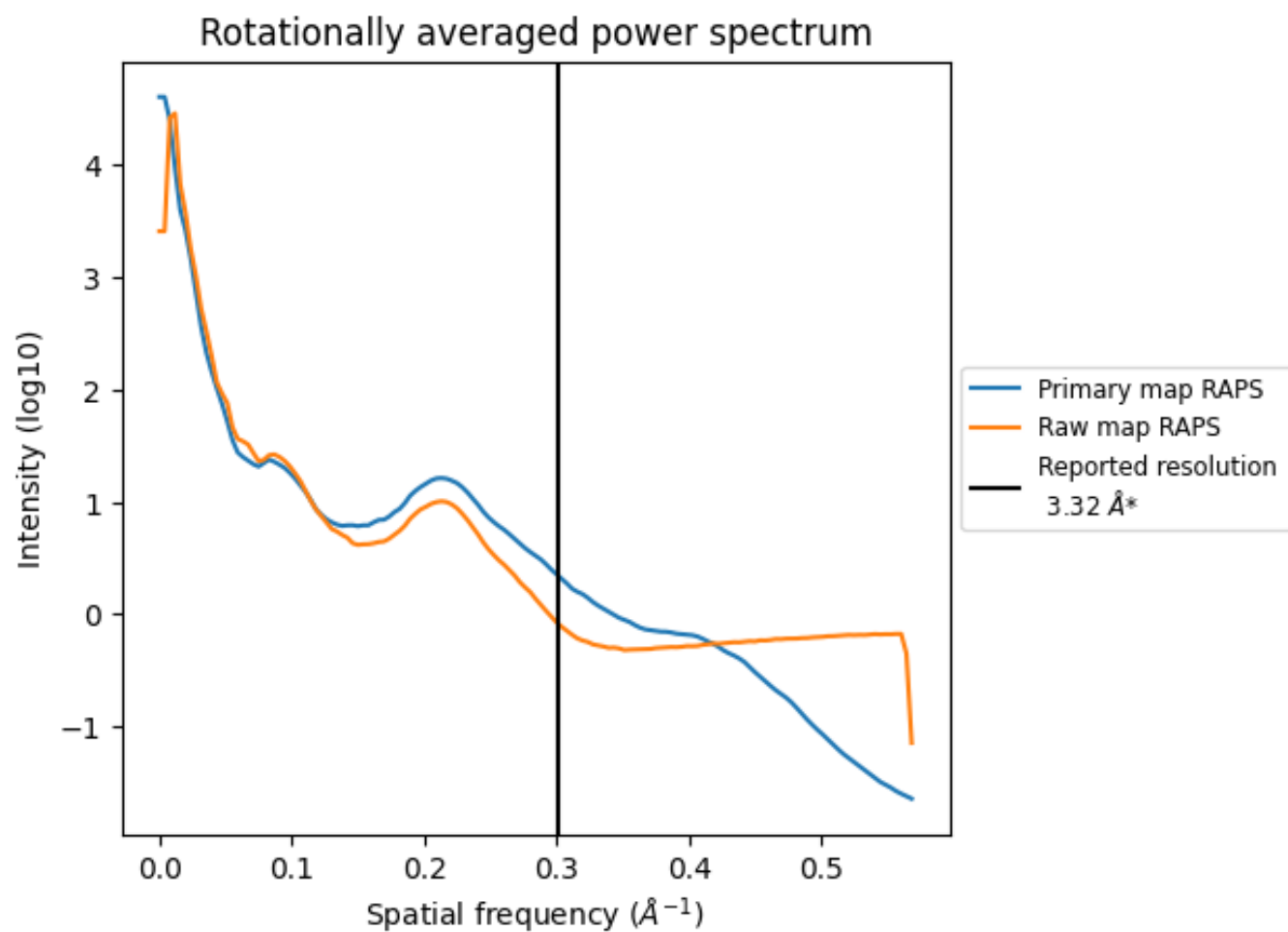
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 8 nm^3 ; this corresponds to an approximate mass of 8 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 ⓘ

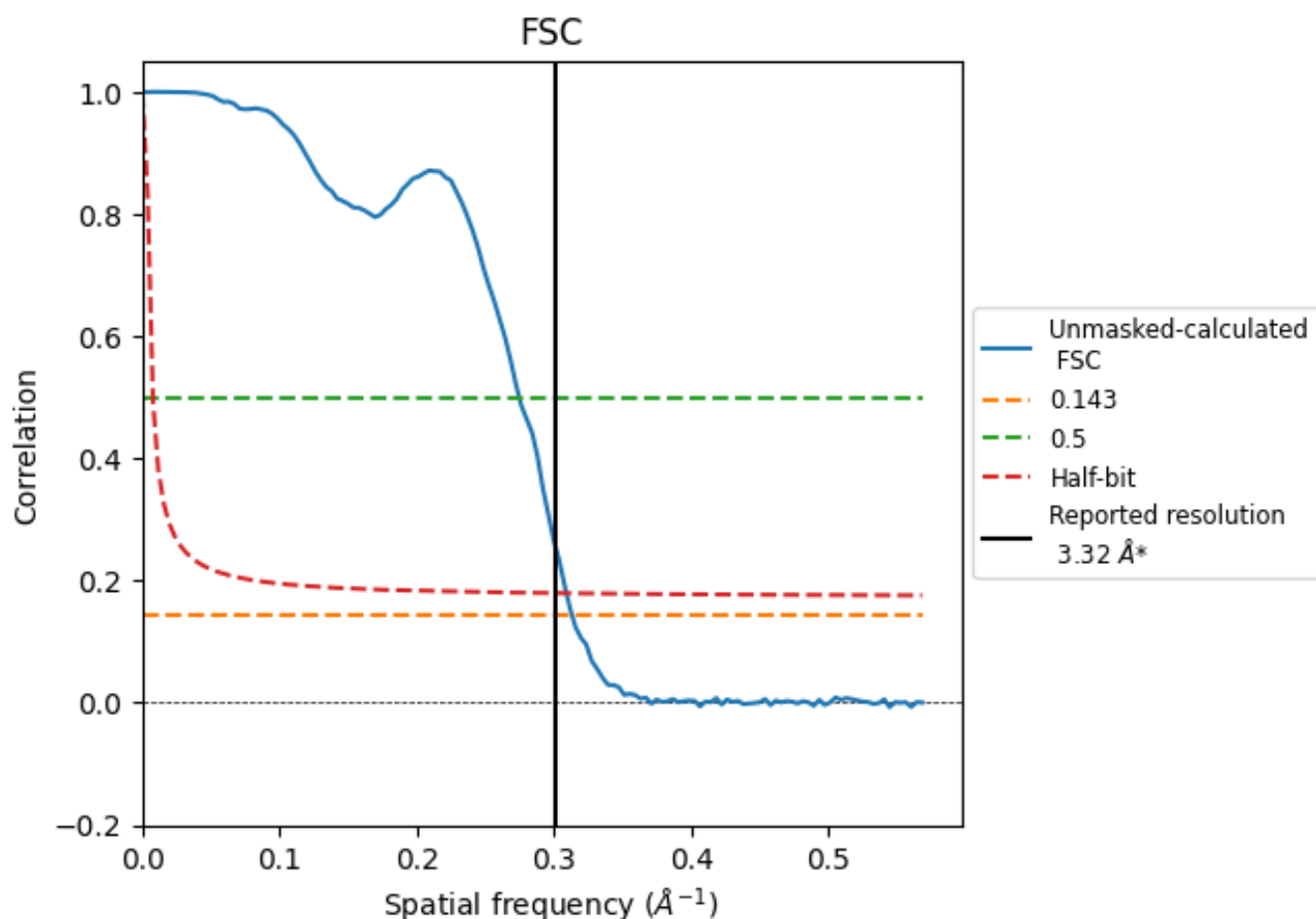


*Reported resolution corresponds to spatial frequency of 0.301 \AA^{-1}

8 Fourier-Shell correlation [i](#)

Fourier-Shell Correlation (FSC) is the most commonly used method to estimate the resolution of single-particle and subtomogram-averaged maps. The shape of the curve depends on the imposed symmetry, mask and whether or not the two 3D reconstructions used were processed from a common reference. The reported resolution is shown as a black line. A curve is displayed for the half-bit criterion in addition to lines showing the 0.143 gold standard cut-off and 0.5 cut-off.

8.1 FSC [i](#)



*Reported resolution corresponds to spatial frequency of 0.301 \AA^{-1}

8.2 Resolution estimates [i](#)

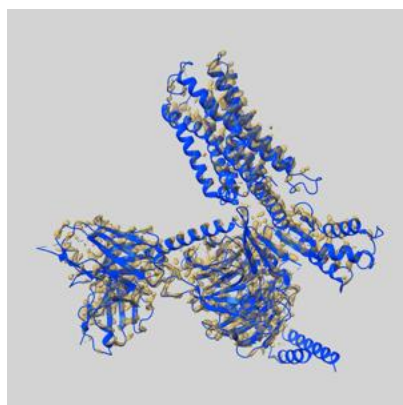
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.32	-	-
Author-provided FSC curve	-	-	-
Unmasked-calculated*	3.19	3.64	3.24

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps.

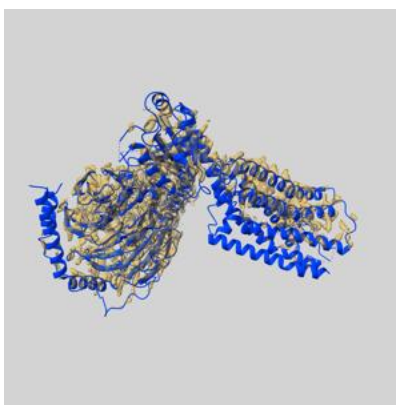
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-71776 and PDB model 9PPW. Per-residue inclusion information can be found in [section 3](#) on [page 6](#).

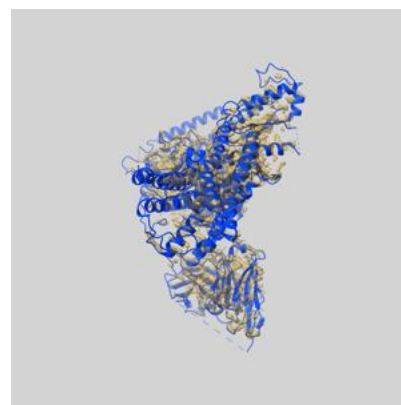
9.1 Map-model overlay [i](#)



X



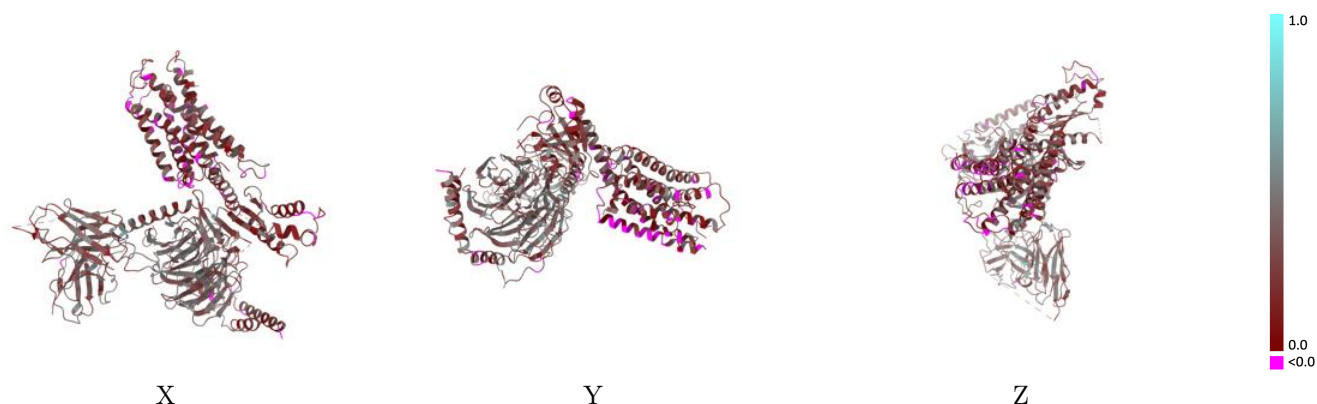
Y



Z

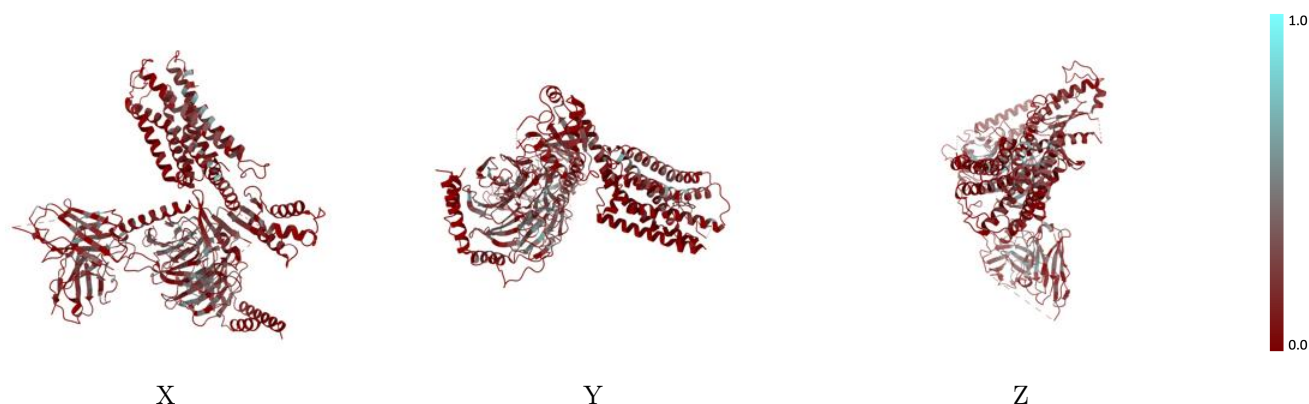
The images above show the 3D surface view of the map at the recommended contour level 0.5 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



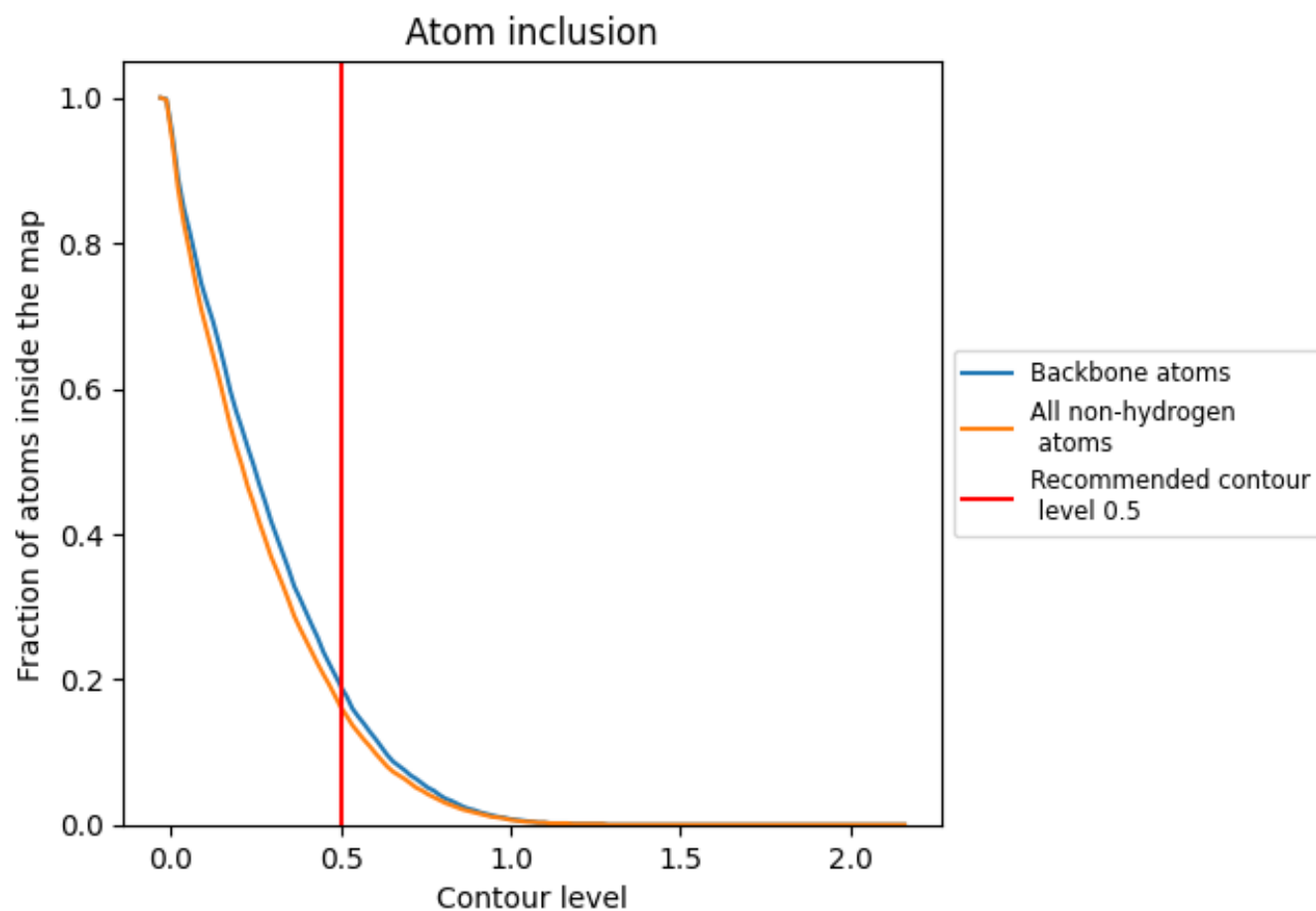
The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.5).

9.4 Atom inclusion ⓘ



At the recommended contour level, 19% of all backbone atoms, 16% 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 (0.5) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	<div></div> 0.1620	<div></div> 0.3030
A	<div></div> 0.1020	<div></div> 0.1960
B	<div></div> 0.1220	<div></div> 0.2760
C	<div></div> 0.2310	<div></div> 0.3710
D	<div></div> 0.0720	<div></div> 0.2830
E	<div></div> 0.1850	<div></div> 0.3530

