



Full wwPDB EM Validation Report ⓘ

Jul 7, 2024 – 05:38 am BST

PDB ID : 7P1K
EMDB ID : EMD-13163
Title : Cryo EM structure of bison NHA2 in nano disc structure
Authors : Matsuoka, R.; Fudim, R.; Jung, S.; Drew, D.
Deposited on : 2021-07-01
Resolution : 3.64 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.dev92
Mogul : 1.8.4, CSD as541be (2020)
MolProbity : 4.02b-467
buster-report : 1.1.7 (2018)
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.37.1

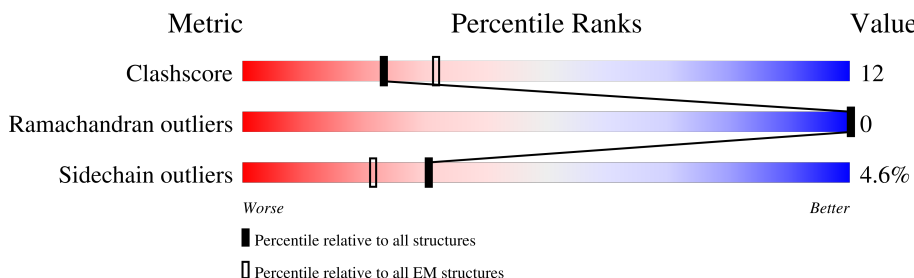
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 3.64 Å.

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



Metric	Whole archive (#Entries)	EM structures (#Entries)
Clashscore	158937	4297
Ramachandran outliers	154571	4023
Sidechain outliers	154315	3826

The table below summarises the geometric issues observed across the polymeric chains and their fit to the map. The red, orange, yellow and green segments of the bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. 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	535	<div> <div>34%</div> <div>60%</div> <div>19%</div> <div>19%</div> </div>
1	B	535	<div> <div>19%</div> <div>59%</div> <div>21%</div> <div>19%</div> </div>

2 Entry composition [i](#)

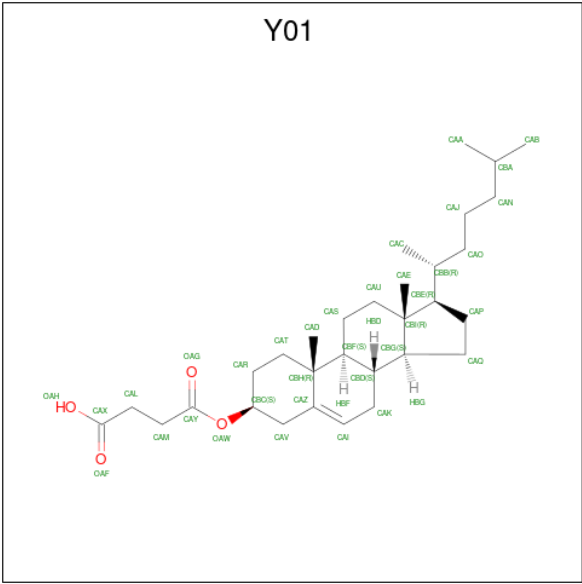
There are 3 unique types of molecules in this entry. The entry contains 7404 atoms, of which 512 are hydrogens and 0 are deuteriums.

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 mitochondrial sodium/hydrogen exchanger 9B2.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	B	433	Total	C	N	O	S	0	0
			3243	2161	516	547	19		
1	A	433	Total	C	N	O	S	0	0
			3243	2161	516	547	19		

- Molecule 2 is CHOLESTEROL HEMISUCCINATE (three-letter code: Y01) (formula: C₃₁H₅₀O₄) (labeled as "Ligand of Interest" by depositor).



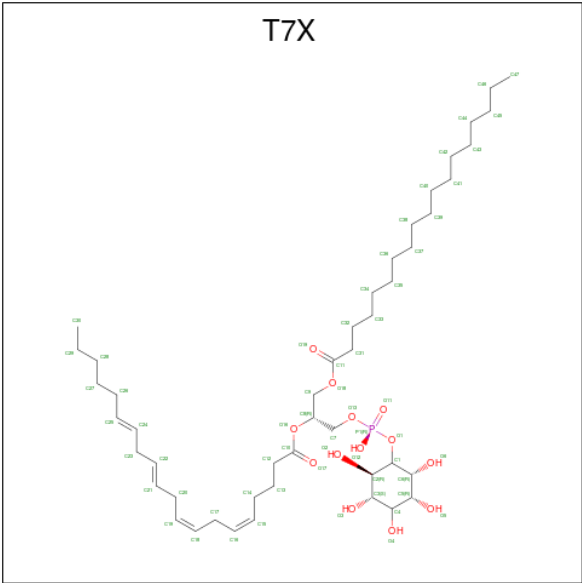
Mol	Chain	Residues	Atoms				AltConf
2	B	1	Total	C	H	O	0
			84	31	49	4	
2	B	1	Total	C	H	O	0
			84	31	49	4	
2	B	1	Total	C	H	O	0
			84	31	49	4	
2	B	1	Total	C	H	O	0
			84	31	49	4	

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Mol	Chain	Residues	Atoms				AltConf
2	A	1	Total	C	H	O	0
			84	31	49	4	
2	A	1	Total	C	H	O	0
			84	31	49	4	
2	A	1	Total	C	H	O	0
			84	31	49	4	
2	A	1	Total	C	H	O	0
			84	31	49	4	

- Molecule 3 is Phosphatidylinositol (three-letter code: T7X) (formula: C₄₇H₈₃O₁₃P) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms					AltConf
3	B	1	Total	C	H	O	P	0
			27	7	10	9	1	
3	B	1	Total	C	H	O	P	0
			96	32	50	13	1	
3	A	1	Total	C	H	O	P	0
			27	7	10	9	1	
3	A	1	Total	C	H	O	P	0
			96	32	50	13	1	



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	362655	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 ($e^-/\text{\AA}^2$)	80	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	Not provided	
Image detector	GATAN K2 QUANTUM (4k x 4k)	Depositor
Maximum map value	0.271	Depositor
Minimum map value	-0.196	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.005	Depositor
Recommended contour level	0.035	Depositor
Map size (Å)	259.776, 259.776, 259.776	wwPDB
Map dimensions	256, 256, 256	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.01475, 1.01475, 1.01475	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: T7X, Y01

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	0/3313	0.41	0/4511
1	B	0.26	0/3313	0.42	0/4511
All	All	0.25	0/6626	0.42	0/9022

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	3243	0	3450	86	0
1	B	3243	0	3450	85	0
2	A	140	196	196	10	0
2	B	140	196	196	8	0
3	A	63	60	0	1	0
3	B	63	60	0	2	0
All	All	6892	512	7292	175	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 12.

All (175) 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:B:175:LEU:HD21	1:B:398:LEU:HD21	1.38	1.03
1:B:175:LEU:CD2	1:B:398:LEU:HD21	1.93	0.97
1:B:221:LEU:HD12	1:B:423:THR:HG22	1.50	0.93
1:A:175:LEU:HD21	1:A:398:LEU:HD21	1.50	0.92
1:A:385:GLU:N	1:A:385:GLU:OE1	2.02	0.91
1:A:157:ASN:HA	1:A:408:LEU:HD13	1.53	0.90
1:A:432:ILE:HD11	1:A:457:LEU:HD21	1.57	0.86
1:A:205:ARG:HH12	1:A:441:PHE:HB2	1.41	0.85
1:B:156:ARG:HG3	1:B:408:LEU:HB2	1.63	0.80
1:A:319:LEU:HD21	1:A:345:LEU:HD22	1.62	0.78
1:A:507:LEU:HD21	1:A:511:LEU:HD22	1.69	0.75
1:B:444:PHE:HB3	1:B:448:GLU:HB2	1.68	0.75
1:A:153:PHE:O	1:A:157:ASN:ND2	2.20	0.74
1:A:232:TRP:CZ2	1:A:482:LEU:HD22	2.24	0.73
1:A:82:LEU:HD23	1:A:85:ARG:HH21	1.55	0.72
1:A:444:PHE:HB3	1:A:448:GLU:HB2	1.69	0.72
1:B:444:PHE:O	1:B:449:LYS:NZ	2.24	0.71
1:B:153:PHE:O	1:B:157:ASN:ND2	2.23	0.71
1:B:213:ILE:HG21	1:B:434:VAL:HG11	1.73	0.71
1:B:166:GLN:O	1:B:167:ILE:HG13	1.92	0.70
1:A:323:ILE:HG23	1:A:341:LEU:HD23	1.74	0.70
1:B:421:VAL:HG22	1:B:495:LEU:HD21	1.74	0.69
1:A:240:LEU:O	1:A:459:LYS:HD3	1.93	0.69
1:B:337:LYS:HD3	1:A:88:THR:HG21	1.75	0.69
1:A:221:LEU:HD12	1:A:423:THR:HG22	1.75	0.68
1:B:323:ILE:HG23	1:B:341:LEU:HD23	1.75	0.68
1:B:136:LEU:H	1:B:136:LEU:HD23	1.58	0.67
1:B:242:ALA:O	1:B:459:LYS:HG3	1.95	0.67
1:A:213:ILE:HG21	1:A:434:VAL:HG11	1.76	0.67
1:A:471:LEU:HD22	1:A:490:LEU:CD1	2.24	0.67
1:A:228:LEU:HG	1:A:485:TYR:HD2	1.59	0.66
1:B:88:THR:HG21	1:A:337:LYS:HD3	1.79	0.65
1:A:156:ARG:HG3	1:A:408:LEU:HB2	1.78	0.64
1:B:432:ILE:HD11	1:B:457:LEU:HD21	1.80	0.64
1:B:142:LEU:HD12	1:B:143:PRO:HD2	1.79	0.64
1:A:136:LEU:H	1:A:136:LEU:HD23	1.63	0.64
1:B:161:ILE:HG23	1:B:164:ASN:HD21	1.63	0.64
1:B:205:ARG:HH12	1:B:441:PHE:HB2	1.63	0.64
1:B:496:SER:O	1:B:500:THR:HG22	1.97	0.63
1:A:507:LEU:CD2	1:A:511:LEU:HD22	2.28	0.63
1:A:382:THR:HG23	1:A:383:ASP:OD1	1.99	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:189:LEU:HG	1:A:385:GLU:OE2	1.99	0.62
1:A:471:LEU:HD22	1:A:490:LEU:HD11	1.83	0.61
1:B:283:THR:HG21	2:B:1201:Y01:HAA1	1.81	0.61
1:B:239:VAL:O	1:B:463:GLN:NE2	2.30	0.60
1:B:409:ILE:O	1:B:413:ARG:NE	2.35	0.60
1:A:175:LEU:CD2	1:A:398:LEU:HD21	2.28	0.59
1:A:248:VAL:O	1:A:252:MET:HG2	2.02	0.59
1:A:231:GLN:NE2	2:A:804:Y01:OAW	2.37	0.58
1:A:142:LEU:HD12	1:A:143:PRO:HD2	1.83	0.58
1:A:496:SER:O	1:A:500:THR:HG22	2.04	0.58
1:B:326:PHE:HB2	1:B:327:PRO:HD3	1.86	0.57
1:A:468:SER:HA	1:A:490:LEU:HD21	1.86	0.57
1:A:217:THR:HG21	1:A:430:ILE:HG21	1.87	0.57
1:A:459:LYS:HG2	1:A:463:GLN:OE1	2.05	0.57
1:B:332:ASP:O	1:B:333:ASN:ND2	2.38	0.57
1:A:82:LEU:HD23	1:A:85:ARG:NH2	2.20	0.56
1:A:260:TYR:OH	1:A:513:PRO:HG3	2.04	0.56
1:B:214:GLU:OE1	1:B:431:ARG:NE	2.40	0.55
1:A:139:LEU:HB2	1:A:140:PRO:HD3	1.89	0.54
1:A:168:LYS:HB3	1:A:171:TRP:CD1	2.43	0.54
1:B:225:LEU:HD12	1:B:419:LEU:HD22	1.90	0.54
1:B:252:MET:CE	1:B:270:LEU:HD13	2.37	0.54
1:B:187:ALA:HB2	1:B:249:VAL:HG11	1.89	0.54
1:B:236:LEU:HD11	1:B:492:VAL:HG11	1.90	0.54
1:A:236:LEU:HD11	1:A:492:VAL:HG11	1.90	0.53
1:A:471:LEU:HD22	1:A:490:LEU:HD12	1.89	0.53
1:A:232:TRP:HZ2	1:A:482:LEU:HD22	1.73	0.53
1:B:248:VAL:O	1:B:252:MET:HG2	2.08	0.53
1:A:262:VAL:HG13	1:A:263:GLU:H	1.74	0.53
1:B:157:ASN:HA	1:B:408:LEU:HD13	1.90	0.53
1:A:326:PHE:HB2	1:A:327:PRO:HD3	1.91	0.53
1:B:164:ASN:HD22	2:B:1206:Y01:HAS1	1.74	0.53
1:A:156:ARG:NH1	1:A:405:ALA:O	2.38	0.53
1:A:396:GLN:HB3	1:A:397:PRO:HD3	1.90	0.53
1:B:175:LEU:CG	1:B:398:LEU:HD21	2.37	0.52
1:A:214:GLU:OE1	1:A:431:ARG:NH2	2.38	0.52
1:A:228:LEU:HG	1:A:485:TYR:CD2	2.44	0.52
1:A:386:LYS:HB3	1:A:386:LYS:NZ	2.24	0.52
1:B:139:LEU:HB2	1:B:140:PRO:HD3	1.91	0.52
2:A:801:Y01:HAC1	2:A:801:Y01:HAU2	1.91	0.52
1:B:262:VAL:HG13	1:B:263:GLU:H	1.75	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:332:ASP:O	1:A:333:ASN:ND2	2.43	0.51
2:B:1204:Y01:HAC1	2:B:1204:Y01:HAU2	1.92	0.51
1:A:193:SER:OG	1:A:375:ARG:HD2	2.11	0.51
1:B:242:ALA:HB1	1:B:462:VAL:HG11	1.93	0.51
1:B:411:ALA:C	1:B:412:LEU:HD13	2.31	0.50
1:B:205:ARG:HH12	1:B:441:PHE:CB	2.24	0.50
1:B:396:GLN:HB3	1:B:397:PRO:HD3	1.94	0.50
1:A:187:ALA:HA	1:A:271:MET:CE	2.41	0.50
1:B:445:ASN:O	1:B:449:LYS:NZ	2.44	0.50
1:A:242:ALA:O	1:A:459:LYS:HG3	2.12	0.50
1:B:490:LEU:HD22	1:B:494:PHE:HE2	1.76	0.49
1:B:240:LEU:HD11	1:B:424:LEU:HD13	1.94	0.49
2:A:803:Y01:HAU2	2:A:803:Y01:HAC1	1.95	0.49
1:B:143:PRO:HD3	1:B:506:LEU:HD12	1.94	0.49
1:B:205:ARG:NH2	1:B:438:MET:O	2.45	0.49
1:B:244:SER:HB2	1:B:460:ALA:H	1.77	0.49
1:A:412:LEU:H	1:A:412:LEU:HD22	1.77	0.49
1:B:191:LEU:HD11	1:B:272:ALA:HB2	1.94	0.49
1:B:275:SER:OG	1:B:367:LEU:HD22	2.12	0.48
2:A:804:Y01:HAC1	2:A:804:Y01:HAU2	1.96	0.48
1:A:187:ALA:HA	1:A:271:MET:HE1	1.95	0.48
1:A:116:GLY:HA2	1:A:165:ILE:HG13	1.96	0.48
1:A:444:PHE:HD1	1:A:448:GLU:HB3	1.79	0.48
1:A:164:ASN:HD22	2:A:803:Y01:HAT2	1.79	0.48
1:A:412:LEU:HD22	1:A:412:LEU:N	2.29	0.47
1:B:88:THR:CG2	1:A:337:LYS:HD3	2.44	0.47
1:B:434:VAL:O	1:B:438:MET:HG2	2.13	0.47
1:B:278:ASP:O	1:B:282:ILE:HG12	2.15	0.47
1:A:253:LEU:HD21	1:A:271:MET:HE3	1.96	0.47
1:B:217:THR:HG21	1:B:430:ILE:HG21	1.97	0.47
1:B:459:LYS:HG2	1:B:463:GLN:CG	2.44	0.47
1:B:399:LEU:O	1:B:403:ILE:HG12	2.15	0.47
1:A:221:LEU:HD13	1:A:225:LEU:HD23	1.96	0.47
1:B:338:ARG:O	1:B:342:VAL:HG22	2.15	0.47
2:B:1201:Y01:HAC1	2:B:1201:Y01:HAU2	1.97	0.47
2:B:1206:Y01:HAC1	2:B:1206:Y01:HAU2	1.96	0.47
1:B:377:TRP:O	1:B:381:LYS:HB2	2.14	0.46
1:A:111:GLY:N	1:A:164:ASN:O	2.46	0.46
1:A:411:ALA:C	1:A:412:LEU:HD13	2.35	0.46
1:B:157:ASN:OD1	1:B:411:ALA:HB2	2.14	0.46
1:B:490:LEU:HD22	1:B:494:PHE:CE2	2.51	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:319:LEU:HD21	1:B:345:LEU:HD22	1.97	0.46
2:A:801:Y01:OAW	2:A:801:Y01:HAD1	2.16	0.46
1:A:466:ILE:HA	1:A:469:VAL:HG23	1.98	0.46
1:A:94:ILE:HD13	2:A:802:Y01:HAQ1	1.97	0.45
1:B:329:SER:HA	1:B:334:LEU:HD22	1.98	0.45
2:B:1205:Y01:HAC1	2:B:1205:Y01:HAU2	1.98	0.45
1:B:507:LEU:CD2	1:B:511:LEU:HD22	2.46	0.45
1:B:348:LEU:HD21	2:A:801:Y01:HAJ2	1.99	0.45
1:A:331:GLN:NE2	1:A:331:GLN:H	2.14	0.45
1:B:331:GLN:HE22	1:A:84:ALA:CB	2.28	0.45
1:B:412:LEU:HD22	1:B:412:LEU:H	1.82	0.45
1:A:479:GLU:OE1	1:A:482:LEU:HD12	2.16	0.45
2:A:802:Y01:HAC1	2:A:802:Y01:HAU2	1.99	0.44
1:B:412:LEU:HD22	1:B:412:LEU:N	2.31	0.44
1:A:244:SER:CB	1:A:460:ALA:H	2.31	0.44
1:A:244:SER:HB2	1:A:460:ALA:H	1.82	0.44
1:B:166:GLN:C	1:B:167:ILE:HG13	2.38	0.44
1:B:90:VAL:O	1:B:94:ILE:HG22	2.18	0.43
1:B:174:ALA:CB	3:B:1203:T7X:O2	2.66	0.43
1:B:161:ILE:HA	1:B:164:ASN:OD1	2.17	0.43
1:A:338:ARG:HB3	1:A:377:TRP:CH2	2.54	0.43
1:B:275:SER:CB	1:B:367:LEU:HD22	2.48	0.43
1:B:221:LEU:HD22	1:B:221:LEU:HA	1.91	0.43
1:A:205:ARG:NH2	1:A:438:MET:O	2.52	0.43
1:A:468:SER:CA	1:A:490:LEU:HD21	2.49	0.43
1:A:174:ALA:HB3	3:A:806:T7X:O2	2.20	0.42
1:B:362:GLY:O	1:B:366:THR:HG22	2.20	0.42
1:B:235:MET:SD	1:B:289:LEU:HD23	2.59	0.42
1:B:337:LYS:HD3	1:A:88:THR:CG2	2.45	0.42
1:A:434:VAL:O	1:A:438:MET:HG2	2.20	0.42
1:B:164:ASN:OD1	1:B:165:ILE:HG22	2.20	0.42
1:A:137:PRO:HB2	1:A:140:PRO:HD2	2.02	0.42
1:A:170:LYS:HG2	1:A:170:LYS:O	2.20	0.42
1:B:97:TRP:CZ2	2:B:1205:Y01:HAD3	2.55	0.41
1:B:168:LYS:HG3	1:B:169:HIS:N	2.35	0.41
1:B:170:LYS:O	1:B:170:LYS:HG2	2.20	0.41
1:A:168:LYS:HB3	1:A:171:TRP:HD1	1.83	0.41
1:A:185:VAL:HG23	1:A:370:ALA:HB2	2.01	0.41
1:B:283:THR:HG21	2:B:1201:Y01:CAA	2.46	0.41
1:A:168:LYS:HG3	1:A:169:HIS:N	2.35	0.41
1:A:125:ILE:HD11	1:A:397:PRO:HG2	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:90:VAL:O	1:A:94:ILE:HG22	2.20	0.41
1:A:94:ILE:HD13	2:A:802:Y01:CAQ	2.51	0.41
1:A:432:ILE:HD11	1:A:457:LEU:CD2	2.40	0.41
1:B:180:LEU:O	1:B:183:ILE:HG22	2.19	0.41
1:B:136:LEU:O	1:B:136:LEU:HG	2.19	0.41
1:B:161:ILE:HG23	1:B:164:ASN:ND2	2.32	0.41
1:A:481:GLN:HG3	1:A:485:TYR:HE1	1.85	0.41
1:B:407:VAL:HG12	1:B:410:THR:HG23	2.03	0.41
1:B:228:LEU:HG	1:B:485:TYR:HD2	1.86	0.40
1:A:125:ILE:CD1	1:A:397:PRO:HG2	2.52	0.40
1:B:175:LEU:HD13	3:B:1203:T7X:O12	2.21	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	429/535 (80%)	411 (96%)	18 (4%)	0	100	100
1	B	429/535 (80%)	411 (96%)	18 (4%)	0	100	100
All	All	858/1070 (80%)	822 (96%)	36 (4%)	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	347/436 (80%)	331 (95%)	16 (5%)	27	60
1	B	347/436 (80%)	331 (95%)	16 (5%)	27	60
All	All	694/872 (80%)	662 (95%)	32 (5%)	31	60

All (32) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	113	ASN
1	B	165	ILE
1	B	168	LYS
1	B	221	LEU
1	B	262	VAL
1	B	280	LEU
1	B	300	PHE
1	B	356	PHE
1	B	358	PHE
1	B	372	LEU
1	B	407	VAL
1	B	412	LEU
1	B	449	LYS
1	B	456	TRP
1	B	507	LEU
1	B	516	LEU
1	A	150	LEU
1	A	168	LYS
1	A	221	LEU
1	A	262	VAL
1	A	280	LEU
1	A	300	PHE
1	A	331	GLN
1	A	356	PHE
1	A	372	LEU
1	A	383	ASP
1	A	385	GLU
1	A	407	VAL
1	A	412	LEU
1	A	459	LYS
1	A	511	LEU
1	A	516	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (4) such sidechains are listed below:

Mol	Chain	Res	Type
1	B	113	ASN
1	B	333	ASN
1	A	331	GLN
1	A	333	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 monosaccharides in this entry.

5.6 Ligand geometry ⓘ

12 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
2	Y01	A	804	-	38,38,38	2.50	15 (39%)	57,57,57	1.87	16 (28%)
2	Y01	A	803	-	38,38,38	2.47	15 (39%)	57,57,57	1.73	14 (24%)
2	Y01	B	1204	-	38,38,38	2.54	15 (39%)	57,57,57	1.62	9 (15%)
3	T7X	B	1203	-	46,46,61	1.49	8 (17%)	56,58,73	1.11	3 (5%)
2	Y01	B	1205	-	38,38,38	2.46	15 (39%)	57,57,57	1.65	13 (22%)
3	T7X	A	805	-	17,17,61	0.74	0	25,26,73	0.80	0
2	Y01	A	802	-	38,38,38	2.45	15 (39%)	57,57,57	1.65	11 (19%)
2	Y01	B	1201	-	38,38,38	2.46	16 (42%)	57,57,57	1.91	15 (26%)
3	T7X	A	806	-	46,46,61	1.49	8 (17%)	56,58,73	1.15	3 (5%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	Y01	A	801	-	38,38,38	2.54	15 (39%)	57,57,57	1.59	11 (19%)
2	Y01	B	1206	-	38,38,38	2.46	15 (39%)	57,57,57	1.72	13 (22%)
3	T7X	B	1202	-	17,17,61	0.75	0	25,26,73	0.81	0

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	Y01	A	804	-	-	9/19/77/77	0/4/4/4
2	Y01	A	803	-	-	7/19/77/77	0/4/4/4
2	Y01	B	1204	-	-	7/19/77/77	0/4/4/4
3	T7X	B	1203	-	-	20/41/65/80	0/1/1/1
2	Y01	B	1205	-	-	4/19/77/77	0/4/4/4
3	T7X	A	805	-	-	1/8/32/80	0/1/1/1
2	Y01	A	802	-	-	4/19/77/77	0/4/4/4
2	Y01	B	1201	-	-	9/19/77/77	0/4/4/4
3	T7X	A	806	-	-	20/41/65/80	0/1/1/1
2	Y01	A	801	-	-	8/19/77/77	0/4/4/4
2	Y01	B	1206	-	-	4/19/77/77	0/4/4/4
3	T7X	B	1202	-	-	7/8/32/80	0/1/1/1

All (137) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	1204	Y01	CAK-CBD	5.80	1.63	1.53
2	A	804	Y01	CAK-CBD	5.72	1.62	1.53
2	A	801	Y01	CAK-CBD	5.71	1.62	1.53
2	B	1201	Y01	CAK-CBD	5.56	1.62	1.53
2	A	802	Y01	CAK-CBD	5.22	1.62	1.53
2	A	803	Y01	CAK-CBD	5.21	1.62	1.53
2	B	1206	Y01	CAK-CBD	5.19	1.61	1.53
2	B	1205	Y01	CAK-CBD	5.16	1.61	1.53
2	A	803	Y01	CBI-CBE	-4.87	1.45	1.55
2	A	801	Y01	CBI-CBE	-4.86	1.45	1.55
2	B	1206	Y01	CBI-CBE	-4.84	1.45	1.55
2	A	802	Y01	CBI-CBE	-4.83	1.45	1.55
2	B	1204	Y01	CBI-CBE	-4.83	1.45	1.55

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	1205	Y01	CBI-CBE	-4.83	1.45	1.55
2	A	804	Y01	CBI-CBE	-4.74	1.46	1.55
2	B	1201	Y01	CBI-CBE	-4.73	1.46	1.55
2	B	1204	Y01	CAK-CAI	4.49	1.59	1.50
2	A	801	Y01	CAQ-CAP	4.47	1.66	1.54
2	B	1204	Y01	CAQ-CAP	4.45	1.66	1.54
2	A	801	Y01	CAK-CAI	4.45	1.59	1.50
2	A	804	Y01	CAQ-CAP	4.45	1.66	1.54
2	A	802	Y01	CAQ-CAP	4.45	1.66	1.54
2	B	1205	Y01	CAQ-CAP	4.44	1.66	1.54
2	A	803	Y01	CAQ-CAP	4.44	1.66	1.54
2	B	1206	Y01	CAQ-CAP	4.40	1.66	1.54
2	B	1201	Y01	CAQ-CAP	4.37	1.66	1.54
2	A	804	Y01	CAK-CAI	4.33	1.59	1.50
2	B	1206	Y01	CAK-CAI	4.28	1.59	1.50
2	A	803	Y01	CAK-CAI	4.26	1.59	1.50
2	B	1201	Y01	CAK-CAI	4.18	1.59	1.50
2	B	1204	Y01	CBH-CAZ	-4.13	1.44	1.52
2	A	802	Y01	CAK-CAI	4.10	1.59	1.50
2	A	801	Y01	CBH-CAZ	-4.06	1.44	1.52
2	B	1205	Y01	CAK-CAI	4.06	1.58	1.50
2	A	804	Y01	OAW-CAY	3.97	1.45	1.34
2	B	1201	Y01	OAW-CAY	3.95	1.45	1.34
2	A	803	Y01	CAV-CAZ	3.91	1.60	1.51
2	A	804	Y01	CAV-CAZ	3.90	1.60	1.51
2	B	1206	Y01	CAV-CAZ	3.88	1.60	1.51
2	B	1205	Y01	CAV-CAZ	3.87	1.60	1.51
2	B	1206	Y01	OAW-CAY	3.87	1.45	1.34
2	A	801	Y01	OAW-CAY	3.86	1.45	1.34
2	B	1204	Y01	OAW-CAY	3.84	1.45	1.34
2	B	1205	Y01	OAW-CAY	3.82	1.45	1.34
2	A	802	Y01	OAW-CAY	3.82	1.45	1.34
2	A	803	Y01	OAW-CAY	3.82	1.45	1.34
2	A	802	Y01	CAV-CAZ	3.80	1.59	1.51
2	A	801	Y01	CAV-CAZ	3.75	1.59	1.51
2	B	1201	Y01	CBB-CBE	3.74	1.60	1.54
3	B	1203	T7X	C16-C15	3.71	1.53	1.31
2	B	1204	Y01	CAV-CAZ	3.71	1.59	1.51
3	B	1203	T7X	C19-C18	3.70	1.53	1.31
3	A	806	T7X	C22-C21	3.70	1.53	1.31
3	A	806	T7X	C25-C24	3.70	1.53	1.31
3	B	1203	T7X	C22-C21	3.69	1.53	1.31

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	1203	T7X	C25-C24	3.69	1.53	1.31
3	A	806	T7X	C16-C15	3.69	1.53	1.31
3	A	806	T7X	C19-C18	3.68	1.53	1.31
2	A	804	Y01	CBB-CBE	3.67	1.60	1.54
2	B	1201	Y01	CAV-CAZ	3.67	1.59	1.51
2	B	1204	Y01	CBB-CBE	3.60	1.60	1.54
2	A	801	Y01	CBB-CBE	3.60	1.60	1.54
2	A	802	Y01	CBB-CBE	3.60	1.60	1.54
2	B	1206	Y01	CBB-CBE	3.58	1.60	1.54
2	B	1205	Y01	CBB-CBE	3.58	1.60	1.54
2	A	803	Y01	CBB-CBE	3.55	1.60	1.54
2	B	1205	Y01	CBH-CAZ	-3.52	1.45	1.52
2	B	1201	Y01	CBH-CAZ	-3.46	1.46	1.52
2	A	803	Y01	CBH-CAZ	-3.45	1.46	1.52
2	A	804	Y01	CBH-CAZ	-3.44	1.46	1.52
2	B	1206	Y01	CBH-CAZ	-3.44	1.46	1.52
2	A	802	Y01	CBH-CAZ	-3.39	1.46	1.52
2	A	803	Y01	CAD-CBH	3.36	1.60	1.54
2	B	1206	Y01	CAD-CBH	3.35	1.60	1.54
2	A	801	Y01	CAD-CBH	3.32	1.60	1.54
2	B	1205	Y01	CAD-CBH	3.30	1.60	1.54
2	B	1201	Y01	CAD-CBH	3.28	1.60	1.54
2	A	804	Y01	CAD-CBH	3.27	1.60	1.54
2	A	802	Y01	CAD-CBH	3.26	1.60	1.54
2	B	1204	Y01	CAD-CBH	3.26	1.60	1.54
2	B	1204	Y01	CAS-CBF	-3.20	1.48	1.53
2	A	801	Y01	CAS-CBF	-3.16	1.48	1.53
2	B	1205	Y01	OAW-CBC	-3.06	1.38	1.46
2	A	802	Y01	OAW-CBC	-3.05	1.39	1.46
2	A	803	Y01	OAW-CBC	-3.05	1.39	1.46
2	B	1205	Y01	CAS-CBF	-2.98	1.48	1.53
2	A	801	Y01	OAW-CBC	-2.98	1.39	1.46
2	B	1206	Y01	OAW-CBC	-2.98	1.39	1.46
2	B	1204	Y01	OAW-CBC	-2.97	1.39	1.46
2	A	804	Y01	CAS-CBF	-2.93	1.48	1.53
2	A	802	Y01	CBD-CBG	-2.91	1.48	1.53
2	B	1204	Y01	CAU-CBI	2.90	1.59	1.54
2	B	1201	Y01	CBD-CBG	-2.89	1.48	1.53
2	A	801	Y01	CAU-CBI	2.89	1.59	1.54
2	A	804	Y01	CAU-CBI	2.89	1.59	1.54
2	A	802	Y01	CAU-CBI	2.88	1.59	1.54
2	B	1205	Y01	CBD-CBG	-2.88	1.48	1.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	1205	Y01	CAU-CBI	2.85	1.59	1.54
2	A	803	Y01	CAS-CBF	-2.85	1.49	1.53
2	A	803	Y01	CBD-CBG	-2.85	1.48	1.53
2	B	1206	Y01	CBD-CBG	-2.83	1.48	1.53
2	A	802	Y01	CAS-CBF	-2.83	1.49	1.53
2	A	801	Y01	CBD-CBG	-2.82	1.48	1.53
2	B	1206	Y01	CAS-CBF	-2.81	1.49	1.53
2	B	1201	Y01	OAW-CBC	-2.79	1.39	1.46
2	B	1201	Y01	CAU-CBI	2.78	1.59	1.54
2	A	804	Y01	OAW-CBC	-2.74	1.39	1.46
2	B	1204	Y01	CBD-CBG	-2.72	1.48	1.53
2	B	1201	Y01	CAS-CBF	-2.71	1.49	1.53
2	B	1206	Y01	CAU-CBI	2.68	1.58	1.54
2	A	804	Y01	CBD-CBG	-2.67	1.48	1.53
2	A	803	Y01	CAU-CBI	2.67	1.58	1.54
3	A	806	T7X	O16-C8	-2.50	1.40	1.46
3	B	1203	T7X	O16-C8	-2.44	1.40	1.46
3	B	1203	T7X	O18-C11	2.42	1.40	1.33
2	A	804	Y01	CAT-CAR	-2.38	1.48	1.53
2	A	803	Y01	CAT-CAR	-2.36	1.48	1.53
3	A	806	T7X	O18-C11	2.35	1.40	1.33
2	B	1206	Y01	CAT-CAR	-2.35	1.48	1.53
2	A	804	Y01	CAQ-CBG	2.34	1.59	1.54
2	A	801	Y01	CAQ-CBG	2.34	1.59	1.54
2	B	1204	Y01	CAQ-CBG	2.32	1.59	1.54
2	A	802	Y01	CAT-CAR	-2.31	1.48	1.53
2	B	1205	Y01	CAT-CAR	-2.31	1.48	1.53
2	A	803	Y01	CAQ-CBG	2.29	1.59	1.54
2	B	1206	Y01	CAQ-CBG	2.29	1.59	1.54
2	B	1201	Y01	CAQ-CBG	2.25	1.59	1.54
2	A	801	Y01	CAT-CAR	-2.20	1.48	1.53
2	B	1205	Y01	CAQ-CBG	2.20	1.58	1.54
2	B	1204	Y01	CAT-CAR	-2.18	1.48	1.53
2	A	802	Y01	CAQ-CBG	2.17	1.58	1.54
3	B	1203	T7X	O16-C10	2.15	1.40	1.34
3	A	806	T7X	O16-C10	2.14	1.40	1.34
2	B	1201	Y01	CAT-CAR	-2.13	1.48	1.53
3	B	1203	T7X	O18-C9	-2.13	1.40	1.45
3	A	806	T7X	O18-C9	-2.11	1.40	1.45
2	B	1201	Y01	CBH-CBF	2.00	1.59	1.56

All (108) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	804	Y01	CAV-CAZ-CBH	5.54	123.79	116.42
2	B	1204	Y01	CAP-CAQ-CBG	-5.23	94.76	105.13
2	B	1205	Y01	CAP-CAQ-CBG	-5.13	94.96	105.13
2	B	1201	Y01	CAP-CAQ-CBG	-5.08	95.06	105.13
2	A	801	Y01	CAP-CAQ-CBG	-5.08	95.07	105.13
2	A	804	Y01	CAP-CAQ-CBG	-4.96	95.31	105.13
2	A	802	Y01	CAP-CAQ-CBG	-4.90	95.42	105.13
2	B	1206	Y01	CAP-CAQ-CBG	-4.88	95.45	105.13
2	A	803	Y01	CAP-CAQ-CBG	-4.86	95.50	105.13
2	B	1201	Y01	CAV-CAZ-CBH	4.30	122.14	116.42
2	A	801	Y01	OAW-CAY-CAM	4.17	120.50	111.50
2	B	1201	Y01	OAW-CAY-CAM	4.11	120.36	111.50
2	B	1204	Y01	OAW-CAY-CAM	4.05	120.24	111.50
2	B	1201	Y01	CAR-CAT-CBH	3.97	121.34	112.74
2	A	804	Y01	OAW-CAY-CAM	3.91	119.92	111.50
3	B	1203	T7X	O16-C10-C12	3.89	119.88	111.50
2	B	1206	Y01	OAW-CAY-CAM	3.80	119.70	111.50
3	A	806	T7X	O16-C10-C12	3.78	119.65	111.50
2	A	802	Y01	OAW-CAY-CAM	3.74	119.55	111.50
2	A	803	Y01	OAW-CAY-CAM	3.71	119.50	111.50
2	A	803	Y01	CBD-CAK-CAI	-3.69	107.42	112.73
2	B	1205	Y01	OAW-CAY-CAM	3.69	119.46	111.50
2	B	1206	Y01	CBD-CAK-CAI	-3.54	107.65	112.73
2	A	802	Y01	CAQ-CBG-CBD	-3.41	113.47	119.08
2	A	804	Y01	CAV-CAZ-CAI	-3.31	115.84	120.61
2	B	1206	Y01	CAU-CAS-CBF	3.28	118.80	113.11
2	A	802	Y01	CBD-CAK-CAI	-3.21	108.12	112.73
2	B	1201	Y01	CAV-CAZ-CAI	-3.19	116.01	120.61
3	A	806	T7X	O18-C11-C31	3.18	119.72	111.38
3	B	1203	T7X	O18-C11-C31	3.18	119.72	111.38
2	A	803	Y01	CAU-CAS-CBF	3.14	118.56	113.11
2	A	803	Y01	CAQ-CBG-CBD	-3.12	113.95	119.08
2	B	1205	Y01	CAV-CAZ-CAI	-3.06	116.19	120.61
2	B	1206	Y01	CAQ-CBG-CBD	-3.04	114.07	119.08
2	A	802	Y01	CAV-CAZ-CAI	-3.03	116.24	120.61
2	B	1201	Y01	CAQ-CBG-CBD	-3.01	114.12	119.08
2	B	1201	Y01	CBC-CAV-CAZ	-3.00	106.85	111.52
2	A	804	Y01	CBI-CBE-CBB	-2.99	114.81	119.49
2	A	803	Y01	CBH-CBF-CBD	-2.98	108.26	112.73
2	B	1201	Y01	CBH-CBF-CBD	-2.96	108.29	112.73
2	B	1206	Y01	CBH-CBF-CBD	-2.96	108.30	112.73
2	B	1205	Y01	CBD-CAK-CAI	-2.93	108.53	112.73
2	B	1205	Y01	CAQ-CBG-CBD	-2.91	114.29	119.08

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	1201	Y01	CAU-CAS-CBF	2.89	118.13	113.11
2	B	1204	Y01	CBI-CBE-CBB	-2.89	114.96	119.49
2	A	803	Y01	CBI-CBE-CBB	-2.88	114.98	119.49
2	B	1206	Y01	CBI-CBE-CBB	-2.80	115.10	119.49
2	A	801	Y01	CBI-CBE-CBB	-2.77	115.15	119.49
2	A	802	Y01	CAU-CAS-CBF	2.74	117.86	113.11
2	B	1201	Y01	CBI-CBE-CBB	-2.71	115.24	119.49
2	B	1204	Y01	CBC-CAV-CAZ	-2.70	107.33	111.52
2	B	1205	Y01	CBI-CBE-CBB	-2.69	115.27	119.49
2	A	804	Y01	CBH-CBF-CBD	-2.68	108.71	112.73
2	B	1206	Y01	CAV-CAZ-CAI	-2.68	116.75	120.61
2	B	1204	Y01	CAV-CAZ-CBH	2.65	119.94	116.42
2	A	803	Y01	CAV-CAZ-CAI	-2.65	116.79	120.61
2	A	801	Y01	CAV-CAZ-CBH	2.63	119.92	116.42
2	B	1204	Y01	CBH-CBF-CBD	-2.62	108.81	112.73
2	A	801	Y01	CBH-CBF-CBD	-2.60	108.84	112.73
2	B	1206	Y01	CAK-CBD-CBF	-2.51	106.67	109.71
2	B	1205	Y01	CAK-CBD-CBG	-2.51	107.27	110.91
2	B	1205	Y01	CAU-CAS-CBF	2.47	117.39	113.11
2	B	1201	Y01	CAT-CBH-CAZ	2.47	113.27	108.75
2	A	804	Y01	CAR-CAT-CBH	2.46	118.08	112.74
2	A	803	Y01	CAK-CBD-CBF	-2.46	106.73	109.71
2	B	1205	Y01	CBF-CBH-CAZ	2.45	113.50	109.65
2	A	801	Y01	CAQ-CBG-CBD	-2.43	115.07	119.08
2	A	802	Y01	CBI-CBE-CBB	-2.41	115.71	119.49
2	A	804	Y01	CAT-CBH-CAZ	2.41	113.17	108.75
2	B	1201	Y01	CAQ-CAP-CBE	2.40	109.90	105.13
2	A	802	Y01	CAK-CBD-CBG	-2.39	107.44	110.91
2	A	804	Y01	CBI-CBG-CBD	-2.37	110.87	114.38
2	A	803	Y01	CBC-CAV-CAZ	-2.37	107.83	111.52
2	A	801	Y01	CBC-CAV-CAZ	-2.37	107.84	111.52
2	A	802	Y01	CBC-CAV-CAZ	-2.36	107.85	111.52
2	A	804	Y01	CAQ-CAP-CBE	2.35	109.80	105.13
2	A	804	Y01	CBF-CBH-CAZ	-2.33	106.00	109.65
2	A	804	Y01	CAQ-CBG-CBD	-2.31	115.27	119.08
2	B	1206	Y01	CAQ-CAP-CBE	2.30	109.68	105.13
2	A	801	Y01	CAU-CAS-CBF	2.30	117.09	113.11
2	A	804	Y01	CAJ-CAO-CBB	-2.29	108.44	115.03
3	B	1203	T7X	O12-P1-O11	-2.29	100.92	112.24
2	A	804	Y01	CAS-CBF-CBD	-2.29	108.46	111.75
2	A	803	Y01	CAQ-CAP-CBE	2.27	109.64	105.13
2	B	1206	Y01	CBC-CAV-CAZ	-2.27	107.99	111.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	1206	Y01	CAV-CAZ-CBH	2.26	119.42	116.42
3	A	806	T7X	O12-P1-O11	-2.25	101.10	112.24
2	B	1204	Y01	CAQ-CAP-CBE	2.24	109.58	105.13
2	B	1201	Y01	CAR-CBC-CAV	-2.22	107.68	110.99
2	A	802	Y01	CAV-CAZ-CBH	2.20	119.34	116.42
2	B	1204	Y01	CBF-CBH-CAZ	-2.19	106.22	109.65
2	B	1205	Y01	CAQ-CAP-CBE	2.18	109.45	105.13
2	B	1204	Y01	CAQ-CBG-CBD	-2.16	115.52	119.08
2	A	801	Y01	CAQ-CAP-CBE	2.16	109.42	105.13
2	A	804	Y01	CAU-CAS-CBF	2.13	116.81	113.11
2	A	803	Y01	CAV-CAZ-CBH	2.11	119.22	116.42
2	B	1201	Y01	CAC-CBB-CBE	-2.11	109.70	112.92
2	B	1206	Y01	CAJ-CAO-CBB	-2.10	108.99	115.03
2	B	1205	Y01	CAV-CAZ-CBH	2.09	119.19	116.42
2	A	804	Y01	CAR-CBC-CAV	-2.07	107.90	110.99
2	B	1205	Y01	CBC-CAV-CAZ	-2.07	108.31	111.52
2	B	1201	Y01	CAS-CBF-CBD	-2.06	108.79	111.75
2	A	803	Y01	CAM-CAL-CAX	-2.05	109.19	113.60
2	A	802	Y01	CAQ-CAP-CBE	2.04	109.18	105.13
2	B	1205	Y01	CAM-CAL-CAX	-2.01	109.27	113.60
2	A	801	Y01	CAR-CAT-CBH	2.01	117.09	112.74
2	A	803	Y01	CAJ-CAO-CBB	-2.00	109.27	115.03
2	A	801	Y01	CAT-CAR-CBC	2.00	113.74	110.33

There are no chirality outliers.

All (100) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	B	1201	Y01	CAV-CBC-OAW-CAY
2	B	1204	Y01	CAM-CAY-OAW-CBC
2	A	801	Y01	OAG-CAY-OAW-CBC
2	A	801	Y01	CAM-CAY-OAW-CBC
2	A	804	Y01	CAV-CBC-OAW-CAY
3	B	1202	T7X	C2-C1-O1-P1
3	B	1202	T7X	C6-C1-O1-P1
3	B	1202	T7X	C1-O1-P1-O13
3	B	1202	T7X	C7-O13-P1-O11
3	B	1202	T7X	C7-O13-P1-O12
3	B	1203	T7X	C7-O13-P1-O12
3	B	1203	T7X	O13-C7-C8-O16
3	B	1203	T7X	C14-C15-C16-C17
3	B	1203	T7X	C18-C19-C20-C21

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Mol	Chain	Res	Type	Atoms
3	A	805	T7X	C7-O13-P1-O12
3	A	806	T7X	C14-C15-C16-C17
3	A	806	T7X	C18-C19-C20-C21
3	B	1203	T7X	O19-C11-O18-C9
2	B	1204	Y01	OAG-CAY-OAW-CBC
2	A	803	Y01	CAX-CAL-CAM-CAY
3	B	1203	T7X	C31-C11-O18-C9
3	B	1203	T7X	C23-C24-C25-C26
3	A	806	T7X	C17-C18-C19-C20
3	A	806	T7X	C23-C24-C25-C26
2	A	804	Y01	OAG-CAY-OAW-CBC
3	A	806	T7X	O19-C11-O18-C9
2	A	804	Y01	CAJ-CAO-CBB-CBE
3	A	806	T7X	C31-C11-O18-C9
2	A	804	Y01	CAM-CAY-OAW-CBC
2	A	804	Y01	CAJ-CAO-CBB-CAC
2	B	1206	Y01	CAJ-CAO-CBB-CBE
2	A	803	Y01	CAJ-CAO-CBB-CBE
2	B	1201	Y01	CAM-CAY-OAW-CBC
3	A	806	T7X	O13-C7-C8-O16
2	B	1206	Y01	CAJ-CAO-CBB-CAC
2	A	803	Y01	CAJ-CAO-CBB-CAC
3	B	1203	T7X	C10-C12-C13-C14
3	A	806	T7X	C10-C12-C13-C14
2	B	1201	Y01	OAG-CAY-OAW-CBC
2	B	1201	Y01	CAO-CAJ-CAN-CBA
2	B	1205	Y01	CAM-CAY-OAW-CBC
2	B	1204	Y01	CAO-CAJ-CAN-CBA
2	A	801	Y01	CAO-CAJ-CAN-CBA
3	B	1203	T7X	C7-O13-P1-O1
3	A	806	T7X	C7-O13-P1-O1
2	B	1205	Y01	OAG-CAY-OAW-CBC
3	B	1203	T7X	C1-O1-P1-O13
3	A	806	T7X	C1-O1-P1-O13
3	B	1203	T7X	C12-C10-O16-C8
3	A	806	T7X	C12-C10-O16-C8
3	B	1203	T7X	O17-C10-O16-C8
3	A	806	T7X	O17-C10-O16-C8
3	B	1203	T7X	C17-C18-C19-C20
2	A	802	Y01	OAG-CAY-OAW-CBC
2	A	802	Y01	CAM-CAY-OAW-CBC
2	A	803	Y01	CAM-CAY-OAW-CBC

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Mol	Chain	Res	Type	Atoms
3	A	806	T7X	O13-C7-C8-C9
3	A	806	T7X	C20-C21-C22-C23
3	B	1203	T7X	O13-C7-C8-C9
2	A	803	Y01	OAG-CAY-OAW-CBC
3	B	1202	T7X	C1-O1-P1-O11
3	B	1203	T7X	C22-C23-C24-C25
3	A	806	T7X	C22-C23-C24-C25
3	B	1203	T7X	O16-C8-C9-O18
3	A	806	T7X	O16-C8-C9-O18
3	A	806	T7X	C25-C26-C27-C28
3	B	1203	T7X	C20-C21-C22-C23
3	B	1203	T7X	C7-O13-P1-O11
3	A	806	T7X	C7-O13-P1-O12
3	B	1203	T7X	C25-C26-C27-C28
2	B	1204	Y01	CAM-CAL-CAX-OAH
2	B	1205	Y01	CAM-CAL-CAX-OAH
2	A	803	Y01	CAM-CAL-CAX-OAH
2	B	1206	Y01	CAM-CAL-CAX-OAF
2	A	801	Y01	CAM-CAL-CAX-OAF
3	B	1202	T7X	C7-O13-P1-O1
2	B	1206	Y01	CAM-CAL-CAX-OAH
2	A	801	Y01	CAM-CAL-CAX-OAH
2	B	1201	Y01	CAM-CAL-CAX-OAF
2	B	1201	Y01	CAM-CAL-CAX-OAH
2	A	802	Y01	CAM-CAL-CAX-OAH
2	B	1205	Y01	CAM-CAL-CAX-OAF
2	A	803	Y01	CAM-CAL-CAX-OAF
2	B	1204	Y01	CAM-CAL-CAX-OAF
2	A	802	Y01	CAM-CAL-CAX-OAF
2	A	804	Y01	CAM-CAL-CAX-OAF
2	A	804	Y01	CAM-CAL-CAX-OAH
2	A	804	Y01	CAL-CAM-CAY-OAW
2	B	1201	Y01	CAL-CAM-CAY-OAW
2	A	801	Y01	CAL-CAM-CAY-OAW
3	A	806	T7X	C7-C8-C9-O18
2	A	801	Y01	CAX-CAL-CAM-CAY
3	A	806	T7X	C13-C14-C15-C16
2	B	1204	Y01	CAL-CAM-CAY-OAW
2	B	1201	Y01	CAL-CAM-CAY-OAG
2	A	804	Y01	CAL-CAM-CAY-OAG
2	A	801	Y01	CAL-CAM-CAY-OAG
3	B	1203	T7X	C7-C8-C9-O18

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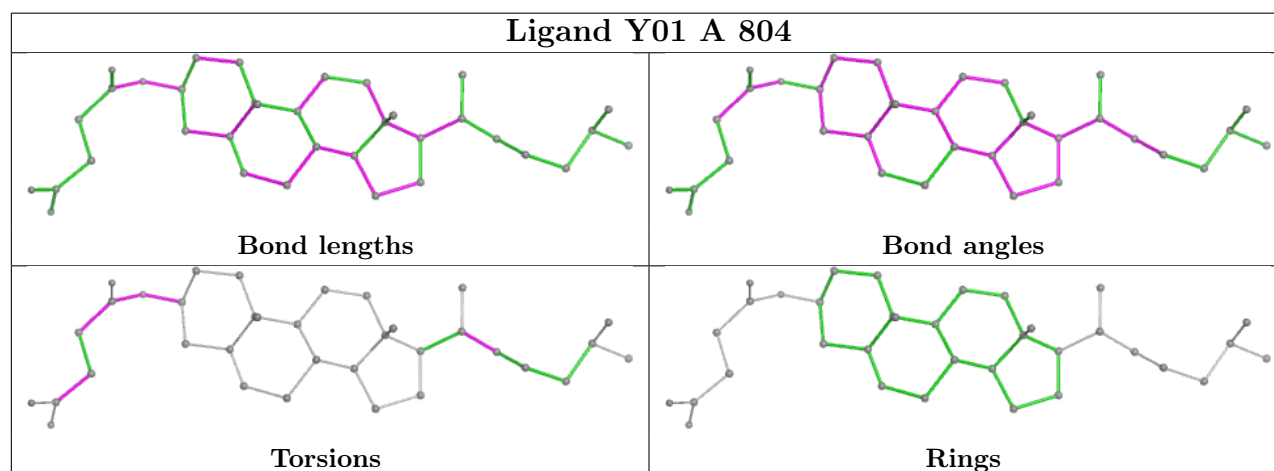
Mol	Chain	Res	Type	Atoms
2	B	1201	Y01	CAJ-CAN-CBA-CAB
2	B	1204	Y01	CAL-CAM-CAY-OAG

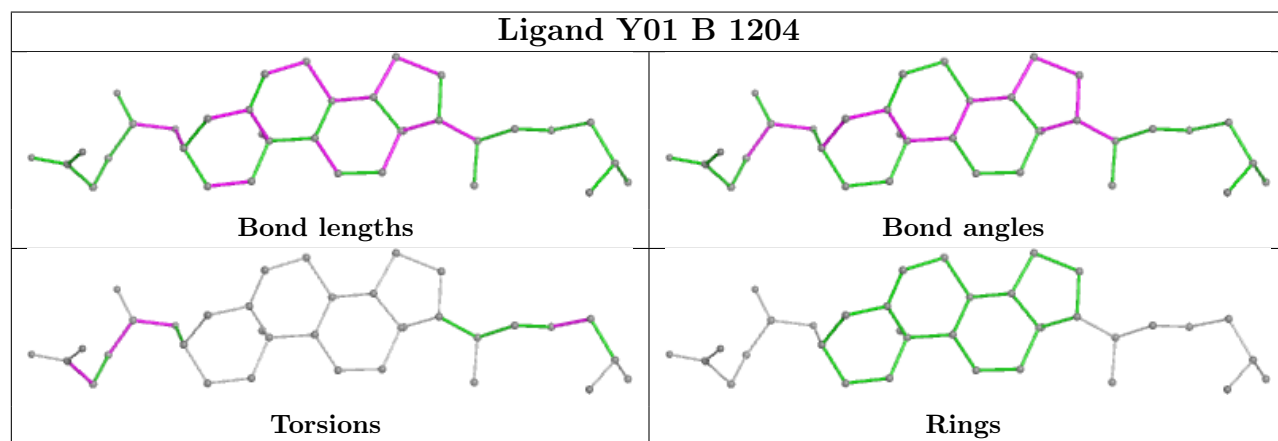
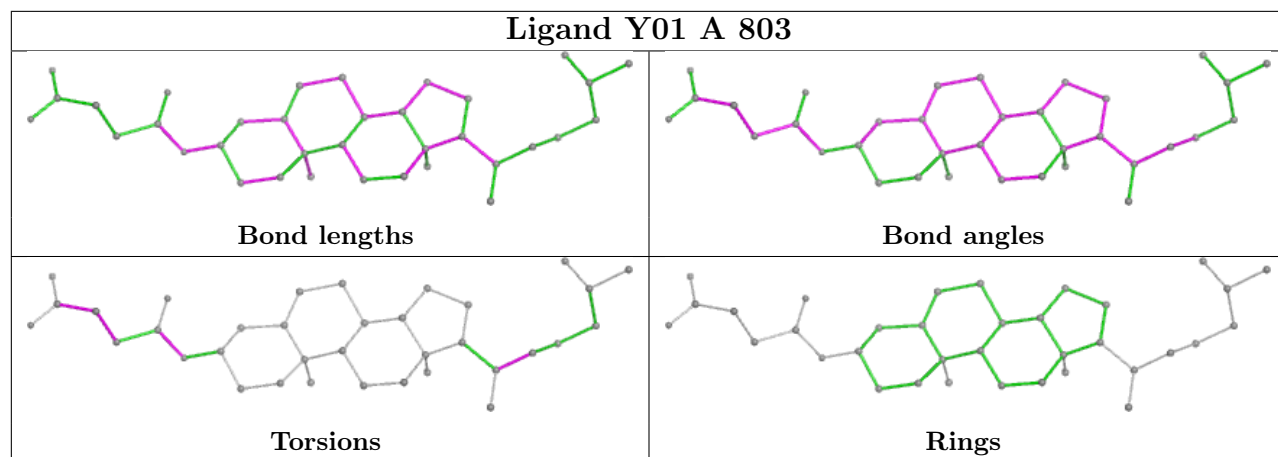
There are no ring outliers.

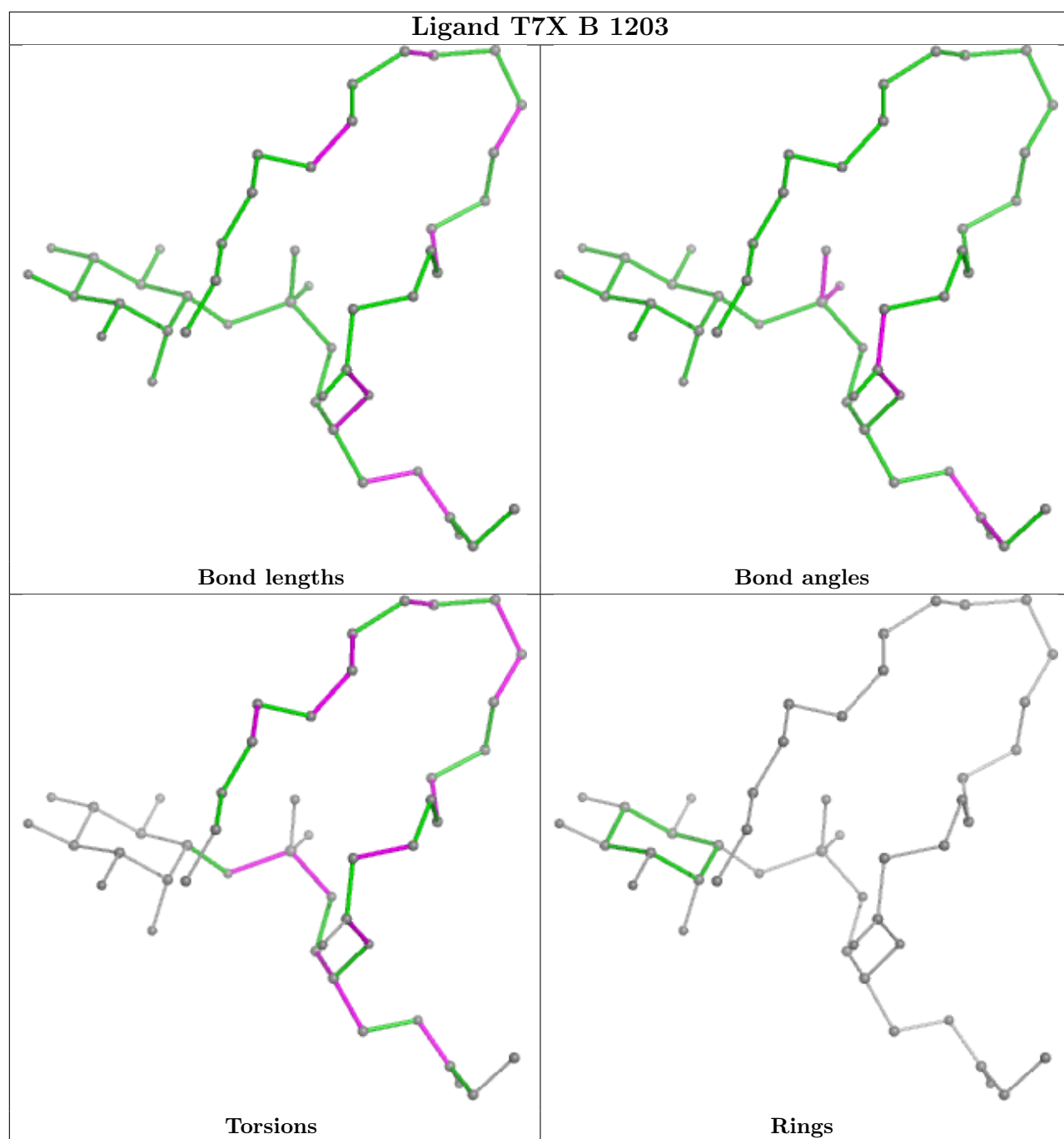
10 monomers are involved in 21 short contacts:

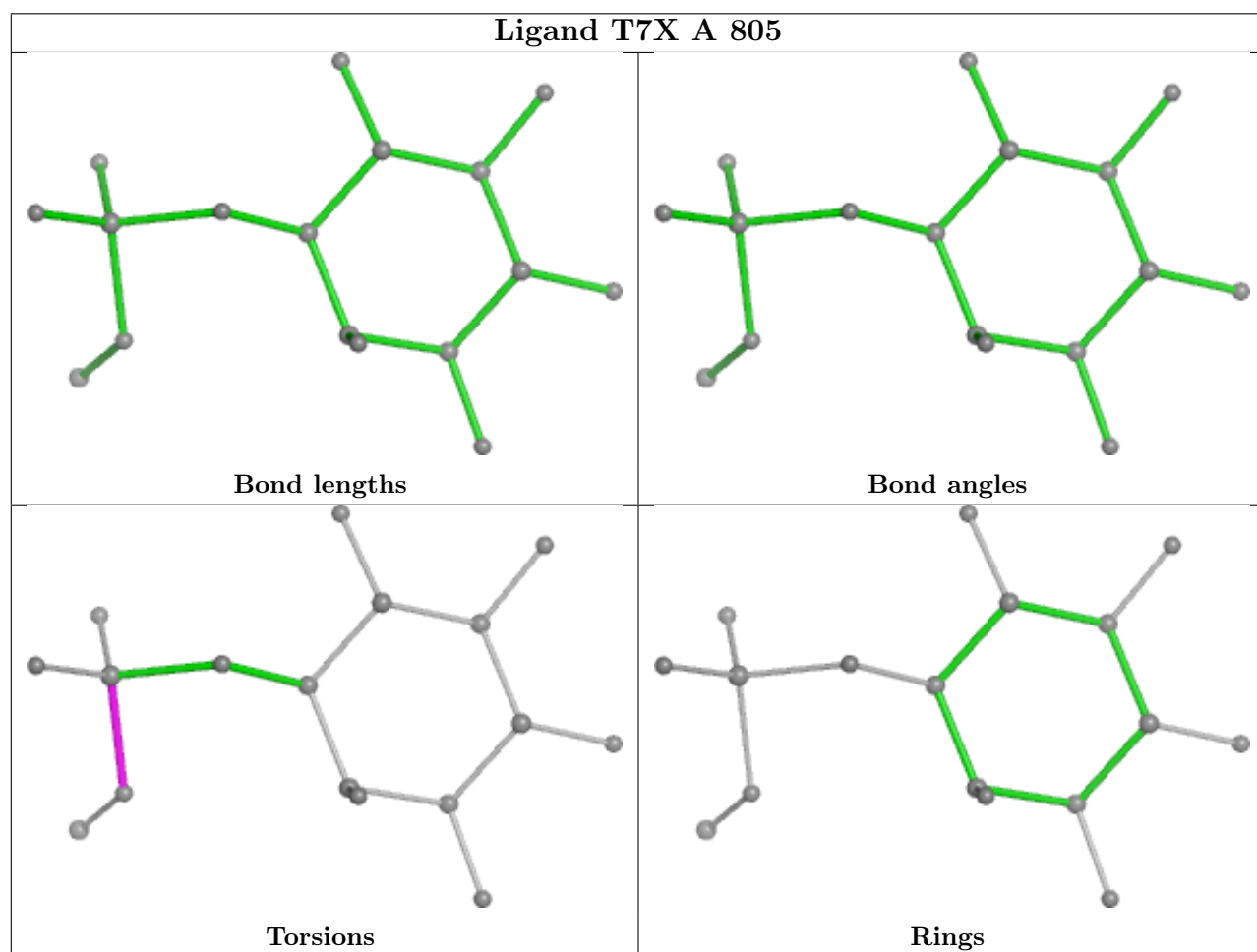
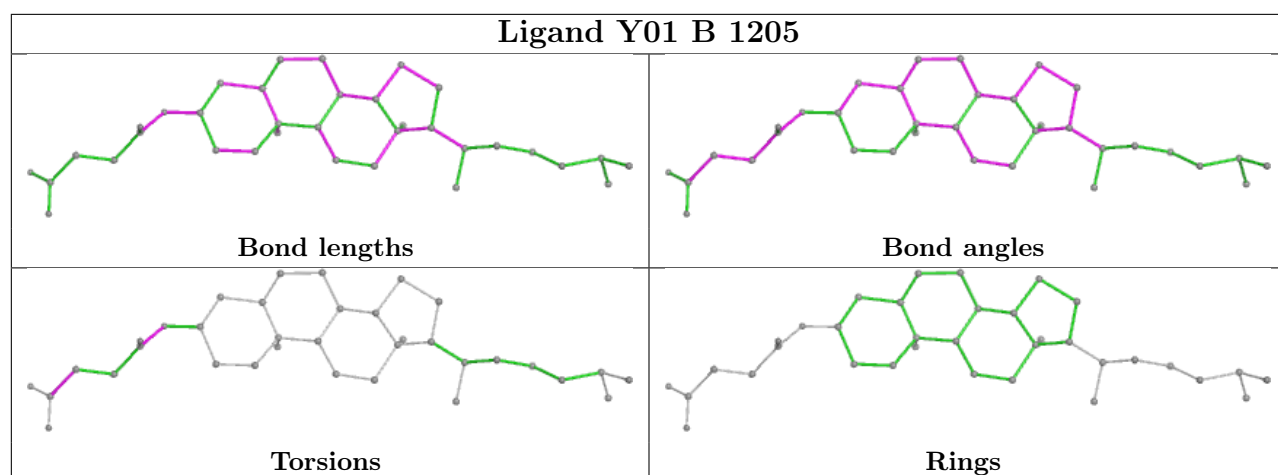
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	804	Y01	2	0
2	A	803	Y01	2	0
2	B	1204	Y01	1	0
3	B	1203	T7X	2	0
2	B	1205	Y01	2	0
2	A	802	Y01	3	0
2	B	1201	Y01	3	0
3	A	806	T7X	1	0
2	A	801	Y01	3	0
2	B	1206	Y01	2	0

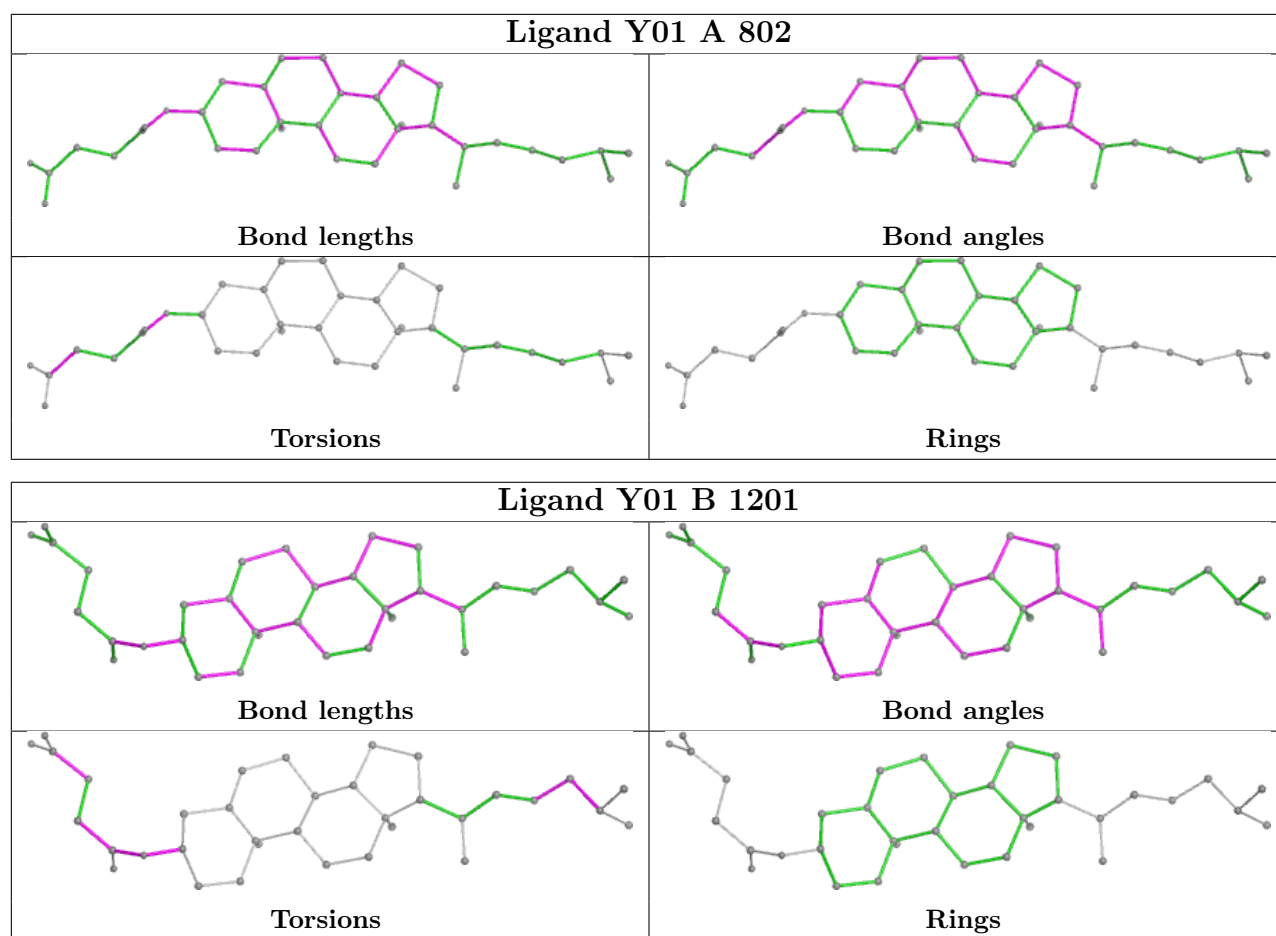
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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



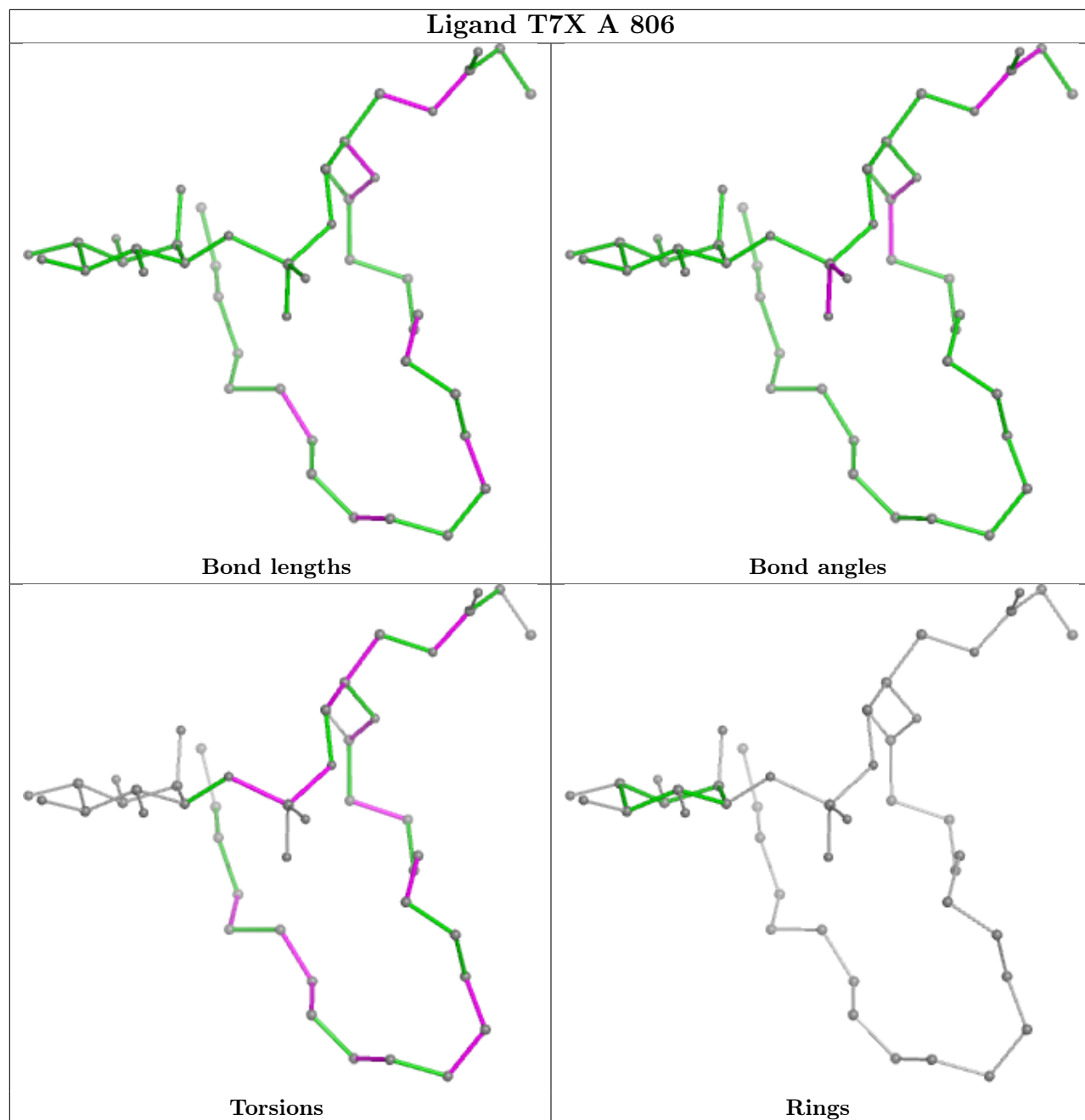




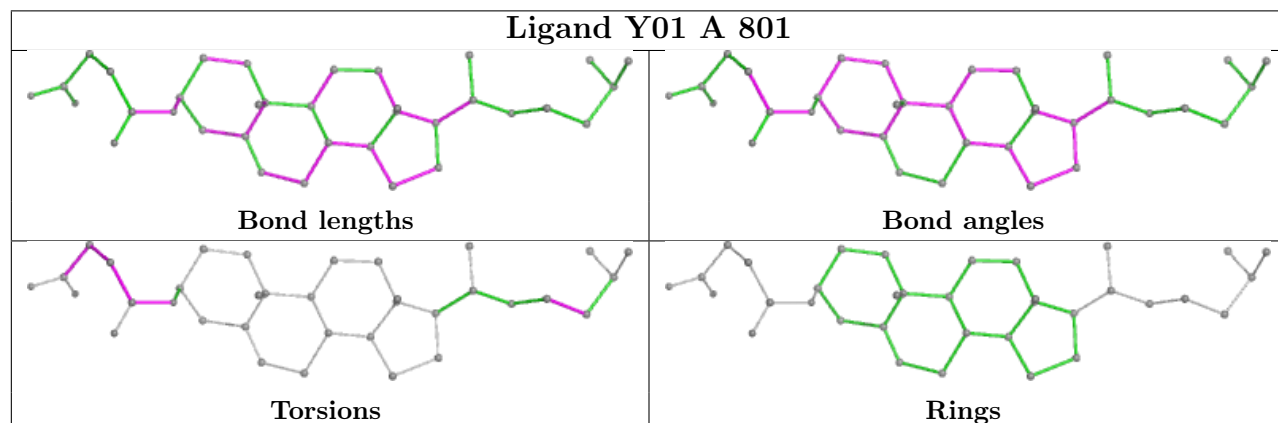


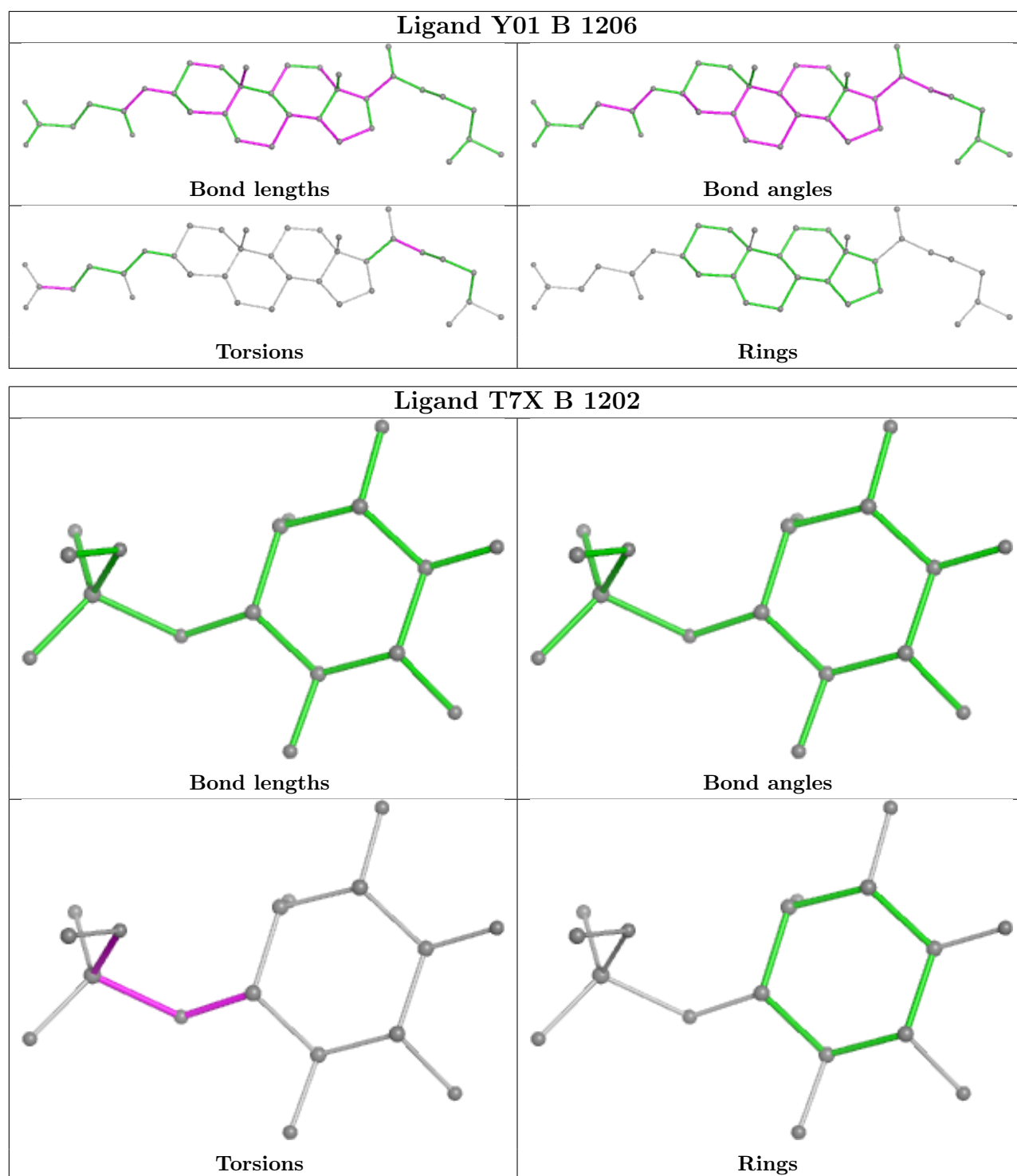


Ligand T7X A 806



Ligand Y01 A 801





5.7 Other polymers ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

There are no chain breaks in this entry.

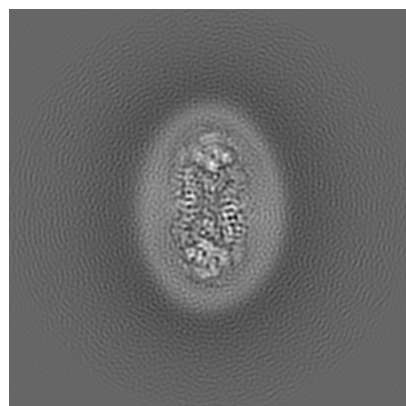
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-13163. These allow visual inspection of the internal detail of the map and identification of artifacts.

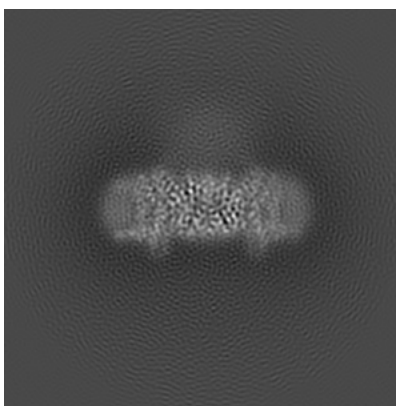
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

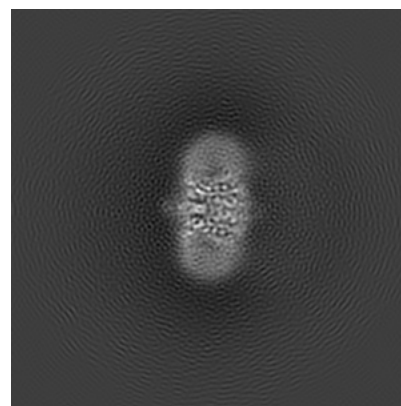
6.1.1 Primary map



X

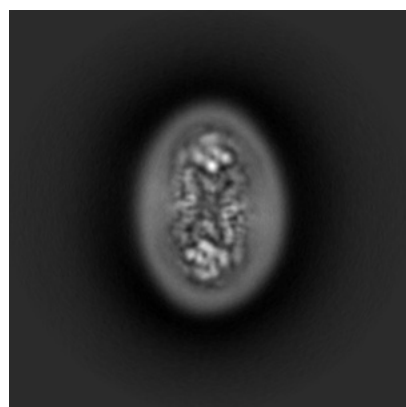


Y

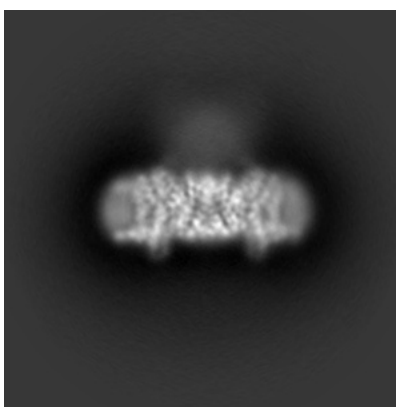


Z

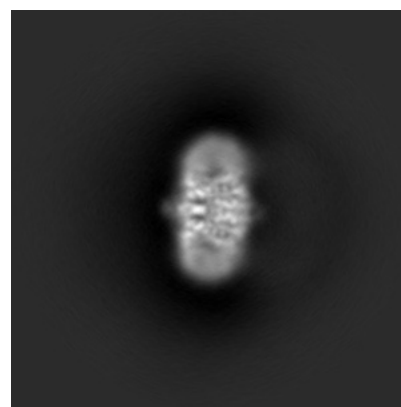
6.1.2 Raw map



X



Y

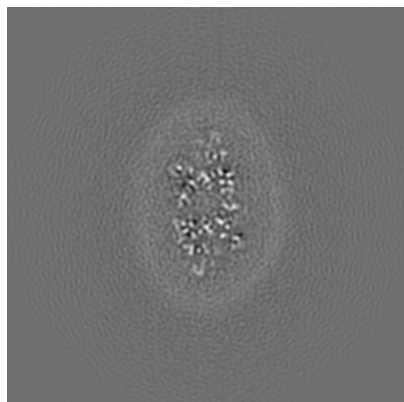


Z

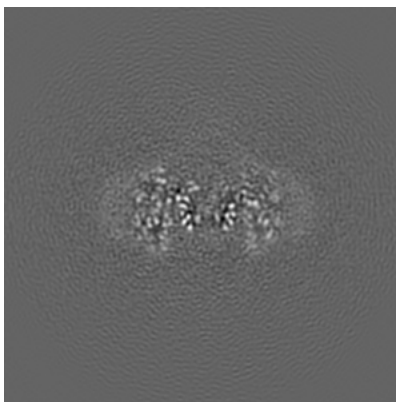
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

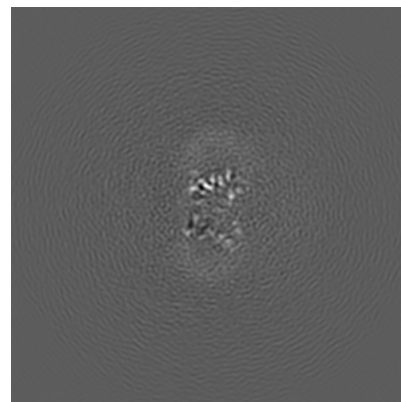
6.2.1 Primary map



X Index: 128

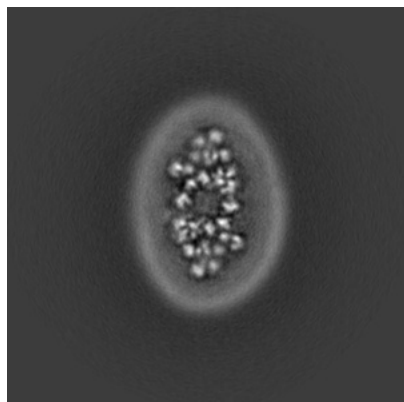


Y Index: 128

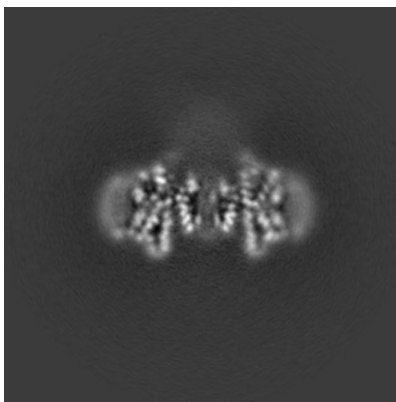


Z Index: 128

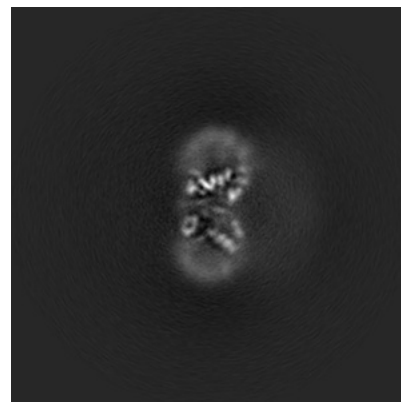
6.2.2 Raw map



X Index: 128



Y Index: 128

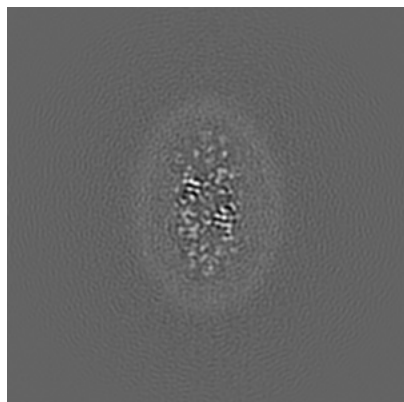


Z Index: 128

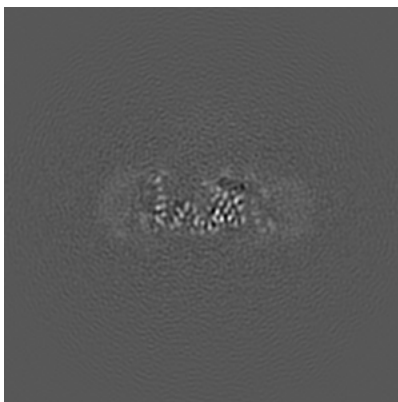
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

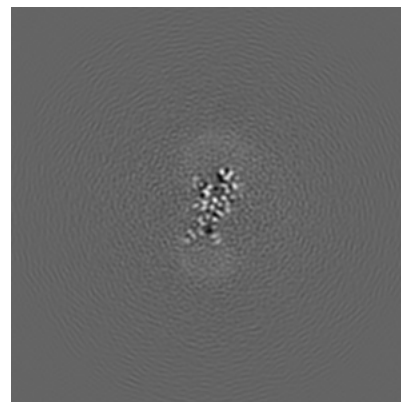
6.3.1 Primary map



X Index: 121

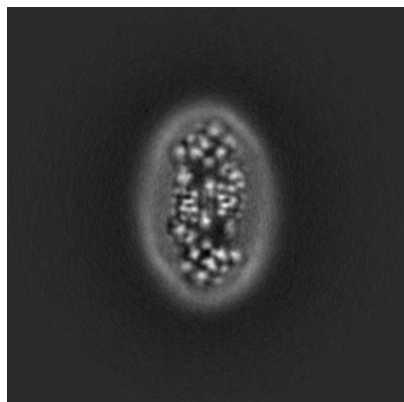


Y Index: 117

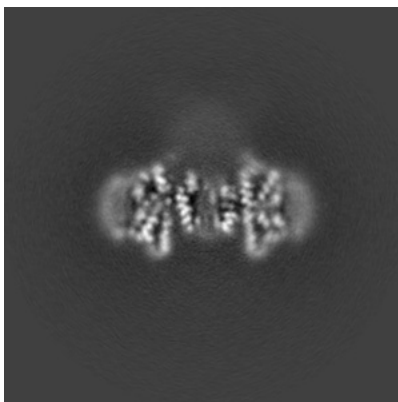


Z Index: 114

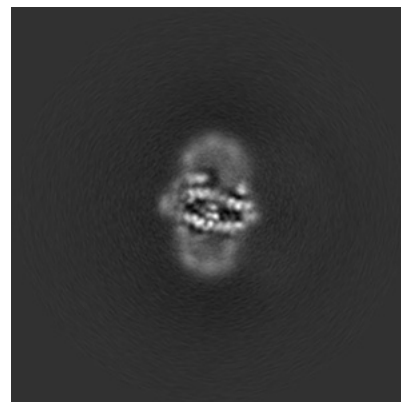
6.3.2 Raw map



X Index: 115



Y Index: 129

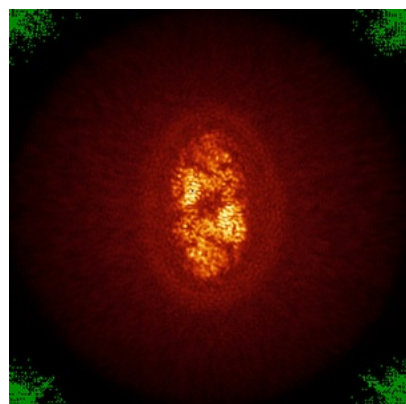


Z Index: 99

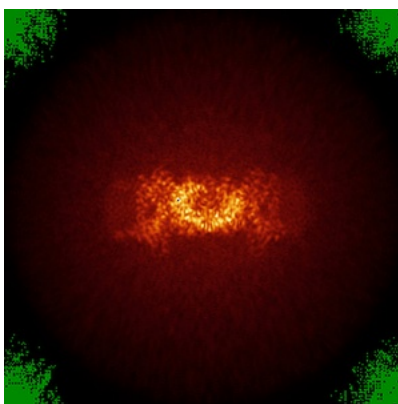
The images above show the largest variance slices of the map in three orthogonal directions.

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

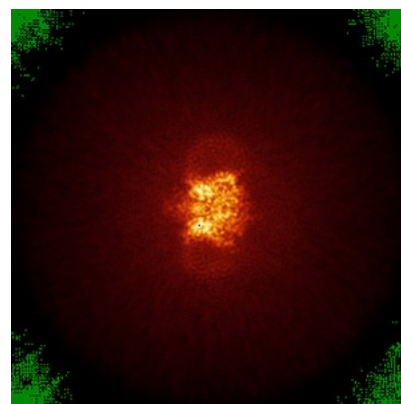
6.4.1 Primary map



X

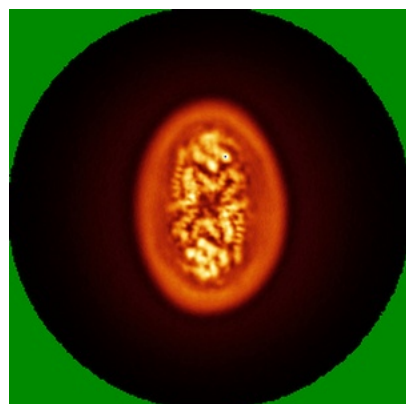


Y

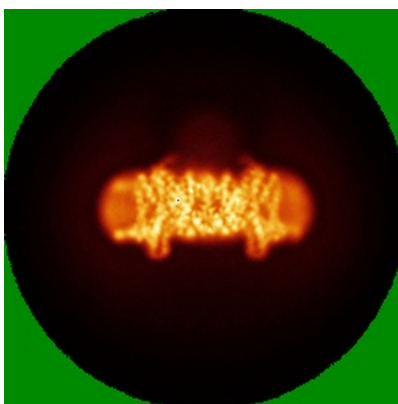


Z

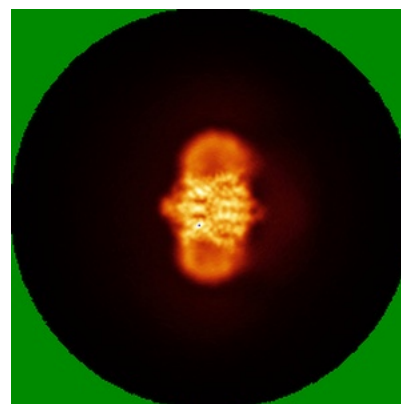
6.4.2 Raw map



X



Y

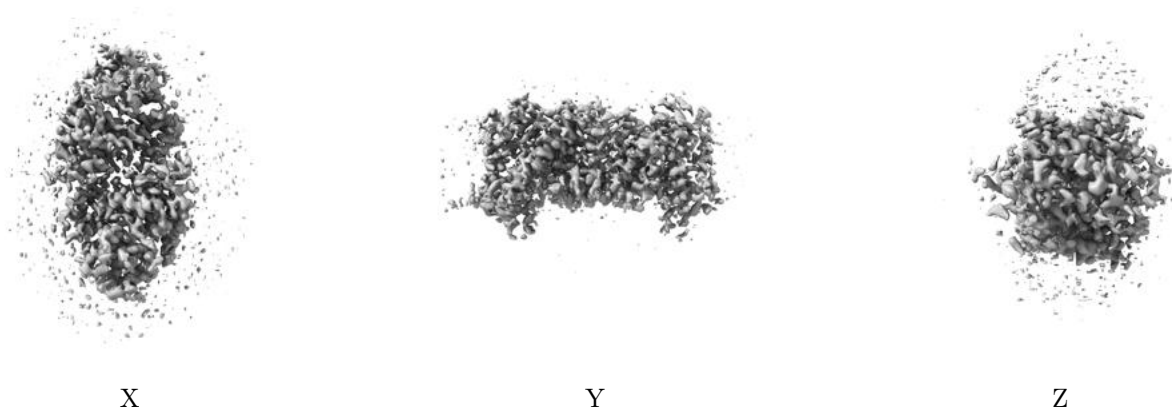


Z

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.

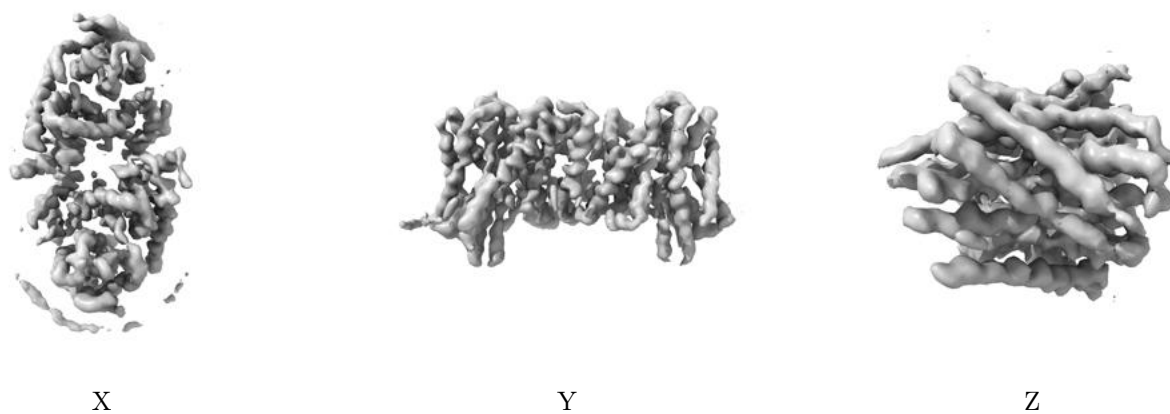
6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.035. 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.

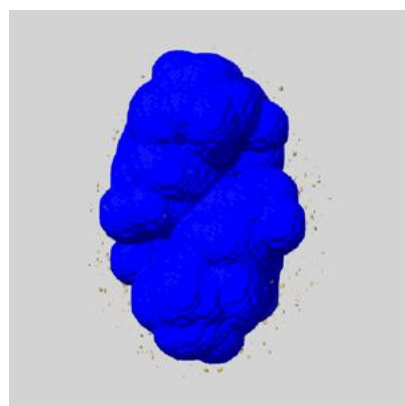
6.6 Mask visualisation [i](#)

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

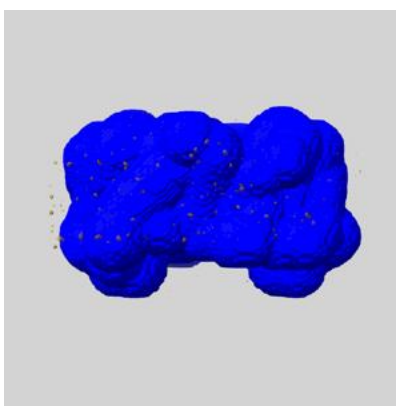
A mask typically either:

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

6.6.1 emd_13163_msk_1.map [i](#)



X



Y

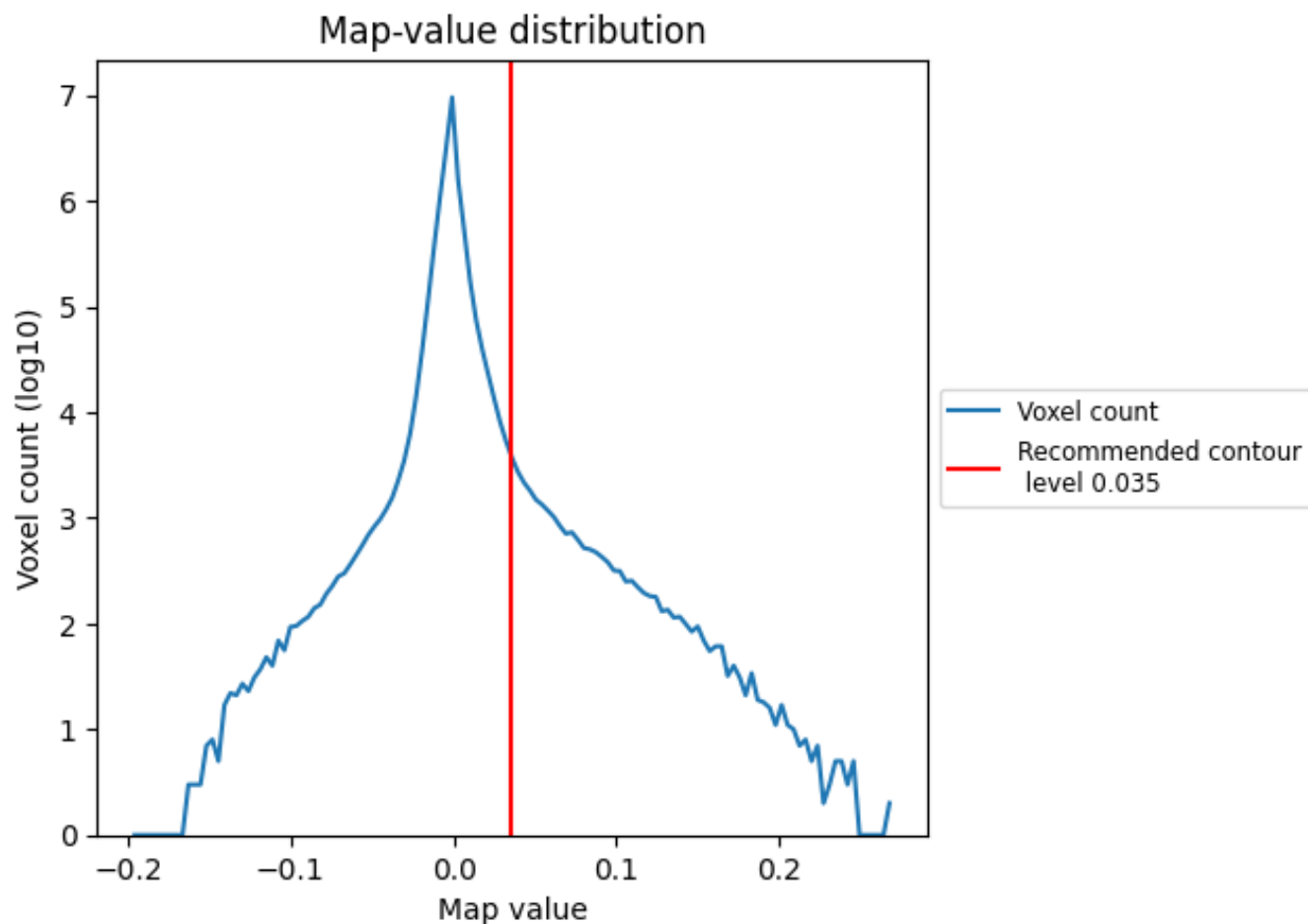


Z

7 Map analysis [i](#)

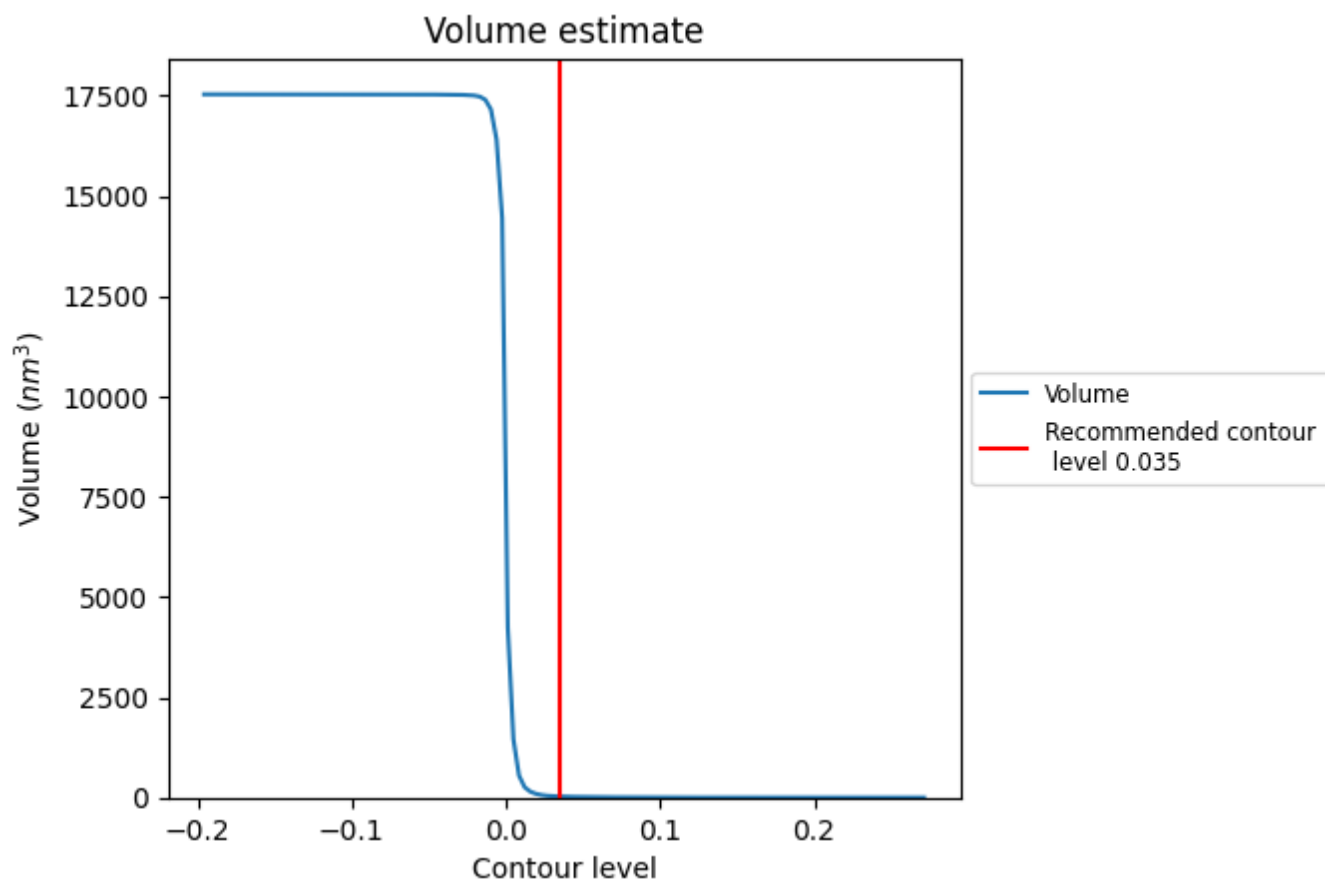
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution [i](#)



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

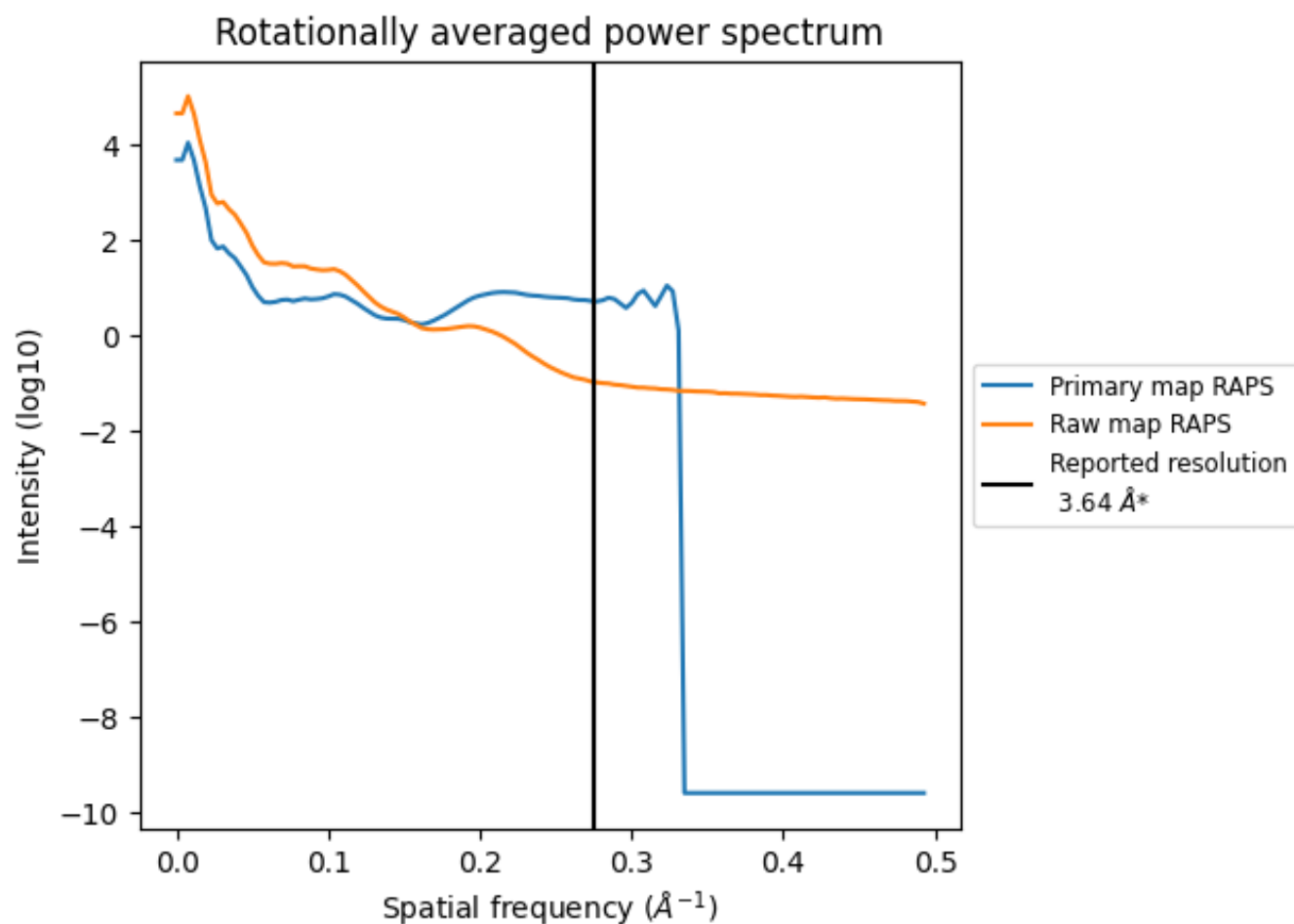
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 26 nm³; this corresponds to an approximate mass of 24 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 ⓘ

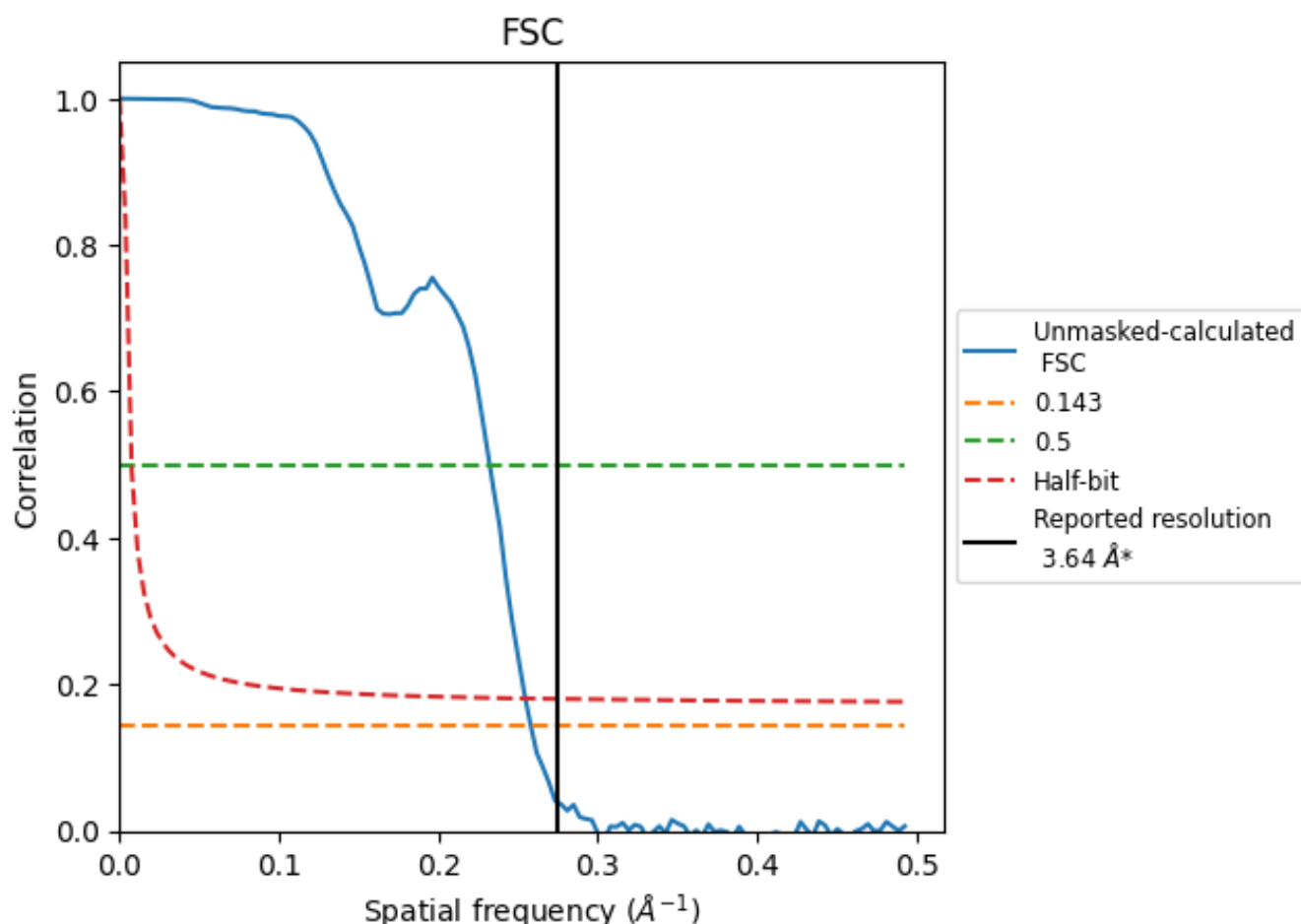


*Reported resolution corresponds to spatial frequency of 0.275 \AA^{-1}

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 0.275 \AA^{-1}

8.2 Resolution estimates [i](#)

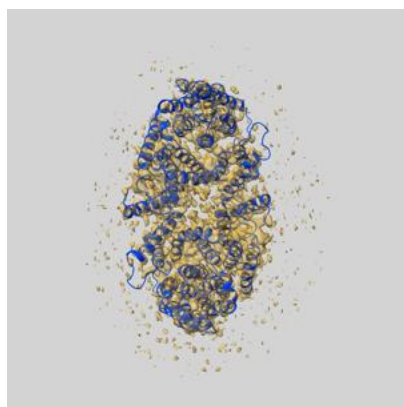
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.64	-	-
Author-provided FSC curve	-	-	-
Unmasked-calculated*	3.87	4.31	3.93

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

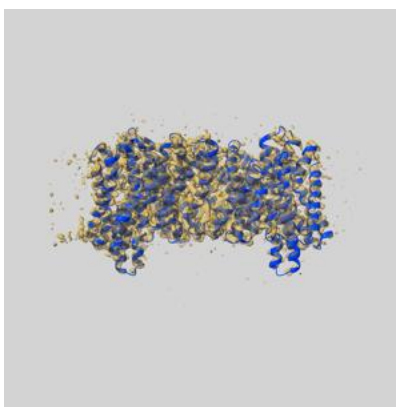
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-13163 and PDB model 7P1K. Per-residue inclusion information can be found in section [3](#) on page [5](#).

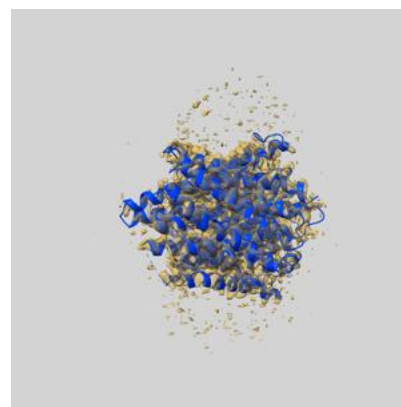
9.1 Map-model overlay [i](#)



X



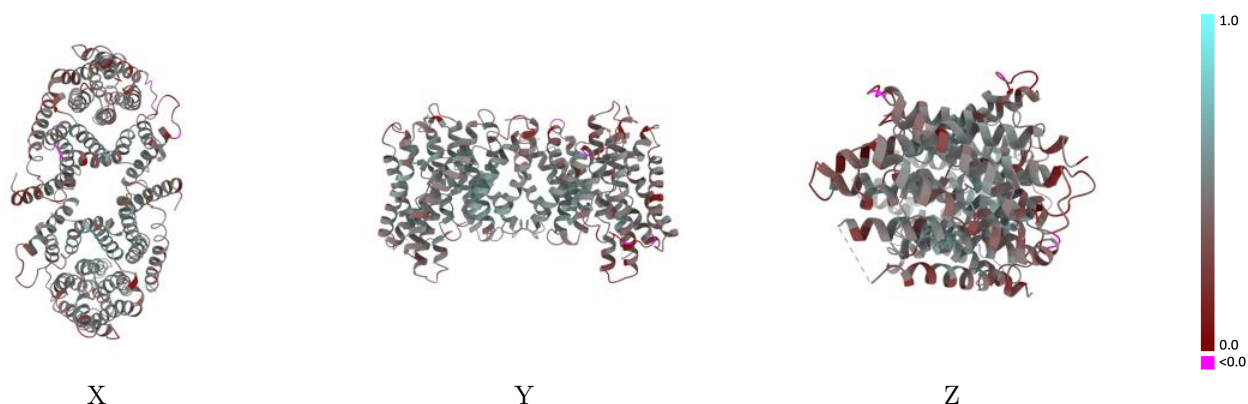
Y



Z

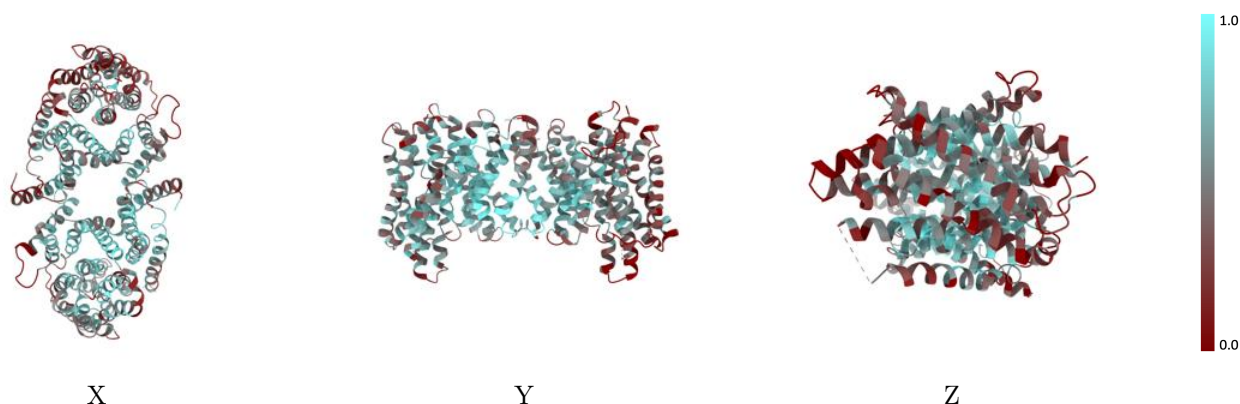
The images above show the 3D surface view of the map at the recommended contour level 0.035 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



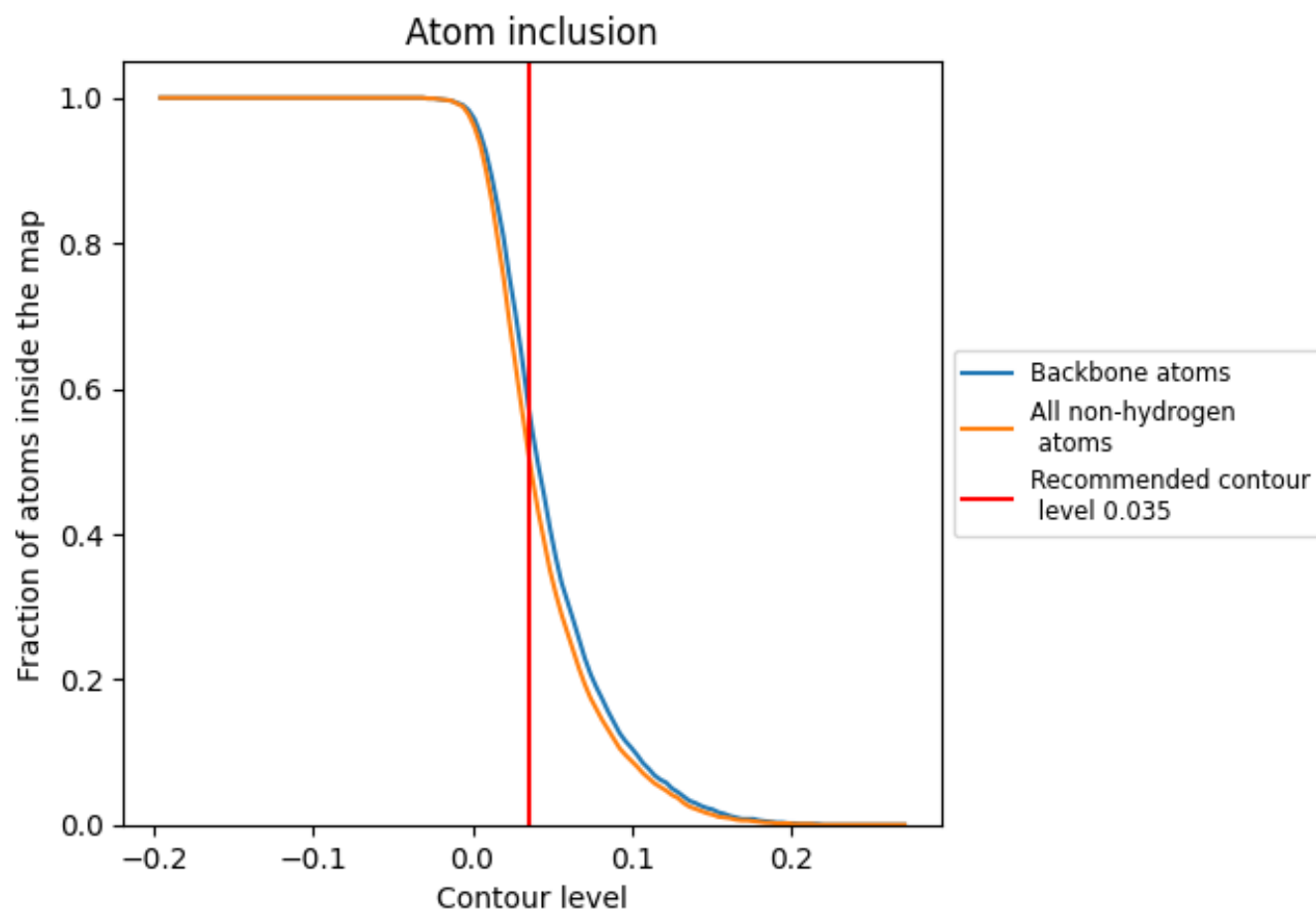
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.035).

9.4 Atom inclusion [i](#)



At the recommended contour level, 58% of all backbone atoms, 51% 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 (0.035) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	<div></div> 0.5130	<div></div> 0.4300
A	<div></div> 0.4590	<div></div> 0.4110
B	<div></div> 0.5700	<div></div> 0.4490

