



Full wwPDB EM Validation Report ⓘ

Mar 25, 2026 – 11:08 AM UTC

PDB ID : 8K66 / pdb_00008k66
EMDB ID : EMD-36918
Title : Cryo-EM structure of Oryza sativa HKT2;1 at 2.5 angstrom
Authors : Wang, X.; Shen, X.; Qu, Y.; Wang, C.; Shen, H.
Deposited on : 2023-07-25
Resolution : 2.53 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

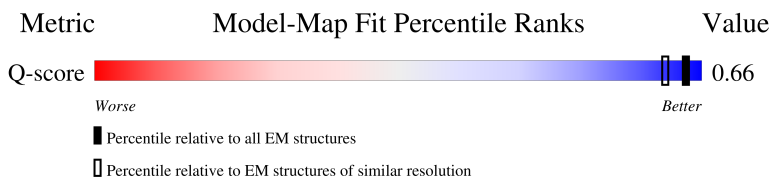
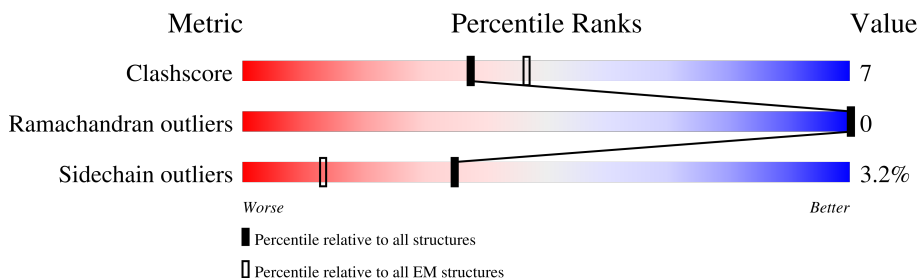
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 2.53 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	7309 (2.03 - 3.03)

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	543	
1	B	543	

2 Entry composition

There are 8 unique types of molecules in this entry. The entry contains 7620 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.

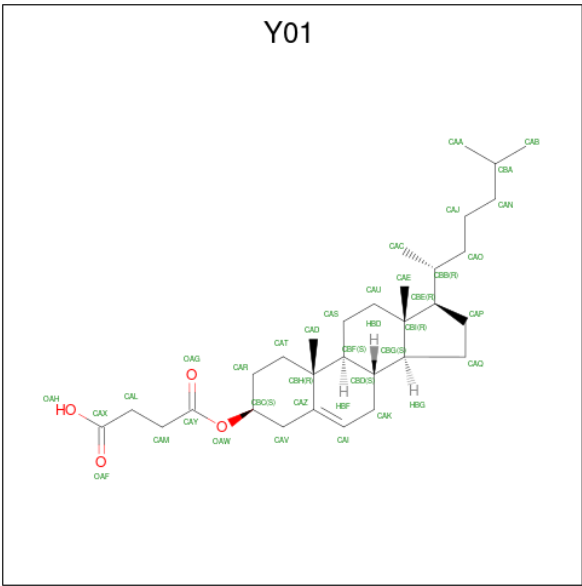
- Molecule 1 is a protein called Cation transporter HKT2;1.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	443	Total	C	N	O	S	1	0
			3514	2349	558	590	17		
1	B	443	Total	C	N	O	S	1	0
			3514	2349	558	590	17		

There are 26 discrepancies between the modelled and reference sequences:

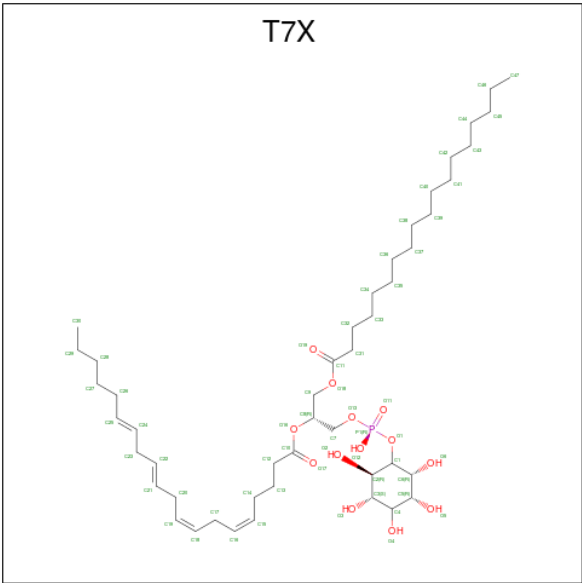
Chain	Residue	Modelled	Actual	Comment	Reference
A	-12	MET	-	initiating methionine	UNP Q0D9S3
A	-11	ALA	-	expression tag	UNP Q0D9S3
A	-10	ASP	-	expression tag	UNP Q0D9S3
A	-9	TYR	-	expression tag	UNP Q0D9S3
A	-8	LYS	-	expression tag	UNP Q0D9S3
A	-7	ASP	-	expression tag	UNP Q0D9S3
A	-6	ASP	-	expression tag	UNP Q0D9S3
A	-5	ASP	-	expression tag	UNP Q0D9S3
A	-4	ASP	-	expression tag	UNP Q0D9S3
A	-3	LYS	-	expression tag	UNP Q0D9S3
A	-2	GLY	-	expression tag	UNP Q0D9S3
A	-1	GLY	-	expression tag	UNP Q0D9S3
A	0	ARG	-	expression tag	UNP Q0D9S3
B	-12	MET	-	initiating methionine	UNP Q0D9S3
B	-11	ALA	-	expression tag	UNP Q0D9S3
B	-10	ASP	-	expression tag	UNP Q0D9S3
B	-9	TYR	-	expression tag	UNP Q0D9S3
B	-8	LYS	-	expression tag	UNP Q0D9S3
B	-7	ASP	-	expression tag	UNP Q0D9S3
B	-6	ASP	-	expression tag	UNP Q0D9S3
B	-5	ASP	-	expression tag	UNP Q0D9S3
B	-4	ASP	-	expression tag	UNP Q0D9S3
B	-3	LYS	-	expression tag	UNP Q0D9S3
B	-2	GLY	-	expression tag	UNP Q0D9S3
B	-1	GLY	-	expression tag	UNP Q0D9S3
B	0	ARG	-	expression tag	UNP Q0D9S3

- Molecule 2 is CHOLESTEROL HEMISUCCINATE (CCD ID: Y01) (formula: C₃₁H₅₀O₄).



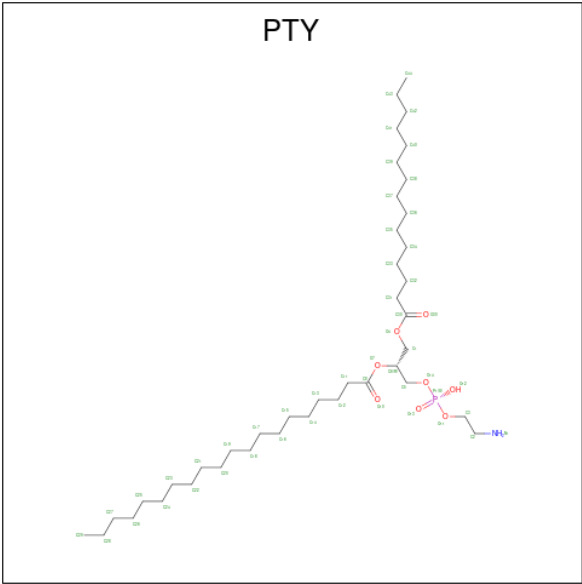
Mol	Chain	Residues	Atoms			AltConf
2	A	1	Total	C	O	0
			35	31	4	
2	A	1	Total	C	O	0
			35	31	4	
2	B	1	Total	C	O	0
			35	31	4	
2	B	1	Total	C	O	0
			35	31	4	

- Molecule 3 is Phosphatidylinositol (CCD ID: T7X) (formula: C₄₇H₈₃O₁₃P).



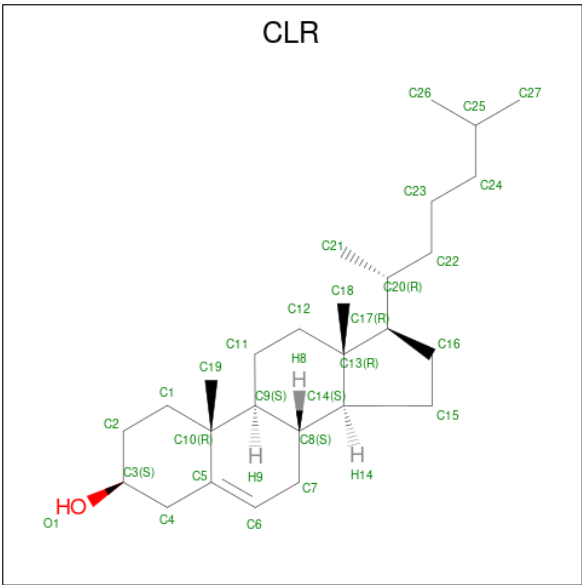
Mol	Chain	Residues	Atoms				AltConf
3	A	1	Total	C	O	P	0
			46	32	13	1	
3	B	1	Total	C	O	P	0
			46	32	13	1	

- Molecule 4 is PHOSPHATIDYLETHANOLAMINE (CCD ID: PTY) (formula: C₄₀H₈₀NO₈P).



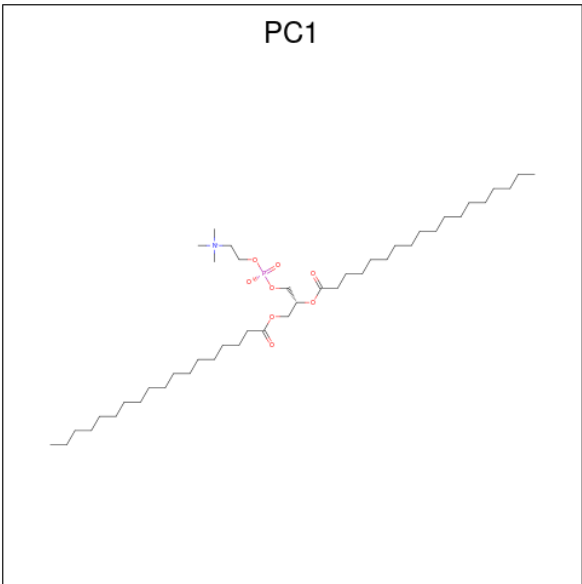
Mol	Chain	Residues	Atoms					AltConf
4	A	1	Total	C	N	O	P	0
			34	24	1	8	1	
4	B	1	Total	C	N	O	P	0
			34	24	1	8	1	

- Molecule 5 is CHOLESTEROL (CCD ID: CLR) (formula: C₂₇H₄₆O).



Mol	Chain	Residues	Atoms			AltConf
5	A	1	Total	C	O	0
			28	27	1	
5	B	1	Total	C	O	0
			28	27	1	

- Molecule 6 is 1,2-DIACYL-SN-GLYCERO-3-PHOSPHOCHOLINE (CCD ID: PC1) (formula: C₄₄H₈₈NO₈P).



Mol	Chain	Residues	Atoms					AltConf
6	A	1	Total	C	N	O	P	0
			51	41	1	8	1	

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Mol	Chain	Residues	Atoms					AltConf
6	B	1	Total	C	N	O	P	0
			51	41	1	8	1	

- Molecule 7 is SODIUM ION (CCD ID: NA) (formula: Na).

Mol	Chain	Residues	Atoms		AltConf
7	A	2	Total	Na	0
			2	2	
7	B	2	Total	Na	0
			2	2	

- Molecule 8 is water.

Mol	Chain	Residues	Atoms		AltConf
8	A	65	Total	O	0
			65	65	
8	B	65	Total	O	0
			65	65	



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	501277	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	50	Depositor
Minimum defocus (nm)	1200	Depositor
Maximum defocus (nm)	2200	Depositor
Magnification	Not provided	
Image detector	GATAN K3 (6k x 4k)	Depositor
Maximum map value	0.079	Depositor
Minimum map value	-0.048	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.001	Depositor
Recommended contour level	0.0155	Depositor
Map size (Å)	258.552, 258.552, 258.552	wwPDB
Map dimensions	480, 480, 480	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	0.53865, 0.53865, 0.53865	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: NA, PC1, T7X, CLR, Y01, PTY

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	0.24	0/3605	0.40	0/4893
1	B	0.21	0/3605	0.39	0/4893
All	All	0.23	0/7210	0.40	0/9786

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	3514	0	3674	54	0
1	B	3514	0	3674	52	0
2	A	70	0	98	4	0
2	B	70	0	98	3	0
3	A	46	0	0	1	0
3	B	46	0	0	0	0
4	A	34	0	41	1	0
4	B	34	0	41	1	0
5	A	28	0	46	3	0
5	B	28	0	46	1	0
6	A	51	0	76	3	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
6	B	51	0	76	2	0
7	A	2	0	0	0	0
7	B	2	0	0	0	0
8	A	65	0	0	10	0
8	B	65	0	0	9	0
All	All	7620	0	7870	115	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 (115) 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:478:ARG:NH1	8:A:701:HOH:O	2.00	0.93
1:B:273:ASN:ND2	8:B:802:HOH:O	2.05	0.89
1:A:382:LEU:HD11	8:A:719:HOH:O	1.78	0.83
1:A:245:LEU:O	8:A:702:HOH:O	2.01	0.79
1:A:188:LEU:HD22	1:A:306:LEU:HD23	1.65	0.77
1:B:245:LEU:O	8:B:801:HOH:O	2.05	0.74
1:B:27:VAL:HG23	4:B:705:PTY:H372	1.76	0.68
1:B:474:TYR:O	8:B:803:HOH:O	2.11	0.68
1:A:88:SER:HB2	1:A:243:VAL:O	1.95	0.66
1:A:474:TYR:O	8:A:703:HOH:O	2.13	0.66
1:A:476:CYS:SG	1:A:488[B]:CYS:HB2	2.36	0.65
1:B:476:CYS:SG	1:B:488[B]:CYS:HB2	2.36	0.64
1:A:88:SER:CB	1:A:243:VAL:O	2.46	0.63
1:B:478:ARG:NH2	8:B:811:HOH:O	2.34	0.61
1:A:87:SER:O	1:A:469:GLY:CA	2.49	0.60
1:A:224:LYS:NZ	1:A:250:GLU:OE2	2.21	0.60
1:A:88:SER:O	1:A:88:SER:OG	2.20	0.59
1:B:88:SER:O	1:B:88:SER:OG	2.20	0.57
1:A:476:CYS:O	1:A:480:GLN:HG2	2.06	0.54
1:A:200:HIS:CE1	8:A:730:HOH:O	2.60	0.54
1:A:125:ARG:NH1	1:A:306:LEU:O	2.41	0.54
1:A:285:TRP:CE2	1:A:289:LYS:HD2	2.43	0.54
1:B:476:CYS:O	1:B:480:GLN:HG2	2.07	0.54
1:A:48:PHE:HD1	1:A:84:LEU:HD13	1.73	0.54
1:A:25:ASN:O	1:A:29:LEU:HG	2.08	0.53
1:A:300:ILE:HG13	1:A:301:LYS:H	1.74	0.53
1:B:103:VAL:O	1:B:107:LEU:HG	2.09	0.53
1:A:90:ILE:CG2	8:A:758:HOH:O	2.58	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:200:HIS:CE1	8:B:830:HOH:O	2.62	0.52
1:A:90:ILE:HG22	8:A:758:HOH:O	2.11	0.51
1:A:220:PRO:HA	1:A:223:LYS:HG2	1.93	0.51
1:A:475:SER:HB3	1:A:478:ARG:HD3	1.93	0.51
1:B:87:SER:O	1:B:469:GLY:CA	2.59	0.51
1:B:90:ILE:O	1:B:493:TYR:HB2	2.10	0.51
1:B:322:SER:HA	2:B:702:Y01:HAC2	1.93	0.51
1:A:24:VAL:O	1:A:28:VAL:HG13	2.10	0.50
1:B:48:PHE:HD1	1:B:84:LEU:HD13	1.75	0.50
1:A:322:SER:HA	2:A:601:Y01:HAC2	1.94	0.50
1:A:27:VAL:HG23	4:A:604:PTY:H372	1.92	0.50
1:A:331:LEU:HD22	1:A:388:LEU:HD22	1.94	0.50
1:B:125:ARG:HD3	1:B:185:ARG:HD2	1.93	0.50
1:A:206:LEU:HD12	5:A:605:CLR:H22	1.93	0.50
1:B:365:ARG:HA	1:B:366:HIS:CG	2.48	0.49
1:B:331:LEU:HD22	1:B:388:LEU:HD22	1.94	0.49
1:A:123:MET:HE3	1:A:189:GLY:HA3	1.95	0.48
1:A:365:ARG:HA	1:A:366:HIS:CG	2.47	0.48
1:B:220:PRO:HA	1:B:223:LYS:HG2	1.95	0.48
6:A:606:PC1:H142	6:A:606:PC1:H111	1.64	0.48
1:A:326:GLY:HA3	6:B:701:PC1:H3A2	1.96	0.48
1:B:25:ASN:O	1:B:29:LEU:HG	2.14	0.48
1:B:63:LYS:HD3	1:B:63:LYS:HA	1.55	0.48
1:A:200:HIS:HE1	8:A:730:HOH:O	1.97	0.47
1:B:365:ARG:NH1	1:B:392:PRO:O	2.48	0.47
1:B:51:ILE:HB	1:B:84:LEU:HD11	1.95	0.47
1:A:294:ARG:O	1:A:298:LEU:HG	2.14	0.47
1:B:246:VAL:HG11	1:B:252:MET:HE3	1.97	0.47
1:A:88:SER:HB3	1:A:243:VAL:O	2.14	0.47
1:A:248:THR:O	8:A:704:HOH:O	2.21	0.46
1:A:252:MET:HG3	1:A:369:GLU:HB3	1.96	0.46
1:A:365:ARG:NH1	1:A:392:PRO:O	2.48	0.46
1:A:414:LYS:HG2	1:A:415:LEU:H	1.80	0.46
1:A:90:ILE:HD13	1:A:94:MET:SD	2.56	0.45
1:B:184:LEU:HB3	1:B:306:LEU:HD21	1.97	0.45
6:A:606:PC1:H321	6:A:606:PC1:H32	1.75	0.45
1:B:22:TYR:HD1	1:B:24:VAL:H	1.65	0.45
1:B:68:GLU:HA	1:B:70:ARG:NH2	2.32	0.45
1:B:294:ARG:O	1:B:298:LEU:HG	2.15	0.45
6:B:701:PC1:H142	6:B:701:PC1:H111	1.64	0.45
2:B:702:Y01:HAA1	2:B:702:Y01:HAJ2	1.85	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:450:LEU:HB2	8:A:706:HOH:O	2.18	0.44
1:B:125:ARG:NH1	1:B:307:GLN:O	2.41	0.44
1:A:430:ILE:HD11	1:A:465:TYR:CE2	2.52	0.44
1:B:122:LEU:HA	1:B:125:ARG:HD2	2.00	0.44
1:B:430:ILE:HD11	1:B:465:TYR:CE2	2.52	0.44
1:A:93:GLU:O	1:A:96:VAL:HG22	2.17	0.44
1:B:123:MET:HE3	1:B:189:GLY:HA3	1.98	0.44
1:A:299:MET:HG2	1:A:306:LEU:HD21	1.99	0.44
1:A:315:LEU:HB3	1:A:316:PRO:HD3	2.00	0.44
6:A:606:PC1:H3A2	1:B:326:GLY:HA3	2.00	0.44
1:A:51:ILE:HB	1:A:84:LEU:HD11	1.99	0.43
1:B:315:LEU:HB3	1:B:316:PRO:HD3	2.00	0.43
2:A:601:Y01:HAA1	2:A:601:Y01:HAJ2	1.85	0.43
1:B:88:SER:HB2	1:B:243:VAL:O	2.17	0.43
1:B:88:SER:CB	1:B:243:VAL:O	2.66	0.43
1:B:457:MET:HE3	1:B:457:MET:HB3	1.94	0.43
2:A:601:Y01:HAE2	2:A:601:Y01:HBB	1.71	0.43
1:B:450:LEU:HB2	8:B:804:HOH:O	2.18	0.43
1:A:23:PHE:O	1:A:27:VAL:HG12	2.18	0.43
1:B:382:LEU:HD22	8:B:818:HOH:O	2.19	0.43
1:B:293:LEU:HD23	1:B:293:LEU:HA	1.91	0.43
1:B:93:GLU:O	1:B:96:VAL:HG22	2.19	0.42
1:A:313:PRO:HB2	1:A:316:PRO:HD2	2.02	0.42
1:B:313:PRO:HB2	1:B:316:PRO:HD2	2.02	0.42
2:A:601:Y01:HAO2	2:A:601:Y01:HAP1	1.73	0.42
5:A:605:CLR:H213	5:A:605:CLR:H232	1.84	0.42
1:B:187:PHE:HB3	1:B:299:MET:HE1	2.02	0.41
1:B:122:LEU:HD12	1:B:125:ARG:HH21	1.85	0.41
1:A:285:TRP:CZ2	1:A:289:LYS:HD2	2.54	0.41
1:A:290:VAL:HG23	1:A:291:THR:HG23	2.02	0.41
1:B:39:HIS:HD2	1:B:41:PHE:HB3	1.85	0.41
1:B:69:PHE:CZ	1:B:71:PRO:HB3	2.56	0.41
1:A:293:LEU:HD12	1:A:293:LEU:HA	1.92	0.41
1:B:39:HIS:CD2	1:B:41:PHE:H	2.38	0.41
1:A:244:GLY:HA2	1:A:369:GLU:HG3	2.02	0.41
2:B:702:Y01:HAO2	2:B:702:Y01:HAP1	1.73	0.41
1:A:528:ARG:HD3	1:B:398:ALA:HB3	2.02	0.40
1:B:200:HIS:HE1	8:B:830:HOH:O	1.99	0.40
1:A:439:ILE:O	1:A:442:ARG:NH1	2.45	0.40
1:B:286:PHE:CD2	5:B:706:CLR:H271	2.56	0.40
1:B:448:ASP:OD1	8:B:804:HOH:O	2.22	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:39:HIS:HD2	1:A:41:PHE:HB3	1.86	0.40
1:B:439:ILE:O	1:B:442:ARG:NH1	2.45	0.40
1:A:304:GLU:H	1:A:304:GLU:CD	2.30	0.40
3:A:603:T7X:C19	5:A:605:CLR:H6	2.52	0.40
1:B:60:MET:HG2	1:B:76:MET:HG3	2.03	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	438/543 (81%)	431 (98%)	7 (2%)	0	100	100
1	B	438/543 (81%)	431 (98%)	7 (2%)	0	100	100
All	All	876/1086 (81%)	862 (98%)	14 (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	391/478 (82%)	378 (97%)	13 (3%)	33	58
1	B	391/478 (82%)	379 (97%)	12 (3%)	35	60
All	All	782/956 (82%)	757 (97%)	25 (3%)	35	60

All (25) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	63	LYS
1	A	84	LEU
1	A	87	SER
1	A	90	ILE
1	A	213	ARG
1	A	215	SER
1	A	252	MET
1	A	305	GLU
1	A	372	ILE
1	A	414	LYS
1	A	415	LEU
1	A	487	ILE
1	A	529	LEU
1	B	63	LYS
1	B	84	LEU
1	B	87	SER
1	B	90	ILE
1	B	180	ARG
1	B	215	SER
1	B	252	MET
1	B	301	LYS
1	B	372	ILE
1	B	415	LEU
1	B	487	ILE
1	B	529	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (16) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	25	ASN
1	A	39	HIS
1	A	200	HIS
1	A	302	ASN
1	A	370	ASN
1	A	420	GLN
1	A	421	ASN
1	A	447	ASN
1	A	456	ASN
1	B	25	ASN
1	B	31	HIS
1	B	39	HIS

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Mol	Chain	Res	Type
1	B	200	HIS
1	B	420	GLN
1	B	421	ASN
1	B	456	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](#)

Of 16 ligands modelled in this entry, 4 are monoatomic - leaving 12 for Mogul analysis.

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	$\# Z > 2$
2	Y01	A	601	-	38,38,38	0.73	0	57,57,57	1.34	7 (12%)
2	Y01	B	702	-	38,38,38	0.72	0	57,57,57	1.34	7 (12%)
5	CLR	B	706	-	31,31,31	0.36	0	48,48,48	1.05	5 (10%)
5	CLR	A	605	-	31,31,31	0.30	0	48,48,48	0.36	0
3	T7X	A	603	-	46,46,61	0.98	5 (10%)	55,58,73	1.07	2 (3%)
2	Y01	A	602	-	38,38,38	0.79	1 (2%)	57,57,57	1.27	9 (15%)
2	Y01	B	703	-	38,38,38	0.79	1 (2%)	57,57,57	1.27	9 (15%)
6	PC1	B	701	-	50,50,53	0.99	4 (8%)	56,58,61	1.05	2 (3%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
6	PC1	A	606	-	50,50,53	0.99	4 (8%)	56,58,61	1.05	2 (3%)
4	PTY	B	705	-	33,33,49	1.06	4 (12%)	36,38,54	1.12	2 (5%)
3	T7X	B	704	-	46,46,61	0.98	5 (10%)	55,58,73	1.07	2 (3%)
4	PTY	A	604	-	33,33,49	1.05	4 (12%)	36,38,54	1.12	2 (5%)

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
2	Y01	A	601	-	-	12/19/77/77	0/4/4/4
2	Y01	B	702	-	-	12/19/77/77	0/4/4/4
5	CLR	B	706	-	-	8/10/68/68	0/4/4/4
5	CLR	A	605	-	-	4/10/68/68	0/4/4/4
3	T7X	A	603	-	-	16/41/65/80	0/1/1/1
2	Y01	A	602	-	-	9/19/77/77	0/4/4/4
2	Y01	B	703	-	-	9/19/77/77	0/4/4/4
6	PC1	B	701	-	-	16/54/54/57	-
6	PC1	A	606	-	-	16/54/54/57	-
4	PTY	B	705	-	-	17/37/37/53	-
3	T7X	B	704	-	-	16/41/65/80	0/1/1/1
4	PTY	A	604	-	-	17/37/37/53	-

All (28) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	B	701	PC1	O21-C2	-2.82	1.40	1.46
3	A	603	T7X	O16-C8	-2.82	1.40	1.46
3	B	704	T7X	O16-C8	-2.81	1.40	1.46
6	A	606	PC1	O21-C2	-2.80	1.40	1.46
4	B	705	PTY	O7-C6	-2.69	1.40	1.46
4	A	604	PTY	O7-C6	-2.66	1.40	1.46
4	B	705	PTY	O4-C1	-2.45	1.39	1.45
3	B	704	T7X	O18-C11	2.45	1.40	1.33
3	A	603	T7X	O18-C11	2.43	1.40	1.33
4	A	604	PTY	O4-C1	-2.41	1.39	1.45
6	B	701	PC1	O31-C31	2.35	1.40	1.33
6	A	606	PC1	O31-C31	2.33	1.40	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	B	701	PC1	O31-C3	-2.27	1.40	1.45
6	A	606	PC1	O31-C3	-2.24	1.40	1.45
4	A	604	PTY	O4-C30	2.22	1.39	1.33
4	B	705	PTY	O4-C30	2.21	1.39	1.33
3	A	603	T7X	O18-C9	-2.20	1.40	1.45
3	B	704	T7X	O18-C9	-2.16	1.40	1.45
2	A	602	Y01	OAW-CBC	-2.13	1.41	1.46
2	B	703	Y01	OAW-CBC	-2.13	1.41	1.46
4	B	705	PTY	O7-C8	2.11	1.40	1.34
3	B	704	T7X	P1-O1	2.08	1.65	1.59
4	A	604	PTY	O7-C8	2.06	1.40	1.34
6	B	701	PC1	O21-C21	2.04	1.40	1.34
3	A	603	T7X	P1-O1	2.04	1.65	1.59
6	A	606	PC1	O21-C21	2.02	1.40	1.34
3	B	704	T7X	O16-C10	2.02	1.40	1.34
3	A	603	T7X	O16-C10	2.02	1.40	1.34

All (49) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	702	Y01	CBI-CBE-CBB	-4.56	112.46	119.50
2	A	601	Y01	CBI-CBE-CBB	-4.54	112.49	119.50
4	A	604	PTY	O7-C8-C11	4.07	120.28	111.48
4	B	705	PTY	O7-C8-C11	4.05	120.24	111.48
3	B	704	T7X	O16-C10-C12	3.76	119.61	111.48
3	A	603	T7X	O16-C10-C12	3.74	119.56	111.48
6	B	701	PC1	O21-C21-C22	3.70	119.48	111.48
6	A	606	PC1	O21-C21-C22	3.68	119.44	111.48
2	A	602	Y01	CBI-CBE-CBB	-2.89	115.03	119.50
2	B	703	Y01	CBI-CBE-CBB	-2.88	115.05	119.50
3	A	603	T7X	O18-C11-C31	2.79	120.33	111.83
3	B	704	T7X	O18-C11-C31	2.76	120.27	111.83
6	B	701	PC1	O31-C31-C32	2.73	120.15	111.83
6	A	606	PC1	O31-C31-C32	2.72	120.12	111.83
2	A	602	Y01	OAW-CAY-OAG	-2.65	117.51	123.70
5	B	706	CLR	C14-C8-C9	-2.65	105.63	109.09
2	B	703	Y01	OAW-CAY-OAG	-2.64	117.53	123.70
2	B	702	Y01	CBI-CBG-CBD	-2.63	110.68	114.41
2	A	601	Y01	CBI-CBG-CBD	-2.59	110.73	114.41
5	B	706	CLR	C11-C9-C10	2.59	116.28	113.08
2	A	601	Y01	OAW-CAY-OAG	-2.50	117.87	123.70
2	B	702	Y01	CAS-CAU-CBI	-2.48	108.55	112.74

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	702	Y01	OAW-CAY-OAG	-2.47	117.92	123.70
2	A	601	Y01	CAS-CAU-CBI	-2.43	108.64	112.74
4	B	705	PTY	O4-C30-C31	2.38	119.11	111.83
2	B	703	Y01	CBI-CBG-CBD	-2.38	111.04	114.41
4	A	604	PTY	O4-C30-C31	2.37	119.08	111.83
2	A	602	Y01	CBI-CBG-CBD	-2.37	111.04	114.41
2	A	601	Y01	CAJ-CAO-CBB	-2.35	108.51	115.08
2	B	702	Y01	CBD-CAK-CAI	-2.33	109.53	112.76
2	B	702	Y01	CAJ-CAO-CBB	-2.33	108.57	115.08
2	A	601	Y01	CBD-CAK-CAI	-2.32	109.55	112.76
5	B	706	CLR	C12-C11-C9	2.31	117.07	113.14
2	A	602	Y01	OAW-CAY-CAM	2.31	116.48	111.48
2	A	602	Y01	CAS-CAU-CBI	-2.31	108.84	112.74
2	B	703	Y01	CAS-CAU-CBI	-2.30	108.86	112.74
2	B	703	Y01	OAW-CAY-CAM	2.29	116.44	111.48
2	B	703	Y01	CAR-CBC-CAV	-2.29	107.80	110.97
2	A	602	Y01	CBC-CAV-CAZ	-2.28	108.08	111.45
2	B	703	Y01	CBC-CAV-CAZ	-2.27	108.10	111.45
2	A	602	Y01	CAR-CBC-CAV	-2.27	107.82	110.97
5	B	706	CLR	C7-C8-C14	2.19	114.03	110.93
2	A	601	Y01	OAW-CAY-CAM	2.13	116.09	111.48
2	B	702	Y01	OAW-CAY-CAM	2.12	116.07	111.48
2	B	703	Y01	CAT-CAR-CBC	-2.06	106.98	110.33
2	A	602	Y01	CAC-CBB-CAO	-2.03	107.19	110.34
2	A	602	Y01	CAT-CAR-CBC	-2.03	107.02	110.33
5	B	706	CLR	C11-C12-C13	2.01	116.13	112.74
2	B	703	Y01	CAC-CBB-CAO	-2.00	107.24	110.34

There are no chirality outliers.

All (152) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	603	T7X	C6-C1-O1-P1
3	A	603	T7X	C7-O13-P1-O11
3	B	704	T7X	C6-C1-O1-P1
3	B	704	T7X	C7-O13-P1-O11
4	A	604	PTY	N1-C2-C3-O11
4	A	604	PTY	C5-O14-P1-O11
4	A	604	PTY	C5-O14-P1-O13
4	B	705	PTY	N1-C2-C3-O11
4	B	705	PTY	C5-O14-P1-O11
4	B	705	PTY	C5-O14-P1-O13

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Mol	Chain	Res	Type	Atoms
6	A	606	PC1	O32-C31-O31-C3
6	A	606	PC1	C32-C31-O31-C3
6	B	701	PC1	O32-C31-O31-C3
6	B	701	PC1	C32-C31-O31-C3
3	A	603	T7X	O19-C11-O18-C9
3	B	704	T7X	O19-C11-O18-C9
5	A	605	CLR	C21-C20-C22-C23
3	A	603	T7X	C31-C11-O18-C9
3	B	704	T7X	C31-C11-O18-C9
5	B	706	CLR	C21-C20-C22-C23
2	A	602	Y01	CAJ-CAO-CBB-CBE
2	B	703	Y01	CAJ-CAO-CBB-CBE
5	A	605	CLR	C17-C20-C22-C23
2	A	602	Y01	CAX-CAL-CAM-CAY
2	B	703	Y01	CAX-CAL-CAM-CAY
2	A	601	Y01	CAC-CBB-CBE-CBI
2	B	702	Y01	CAC-CBB-CBE-CBI
4	A	604	PTY	C8-C11-C12-C13
4	B	705	PTY	C8-C11-C12-C13
2	A	601	Y01	CAO-CBB-CBE-CBI
2	B	702	Y01	CAO-CBB-CBE-CBI
2	A	602	Y01	CAJ-CAO-CBB-CAC
2	B	703	Y01	CAJ-CAO-CBB-CAC
5	B	706	CLR	C17-C20-C22-C23
3	A	603	T7X	C11-C31-C32-C33
3	B	704	T7X	C11-C31-C32-C33
2	A	602	Y01	CAO-CAJ-CAN-CBA
2	B	703	Y01	CAO-CAJ-CAN-CBA
5	A	605	CLR	C20-C22-C23-C24
2	A	602	Y01	CAN-CAJ-CAO-CBB
2	B	703	Y01	CAN-CAJ-CAO-CBB
4	A	604	PTY	C30-C31-C32-C33
4	B	705	PTY	C30-C31-C32-C33
5	B	706	CLR	C13-C17-C20-C22
3	A	603	T7X	C31-C32-C33-C34
3	B	704	T7X	C31-C32-C33-C34
4	A	604	PTY	C34-C35-C36-C37
4	B	705	PTY	C34-C35-C36-C37
6	A	606	PC1	C26-C27-C28-C29
6	B	701	PC1	C26-C27-C28-C29
6	B	701	PC1	C23-C24-C25-C26
6	A	606	PC1	C23-C24-C25-C26

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Mol	Chain	Res	Type	Atoms
6	A	606	PC1	C36-C37-C38-C39
6	B	701	PC1	C36-C37-C38-C39
4	A	604	PTY	C15-C16-C17-C18
4	B	705	PTY	C15-C16-C17-C18
6	A	606	PC1	C24-C25-C26-C27
6	B	701	PC1	C24-C25-C26-C27
2	A	602	Y01	CAM-CAY-OAW-CBC
2	B	703	Y01	CAM-CAY-OAW-CBC
6	A	606	PC1	C2C-C2D-C2E-C2F
6	B	701	PC1	C2C-C2D-C2E-C2F
5	B	706	CLR	C13-C17-C20-C21
3	A	603	T7X	C12-C13-C14-C15
3	B	704	T7X	C12-C13-C14-C15
6	A	606	PC1	C2B-C2C-C2D-C2E
6	B	701	PC1	C2B-C2C-C2D-C2E
2	A	601	Y01	CAJ-CAO-CBB-CBE
2	B	702	Y01	CAJ-CAO-CBB-CBE
3	A	603	T7X	O13-C7-C8-C9
3	B	704	T7X	O13-C7-C8-C9
2	A	602	Y01	OAG-CAY-OAW-CBC
2	B	703	Y01	OAG-CAY-OAW-CBC
4	A	604	PTY	C32-C33-C34-C35
4	B	705	PTY	C32-C33-C34-C35
3	A	603	T7X	C12-C10-O16-C8
3	B	704	T7X	C12-C10-O16-C8
2	A	601	Y01	CAC-CBB-CBE-CAP
2	B	702	Y01	CAC-CBB-CBE-CAP
5	B	706	CLR	C16-C17-C20-C21
6	A	606	PC1	C21-C22-C23-C24
6	B	701	PC1	C21-C22-C23-C24
5	A	605	CLR	C22-C23-C24-C25
3	A	603	T7X	C35-C36-C37-C38
3	B	704	T7X	C35-C36-C37-C38
6	A	606	PC1	C3D-C3E-C3F-C3G
6	B	701	PC1	C3D-C3E-C3F-C3G
3	A	603	T7X	O13-C7-C8-O16
3	B	704	T7X	O13-C7-C8-O16
2	A	601	Y01	CAO-CBB-CBE-CAP
2	B	702	Y01	CAO-CBB-CBE-CAP
5	B	706	CLR	C16-C17-C20-C22
3	A	603	T7X	O17-C10-O16-C8
4	A	604	PTY	C11-C12-C13-C14

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Mol	Chain	Res	Type	Atoms
4	B	705	PTY	C11-C12-C13-C14
6	A	606	PC1	C28-C29-C2A-C2B
6	B	701	PC1	C28-C29-C2A-C2B
4	A	604	PTY	C16-C17-C18-C19
4	B	705	PTY	C16-C17-C18-C19
6	A	606	PC1	C37-C38-C39-C3A
6	B	701	PC1	C37-C38-C39-C3A
3	B	704	T7X	O17-C10-O16-C8
5	B	706	CLR	C23-C24-C25-C27
4	A	604	PTY	O14-C5-C6-O7
4	B	705	PTY	O14-C5-C6-O7
6	B	701	PC1	C39-C3A-C3B-C3C
6	A	606	PC1	C39-C3A-C3B-C3C
4	B	705	PTY	C13-C14-C15-C16
4	A	604	PTY	C13-C14-C15-C16
4	A	604	PTY	C35-C36-C37-C38
4	B	705	PTY	C35-C36-C37-C38
5	B	706	CLR	C23-C24-C25-C26
4	A	604	PTY	C31-C32-C33-C34
4	B	705	PTY	C31-C32-C33-C34
6	A	606	PC1	C27-C28-C29-C2A
6	B	701	PC1	C27-C28-C29-C2A
4	B	705	PTY	C12-C13-C14-C15
4	A	604	PTY	C12-C13-C14-C15
3	A	603	T7X	C33-C34-C35-C36
3	B	704	T7X	C33-C34-C35-C36
2	A	602	Y01	CAM-CAL-CAX-OAH
2	B	703	Y01	CAM-CAL-CAX-OAH
2	B	703	Y01	CAM-CAL-CAX-OAF
4	A	604	PTY	O14-C5-C6-C1
4	B	705	PTY	O14-C5-C6-C1
2	A	602	Y01	CAM-CAL-CAX-OAF
6	A	606	PC1	C22-C23-C24-C25
6	B	701	PC1	C22-C23-C24-C25
2	A	601	Y01	CAO-CAJ-CAN-CBA
2	B	702	Y01	CAO-CAJ-CAN-CBA
4	A	604	PTY	C12-C11-C8-O7
4	B	705	PTY	C12-C11-C8-O7
3	B	704	T7X	O18-C11-C31-C32
3	A	603	T7X	O18-C11-C31-C32
3	A	603	T7X	C32-C33-C34-C35
3	B	704	T7X	C32-C33-C34-C35

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Mol	Chain	Res	Type	Atoms
2	A	601	Y01	CAL-CAM-CAY-OAW
2	B	702	Y01	CAL-CAM-CAY-OAW
2	B	702	Y01	OAG-CAY-OAW-CBC
2	A	601	Y01	OAG-CAY-OAW-CBC
2	A	601	Y01	CAM-CAY-OAW-CBC
2	B	702	Y01	CAM-CAY-OAW-CBC
6	B	701	PC1	C35-C36-C37-C38
3	A	603	T7X	O19-C11-C31-C32
6	A	606	PC1	C35-C36-C37-C38
2	A	601	Y01	CAM-CAL-CAX-OAF
2	A	601	Y01	CAL-CAM-CAY-OAG
2	B	702	Y01	CAL-CAM-CAY-OAG
3	B	704	T7X	O19-C11-C31-C32
2	A	601	Y01	CAJ-CAO-CBB-CAC
2	B	702	Y01	CAJ-CAO-CBB-CAC
2	B	702	Y01	CAM-CAL-CAX-OAF

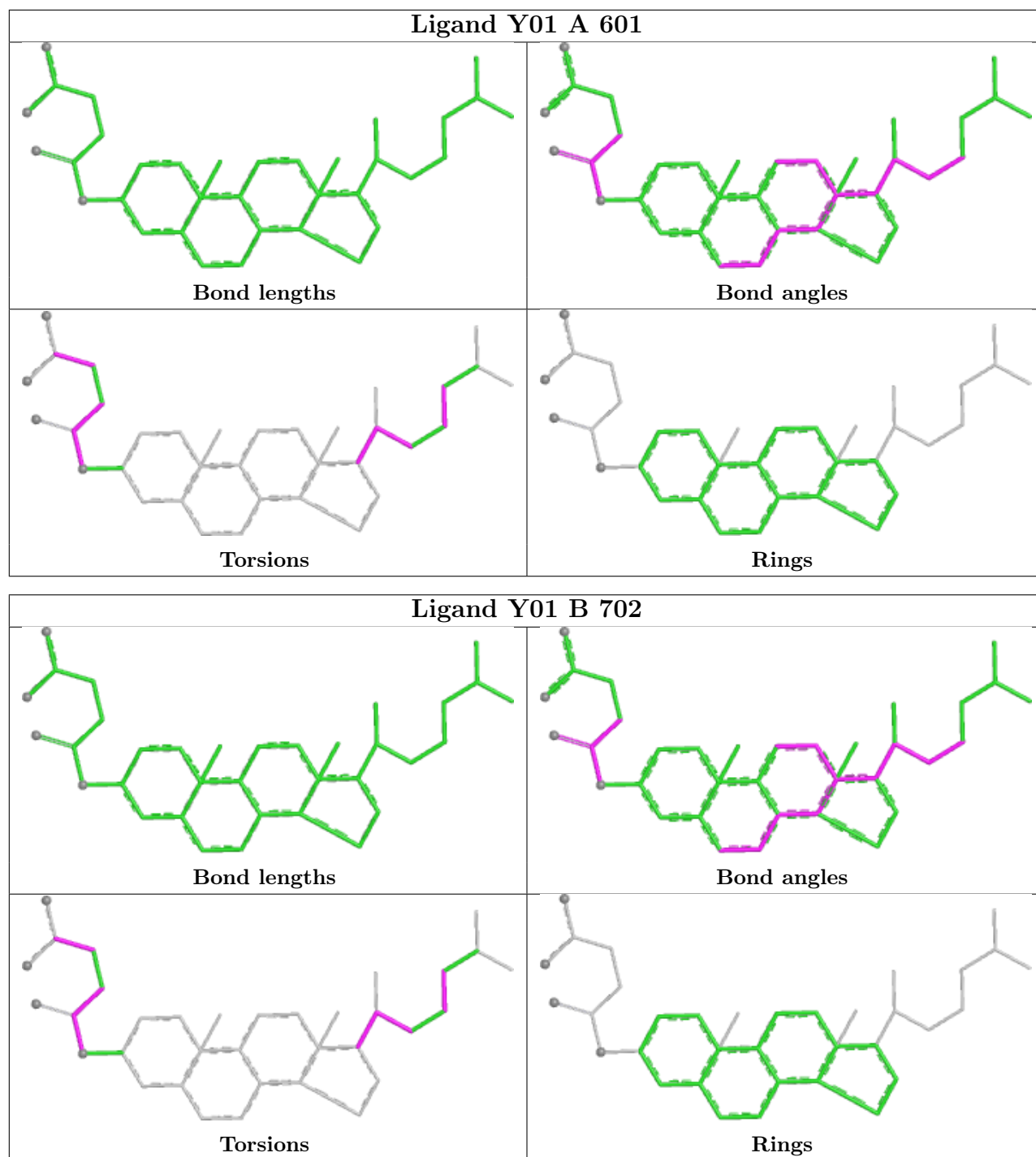
There are no ring outliers.

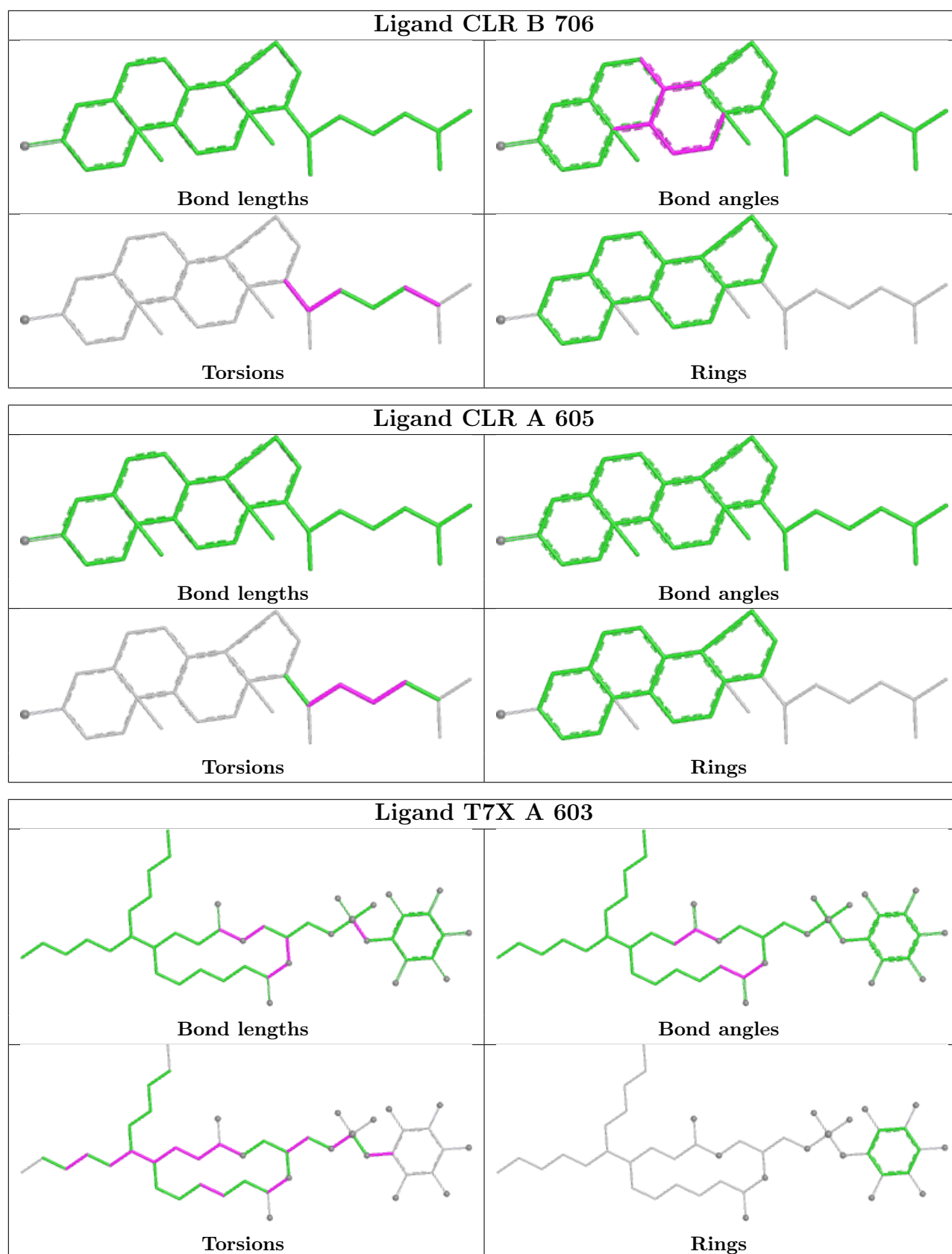
9 monomers are involved in 18 short contacts:

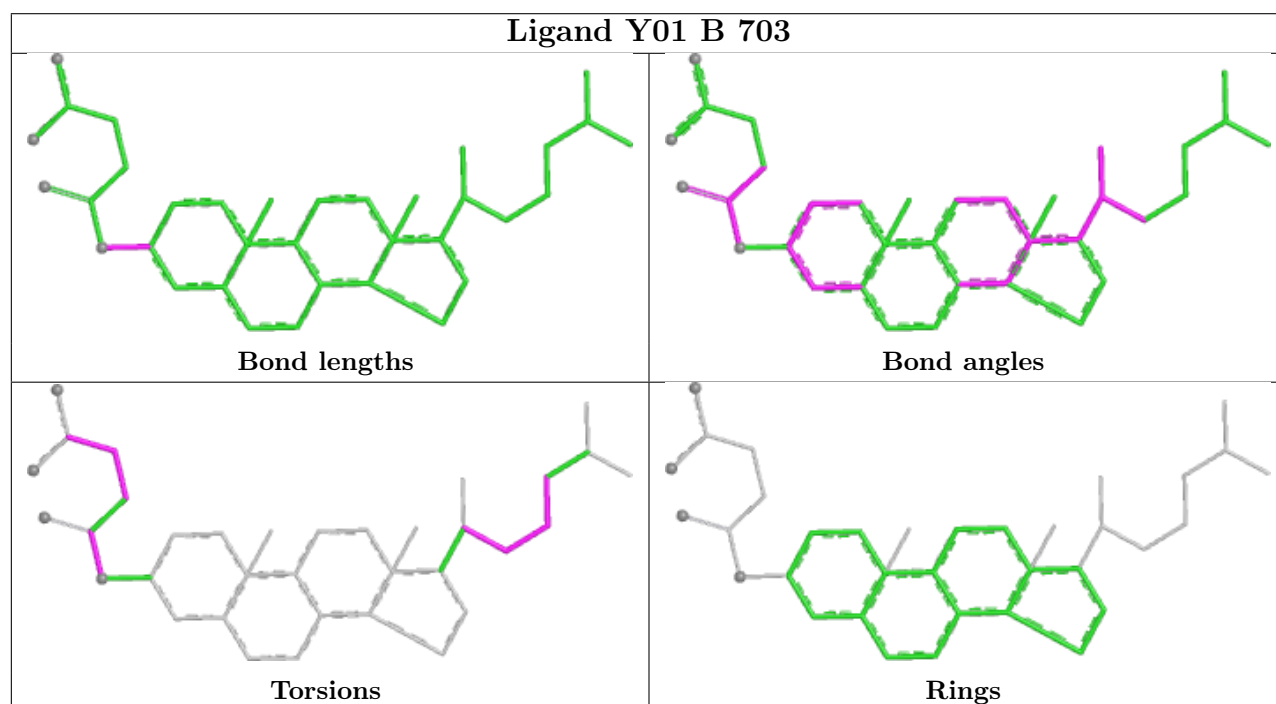
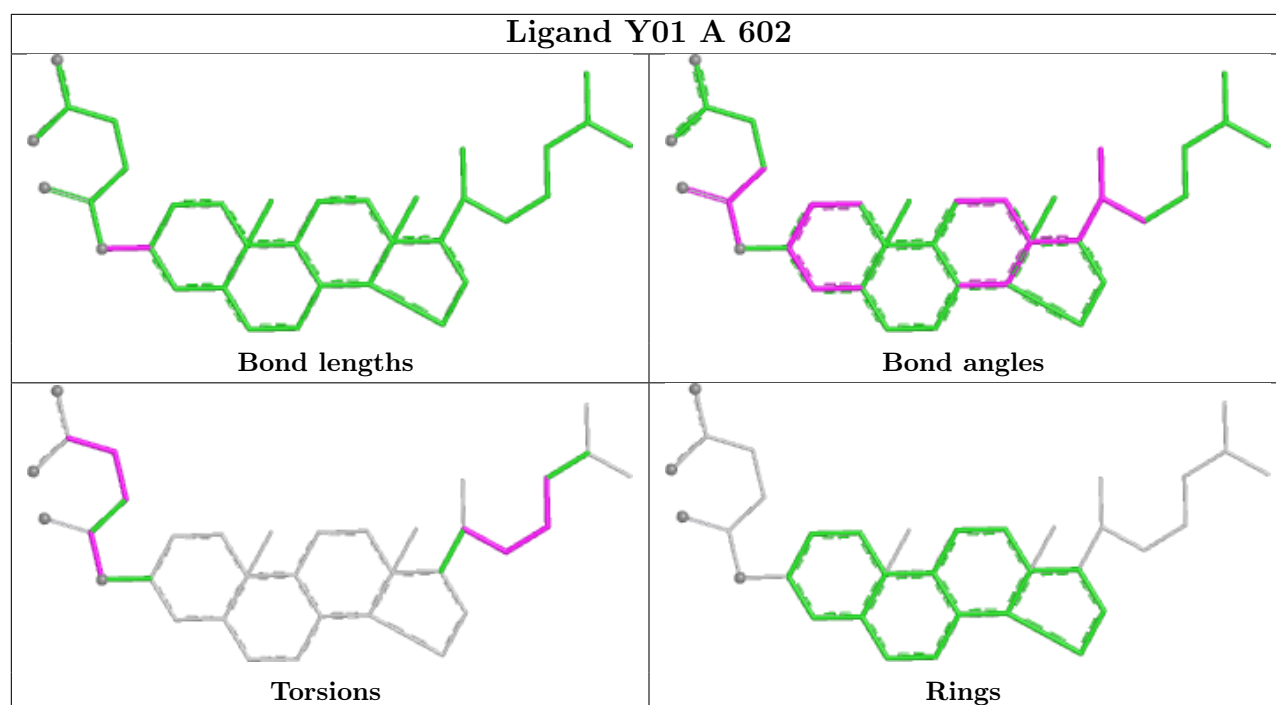
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	601	Y01	4	0
2	B	702	Y01	3	0
5	B	706	CLR	1	0
5	A	605	CLR	3	0
3	A	603	T7X	1	0
6	B	701	PC1	2	0
6	A	606	PC1	3	0
4	B	705	PTY	1	0
4	A	604	PTY	1	0

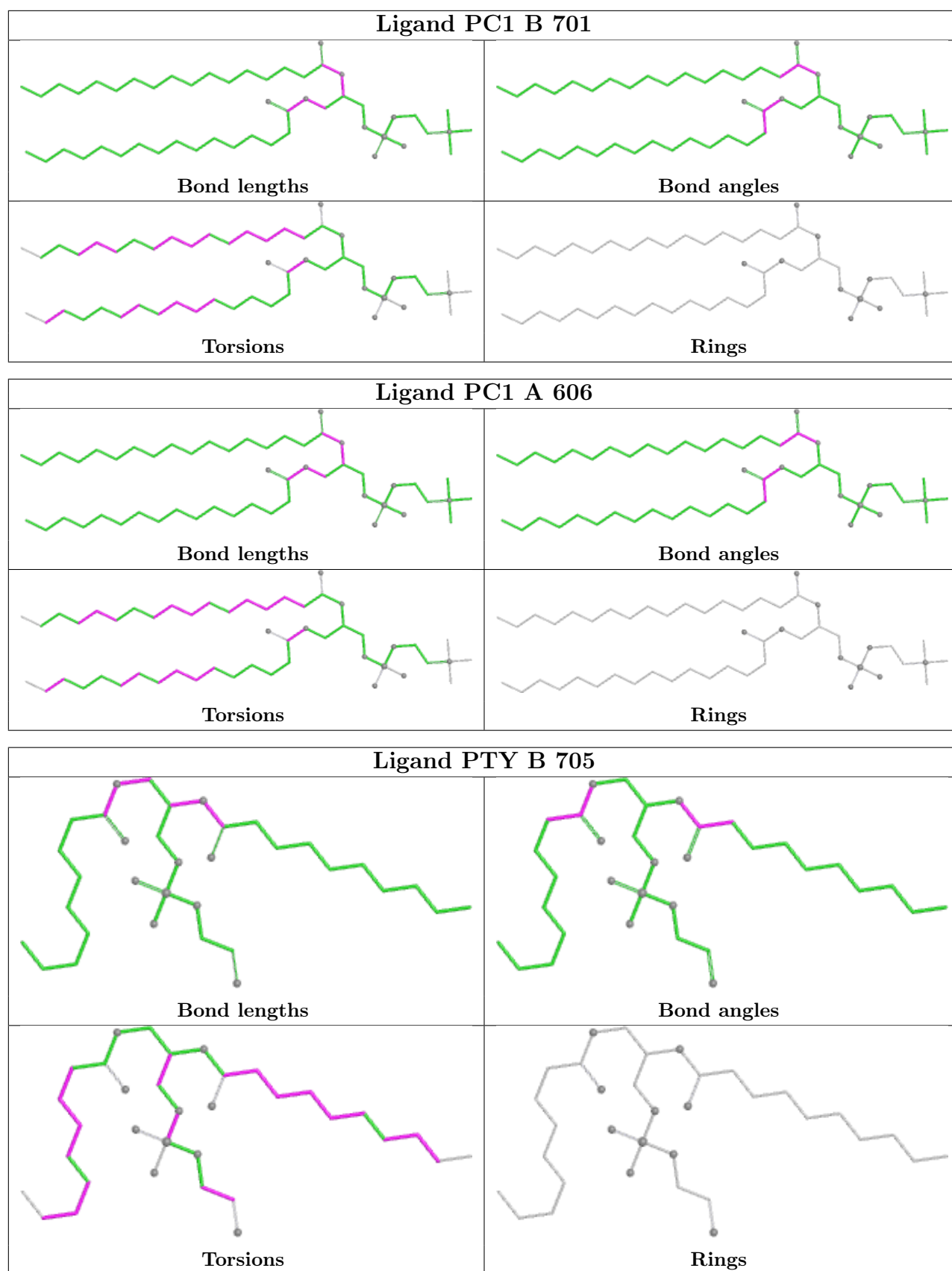
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

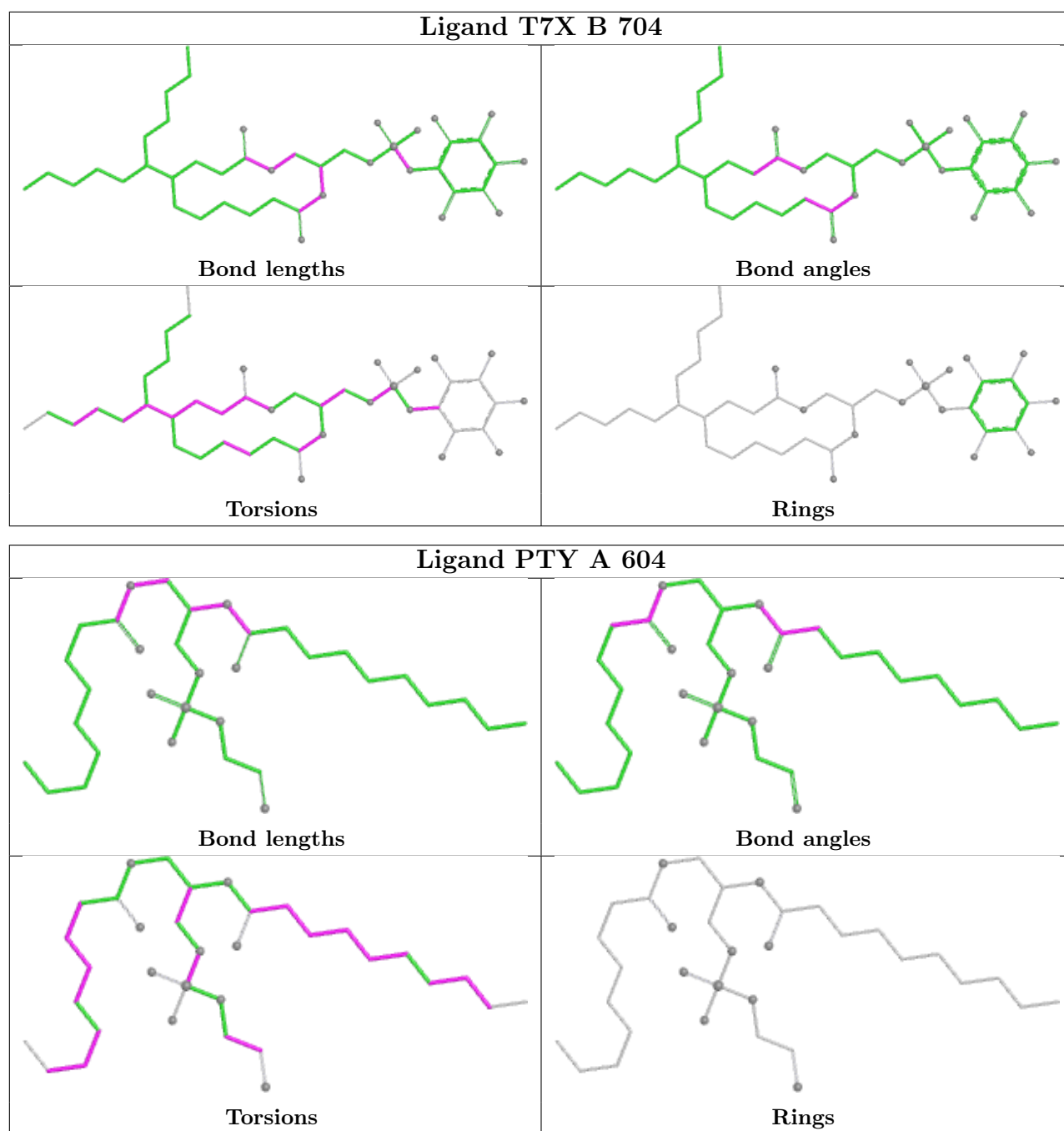
equivalents in the CSD to analyse the geometry.











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.

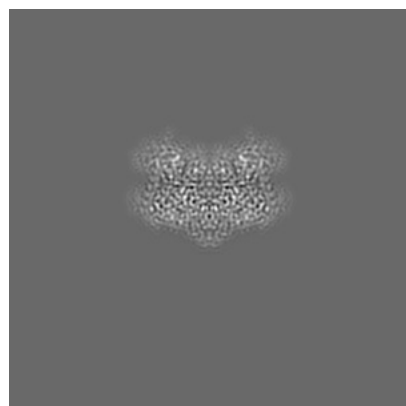
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-36918. These allow visual inspection of the internal detail of the map and identification of artifacts.

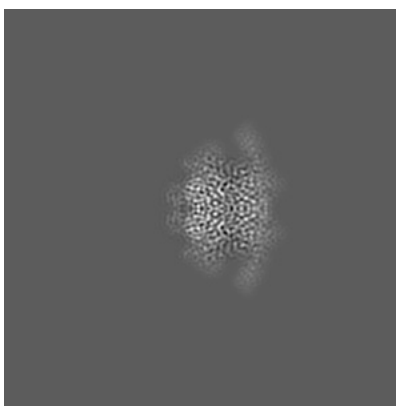
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

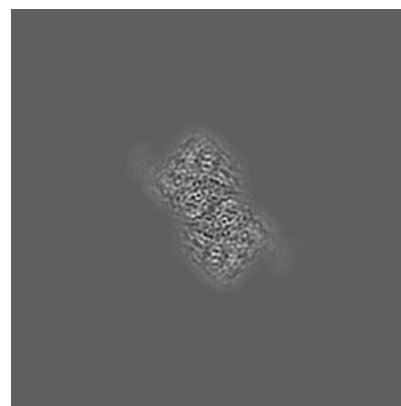
6.1.1 Primary map



X

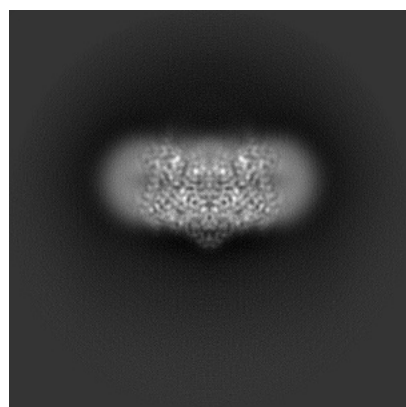


Y

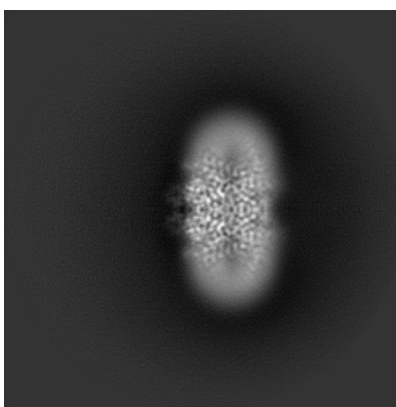


Z

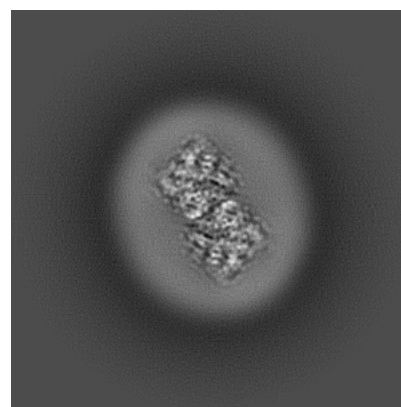
6.1.2 Raw map



X



Y

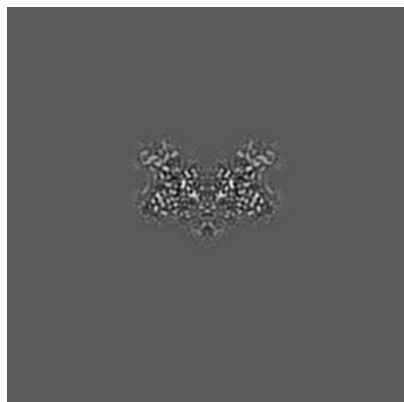


Z

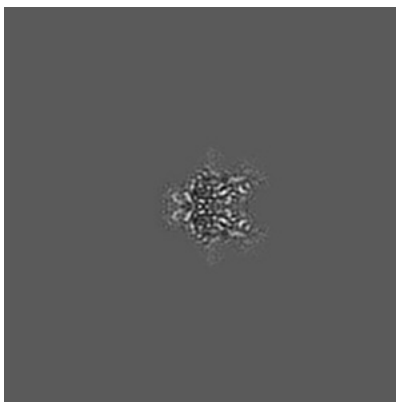
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

6.2.1 Primary map



X Index: 240

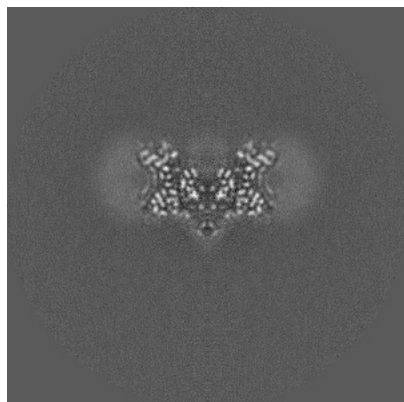


Y Index: 240

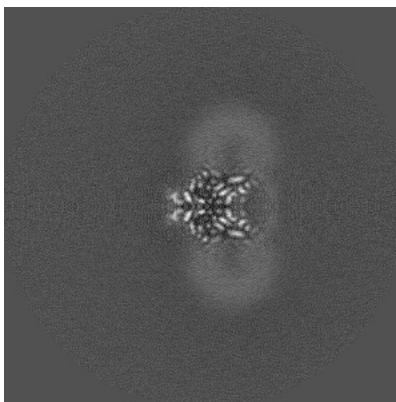


Z Index: 240

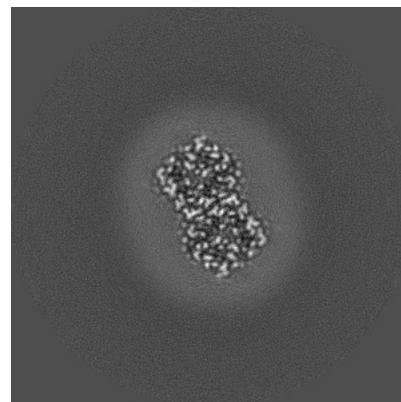
6.2.2 Raw map



X Index: 240



Y Index: 240

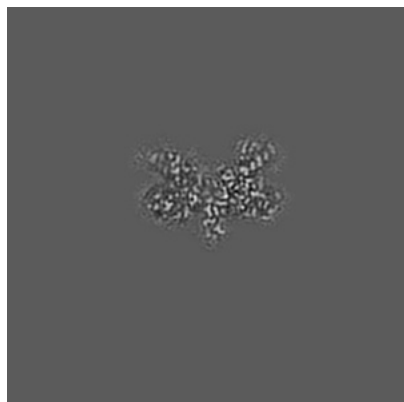


Z Index: 240

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

6.3 Largest variance slices [i](#)

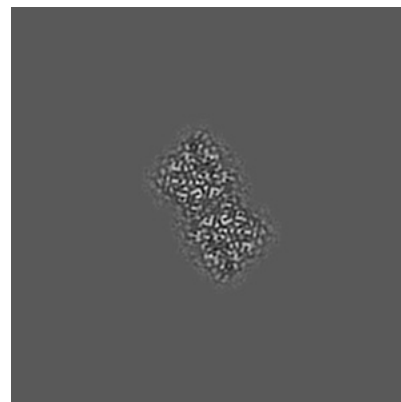
6.3.1 Primary map



X Index: 233

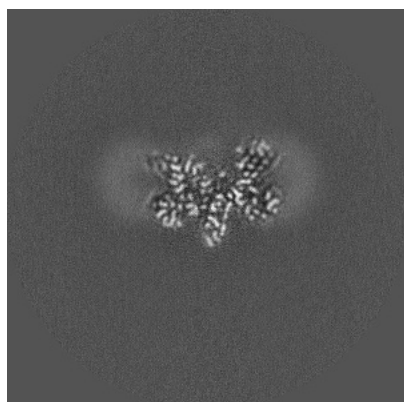


Y Index: 280

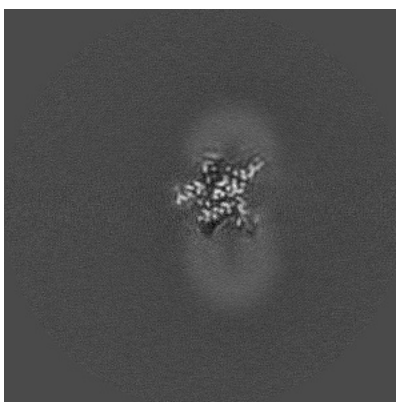


Z Index: 253

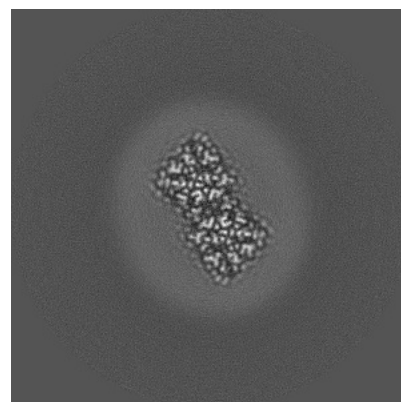
6.3.2 Raw map



X Index: 228



Y Index: 222

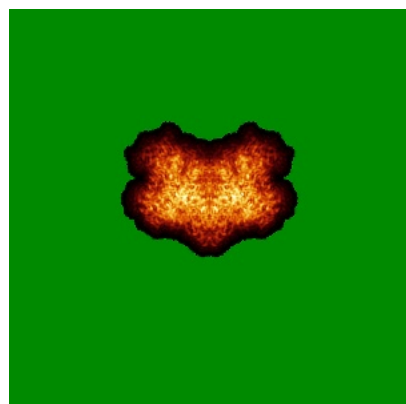


Z Index: 253

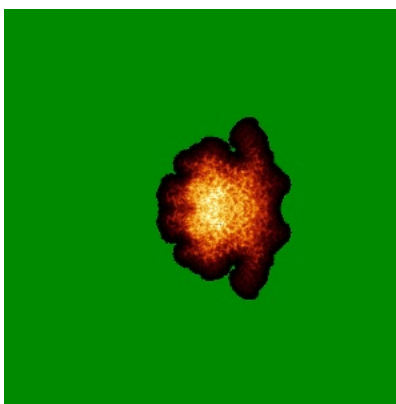
The images above show the largest variance slices of the map in three orthogonal directions.

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

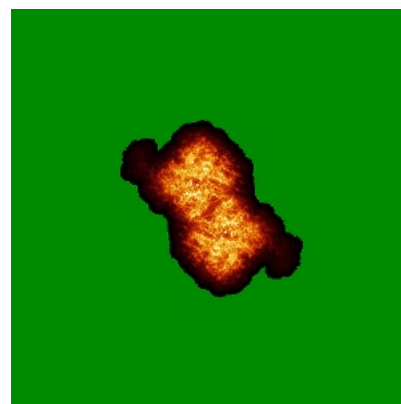
6.4.1 Primary map



X

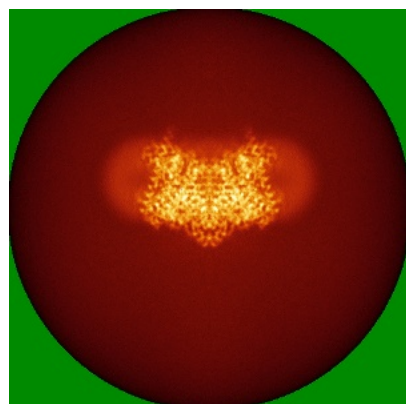


Y

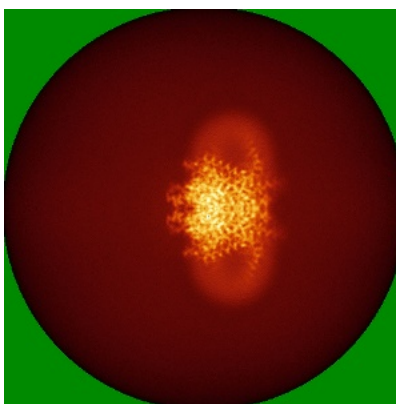


Z

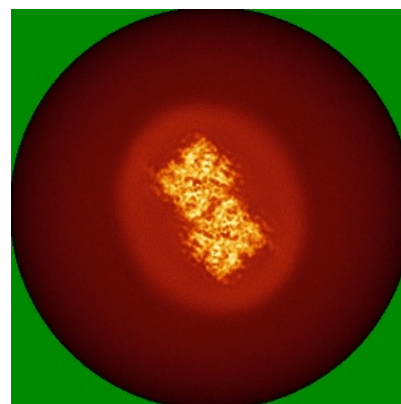
6.4.2 Raw map



X



Y

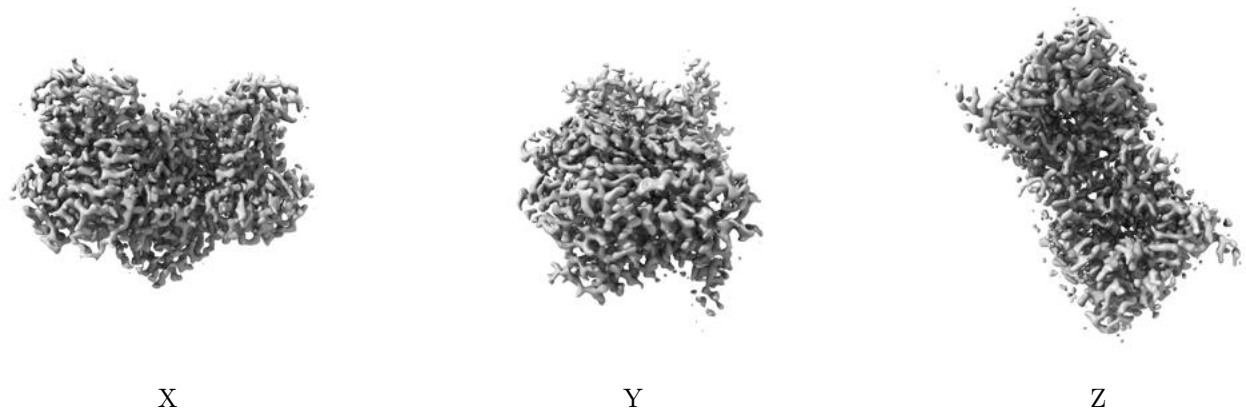


Z

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.

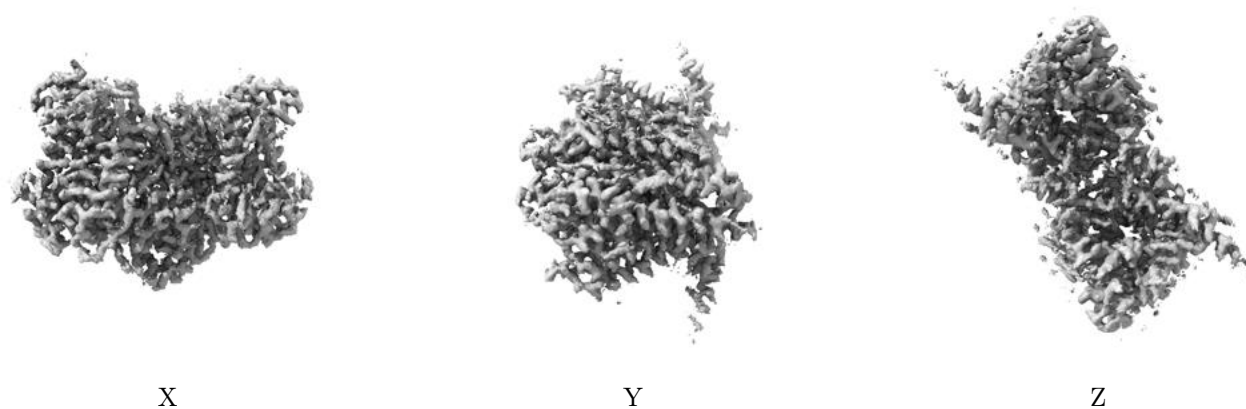
6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.0155. 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.

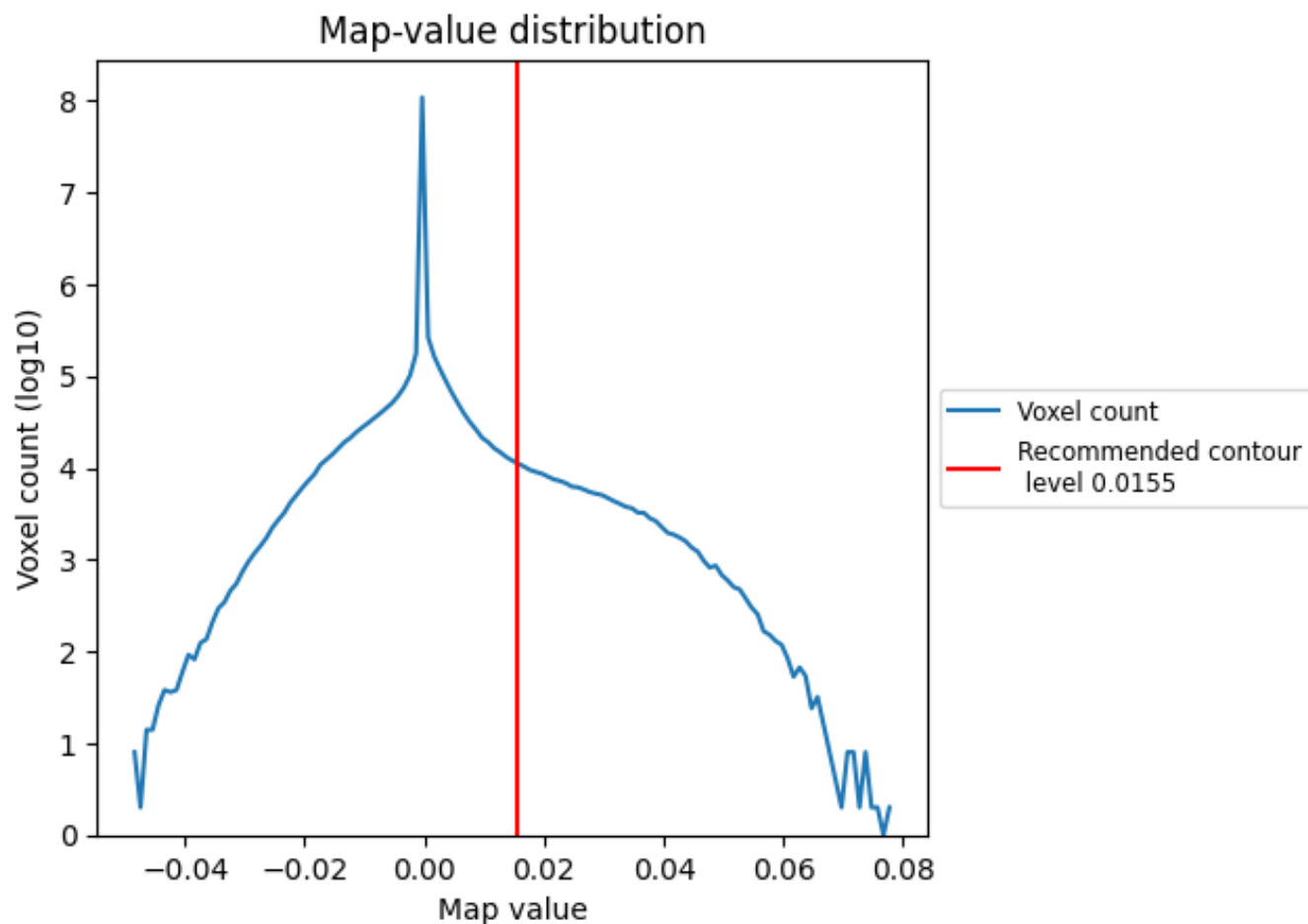
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

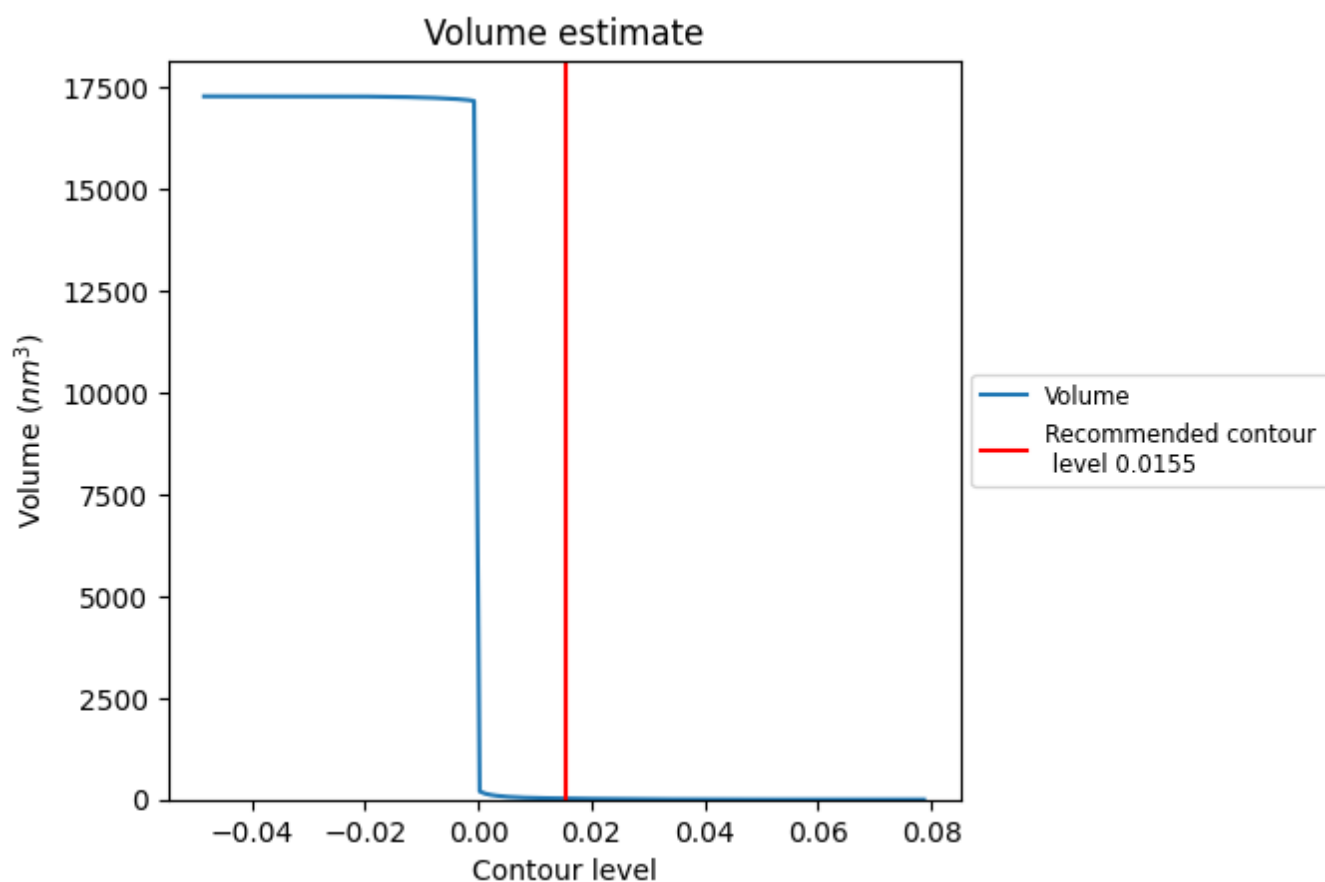
This section contains the results of statistical analysis of the map.

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.

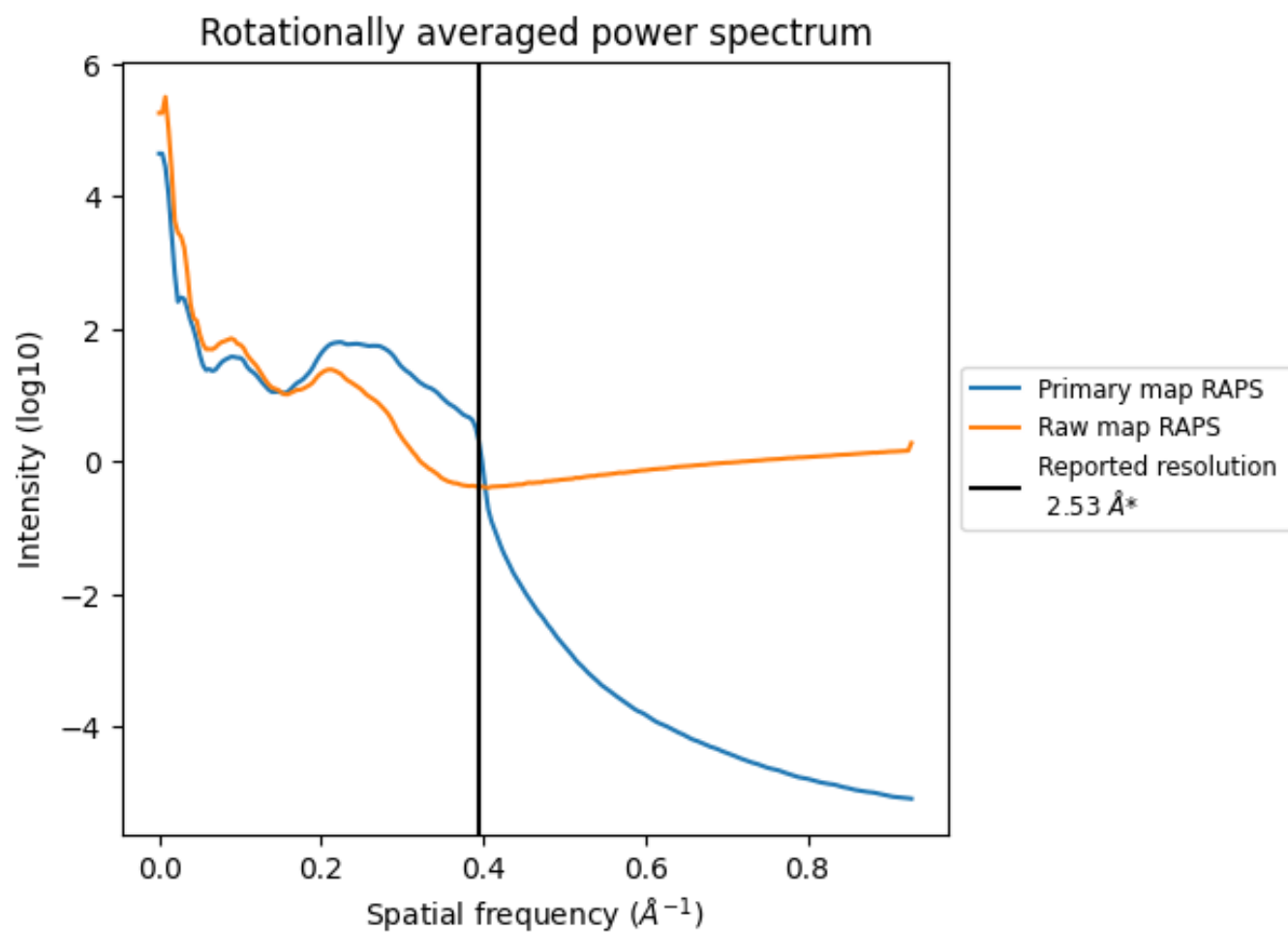
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 26 nm^3 ; this corresponds to an approximate mass of 23 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 ⓘ

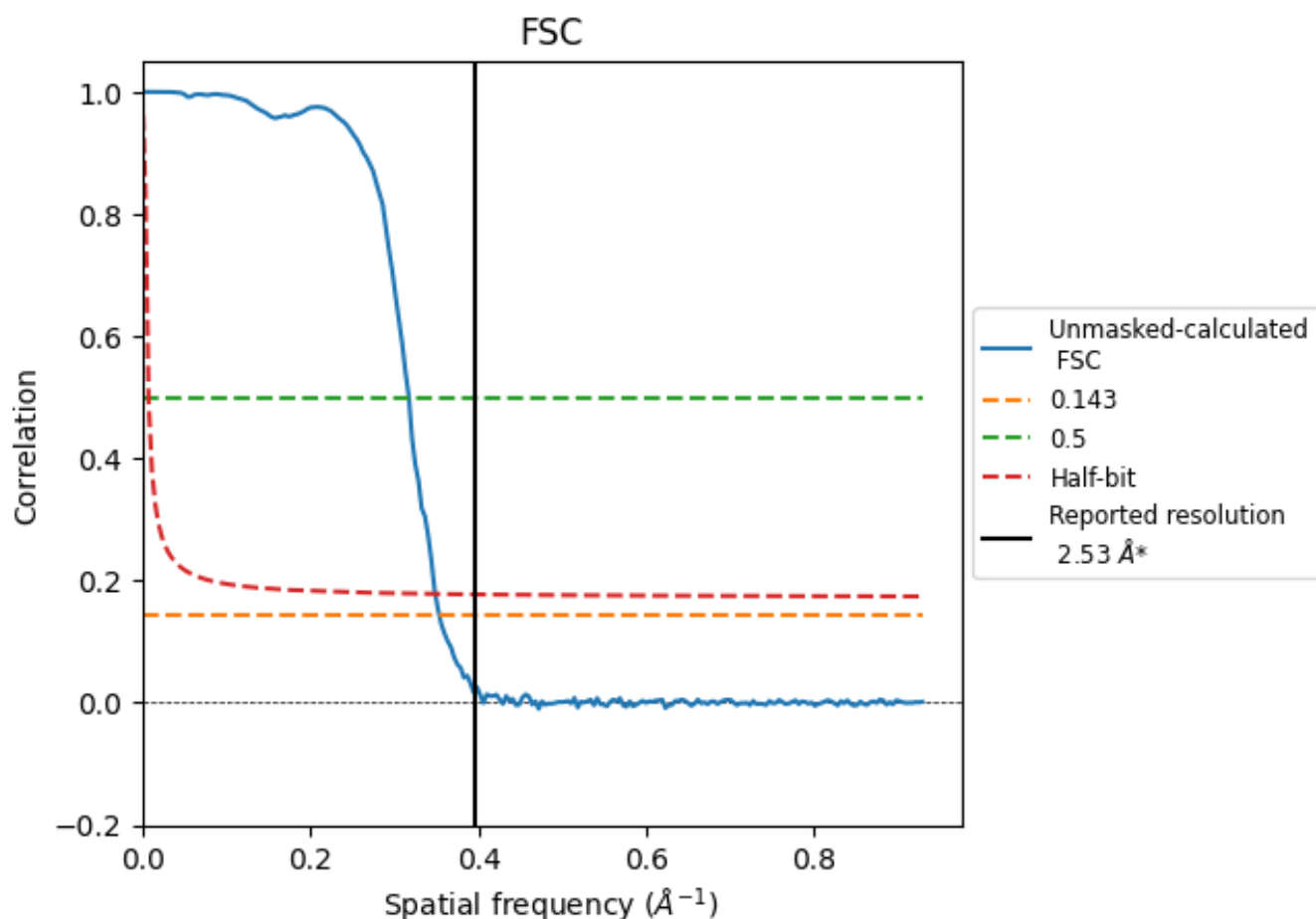


*Reported resolution corresponds to spatial frequency of $0.395 \text{ \AA}^{-1}$

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 0.395 $\text{\AA}^{-1}$

8.2 Resolution estimates [i](#)

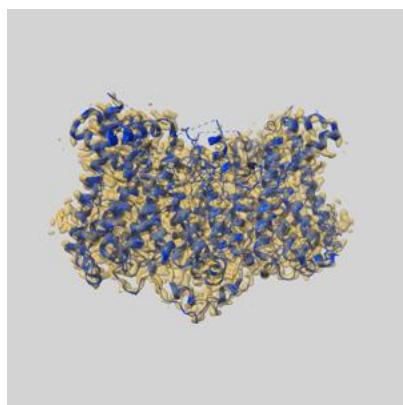
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	2.53	-	-
Author-provided FSC curve	-	-	-
Unmasked-calculated*	2.83	3.15	2.87

*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 2.83 differs from the reported value 2.53 by more than 10 %

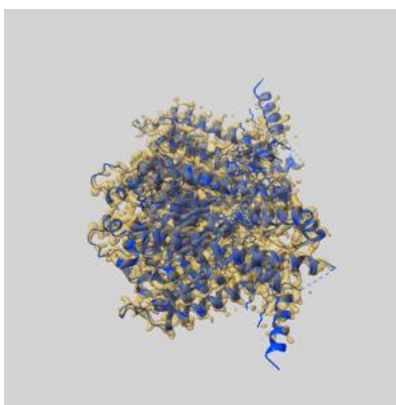
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-36918 and PDB model 8K66. Per-residue inclusion information can be found in section [3](#) on page [8](#).

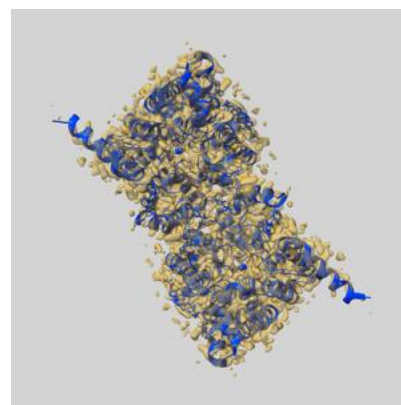
9.1 Map-model overlay [i](#)



X



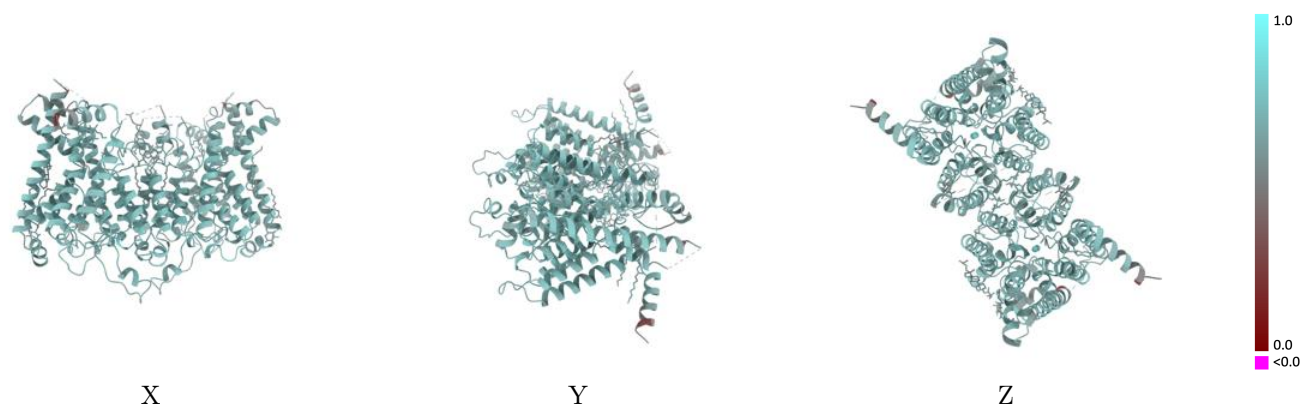
Y



Z

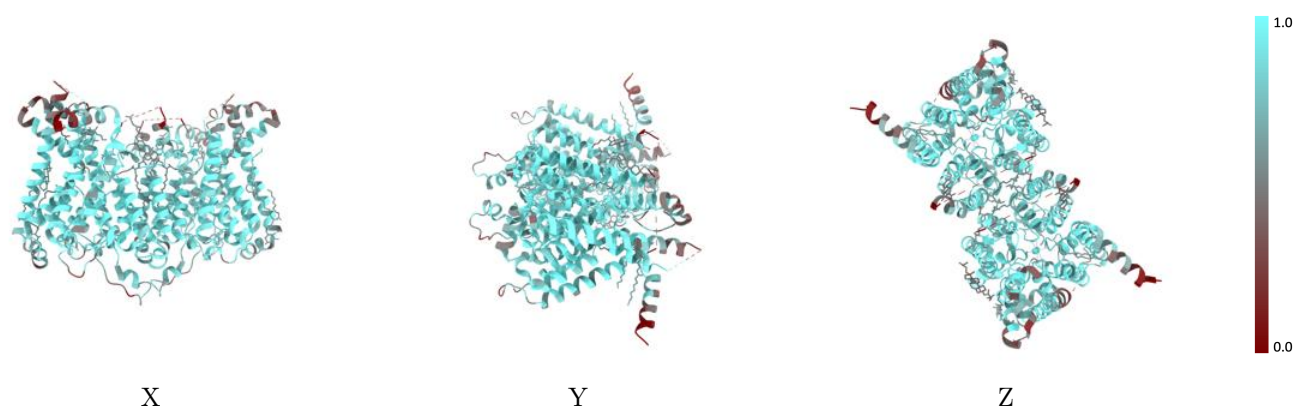
The images above show the 3D surface view of the map at the recommended contour level 0.0155 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



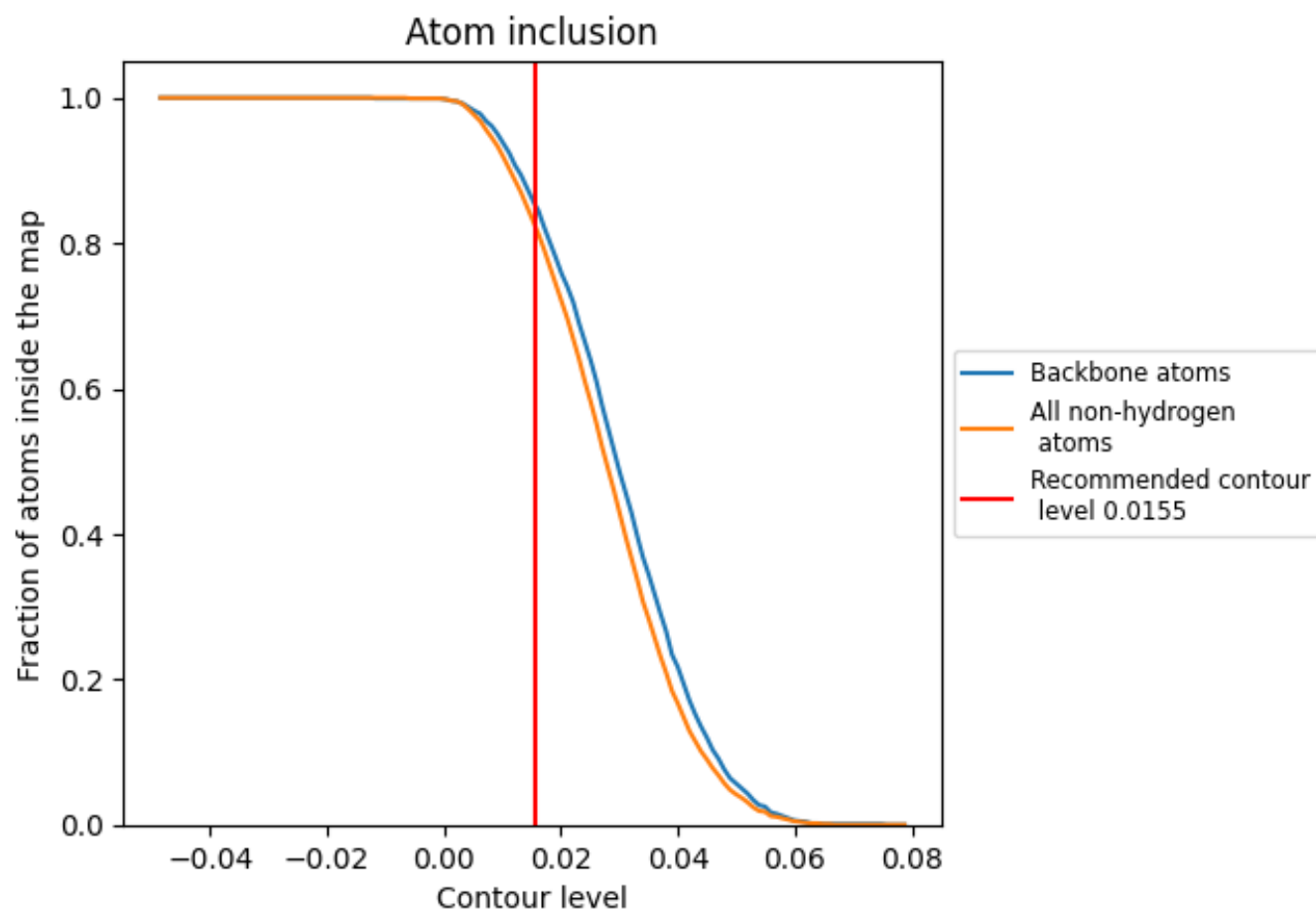
The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.0155).

9.4 Atom inclusion [i](#)



At the recommended contour level, 85% of all backbone atoms, 82% 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 (0.0155) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.8250	0.6600
A	0.8270	0.6590
B	0.8270	0.6600

