



Full wwPDB EM Validation Report ⓘ

Mar 23, 2026 – 11:23 PM UTC

PDB ID : 7E2Z / pdb_00007e2z
EMDB ID : EMD-30973
Title : Aripiprazole-bound serotonin 1A (5-HT1A) receptor-Gi protein complex
Authors : Xu, P.; Huang, S.; Zhang, H.; Mao, C.; Zhou, X.E.; Shen, D.D.; Jiang, Y.;
Zhang, Y.; Xu, H.E.
Deposited on : 2021-02-07
Resolution : 3.10 Å(reported)

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

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

A user guide is available at

<https://www.wwpdb.org/validation/2017/EMValidationReportHelp>
with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

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

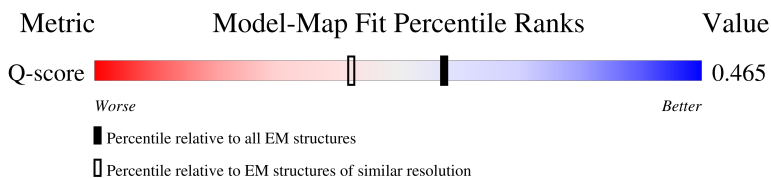
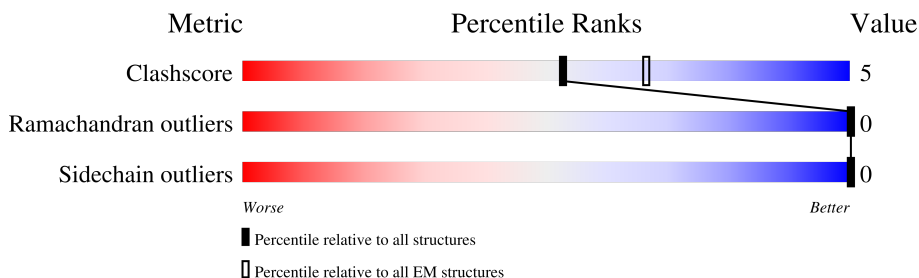
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 3.10 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	14724 (2.60 - 3.60)

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	354	9% 52% 10% 38%
2	B	345	12% 81% 14% 5%
3	G	71	32% 55% 8% 37%
4	R	543	5% 45% 6% 49%

2 Entry composition

There are 7 unique types of molecules in this entry. The entry contains 6997 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
1	A	219	Total	C	N	O	S	0	0
			1766	1126	295	333	12		

There are 4 discrepancies between the modelled and reference sequences:

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

- Molecule 2 is a protein called Guanine nucleotide-binding protein G(I)/G(S)/G(T) subunit beta-1.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	B	328	Total	C	N	O	S	0	0
			2516	1554	452	489	21		

There are 6 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	-4	MET	-	initiating methionine	UNP P62873
B	-3	GLY	-	expression tag	UNP P62873
B	-2	SER	-	expression tag	UNP P62873
B	-1	LEU	-	expression tag	UNP P62873
B	0	LEU	-	expression tag	UNP P62873
B	1	GLN	-	expression tag	UNP P62873

- 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
3	G	45	Total	C	N	O	S	0	0
			347	218	60	66	3		

- Molecule 4 is a protein called Soluble cytochrome b562,5-hydroxytryptamine receptor 1A.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	R	278	Total	C	N	O	S	0	0
			2197	1453	362	365	17		

There are 43 discrepancies between the modelled and reference sequences:

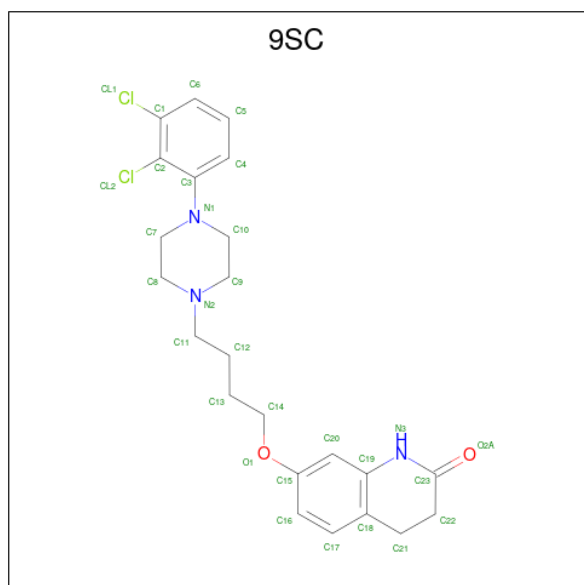
Chain	Residue	Modelled	Actual	Comment	Reference
R	-120	ASP	-	expression tag	UNP P0ABE7
R	-119	TYR	-	expression tag	UNP P0ABE7
R	-118	LYS	-	expression tag	UNP P0ABE7
R	-117	ASP	-	expression tag	UNP P0ABE7
R	-116	ASP	-	expression tag	UNP P0ABE7
R	-115	ASP	-	expression tag	UNP P0ABE7
R	-114	ASP	-	expression tag	UNP P0ABE7
R	-113	ALA	-	expression tag	UNP P0ABE7
R	-112	LYS	-	expression tag	UNP P0ABE7
R	-111	LEU	-	expression tag	UNP P0ABE7
R	-110	GLN	-	expression tag	UNP P0ABE7
R	-109	THR	-	expression tag	UNP P0ABE7
R	-108	MET	-	expression tag	UNP P0ABE7
R	-107	HIS	-	expression tag	UNP P0ABE7
R	-106	HIS	-	expression tag	UNP P0ABE7
R	-105	HIS	-	expression tag	UNP P0ABE7
R	-104	HIS	-	expression tag	UNP P0ABE7
R	-103	HIS	-	expression tag	UNP P0ABE7
R	-102	HIS	-	expression tag	UNP P0ABE7
R	-101	HIS	-	expression tag	UNP P0ABE7
R	-100	HIS	-	expression tag	UNP P0ABE7
R	-99	HIS	-	expression tag	UNP P0ABE7
R	-98	HIS	-	expression tag	UNP P0ABE7
R	-97	HIS	-	expression tag	UNP P0ABE7
R	-96	HIS	-	expression tag	UNP P0ABE7
R	-95	HIS	-	expression tag	UNP P0ABE7
R	-94	HIS	-	expression tag	UNP P0ABE7
R	-93	HIS	-	expression tag	UNP P0ABE7
R	-86	TRP	MET	engineered mutation	UNP P0ABE7
R	9	ILE	HIS	engineered mutation	UNP P0ABE7
R	13	LEU	ARG	engineered mutation	UNP P0ABE7

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
R	14	ALA	-	linker	UNP P0ABE7
R	15	SER	-	linker	UNP P0ABE7
R	16	GLU	-	linker	UNP P0ABE7
R	17	ASN	-	linker	UNP P0ABE7
R	18	LEU	-	linker	UNP P0ABE7
R	19	TYR	-	linker	UNP P0ABE7
R	20	PHE	-	linker	UNP P0ABE7
R	21	GLN	-	linker	UNP P0ABE7
R	22	GLY	-	linker	UNP P0ABE7
R	23	GLY	-	linker	UNP P0ABE7
R	24	THR	-	linker	UNP P0ABE7
R	125	TRP	LEU	engineered mutation	UNP P08908

- Molecule 5 is 7-[4-[4-[2,3-bis(chloranyl)phenyl]piperazin-1-yl]butoxy]-3,4-dihydro-1H-quinolin-2-one (CCD ID: 9SC) (formula: $C_{23}H_{27}Cl_2N_3O_2$) (labeled as "Ligand of Interest" by depositor).



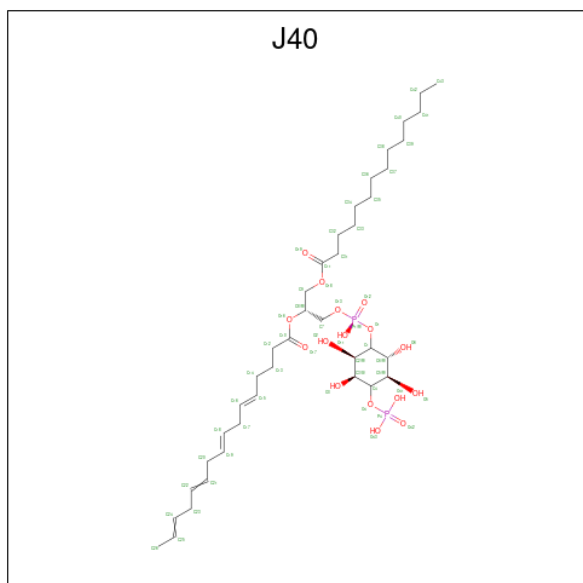
Mol	Chain	Residues	Atoms					AltConf
5	R	1	Total	C	Cl	N	O	0
			30	23	2	3	2	

- Molecule 6 is CHOLESTEROL (CCD ID: CLR) (formula: $C_{27}H_{46}O$).



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

- Molecule 7 is [(2R)-1-[oxidanyl-[(2R,3R,5S,6R)-2,3,5,6-tetrakis(oxidanyl)-4-phosphonooxy-cyclohexyl]oxy-phosphoryl]oxy-3-tetradecanoyloxy-propan-2-yl] (5E,8E)-hexadeca-5,8,11,14-tetraenoate (CCD ID: J40) (formula: C₃₉H₆₈O₁₆P₂).



Mol	Chain	Residues	Atoms				AltConf
			Total	C	O	P	
7	R	1	57	39	16	2	0

4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	154241	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	NONE	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	62	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	49310	Depositor
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor
Maximum map value	0.217	Depositor
Minimum map value	-0.142	Depositor
Average map value	-0.000	Depositor
Map value standard deviation	0.007	Depositor
Recommended contour level	0.03	Depositor
Map size ($\text{\AA}$)	194.68802, 194.68802, 194.68802	wwPDB
Map dimensions	192, 192, 192	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing ($\text{\AA}$)	1.014, 1.014, 1.014	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: 9SC, J40, CLR

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	0.09	0/1795	0.24	0/2407
2	B	0.11	0/2563	0.34	0/3475
3	G	0.10	0/353	0.28	0/477
4	R	0.13	0/2248	0.30	0/3058
All	All	0.11	0/6959	0.30	0/9417

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	1766	0	1768	19	0
2	B	2516	0	2425	29	0
3	G	347	0	350	4	0
4	R	2197	0	2298	23	0
5	R	30	0	0	1	0
6	R	84	0	135	4	0
7	R	57	0	0	1	0
All	All	6997	0	6976	74	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 5.

All (74) 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:B:30:LEU:HD13	3:G:34:ALA:HB1	1.64	0.80
4:R:85:VAL:HG22	4:R:119:CYS:HB3	1.75	0.69
1:A:251:ASP:OD1	1:A:255:ASN:ND2	2.26	0.68
4:R:403:PHE:O	7:R:505:J40:O2	2.16	0.63
2:B:22:ARG:NH1	2:B:258:ASP:O	2.32	0.62
1:A:229:ASP:HA	1:A:232:LEU:HD13	1.81	0.62
2:B:210:LEU:HD22	2:B:255:LEU:HD22	1.83	0.60
1:A:318:GLU:OE2	1:A:345:LYS:NZ	2.35	0.60
1:A:53:MET:HG3	1:A:332:VAL:HG22	1.83	0.59
1:A:10:LYS:O	1:A:14:GLU:HG2	2.03	0.59
2:B:257:ALA:HA	3:G:27:ARG:HH22	1.67	0.58
4:R:63:LEU:HD11	4:R:414:ILE:HD11	1.87	0.56
4:R:88:LEU:HD23	4:R:115:LEU:HD21	1.88	0.56
1:A:206:SER:OG	1:A:211:TRP:NE1	2.39	0.55
1:A:44:SER:HA	1:A:226:ALA:HB2	1.88	0.54
2:B:58:ILE:HG22	2:B:74:SER:HB2	1.89	0.54
2:B:49:ARG:HB2	2:B:338:ILE:HD12	1.89	0.54
2:B:93:ILE:HG12	2:B:133:VAL:HG21	1.89	0.54
2:B:58:ILE:HA	2:B:74:SER:HA	1.89	0.53
3:G:28:ILE:HD12	3:G:32:LYS:HD2	1.89	0.52
4:R:88:LEU:HB3	4:R:115:LEU:HD21	1.92	0.52
1:A:278:ILE:HD11	1:A:283:LEU:HD22	1.91	0.52
1:A:341:ASP:OD1	4:R:225:ARG:NH1	2.42	0.52
1:A:340:THR:HG23	4:R:141:PRO:HG3	1.92	0.51
2:B:294:CYS:HB2	2:B:308:LEU:HB2	1.91	0.51
1:A:325:CYS:SG	1:A:326:SER:N	2.84	0.50
2:B:149:CYS:HB3	2:B:159:THR:HG23	1.93	0.50
2:B:58:ILE:HD11	2:B:330:GLY:HA3	1.93	0.50
2:B:79:LEU:HD23	2:B:93:ILE:HD12	1.93	0.50
4:R:351:MET:HE3	4:R:351:MET:HA	1.94	0.50
4:R:356:LEU:HD23	6:R:503:CLR:H241	1.94	0.50
2:B:51:LEU:HB2	2:B:336:LEU:HB2	1.94	0.49
4:R:78:LEU:HD21	4:R:396:ASN:HB3	1.95	0.49
4:R:223:ARG:O	4:R:227:ARG:HG2	2.13	0.49
2:B:168:LEU:HB3	2:B:178:THR:HB	1.94	0.48
4:R:199:SER:OG	5:R:501:9SC:CL1	2.65	0.48
1:A:243:MET:HG3	1:A:247:MET:HE3	1.97	0.47
2:B:95:LEU:HD13	2:B:100:VAL:HG11	1.96	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:249:THR:HG22	2:B:265:SER:HB3	1.96	0.47
4:R:83:LEU:O	4:R:87:VAL:HG22	2.15	0.47
4:R:81:THR:O	4:R:85:VAL:HG23	2.14	0.47
1:A:342:VAL:O	1:A:346:ASN:ND2	2.41	0.46
4:R:121:THR:HG21	4:R:167:ILE:HD12	1.97	0.46
4:R:122:SER:O	4:R:126:HIS:ND1	2.38	0.46
1:A:185:VAL:HB	1:A:200:ASP:HB3	1.98	0.46
2:B:215:GLU:HG3	2:B:217:MET:HG3	1.96	0.46
4:R:169:ILE:N	4:R:170:PRO:HD2	2.31	0.46
2:B:145:TYR:O	2:B:162:GLY:N	2.48	0.45
3:G:38:MET:O	3:G:42:GLU:HG3	2.16	0.45
1:A:315:ASP:OD1	1:A:316:THR:N	2.50	0.44
1:A:299:ALA:O	1:A:303:ILE:HG12	2.18	0.44
1:A:207:GLU:HG2	1:A:209:LYS:HG2	2.00	0.44
2:B:168:LEU:O	2:B:177:THR:N	2.51	0.44
4:R:159:LEU:O	4:R:163:ILE:HG12	2.17	0.44
2:B:100:VAL:HA	2:B:116:GLY:HA3	2.00	0.44
6:R:503:CLR:H193	6:R:503:CLR:H111	1.84	0.43
2:B:250:CYS:HB2	2:B:264:TYR:HB2	1.99	0.43
2:B:314:ARG:C	2:B:331:SER:HG	2.24	0.43
4:R:357:CYS:HB3	4:R:392:ASN:HB2	2.01	0.43
6:R:502:CLR:H242	6:R:503:CLR:H261	2.01	0.42
4:R:47:ILE:HG12	4:R:90:LEU:HB3	2.01	0.42
6:R:502:CLR:H183	6:R:502:CLR:H20	1.93	0.42
4:R:54:ASN:HB3	4:R:83:LEU:HB2	2.01	0.42
2:B:240:ALA:HA	2:B:254:ASP:HA	2.00	0.42
1:A:51:LYS:HA	1:A:54:LYS:HG2	2.01	0.42
2:B:286:LEU:HD22	2:B:296:VAL:HG22	2.02	0.41
2:B:252:LEU:HD22	2:B:261:LEU:HD12	2.02	0.41
2:B:54:HIS:CE1	2:B:80:ILE:HD12	2.56	0.41
1:A:49:ILE:HB	1:A:53:MET:HE1	2.02	0.41
2:B:27:ASP:OD1	2:B:28:ALA:N	2.53	0.41
4:R:114:ALA:HB2	4:R:172:MET:HE3	2.02	0.41
2:B:180:PHE:HE1	2:B:216:GLY:HA2	1.86	0.41
4:R:84:MET:O	4:R:88:LEU:HB2	2.21	0.41
2:B:168:LEU:HD22	2:B:213:VAL:HG13	2.03	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	213/354 (60%)	211 (99%)	2 (1%)	0	100	100
2	B	326/345 (94%)	315 (97%)	11 (3%)	0	100	100
3	G	43/71 (61%)	43 (100%)	0	0	100	100
4	R	272/543 (50%)	271 (100%)	1 (0%)	0	100	100
All	All	854/1313 (65%)	840 (98%)	14 (2%)	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	195/305 (64%)	195 (100%)	0	100	100
2	B	272/287 (95%)	272 (100%)	0	100	100
3	G	37/58 (64%)	37 (100%)	0	100	100
4	R	237/453 (52%)	237 (100%)	0	100	100
All	All	741/1103 (67%)	741 (100%)	0	100	100

There are no protein residues with a non-rotameric sidechain to report.

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

Mol	Chain	Res	Type
1	A	204	GLN
1	A	269	ASN
2	B	88	ASN
3	G	18	GLN
4	R	54	ASN
4	R	72	ASN
4	R	386	ASN

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 oligosaccharides in this entry.

5.6 Ligand geometry ⓘ

5 ligands are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
6	CLR	R	503	-	31,31,31	1.82	5 (16%)	48,48,48	1.61	10 (20%)
6	CLR	R	502	-	31,31,31	1.83	5 (16%)	48,48,48	1.60	11 (22%)
5	9SC	R	501	-	33,33,33	4.96	14 (42%)	45,45,45	2.66	15 (33%)
7	J40	R	505	-	57,57,57	1.49	11 (19%)	69,72,72	1.22	5 (7%)
6	CLR	R	504	-	31,31,31	1.85	5 (16%)	48,48,48	1.55	13 (27%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
6	CLR	R	503	-	-	4/10/68/68	0/4/4/4
6	CLR	R	502	-	-	4/10/68/68	0/4/4/4
5	9SC	R	501	-	-	7/12/31/31	0/4/4/4
7	J40	R	505	-	-	18/53/77/77	0/1/1/1
6	CLR	R	504	-	-	2/10/68/68	0/4/4/4

All (40) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	R	501	9SC	C19-N3	15.01	1.65	1.39
5	R	501	9SC	C23-N3	13.92	1.51	1.35
5	R	501	9SC	C20-C19	11.87	1.58	1.39
5	R	501	9SC	O2A-C23	8.61	1.40	1.23
5	R	501	9SC	C21-C22	-7.09	1.34	1.52
6	R	503	CLR	C6-C5	6.82	1.47	1.33
6	R	504	CLR	C6-C5	6.81	1.47	1.33
6	R	502	CLR	C6-C5	6.72	1.46	1.33
5	R	501	9SC	C17-C18	5.41	1.48	1.39
5	R	501	9SC	C22-C23	-5.36	1.38	1.50
6	R	502	CLR	O1-C3	-4.47	1.30	1.43
6	R	503	CLR	O1-C3	-4.46	1.30	1.43
6	R	504	CLR	O1-C3	-4.44	1.30	1.43
5	R	501	9SC	C21-C18	-3.84	1.44	1.51
7	R	505	J40	C19-C18	3.79	1.53	1.31
5	R	501	9SC	C19-C18	3.78	1.44	1.40
7	R	505	J40	C22-C21	3.78	1.53	1.31
7	R	505	J40	C16-C15	3.77	1.53	1.31
6	R	502	CLR	C4-C3	3.35	1.58	1.52
6	R	504	CLR	C4-C3	3.34	1.58	1.52
7	R	505	J40	P4-O4	3.30	1.65	1.59
6	R	503	CLR	C4-C3	3.28	1.58	1.52
7	R	505	J40	C24-C25	3.25	1.53	1.29
5	R	501	9SC	C2-CL2	2.92	1.79	1.72
5	R	501	9SC	C16-C17	-2.87	1.34	1.38
5	R	501	9SC	C20-C15	2.79	1.43	1.39
7	R	505	J40	O16-C8	-2.65	1.40	1.46
6	R	502	CLR	C4-C5	-2.44	1.46	1.51
7	R	505	J40	O18-C11	2.39	1.40	1.33

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	R	503	CLR	C4-C5	-2.39	1.46	1.51
6	R	504	CLR	C4-C5	-2.35	1.47	1.51
6	R	502	CLR	C2-C3	2.32	1.57	1.51
6	R	503	CLR	C2-C3	2.27	1.56	1.51
6	R	504	CLR	C2-C3	2.27	1.56	1.51
5	R	501	9SC	C1-CL1	2.27	1.79	1.73
7	R	505	J40	P4-O43	-2.27	1.46	1.54
7	R	505	J40	P4-O41	-2.22	1.46	1.54
7	R	505	J40	O16-C10	2.18	1.40	1.34
7	R	505	J40	O18-C9	-2.14	1.40	1.45
5	R	501	9SC	C3-N1	2.00	1.45	1.41

All (54) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	R	501	9SC	C19-N3-C23	-6.78	116.33	124.45
5	R	501	9SC	C22-C21-C18	6.07	124.06	111.97
5	R	501	9SC	C20-C19-C18	-5.50	114.60	120.86
5	R	501	9SC	C16-C15-C20	-5.40	113.24	120.50
5	R	501	9SC	C17-C16-C15	5.09	125.54	119.73
5	R	501	9SC	C20-C19-N3	4.91	128.28	119.76
5	R	501	9SC	C21-C22-C23	4.46	123.67	113.77
7	R	505	J40	O16-C10-C12	3.99	120.12	111.48
5	R	501	9SC	C19-C20-C15	3.94	125.43	118.03
5	R	501	9SC	C16-C17-C18	3.71	126.24	121.39
5	R	501	9SC	C21-C18-C17	3.70	128.77	121.05
6	R	502	CLR	C12-C11-C9	3.64	119.32	113.14
6	R	503	CLR	C12-C11-C9	3.60	119.25	113.14
6	R	504	CLR	C12-C11-C9	3.55	119.17	113.14
5	R	501	9SC	C17-C18-C19	-3.52	114.95	118.32
6	R	503	CLR	C4-C5-C10	3.45	120.84	116.42
6	R	504	CLR	C4-C5-C10	3.34	120.70	116.42
6	R	502	CLR	C10-C9-C8	-3.20	108.03	112.71
6	R	502	CLR	C4-C5-C10	3.15	120.46	116.42
6	R	503	CLR	C10-C9-C8	-3.01	108.32	112.71
6	R	503	CLR	C17-C13-C14	2.99	103.53	100.10
6	R	502	CLR	C17-C13-C14	2.94	103.47	100.10
6	R	503	CLR	C4-C5-C6	-2.84	116.73	120.57
6	R	504	CLR	C17-C13-C14	2.81	103.33	100.10
6	R	504	CLR	C4-C5-C6	-2.78	116.80	120.57
6	R	502	CLR	C4-C5-C6	-2.75	116.85	120.57
5	R	501	9SC	C10-N1-C7	2.73	117.72	111.57

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	R	503	CLR	C19-C10-C9	-2.72	108.60	111.66
7	R	505	J40	O18-C11-C31	2.72	120.13	111.83
6	R	504	CLR	C19-C10-C9	-2.68	108.66	111.66
6	R	502	CLR	C19-C10-C9	-2.67	108.66	111.66
5	R	501	9SC	C8-C7-N1	-2.64	105.23	110.78
6	R	504	CLR	C7-C8-C9	2.62	112.75	109.72
6	R	504	CLR	C10-C9-C8	-2.61	108.90	112.71
6	R	502	CLR	C1-C2-C3	2.58	113.90	110.48
5	R	501	9SC	C18-C19-N3	-2.58	117.12	119.14
6	R	503	CLR	C7-C8-C9	2.49	112.60	109.72
6	R	503	CLR	C13-C14-C8	-2.40	111.00	114.41
7	R	505	J40	O11-P1-O12	-2.38	101.37	112.44
6	R	504	CLR	C13-C14-C8	-2.31	111.13	114.41
6	R	503	CLR	C1-C2-C3	2.26	113.47	110.48
6	R	504	CLR	C1-C2-C3	2.23	113.43	110.48
5	R	501	9SC	C21-C18-C19	-2.18	116.29	118.54
6	R	502	CLR	C13-C14-C8	-2.16	111.35	114.41
6	R	502	CLR	C7-C8-C9	2.15	112.20	109.72
7	R	505	J40	O43-P4-O4	2.14	114.19	105.85
6	R	502	CLR	C7-C6-C5	-2.13	121.42	125.02
7	R	505	J40	O41-P4-O4	2.13	114.15	105.85
6	R	503	CLR	C2-C3-C4	-2.06	107.39	110.29
6	R	504	CLR	C2-C3-C4	-2.04	107.42	110.29
6	R	502	CLR	C21-C20-C17	-2.03	109.83	112.88
6	R	504	CLR	C15-C16-C17	2.02	109.10	105.14
6	R	504	CLR	C2-C1-C10	2.02	117.08	112.78
6	R	504	CLR	C7-C6-C5	-2.01	121.62	125.02

There are no chirality outliers.

All (35) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	R	501	9SC	C2-C3-N1-C10
7	R	505	J40	C23-C24-C25-C26
6	R	502	CLR	C16-C17-C20-C21
6	R	502	CLR	C13-C17-C20-C21
6	R	502	CLR	C13-C17-C20-C22
6	R	502	CLR	C16-C17-C20-C22
7	R	505	J40	C20-C21-C22-C23
6	R	504	CLR	C17-C20-C22-C23
5	R	501	9SC	C12-C13-C14-O1
7	R	505	J40	C12-C10-O16-C8

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
7	R	505	J40	O17-C10-O16-C8
6	R	503	CLR	C13-C17-C20-C22
7	R	505	J40	C31-C32-C33-C34
5	R	501	9SC	C16-C15-O1-C14
6	R	503	CLR	C13-C17-C20-C21
7	R	505	J40	C38-C39-C40-C41
5	R	501	9SC	C20-C15-O1-C14
7	R	505	J40	C36-C37-C38-C39
6	R	503	CLR	C16-C17-C20-C21
6	R	504	CLR	C21-C20-C22-C23
7	R	505	J40	C13-C14-C15-C16
5	R	501	9SC	C13-C14-O1-C15
6	R	503	CLR	C16-C17-C20-C22
7	R	505	J40	C12-C13-C14-C15
7	R	505	J40	C16-C17-C18-C19
7	R	505	J40	C18-C19-C20-C21
7	R	505	J40	C19-C20-C21-C22
5	R	501	9SC	C4-C3-N1-C10
5	R	501	9SC	C12-C11-N2-C8
7	R	505	J40	O13-C7-C8-O16
7	R	505	J40	C31-C11-O18-C9
7	R	505	J40	C8-C7-O13-P1
7	R	505	J40	O16-C8-C9-O18
7	R	505	J40	O19-C11-O18-C9
7	R	505	J40	C17-C18-C19-C20

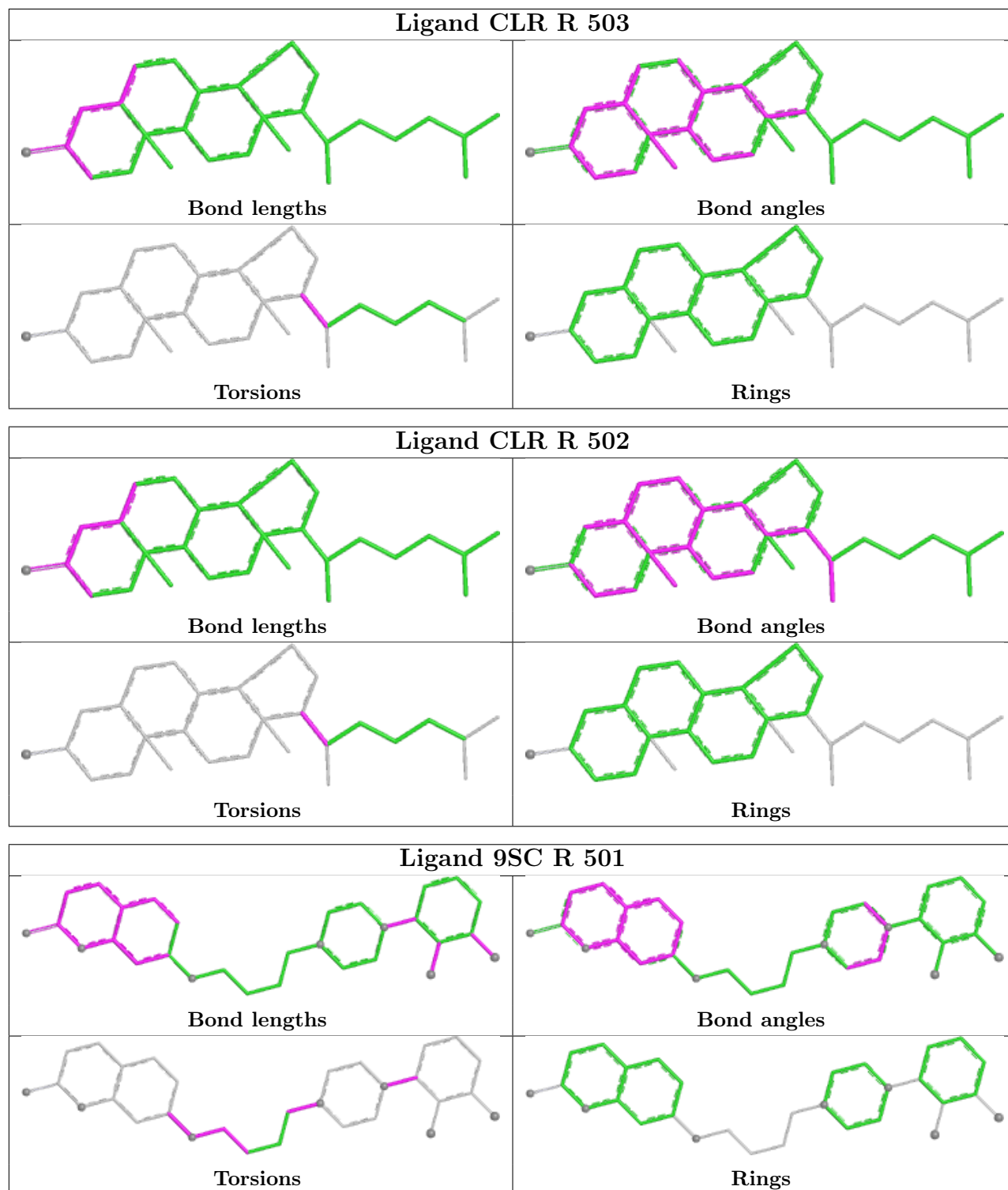
There are no ring outliers.

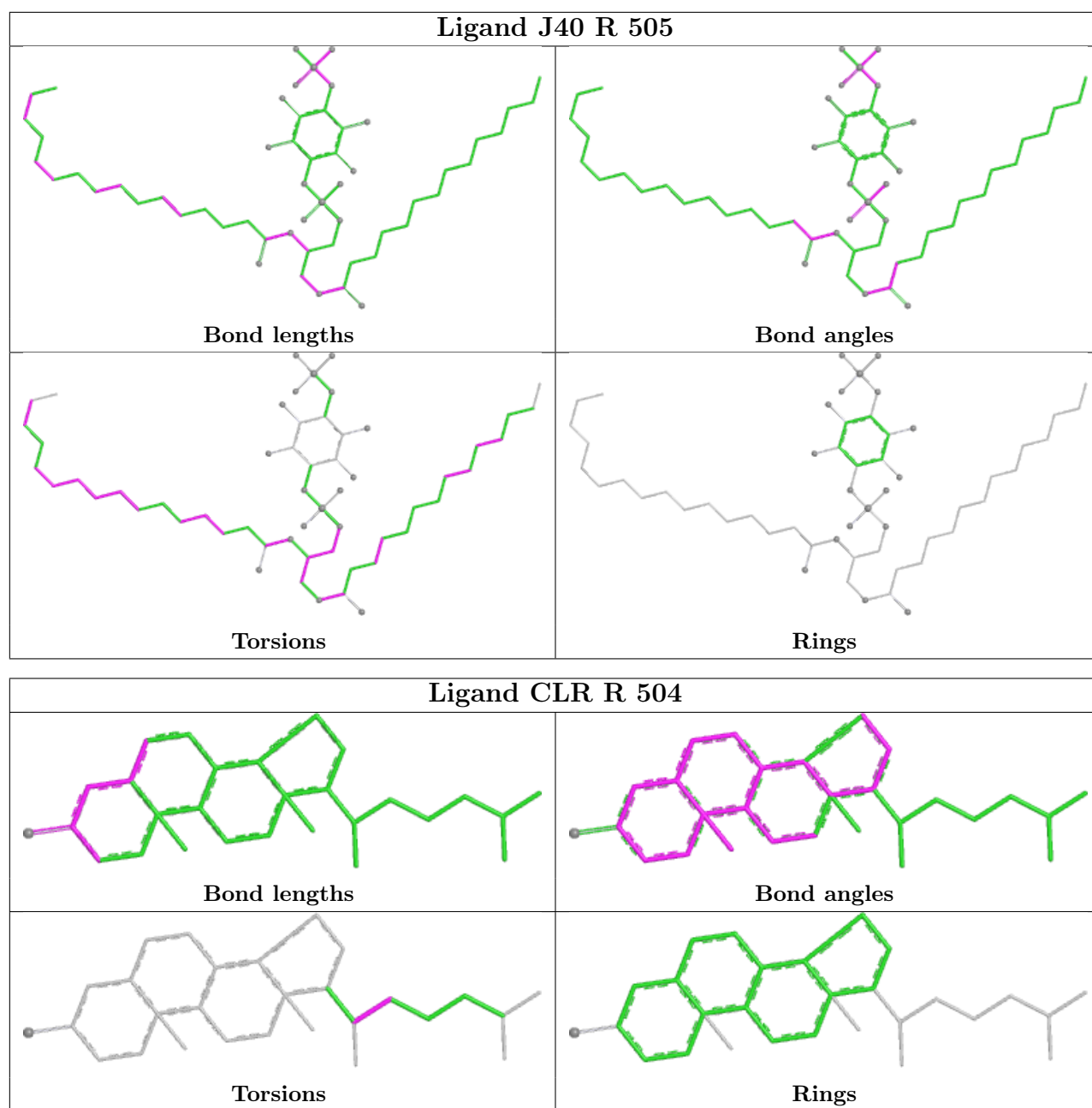
4 monomers are involved in 6 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	R	503	CLR	3	0
6	R	502	CLR	2	0
5	R	501	9SC	1	0
7	R	505	J40	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 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.

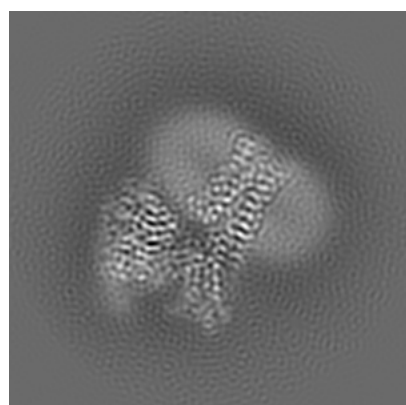
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-30973. These allow visual inspection of the internal detail of the map and identification of artifacts.

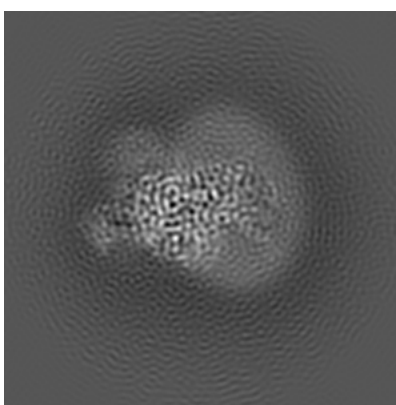
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

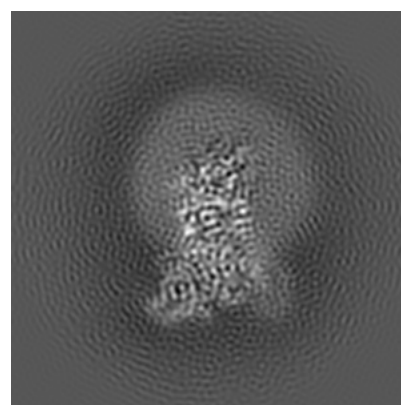
6.1.1 Primary map



X



Y

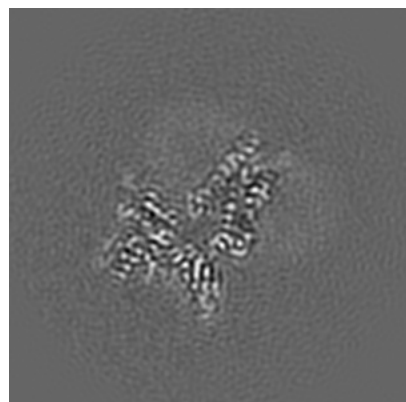


Z

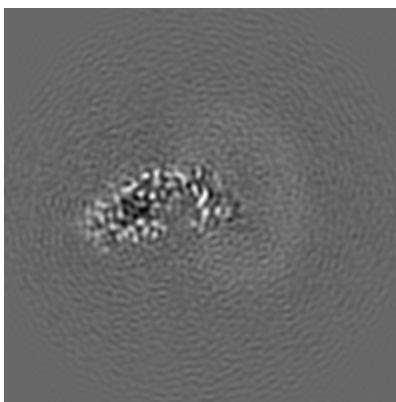
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

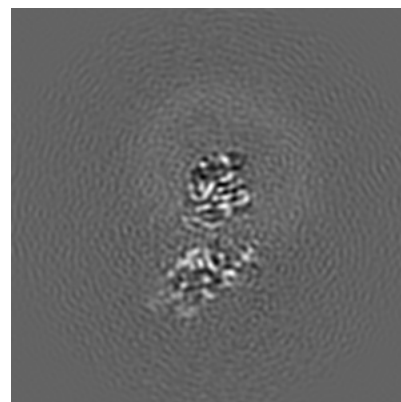
6.2.1 Primary map



X Index: 96



Y Index: 96

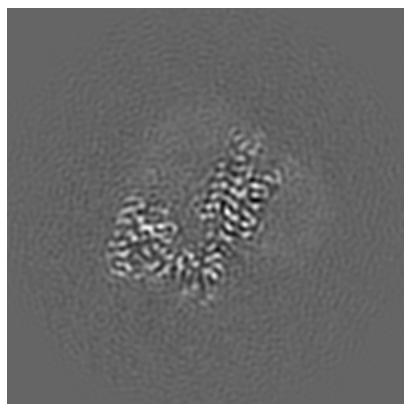


Z Index: 96

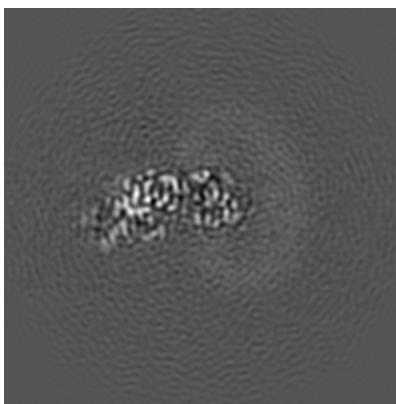
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

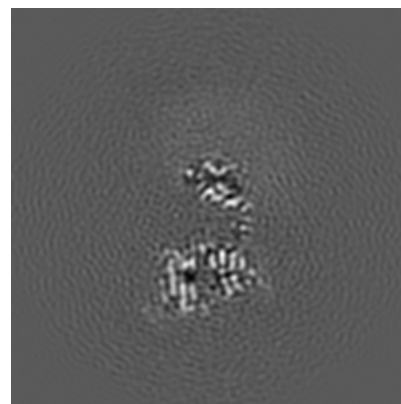
6.3.1 Primary map



X Index: 102



Y Index: 99

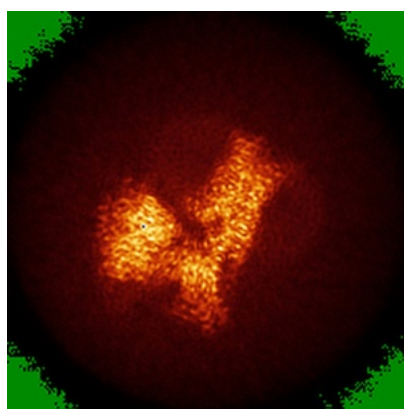


Z Index: 82

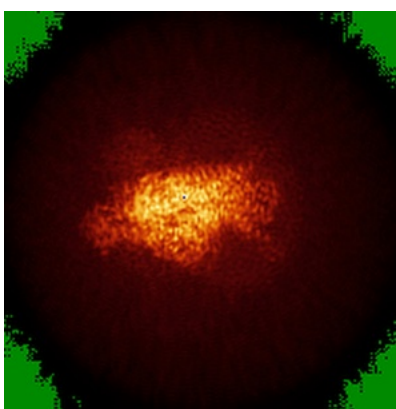
The images above show the largest variance slices of the map in three orthogonal directions.

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

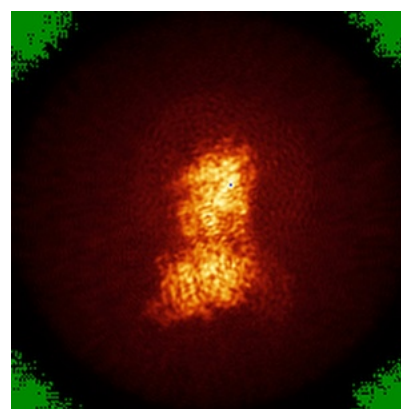
6.4.1 Primary map



X



Y

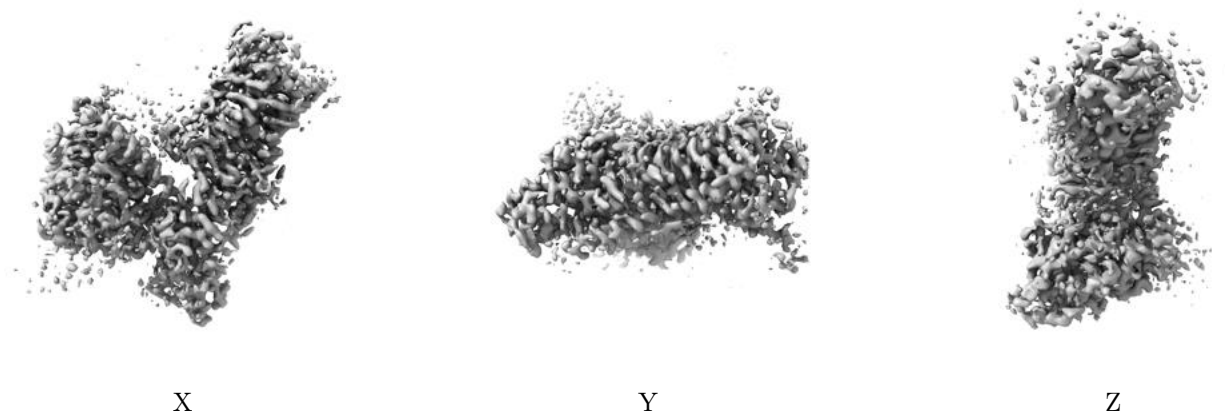


Z

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 0.03. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

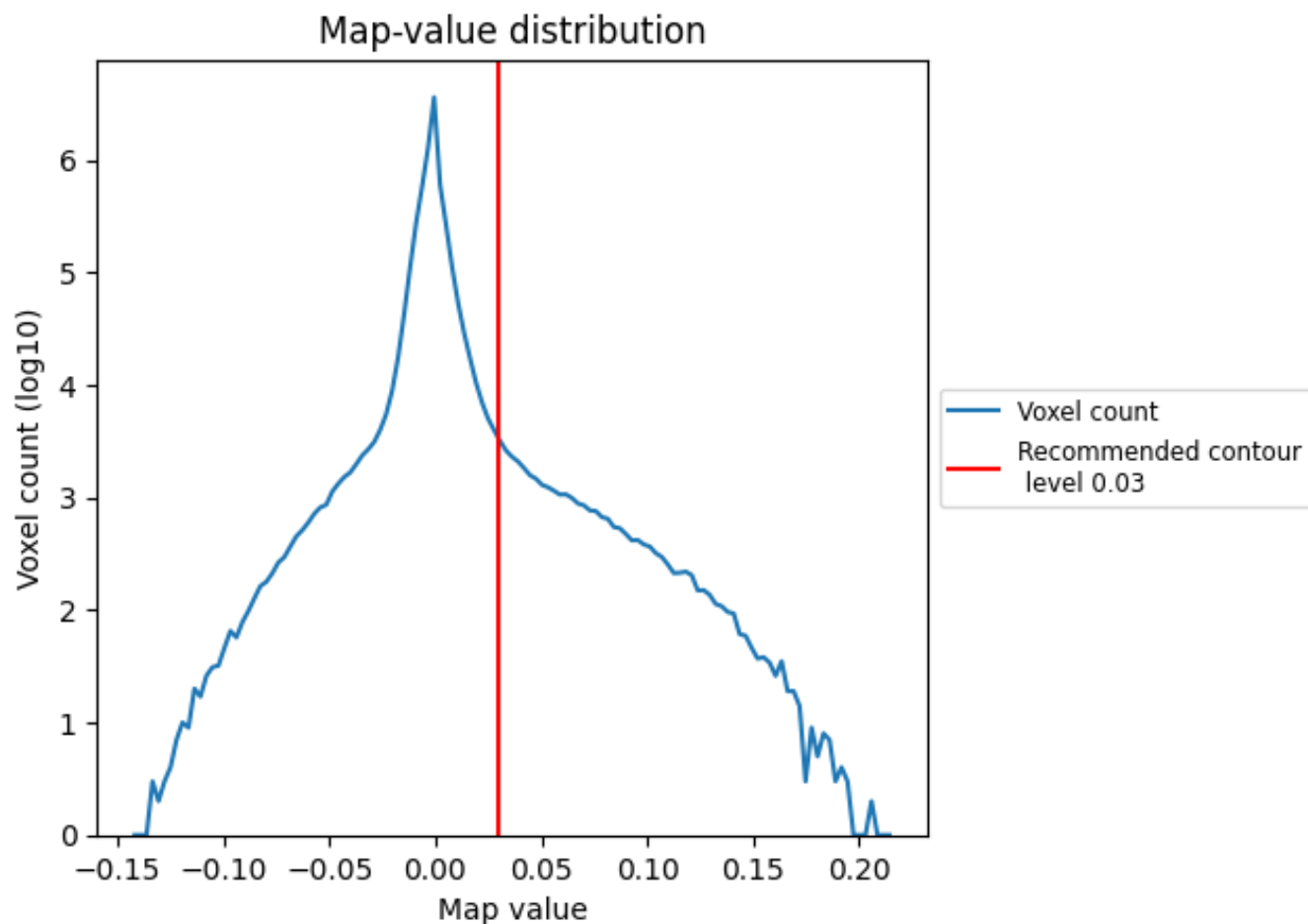
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

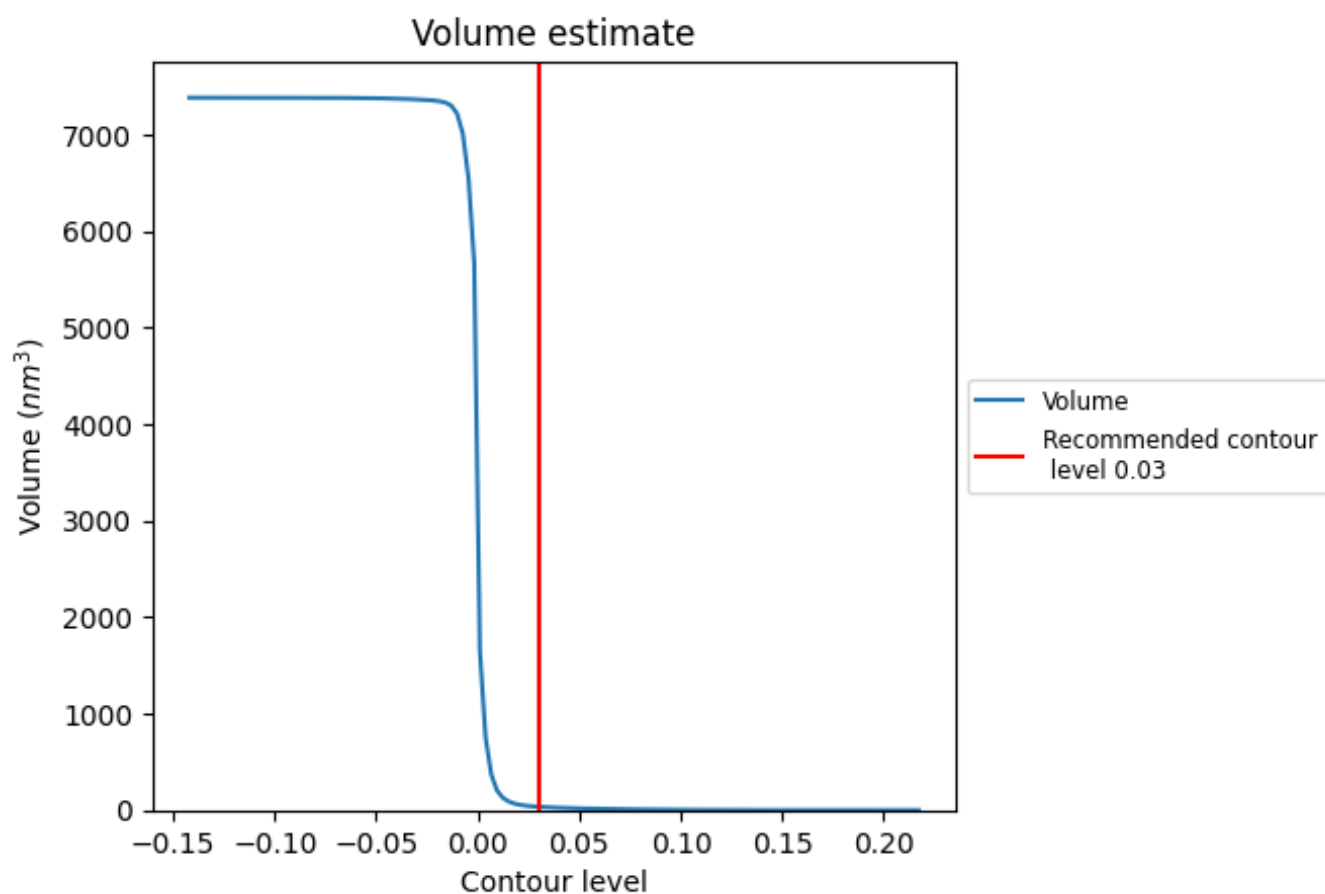
This section contains the results of statistical analysis of the map.

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.

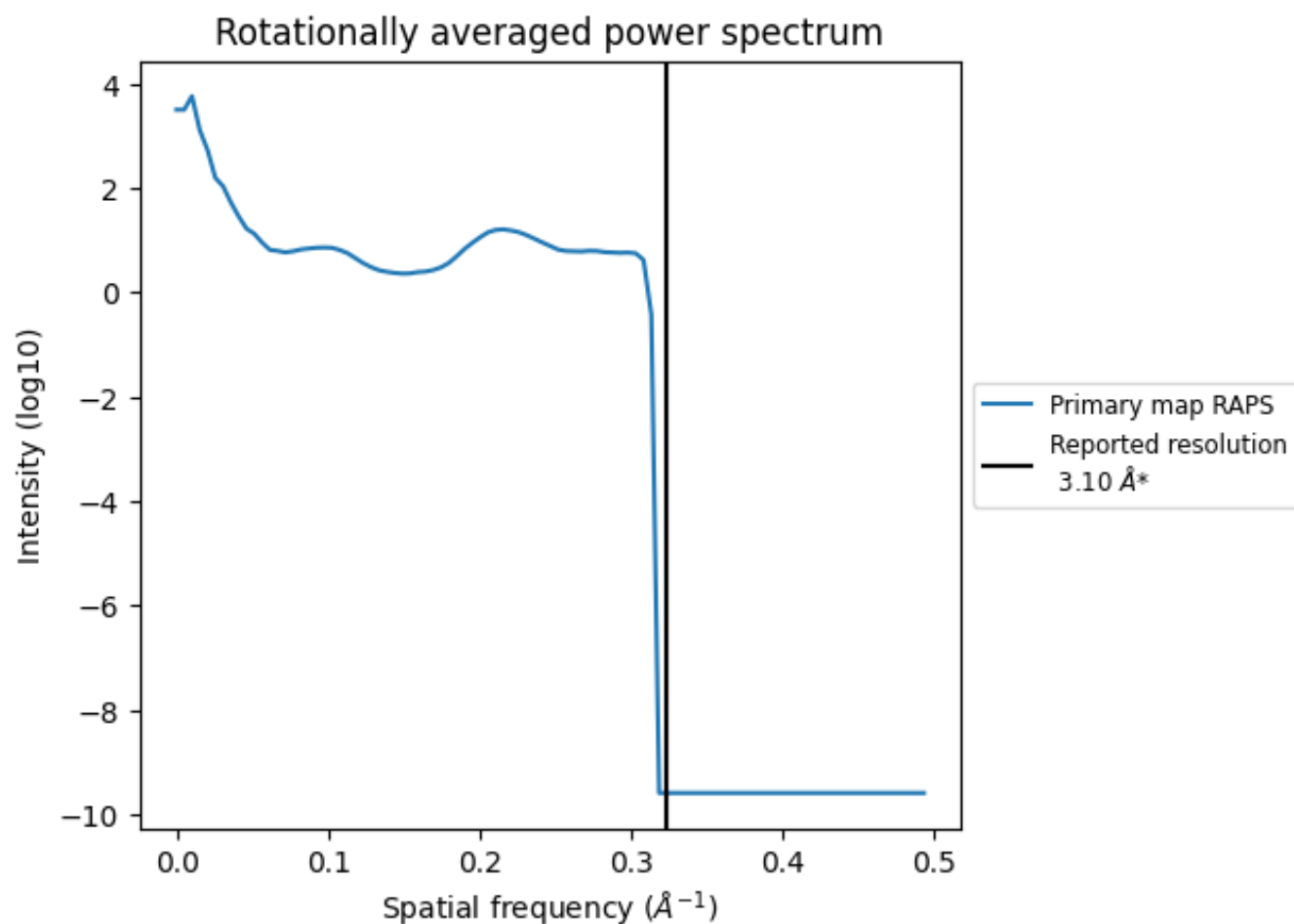
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 35 nm^3 ; this corresponds to an approximate mass of 31 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 0.323 $\text{\AA}^{-1}$

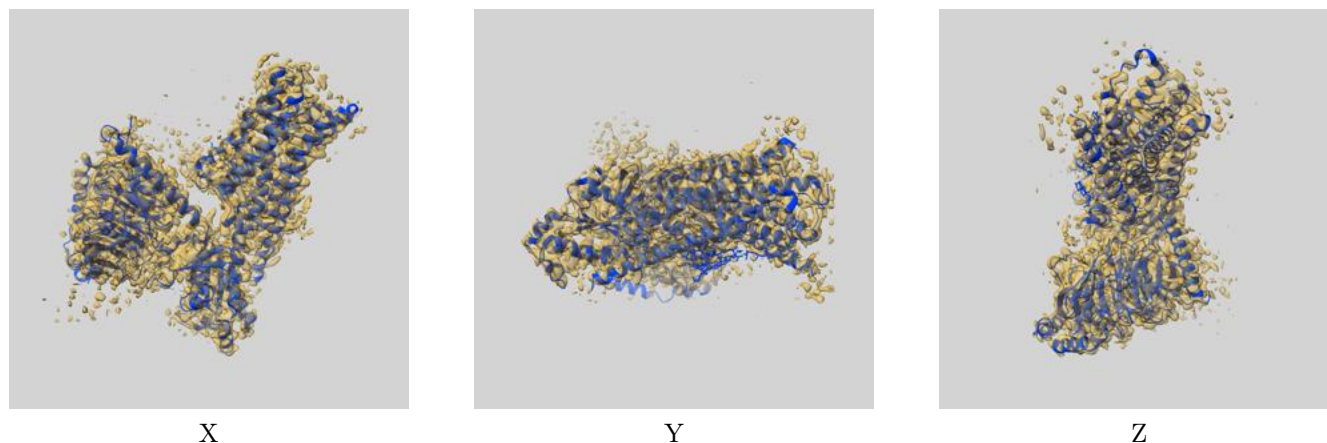
8 Fourier-Shell correlation ⓘ

This section was not generated. No FSC curve or half-maps provided.

9 Map-model fit [i](#)

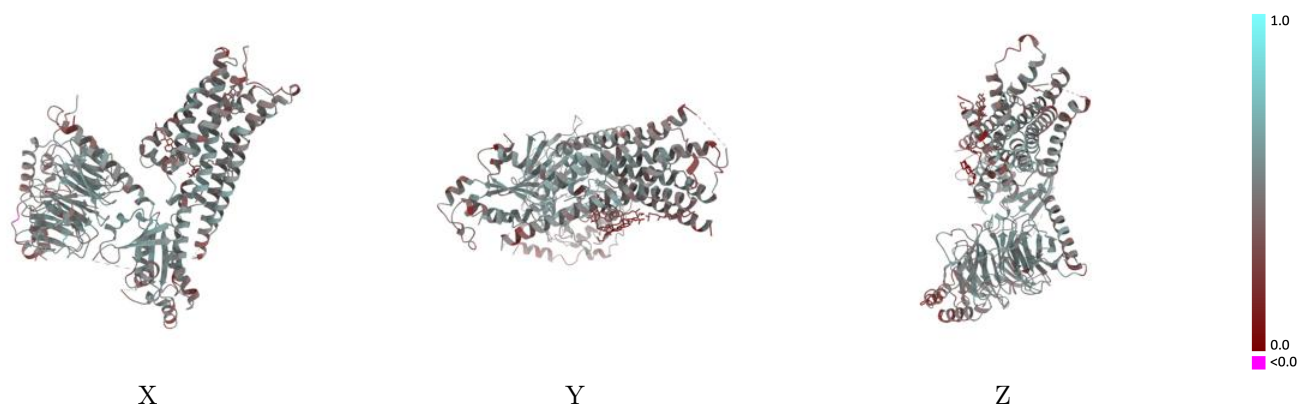
This section contains information regarding the fit between EMDB map EMD-30973 and PDB model 7E2Z. Per-residue inclusion information can be found in section [3](#) on page [8](#).

9.1 Map-model overlay [i](#)



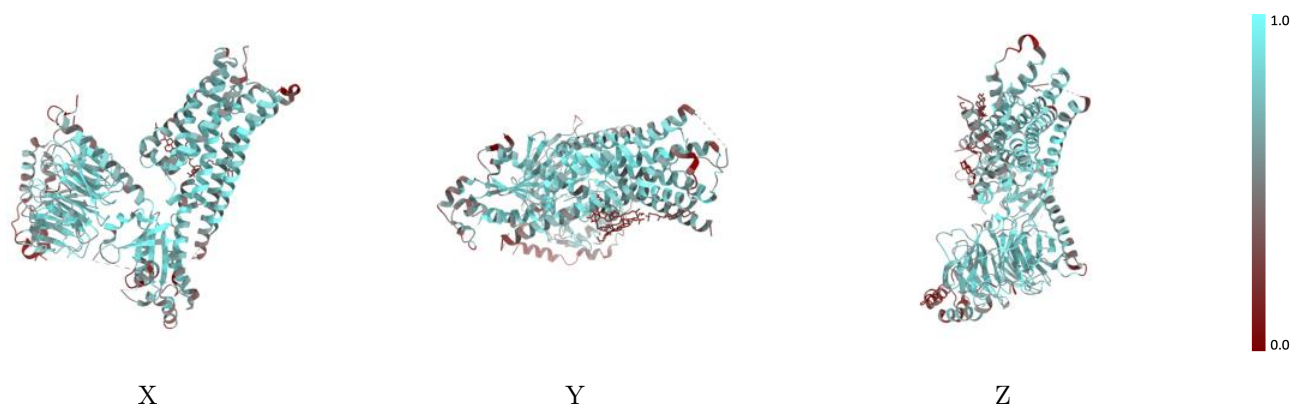
The images above show the 3D surface view of the map at the recommended contour level 0.03 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



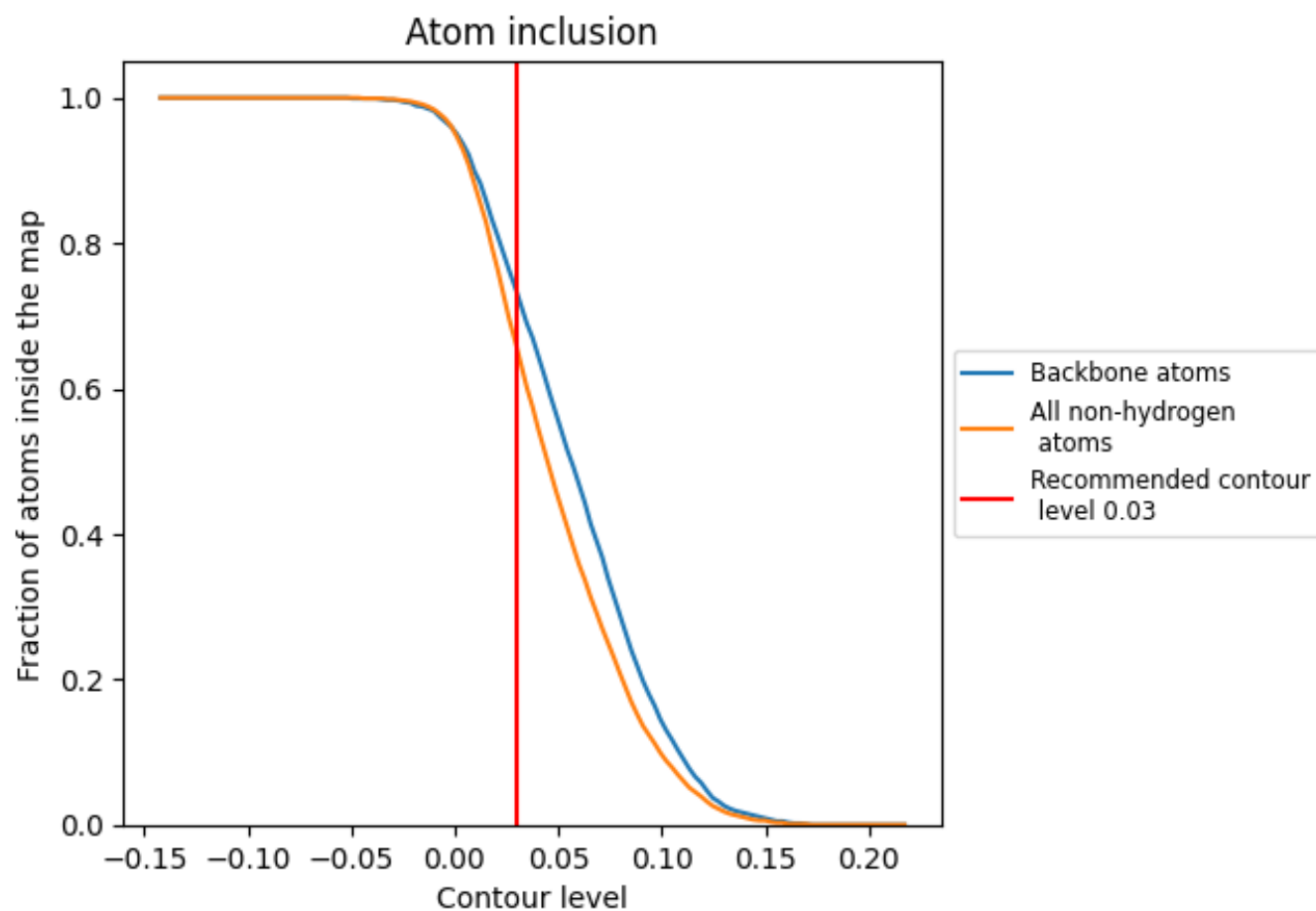
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions at which atoms can be resolved. Low Q-score values may therefore be expected for many entries.

9.3 Atom inclusion mapped to coordinate model [i](#)



The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.03).

9.4 Atom inclusion [i](#)



At the recommended contour level, 73% of all backbone atoms, 66% 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 (0.03) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.6570	0.4650
A	0.6730	0.4910
B	0.6840	0.4800
G	0.3650	0.3500
R	0.6600	0.4470

