



Full wwPDB EM Validation Report ⓘ

Jul 8, 2026 – 04:18 PM JST

PDB ID : 9KVI / pdb_00009kvi
EMDB ID : EMD-62595
Title : A Cryo_EM structure of 5_HT1A complex with DMT
Authors : Yuan, Q.; Li, S.
Deposited on : 2024-12-05
Resolution : 2.54 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:

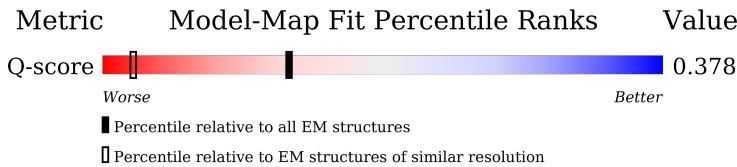
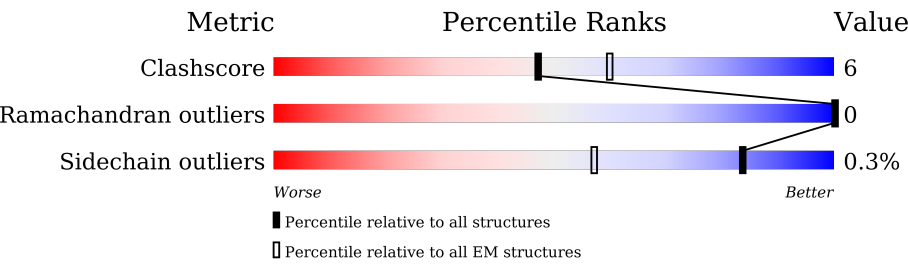
EMDB validation analysis : 0.0.1.dev133
Mogul : 1.8.5 (274361), CSD as541be (2020)
MolProbity : 4-5-2 with Phenix2.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using 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) : 2.50

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 2.54 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	7403 (2.04 - 3.04)

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	5% 57% 5% 37%
2	B	344	7% 80% 16% .
3	E	247	16% 86% 7% 6%
4	G	71	23% 69% 6% 25%

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Mol	Chain	Length	Quality of chain
5	R	398	8% 63% 9% 28%

2 Entry composition

There are 10 unique types of molecules in this entry. The entry contains 8963 atoms, of which 46 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	222	Total	C	N	O	S	0	0
			1786	1136	297	339	14		

There are 7 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	47	ASN	SER	conflict	UNP P63096
A	203	ALA	GLY	conflict	UNP P63096
A	236	ASP	GLU	conflict	UNP P63096
A	237	GLU	ASP	conflict	UNP P63096
A	238	ALA	GLU	conflict	UNP P63096
A	245	ALA	GLU	conflict	UNP P63096
A	326	SER	ALA	conflict	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	332	Total	C	N	O	S	0	0
			2547	1571	457	498	21		

There are 5 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	2	GLY	-	expression tag	UNP P62873
B	3	SER	-	expression tag	UNP P62873
B	4	LEU	-	expression tag	UNP P62873
B	5	LEU	-	expression tag	UNP P62873
B	6	GLN	-	expression tag	UNP P62873

- Molecule 3 is a protein called SCFV16.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	E	232	Total	C	N	O	S	0	0
			1780	1130	295	345	10		

- 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	G	53	Total	C	N	O	S	0	0
			410	257	73	77	3		

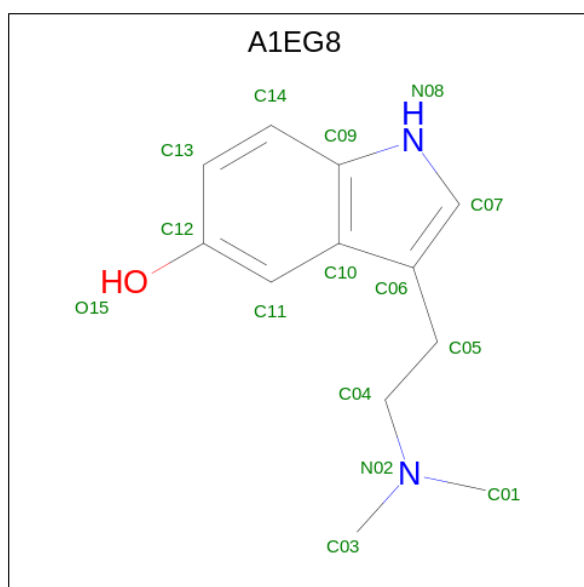
- Molecule 5 is a protein called 5-hydroxytryptamine receptor 1A.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	R	286	Total	C	N	O	S	0	0
			2255	1484	372	382	17		

There is a discrepancy between the modelled and reference sequences:

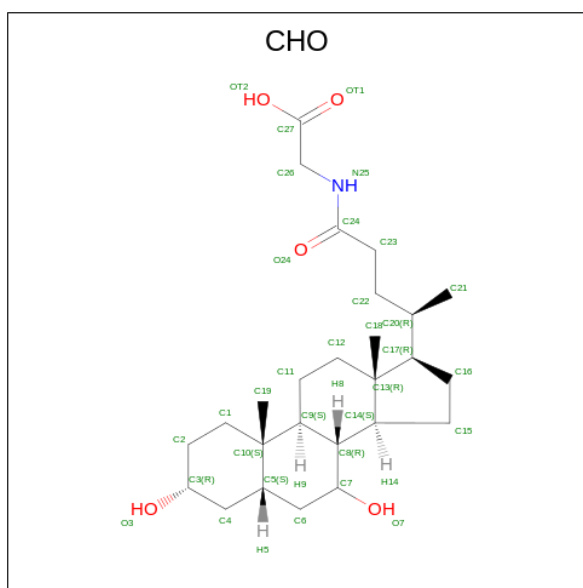
Chain	Residue	Modelled	Actual	Comment	Reference
R	125	TRP	LEU	conflict	UNP P08908

- Molecule 6 is Bufotenin (CCD ID: A1EG8) (formula: $C_{12}H_{16}N_2O$) (labeled as "Ligand of Interest" by depositor).



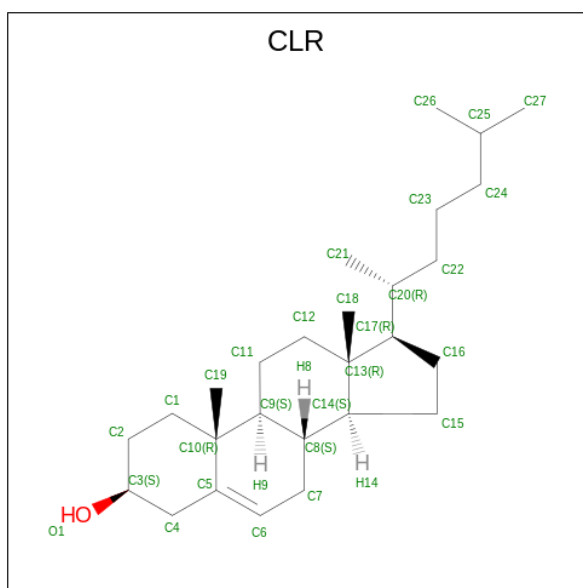
Mol	Chain	Residues	Atoms				AltConf
6	R	1	Total	C	N	O	0
			15	12	2	1	

- Molecule 7 is GLYCOCHENODEOXYCHOLIC ACID (CCD ID: CHO) (formula: $C_{26}H_{43}NO_5$).



Mol	Chain	Residues	Atoms				AltConf
7	R	1	Total	C	N	O	0
			32	26	1	5	

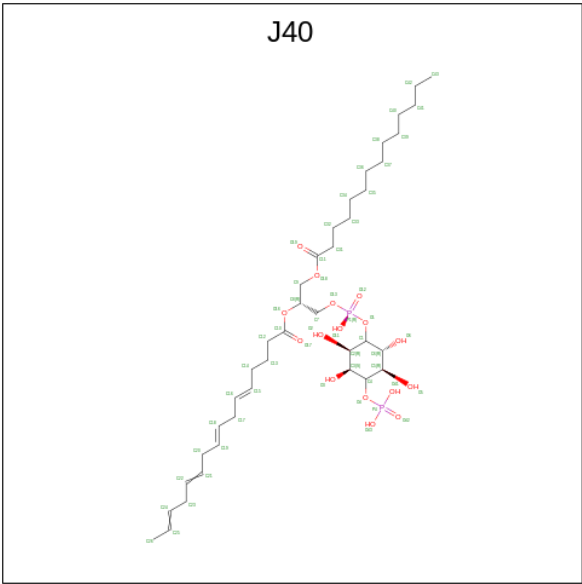
- Molecule 8 is CHOLESTEROL (CCD ID: CLR) (formula: $C_{27}H_{46}O$).



Mol	Chain	Residues	Atoms				AltConf
8	R	1	Total	C	H	O	0
			74	27	46	1	

- Molecule 9 is [(2R)-1-[oxidanyl-[(2R,3R,5S,6R)-2,3,5,6-tetrakis(oxidanyl)-4-phosphonooxy-c

yclohexyl]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	
9	R	1	57	39	16	2	0

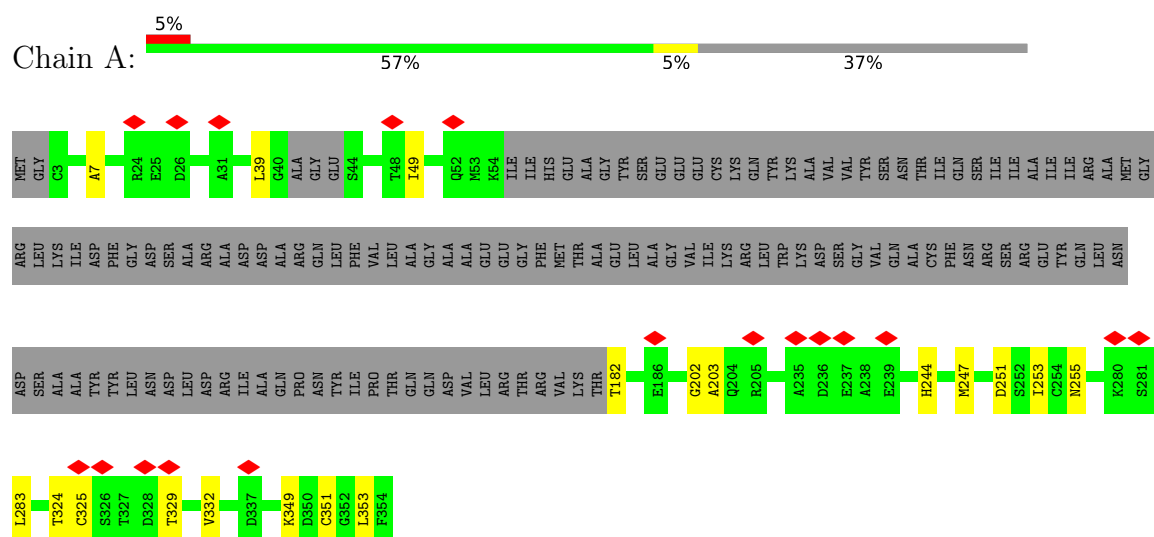
- Molecule 10 is water.

Mol	Chain	Residues	Atoms		AltConf
10	R	7	Total	O	0
			7	7	

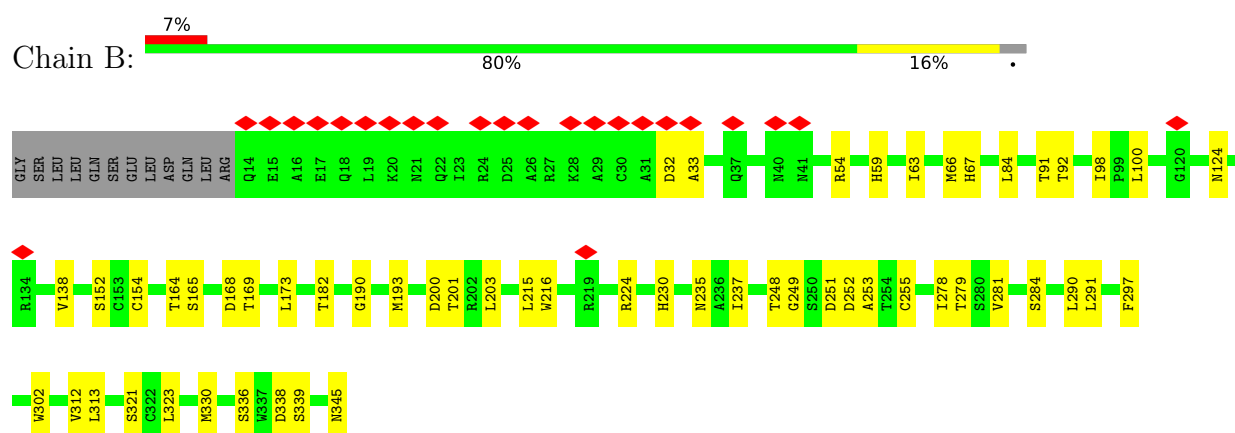
3 Residue-property plots

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.

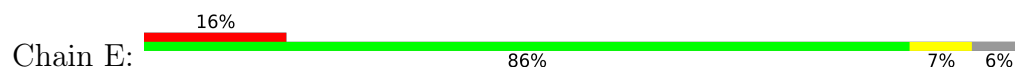
• Molecule 1: Guanine nucleotide-binding protein G(i) subunit alpha-1

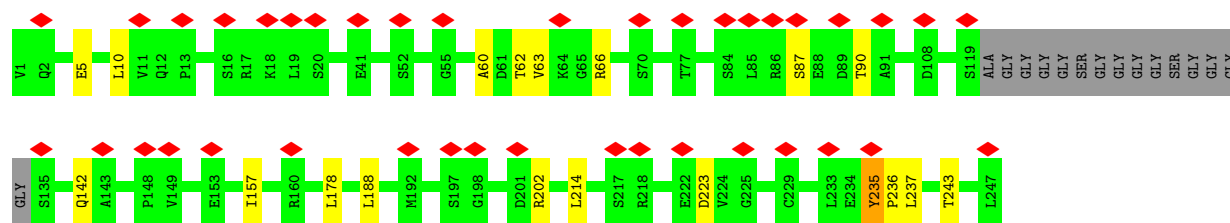


• Molecule 2: Guanine nucleotide-binding protein G(I)/G(S)/G(T) subunit beta-1

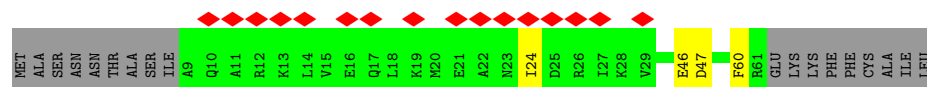


• Molecule 3: SCFV16

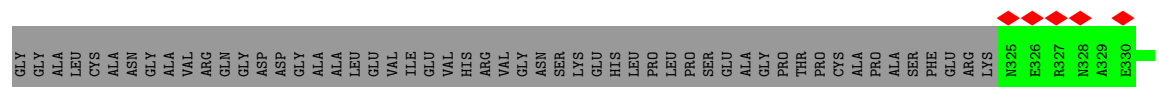
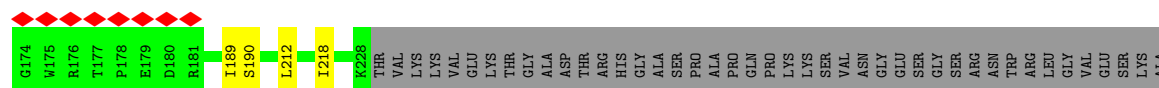
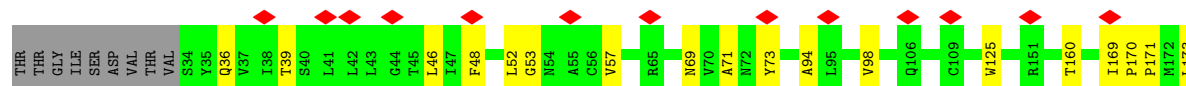




- Molecule 4: Guanine nucleotide-binding protein G(I)/G(S)/G(O) subunit gamma-2



- Molecule 5: 5-hydroxytryptamine receptor 1A



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	195003	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	TFS KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	50	Depositor
Minimum defocus (nm)	8000	Depositor
Maximum defocus (nm)	18000	Depositor
Magnification	Not provided	
Image detector	FEI FALCON III (4k x 4k)	Depositor
Maximum map value	2.644	Depositor
Minimum map value	-1.857	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.061	Depositor
Recommended contour level	0.184	Depositor
Map size (Å)	219.0, 219.0, 219.0	wwPDB
Map dimensions	300, 300, 300	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	0.73, 0.73, 0.73	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: J40, CHO, A1EG8, 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	0.17	0/1815	0.32	0/2434
2	B	0.13	0/2594	0.30	0/3517
3	E	0.09	0/1824	0.25	0/2473
4	G	0.13	0/416	0.27	0/561
5	R	0.14	0/2308	0.28	0/3144
All	All	0.14	0/8957	0.29	0/12129

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

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

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	349	LYS	Mainchain

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	1786	0	1777	16	0
2	B	2547	0	2445	42	0
3	E	1780	0	1720	13	0
4	G	410	0	420	4	0
5	R	2255	0	2336	39	0
6	R	15	0	0	0	0
7	R	32	0	42	0	0
8	R	28	46	46	15	0
9	R	57	0	0	1	0
10	R	7	0	0	3	0
All	All	8917	46	8786	106	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 6.

All (106) 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:324:THR:HG22	1:A:325:CYS:H	1.17	1.04
2:B:255:CYS:SG	2:B:278:ILE:CD1	2.45	1.04
2:B:255:CYS:SG	2:B:278:ILE:HD12	2.04	0.96
1:A:324:THR:HG22	1:A:325:CYS:N	1.79	0.96
5:R:400:TYR:OH	10:R:601:HOH:O	1.85	0.94
2:B:255:CYS:SG	2:B:278:ILE:HD13	2.07	0.93
1:A:324:THR:CG2	1:A:325:CYS:H	1.85	0.90
5:R:387:TRP:NE1	8:R:503:CLR:H193	2.07	0.69
5:R:387:TRP:CD1	8:R:503:CLR:H193	2.28	0.69
2:B:338:ASP:O	2:B:339:SER:OG	2.11	0.68
5:R:36:GLN:NE2	5:R:98:VAL:O	2.26	0.68
5:R:394:LEU:HD23	8:R:503:CLR:C26	2.25	0.67
4:G:46:GLU:N	4:G:46:GLU:OE1	2.29	0.65
3:E:5:GLU:N	3:E:5:GLU:OE1	2.29	0.65
1:A:182:THR:OG1	2:B:124:ASN:ND2	2.28	0.65
3:E:142:GLN:NE2	3:E:243:THR:OG1	2.31	0.64
5:R:394:LEU:HD23	8:R:503:CLR:H261	1.80	0.63
2:B:193:MET:HA	2:B:193:MET:HE2	1.83	0.60
5:R:387:TRP:CD1	8:R:503:CLR:H111	2.37	0.60
2:B:330:MET:O	2:B:345:ASN:ND2	2.36	0.59
3:E:87:SER:O	3:E:90:THR:HG22	2.03	0.59
5:R:391:SER:HB3	8:R:503:CLR:H263	1.84	0.59
2:B:63:ILE:CG1	2:B:336:SER:O	2.52	0.58
2:B:200:ASP:O	2:B:201:THR:OG1	2.16	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:R:405:LYS:NZ	9:R:504:J40:C2	2.67	0.58
3:E:90:THR:O	3:E:90:THR:HG23	2.02	0.57
5:R:125:TRP:HB3	5:R:160:THR:HG22	1.86	0.57
2:B:281:VAL:HG13	2:B:290:LEU:HD11	1.87	0.56
5:R:387:TRP:HB3	8:R:503:CLR:H183	1.89	0.55
5:R:387:TRP:HD1	8:R:503:CLR:H111	1.71	0.55
2:B:98:ILE:HD12	2:B:98:ILE:N	2.21	0.55
1:A:251:ASP:OD1	1:A:255:ASN:ND2	2.41	0.54
2:B:173:LEU:O	2:B:182:THR:N	2.38	0.54
1:A:351:CYS:HB2	1:A:353:LEU:HD12	1.90	0.53
2:B:169:THR:HG22	2:B:190:GLY:C	2.35	0.52
3:E:62:THR:O	3:E:66:ARG:NH2	2.40	0.52
1:A:329:THR:O	1:A:332:VAL:N	2.42	0.51
2:B:98:ILE:HG12	2:B:138:VAL:HG11	1.93	0.51
2:B:237:ILE:HG22	2:B:248:THR:HG22	1.92	0.51
2:B:54:ARG:NH1	4:G:60:PHE:O	2.40	0.51
5:R:212:LEU:HD23	5:R:351:MET:HE2	1.93	0.50
2:B:32:ASP:OD1	2:B:33:ALA:N	2.44	0.50
2:B:279:THR:HG21	2:B:321:SER:HA	1.94	0.49
5:R:387:TRP:HE1	8:R:503:CLR:H193	1.75	0.49
1:A:353:LEU:HD13	5:R:218:ILE:HG21	1.94	0.49
3:E:235:TYR:N	3:E:236:PRO:HD2	2.28	0.48
5:R:386:ASN:ND2	10:R:602:HOH:O	2.46	0.48
5:R:39:THR:HG22	8:R:503:CLR:H6	1.95	0.48
5:R:39:THR:HG22	8:R:503:CLR:C6	2.44	0.47
5:R:170:PRO:N	5:R:171:PRO:HD2	2.30	0.47
2:B:66:MET:SD	2:B:67:HIS:N	2.88	0.47
2:B:154:CYS:SG	2:B:164:THR:HG23	2.55	0.47
3:E:60:ALA:HB3	3:E:63:VAL:HG22	1.97	0.47
5:R:212:LEU:CD2	5:R:351:MET:HE2	2.45	0.47
5:R:69:ASN:O	5:R:73:TYR:N	2.43	0.47
5:R:169:ILE:N	5:R:170:PRO:CD	2.78	0.46
5:R:169:ILE:HG23	5:R:173:LEU:HD13	1.98	0.46
1:A:353:LEU:HD13	5:R:218:ILE:CG2	2.46	0.45
5:R:48:PHE:CE2	5:R:52:LEU:HD11	2.52	0.45
2:B:255:CYS:SG	2:B:278:ILE:HG21	2.56	0.45
2:B:281:VAL:CG1	2:B:290:LEU:HD11	2.47	0.45
5:R:384:ILE:HG12	8:R:503:CLR:H112	1.98	0.45
1:A:7:ALA:HB1	3:E:235:TYR:CE2	2.51	0.45
2:B:152:SER:N	2:B:165:SER:O	2.44	0.45
5:R:71:ALA:HB1	10:R:603:HOH:O	2.15	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:R:404:ASN:OD1	5:R:405:LYS:N	2.49	0.45
2:B:168:ASP:O	2:B:169:THR:OG1	2.27	0.44
2:B:235:ASN:N	2:B:249:GLY:O	2.39	0.44
5:R:394:LEU:O	5:R:398:VAL:HG23	2.16	0.44
5:R:395:LEU:HD11	8:R:503:CLR:H271	2.00	0.44
2:B:215:LEU:HD23	2:B:216:TRP:N	2.32	0.44
1:A:283:LEU:H	1:A:283:LEU:HD23	1.81	0.44
2:B:252:ASP:O	2:B:253:ALA:HB3	2.18	0.44
3:E:235:TYR:O	3:E:237:LEU:N	2.51	0.44
2:B:313:LEU:HD12	2:B:313:LEU:N	2.33	0.44
3:E:178:LEU:HB2	3:E:188:LEU:HD11	1.99	0.44
3:E:202:ARG:NH1	3:E:223:ASP:OD2	2.47	0.44
2:B:323:LEU:C	2:B:323:LEU:HD12	2.43	0.43
5:R:395:LEU:HD11	8:R:503:CLR:C27	2.48	0.43
2:B:290:LEU:HB3	2:B:302:TRP:HB2	1.99	0.43
1:A:202:GLY:O	1:A:203:ALA:HB3	2.19	0.43
5:R:53:GLY:O	5:R:57:VAL:HG23	2.18	0.43
1:A:353:LEU:HD21	5:R:347:LEU:HD21	1.99	0.43
5:R:387:TRP:HB3	8:R:503:CLR:H212	2.01	0.42
2:B:230:HIS:HE2	2:B:248:THR:CB	2.32	0.42
2:B:291:LEU:HD22	2:B:291:LEU:N	2.34	0.42
2:B:284:SER:OG	4:G:47:ASP:OD2	2.32	0.42
2:B:84:LEU:HD23	2:B:100:LEU:HD21	2.00	0.42
3:E:157:ILE:O	3:E:214:LEU:N	2.44	0.42
5:R:347:LEU:O	5:R:348:GLY:C	2.61	0.42
2:B:203:LEU:HD12	2:B:215:LEU:HD21	2.01	0.42
5:R:46:LEU:C	5:R:46:LEU:HD23	2.44	0.42
5:R:398:VAL:HG12	5:R:403:PHE:CZ	2.54	0.42
1:A:49:ILE:CD1	1:A:324:THR:HG21	2.50	0.42
2:B:230:HIS:NE2	2:B:248:THR:OG1	2.48	0.42
5:R:94:ALA:O	5:R:98:VAL:HG12	2.19	0.41
1:A:39:LEU:HD13	1:A:253:ILE:HG12	2.01	0.41
5:R:189:ILE:HG22	5:R:190:SER:N	2.35	0.41
2:B:224:ARG:HD2	4:G:24:ILE:HD11	2.02	0.41
2:B:91:THR:O	2:B:92:THR:OG1	2.31	0.41
2:B:203:LEU:N	2:B:203:LEU:HD23	2.36	0.40
1:A:244:HIS:HA	1:A:247:MET:HG2	2.02	0.40
2:B:297:PHE:N	2:B:297:PHE:CD1	2.88	0.40
2:B:312:VAL:C	2:B:313:LEU:HD12	2.47	0.40
2:B:235:ASN:ND2	2:B:251:ASP:OD1	2.43	0.40
3:E:10:LEU:HD23	3:E:10:LEU:C	2.46	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	216/354 (61%)	211 (98%)	5 (2%)	0	100	100
2	B	330/344 (96%)	321 (97%)	9 (3%)	0	100	100
3	E	228/247 (92%)	224 (98%)	4 (2%)	0	100	100
4	G	51/71 (72%)	50 (98%)	1 (2%)	0	100	100
5	R	282/398 (71%)	275 (98%)	7 (2%)	0	100	100
All	All	1107/1414 (78%)	1081 (98%)	26 (2%)	0	100	100

There are no Ramachandran outliers to report.

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	197/304 (65%)	197 (100%)	0	100	100
2	B	274/286 (96%)	273 (100%)	1 (0%)	84	90
3	E	195/198 (98%)	194 (100%)	1 (0%)	81	88
4	G	43/58 (74%)	43 (100%)	0	100	100
5	R	244/332 (74%)	243 (100%)	1 (0%)	84	90
All	All	953/1178 (81%)	950 (100%)	3 (0%)	84	92

All (3) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	B	59	HIS
3	E	235	TYR
5	R	345	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (11) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	213	HIS
2	B	22	GLN
2	B	124	ASN
2	B	130	ASN
3	E	2	GLN
3	E	12	GLN
3	E	38	GLN
3	E	142	GLN
3	E	179	GLN
5	R	36	GLN
5	R	54	ASN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

4 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
7	CHO	R	502	-	35,35,35	0.54	0	54,54,54	0.90	3 (5%)
9	J40	R	504	-	57,57,57	1.42	9 (15%)	69,72,72	0.98	2 (2%)
8	CLR	R	503	-	31,31,31	0.32	0	48,48,48	0.81	2 (4%)
6	A1EG8	R	501	-	16,16,16	2.31	8 (50%)	22,22,22	0.90	2 (9%)

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
7	CHO	R	502	-	-	0/14/75/75	1/4/4/4
9	J40	R	504	-	-	23/53/77/77	0/1/1/1
8	CLR	R	503	-	-	2/10/68/68	0/4/4/4
6	A1EG8	R	501	-	-	2/5/5/5	0/2/2/2

All (17) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	R	501	A1EG8	C07-C06	4.13	1.43	1.36
6	R	501	A1EG8	O15-C12	3.91	1.46	1.37
9	R	504	J40	C19-C18	3.88	1.54	1.31
9	R	504	J40	C16-C15	3.84	1.54	1.31
9	R	504	J40	C22-C21	3.77	1.53	1.31
6	R	501	A1EG8	C05-C06	3.52	1.56	1.50
9	R	504	J40	O18-C11	3.21	1.42	1.33
9	R	504	J40	C24-C25	3.12	1.52	1.29
6	R	501	A1EG8	C07-N08	-2.88	1.32	1.37
9	R	504	J40	P4-O4	2.58	1.64	1.59
9	R	504	J40	O16-C10	2.58	1.41	1.34
9	R	504	J40	O16-C8	-2.58	1.40	1.46
6	R	501	A1EG8	C10-C09	-2.50	1.38	1.41
6	R	501	A1EG8	C04-C05	2.39	1.57	1.52
6	R	501	A1EG8	C09-N08	2.19	1.41	1.37
6	R	501	A1EG8	C11-C10	2.10	1.43	1.39
9	R	504	J40	P1-O1	2.07	1.65	1.60

All (9) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
9	R	504	J40	O16-C10-C12	3.91	119.94	111.50
9	R	504	J40	O18-C11-C31	2.59	120.04	111.91
8	R	503	CLR	C11-C9-C8	2.57	115.46	111.75
8	R	503	CLR	C12-C11-C9	2.54	117.52	113.11
7	R	502	CHO	C5-C6-C7	2.45	117.16	114.46
6	R	501	A1EG8	C14-C09-C10	-2.39	119.79	122.19
6	R	501	A1EG8	C06-C07-N08	-2.31	107.63	110.31
7	R	502	CHO	C14-C8-C7	2.18	114.70	111.81
7	R	502	CHO	C2-C1-C10	2.07	116.32	112.78

There are no chirality outliers.

All (27) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
9	R	504	J40	C4-O4-P4-O42
9	R	504	J40	C19-C20-C21-C22
9	R	504	J40	C23-C24-C25-C26
9	R	504	J40	C20-C21-C22-C23
9	R	504	J40	O16-C8-C9-O18
6	R	501	A1EG8	C05-C04-N02-C01
8	R	503	CLR	C20-C22-C23-C24
9	R	504	J40	C12-C10-O16-C8
9	R	504	J40	C34-C35-C36-C37
9	R	504	J40	O17-C10-O16-C8
9	R	504	J40	C33-C34-C35-C36
9	R	504	J40	C39-C40-C41-C42
9	R	504	J40	C31-C11-O18-C9
9	R	504	J40	C12-C13-C14-C15
9	R	504	J40	O19-C11-O18-C9
9	R	504	J40	C7-C8-C9-O18
9	R	504	J40	C16-C17-C18-C19
9	R	504	J40	C18-C19-C20-C21
9	R	504	J40	C8-C7-O13-P1
9	R	504	J40	C13-C14-C15-C16
9	R	504	J40	C35-C36-C37-C38
9	R	504	J40	C36-C37-C38-C39
9	R	504	J40	C40-C41-C42-C43
9	R	504	J40	C7-O13-P1-O1
6	R	501	A1EG8	C05-C04-N02-C03
8	R	503	CLR	C17-C20-C22-C23
9	R	504	J40	C4-O4-P4-O43

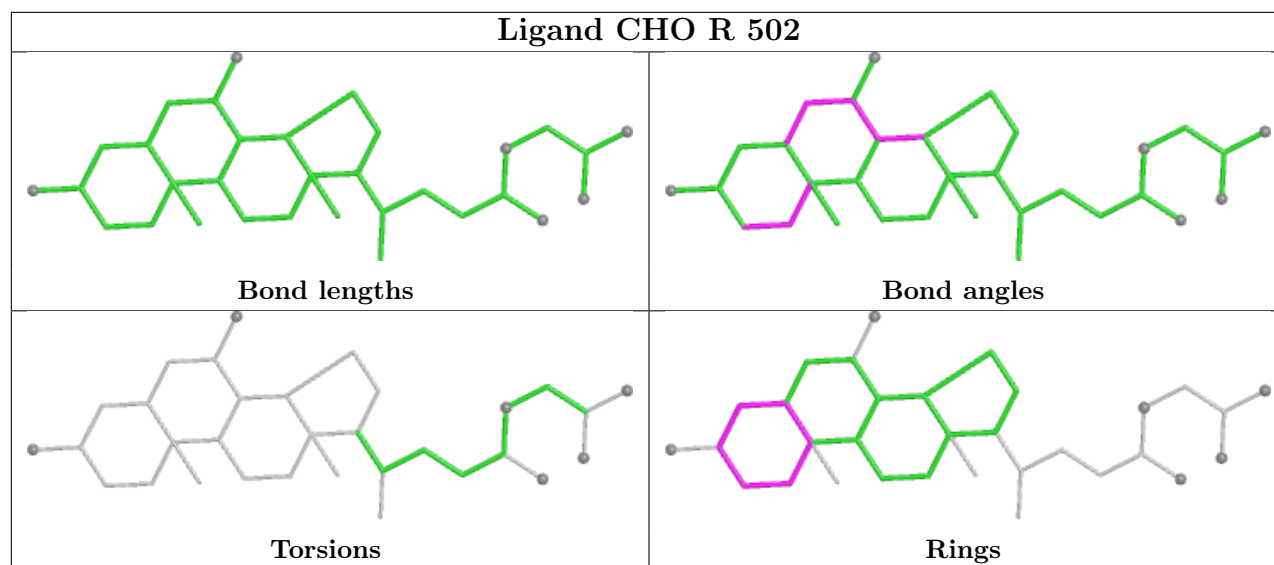
All (1) ring outliers are listed below:

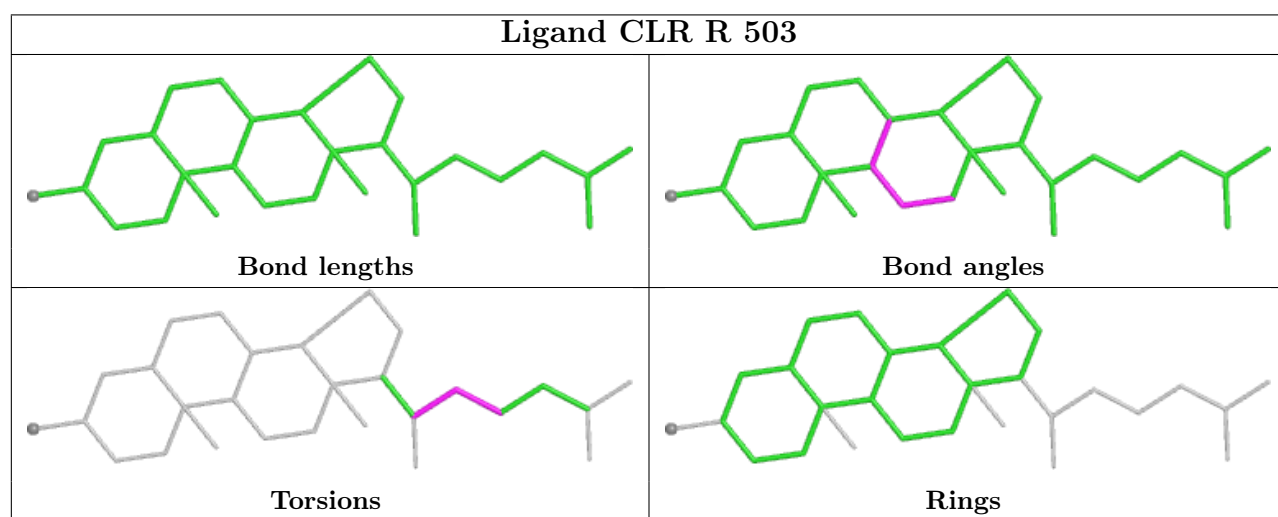
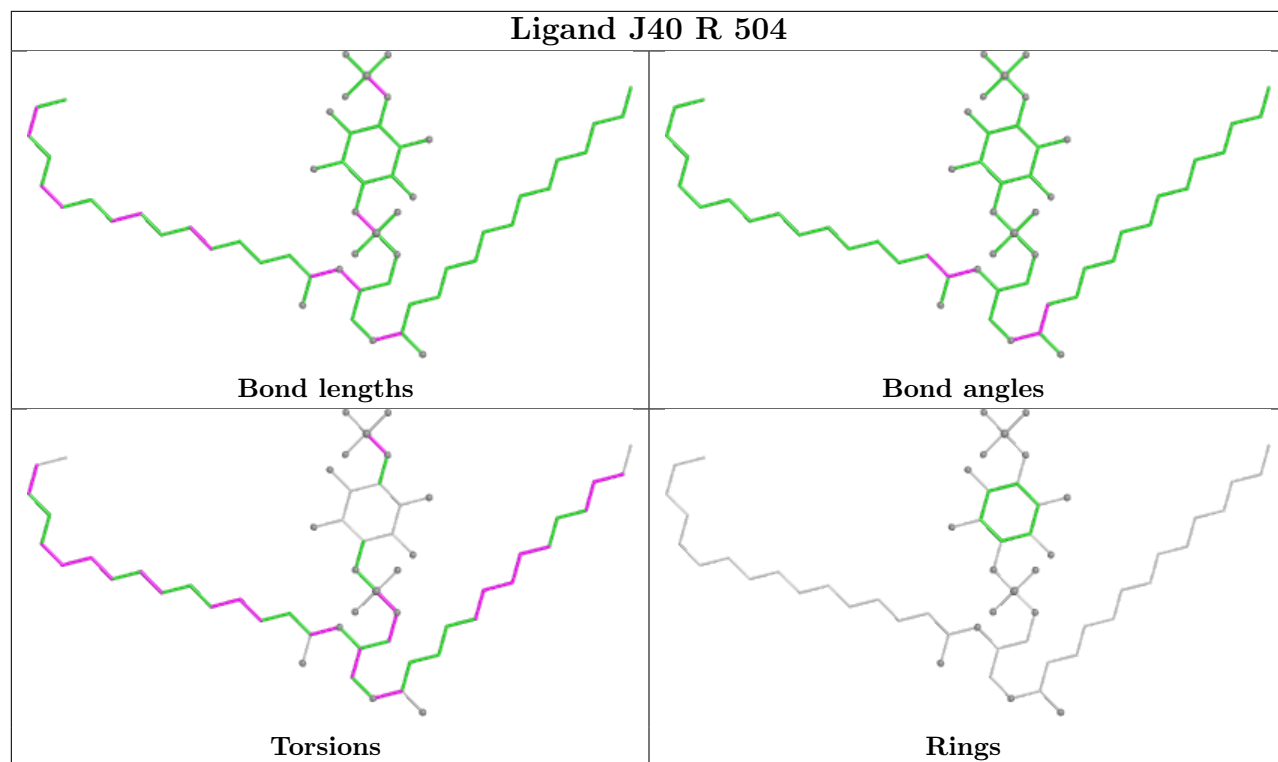
Mol	Chain	Res	Type	Atoms
7	R	502	CHO	C1-C10-C2-C3-C4-C5

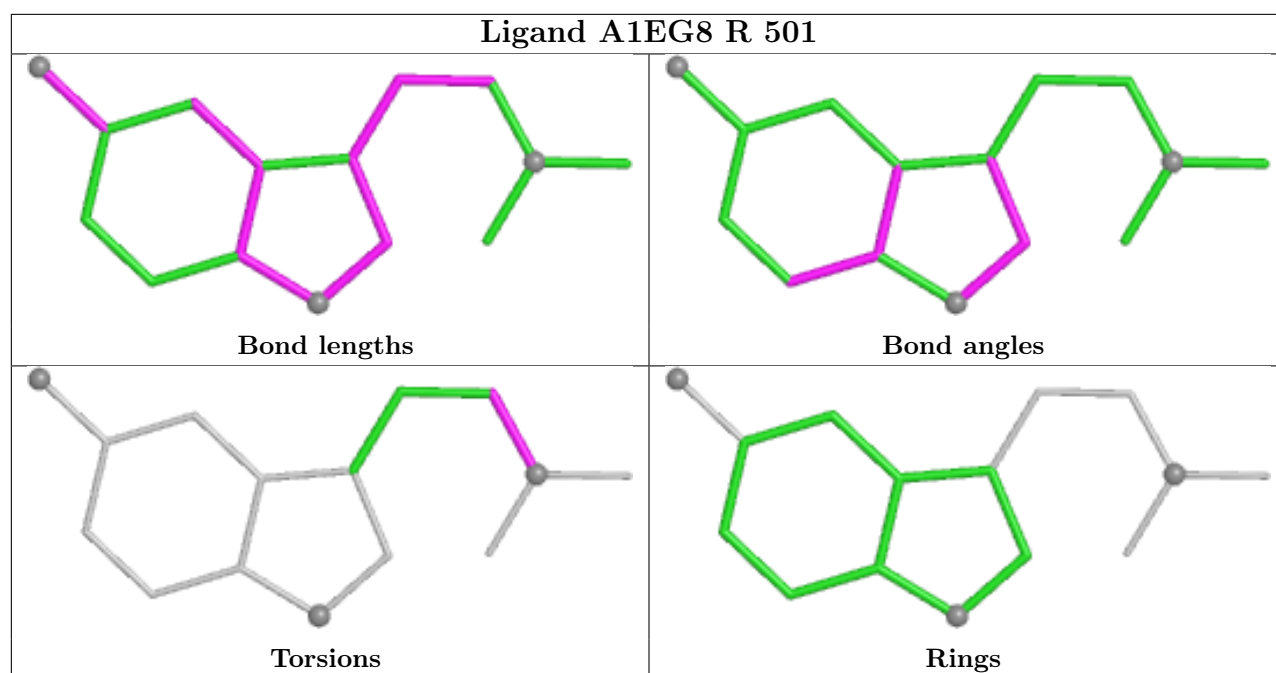
2 monomers are involved in 16 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
9	R	504	J40	1	0
8	R	503	CLR	15	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.

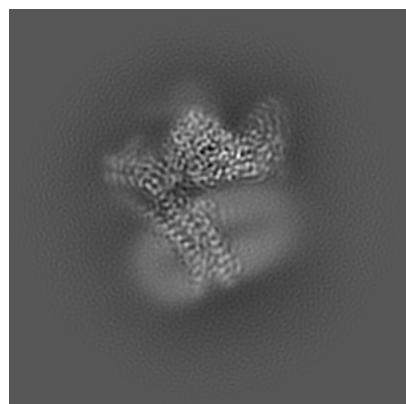
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-62595. These allow visual inspection of the internal detail of the map and identification of artifacts.

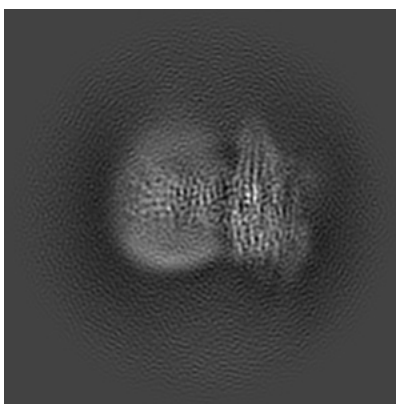
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

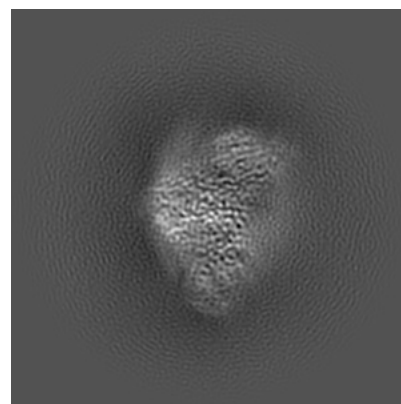
6.1.1 Primary map



X

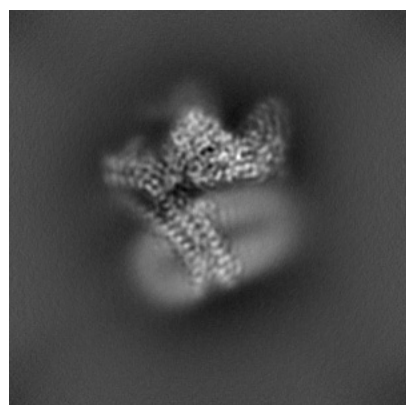


Y

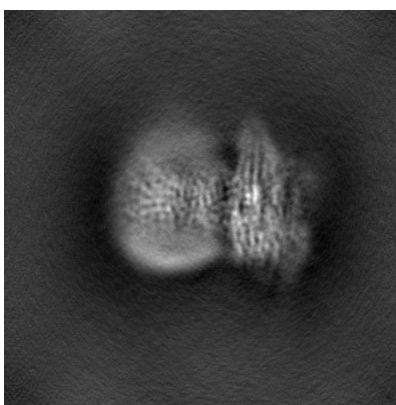


Z

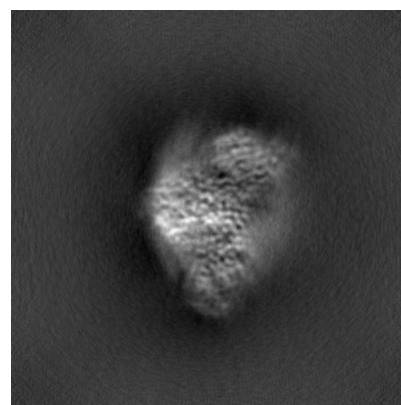
6.1.2 Raw map



X



Y

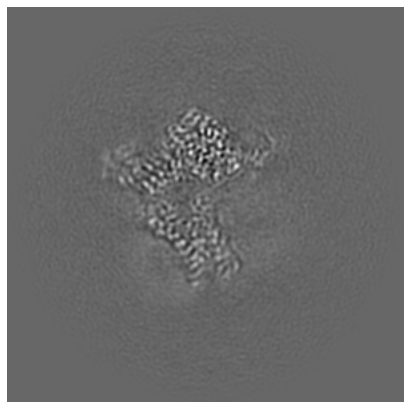


Z

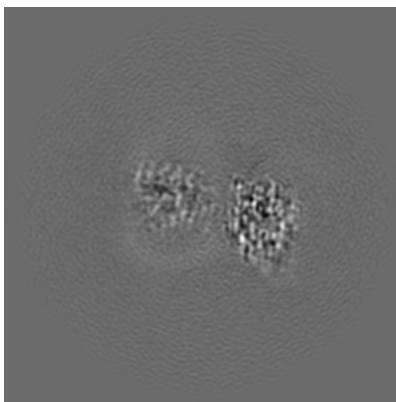
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

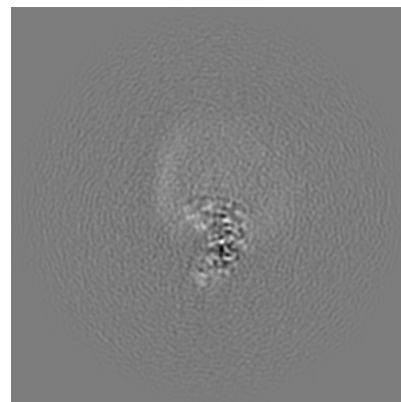
6.2.1 Primary map



X Index: 150

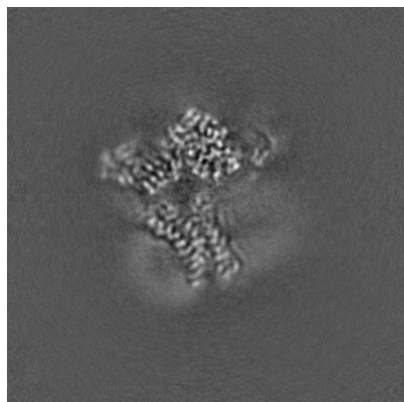


Y Index: 150

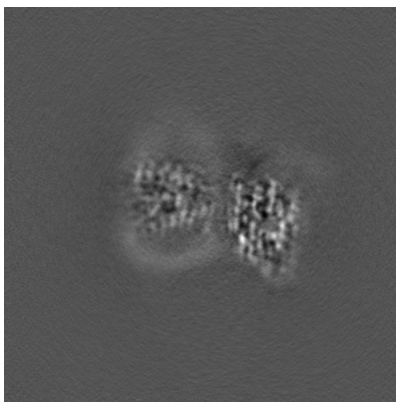


Z Index: 150

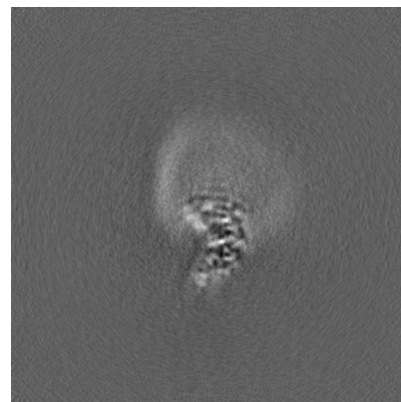
6.2.2 Raw map



X Index: 150



Y Index: 150

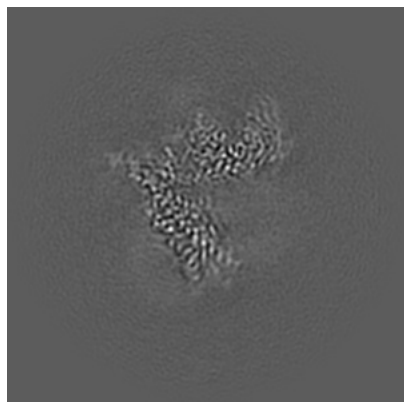


Z Index: 150

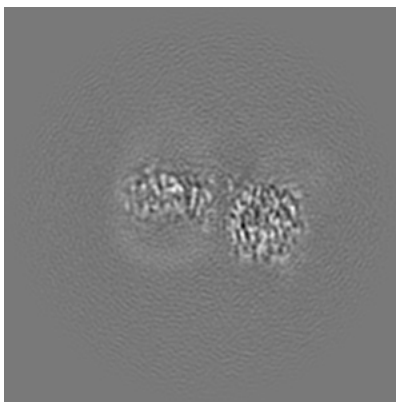
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

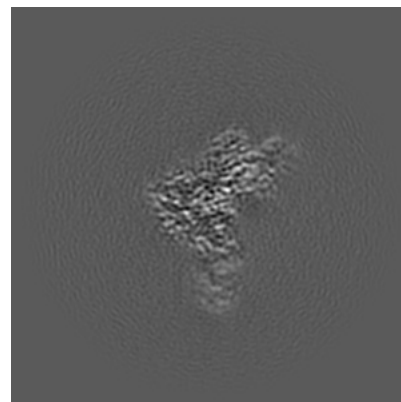
6.3.1 Primary map



X Index: 163

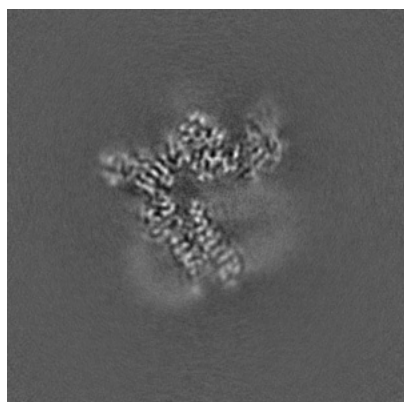


Y Index: 141

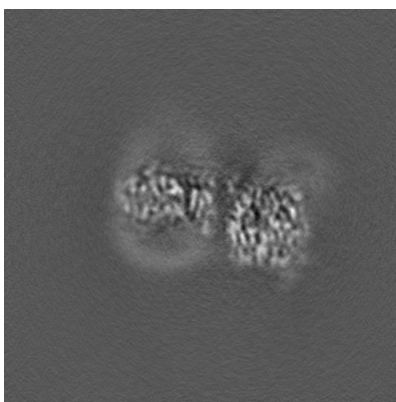


Z Index: 188

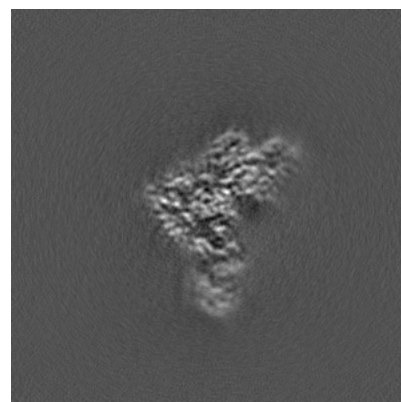
6.3.2 Raw map



X Index: 157



Y Index: 141

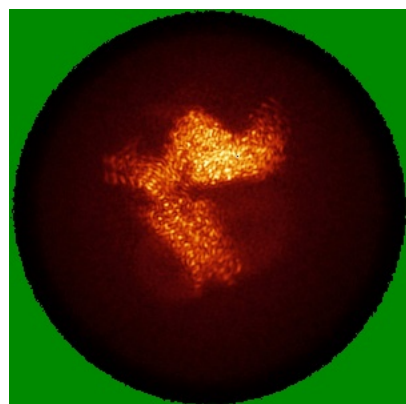


Z Index: 188

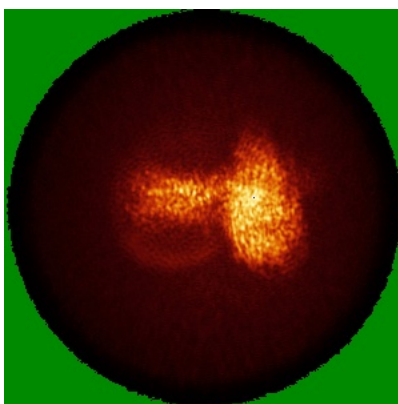
The images above show the largest variance slices of the map in three orthogonal directions.

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

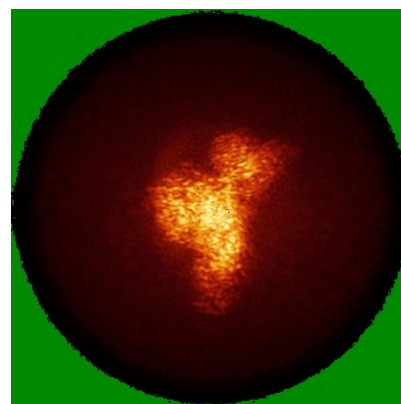
6.4.1 Primary map



X

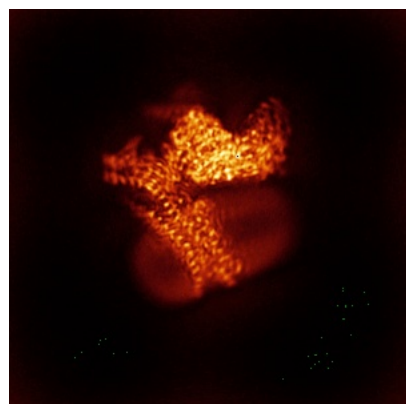


Y

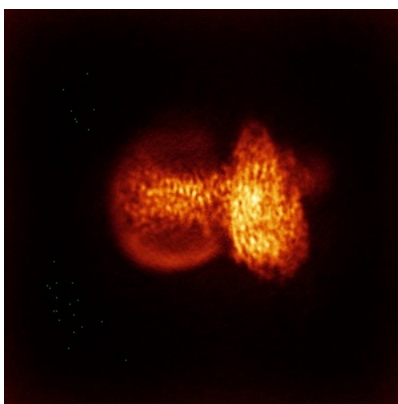


Z

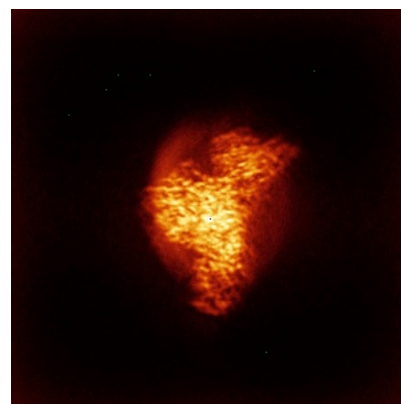
6.4.2 Raw map



X



Y

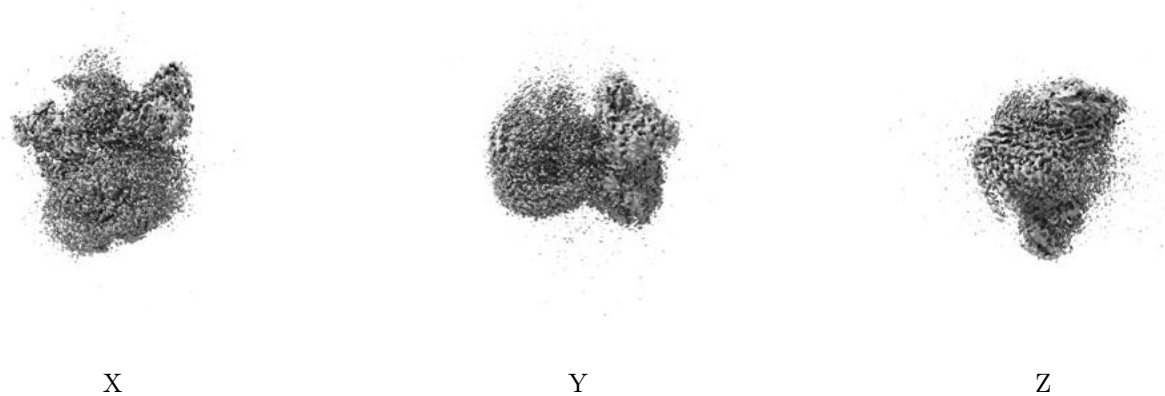


Z

The images above show the map standard deviation projections with false color in three orthogonal directions. Minimum values are shown in green, max in blue, and dark to light orange shades represent small to large values respectively.

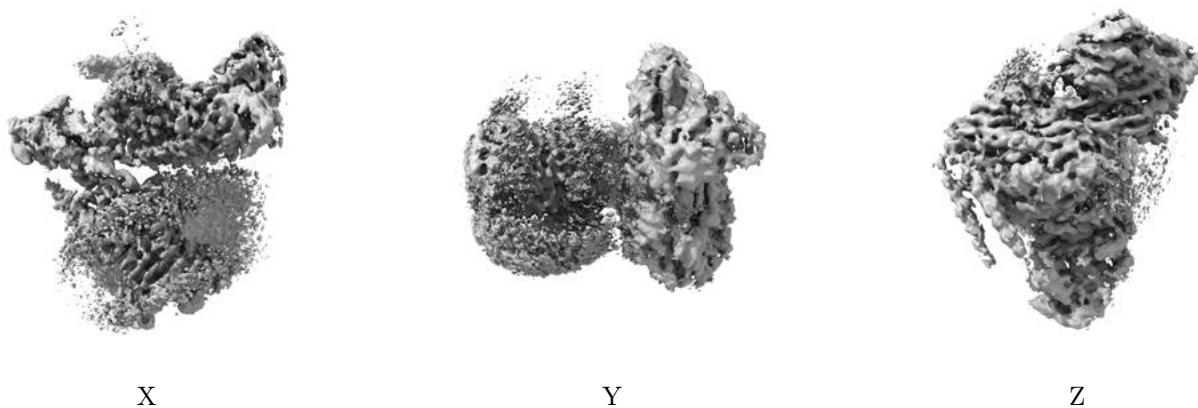
6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.184. 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.

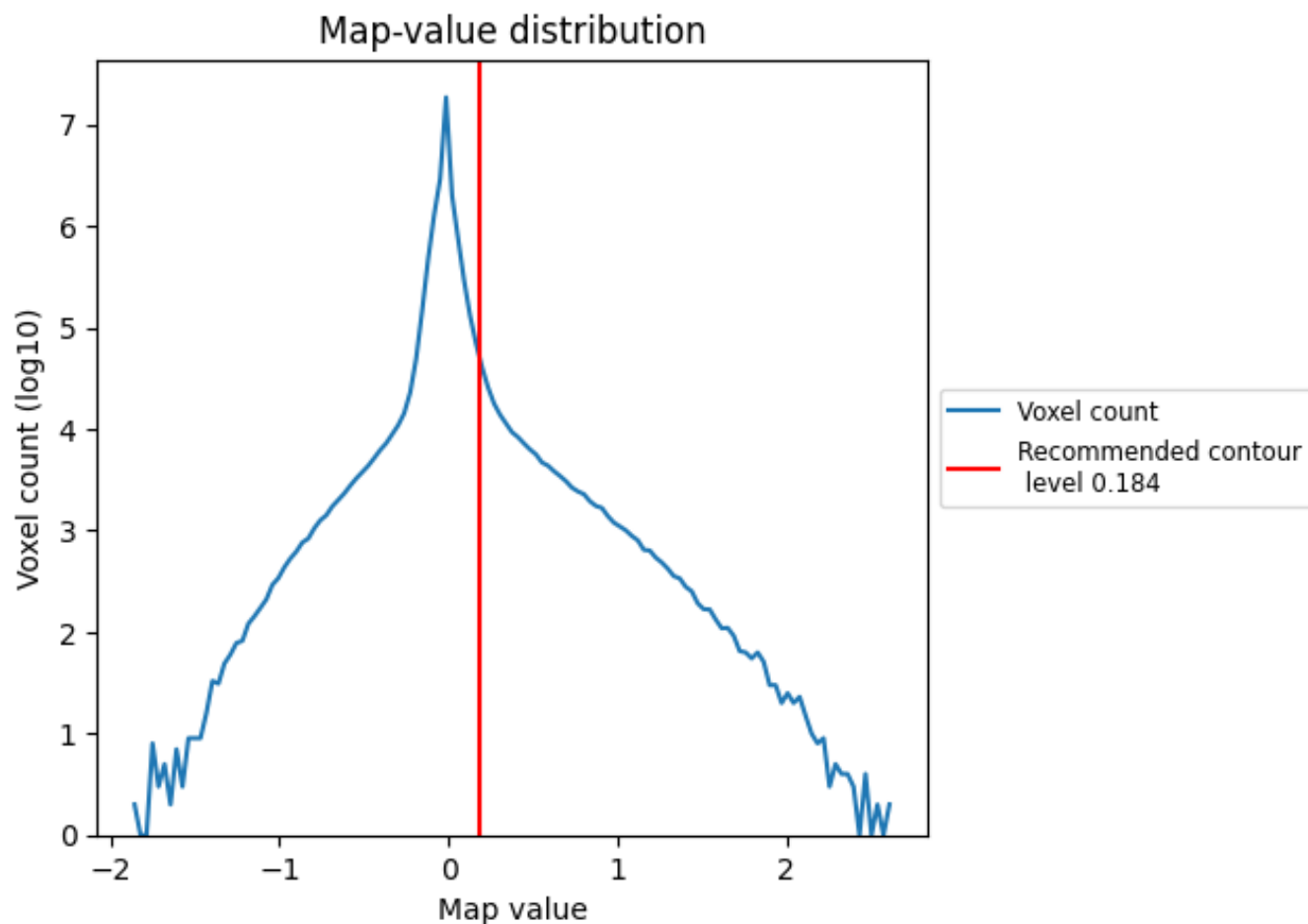
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

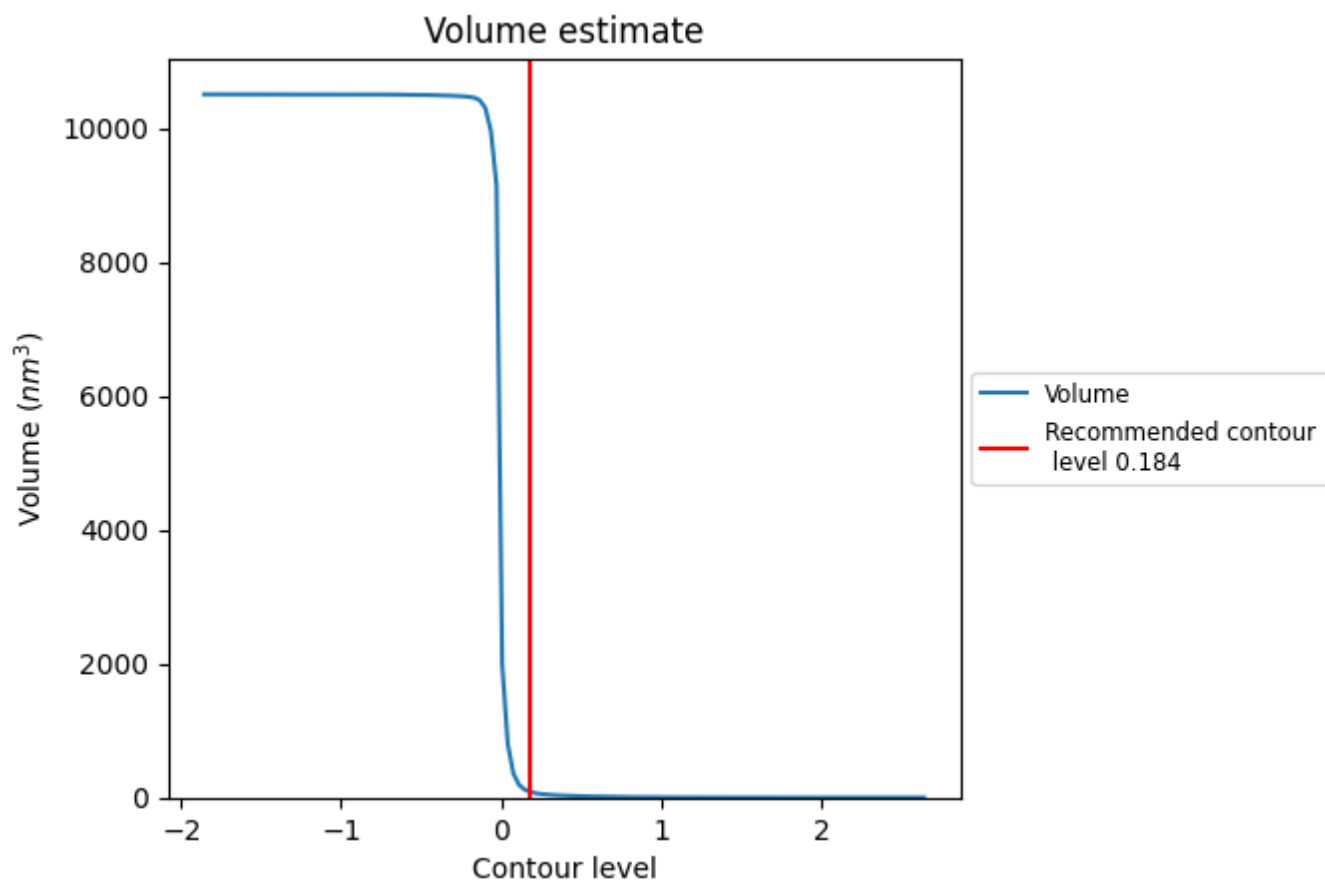
This section contains the results of statistical analysis of the map.

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.

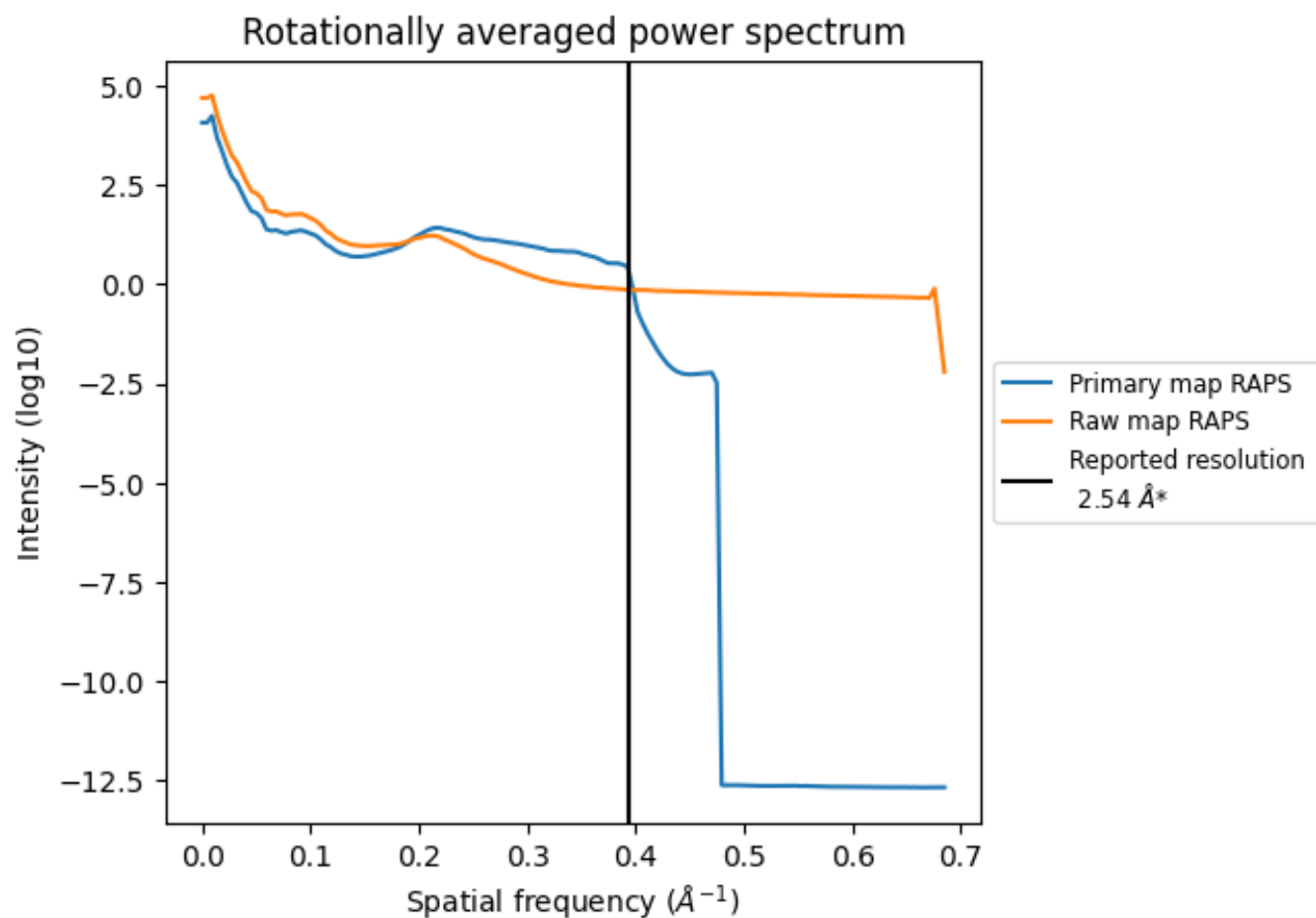
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 84 nm³; this corresponds to an approximate mass of 76 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 ⓘ

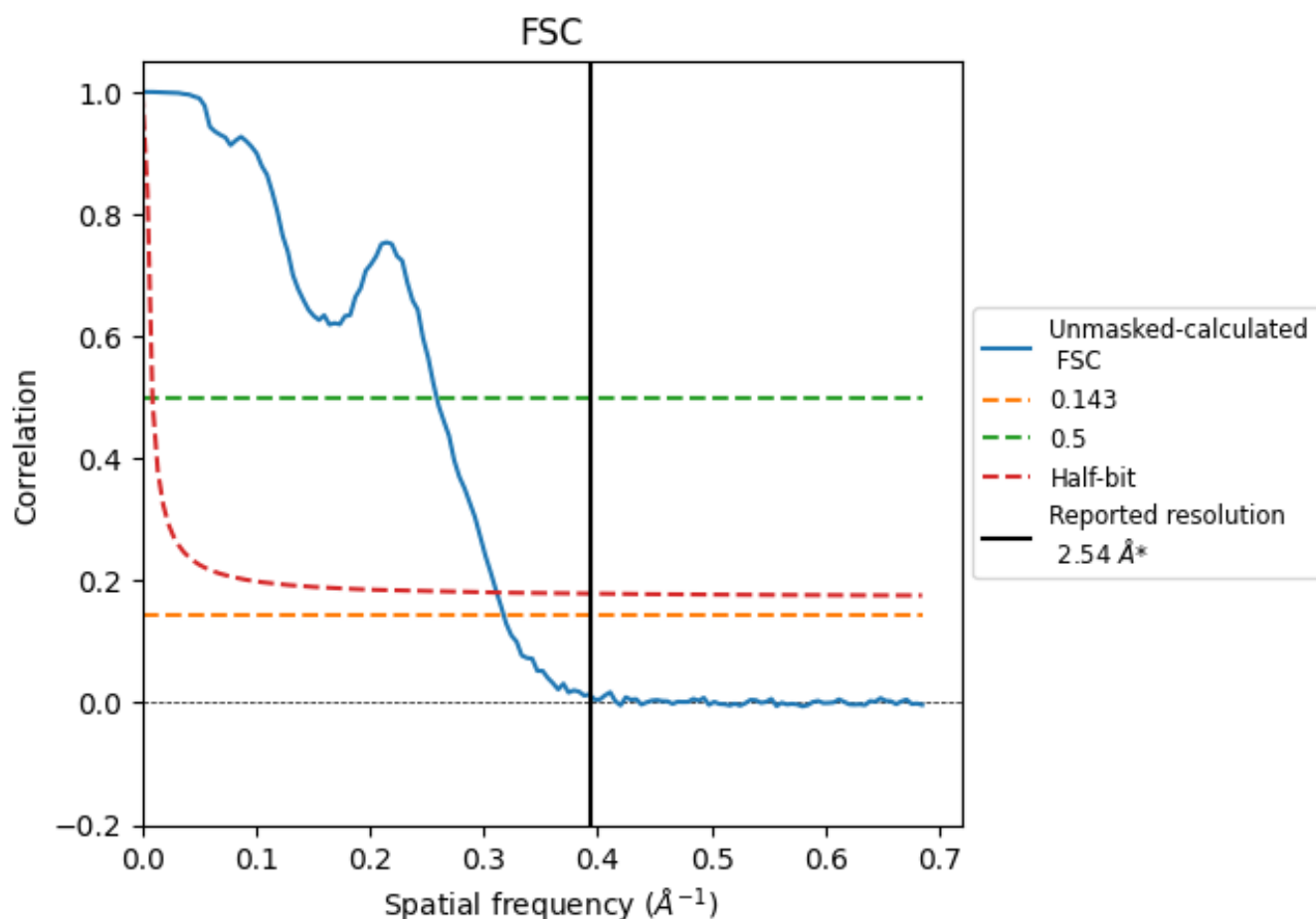


*Reported resolution corresponds to spatial frequency of 0.394 Å⁻¹

8 Fourier-Shell correlation [i](#)

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

8.1 FSC [i](#)



*Reported resolution corresponds to spatial frequency of 0.394 $\text{\AA}^{-1}$

8.2 Resolution estimates [i](#)

Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	2.54	-	-
Author-provided FSC curve	-	-	-
Unmasked-calculated*	3.15	3.87	3.21

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 3.15 differs from the reported value 2.54 by more than 10 %

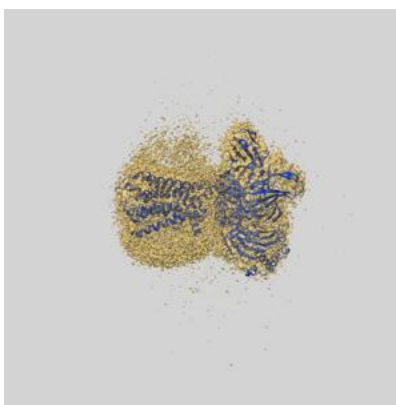
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-62595 and PDB model 9KVI. Per-residue inclusion information can be found in section [3](#) on page [8](#).

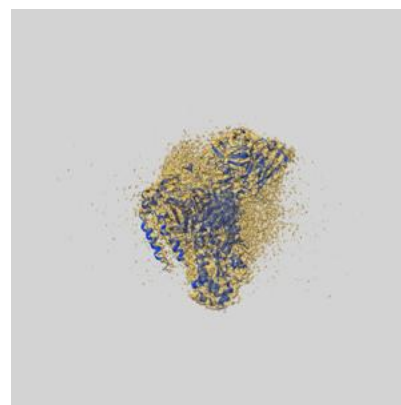
9.1 Map-model overlay [i](#)



X



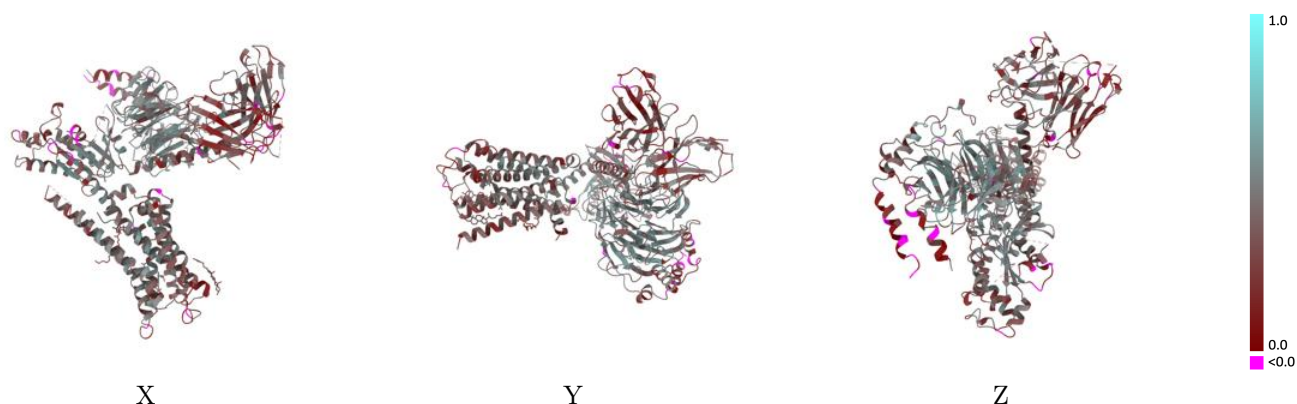
Y



Z

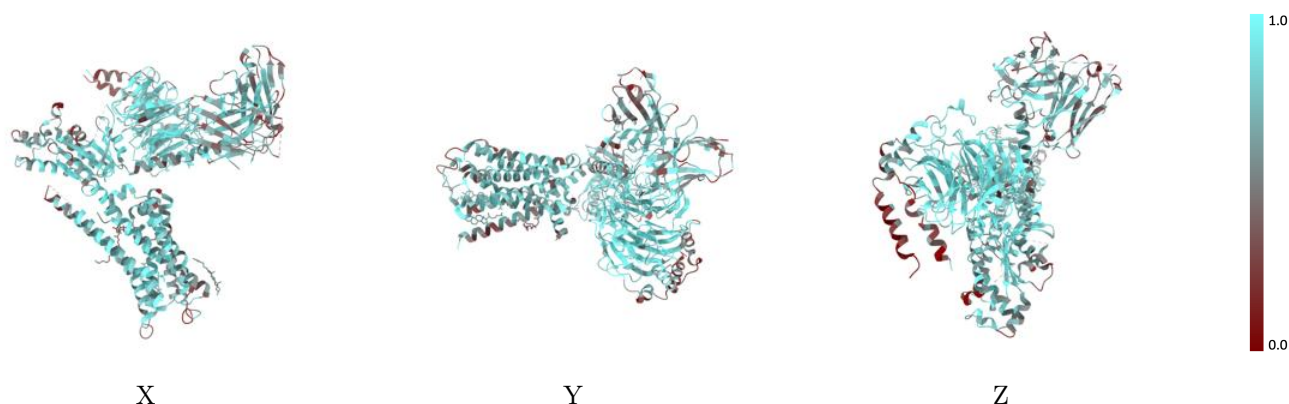
The images above show the 3D surface view of the map at the recommended contour level 0.184 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



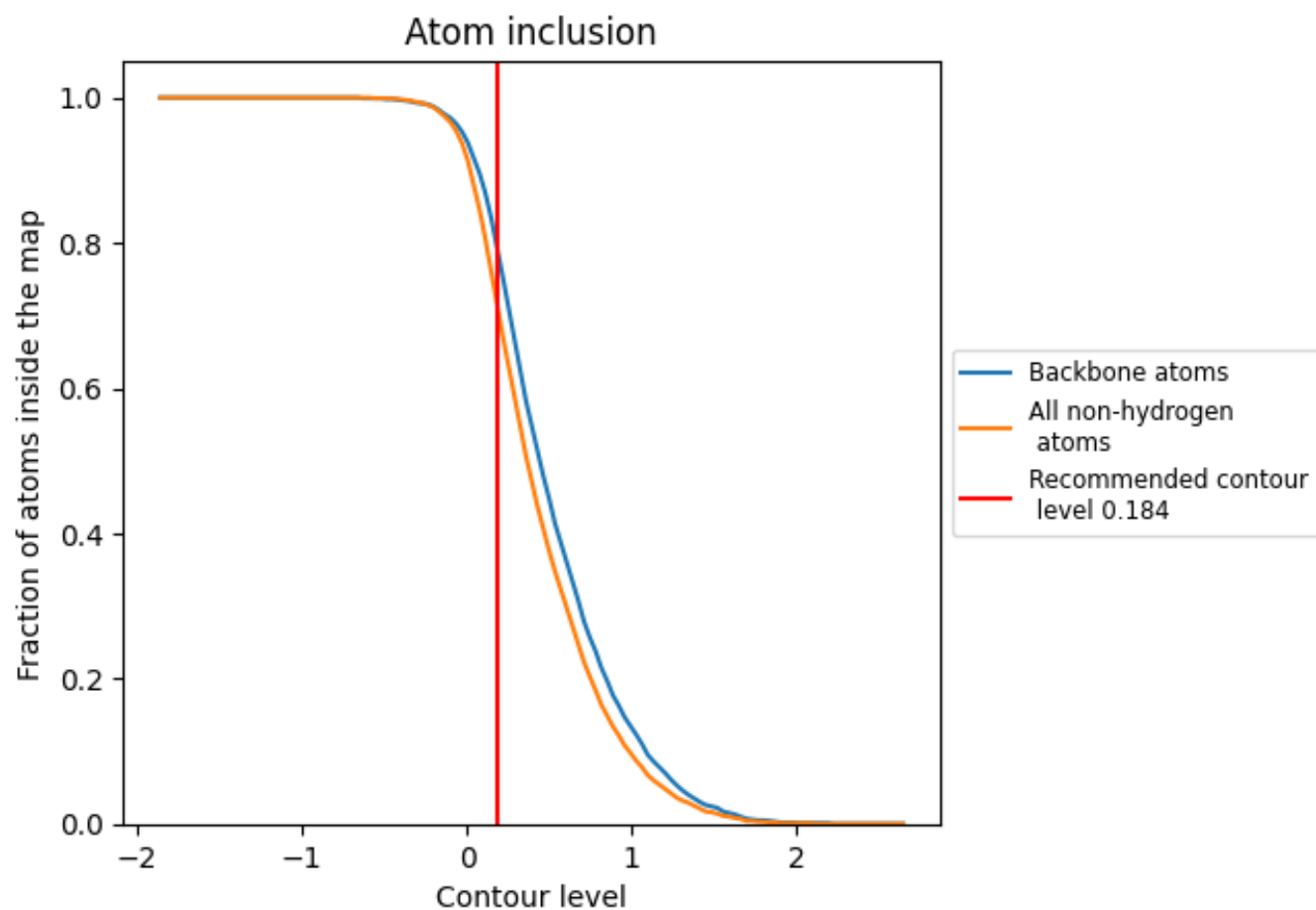
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.184).

9.4 Atom inclusion [i](#)



At the recommended contour level, 79% of all backbone atoms, 72% 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 (0.184) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.7150	0.3780
A	0.7150	0.3960
B	0.8210	0.4480
E	0.6240	0.3060
G	0.5880	0.3110
R	0.6850	0.3540

