



Full wwPDB EM Validation Report ⓘ

Mar 24, 2025 – 03:21 PM EDT

PDB ID : 9DVO
EMDB ID : EMD-47213
Title : Structure of the phosphate exporter XPR1/SLC53A1, Pi and InsP8-bound, intracellular gate open/intracellular gate closed state
Authors : Zhu, Q.; Diver, M.M.
Deposited on : 2024-10-08
Resolution : 3.10 Å(reported)

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

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

A user guide is available at

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

The types of validation reports are described at

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

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

EMDB validation analysis : 0.0.1.dev117
Mogul : 2022.3.0, CSD as543be (2022)
MolProbity : 4.02b-467
buster-report : 1.1.7 (2018)
Percentile statistics : 20231227.v01 (using entries in the PDB archive December 27th 2023)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.41.4

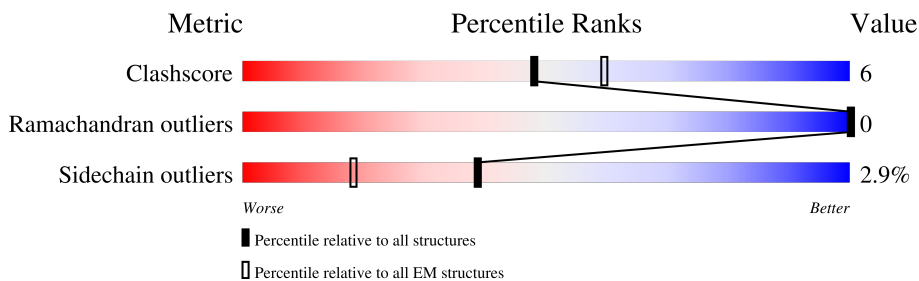
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 3.10 Å.

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



Metric	Whole archive (#Entries)	EM structures (#Entries)
Clashscore	210492	15764
Ramachandran outliers	207382	16835
Sidechain outliers	206894	16415

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	702	<div> <div>16%</div> <div>71%</div> <div>11%</div> <div>18%</div> </div>
1	B	702	<div> <div>16%</div> <div>68%</div> <div>14%</div> <div>18%</div> </div>

2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 19779 atoms, of which 9836 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.

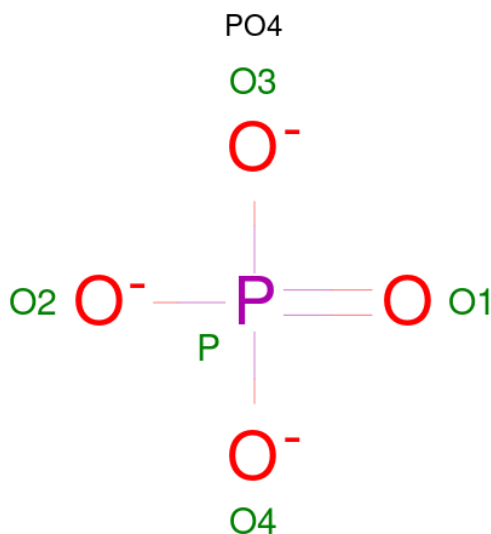
- Molecule 1 is a protein called Solute carrier family 53 member 1.

Mol	Chain	Residues	Atoms						AltConf	Trace
1	A	578	Total	C	H	N	O	S	0	0
			9602	3181	4797	792	811	21		
1	B	574	Total	C	H	N	O	S	0	0
			9555	3165	4775	789	805	21		

There are 12 discrepancies between the modelled and reference sequences:

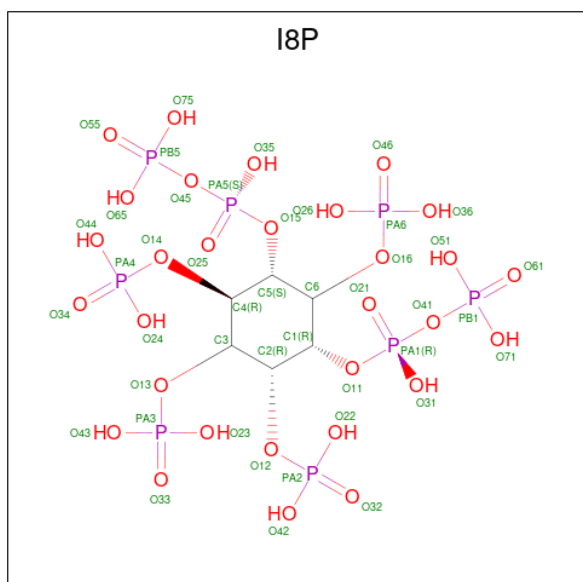
Chain	Residue	Modelled	Actual	Comment	Reference
A	697	LEU	-	expression tag	UNP Q9UBH6
A	698	GLU	-	expression tag	UNP Q9UBH6
A	699	VAL	-	expression tag	UNP Q9UBH6
A	700	LEU	-	expression tag	UNP Q9UBH6
A	701	PHE	-	expression tag	UNP Q9UBH6
A	702	GLN	-	expression tag	UNP Q9UBH6
B	697	LEU	-	expression tag	UNP Q9UBH6
B	698	GLU	-	expression tag	UNP Q9UBH6
B	699	VAL	-	expression tag	UNP Q9UBH6
B	700	LEU	-	expression tag	UNP Q9UBH6
B	701	PHE	-	expression tag	UNP Q9UBH6
B	702	GLN	-	expression tag	UNP Q9UBH6

- Molecule 2 is PHOSPHATE ION (three-letter code: PO4) (formula: O₄P) (labeled as "Ligand of Interest" by depositor).



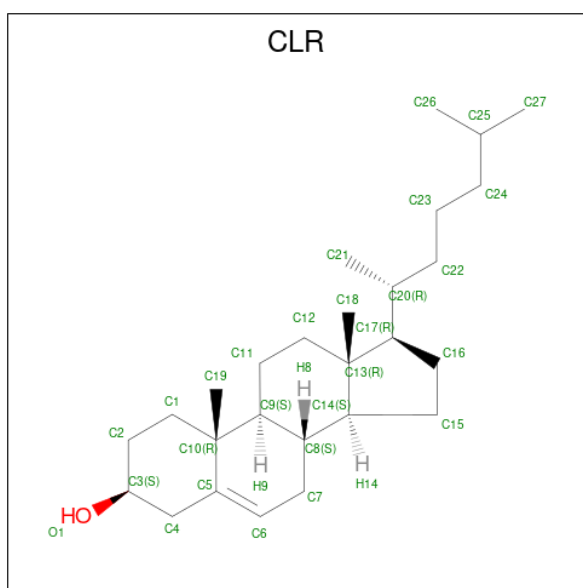
Mol	Chain	Residues	Atoms			AltConf
2	A	1	Total 5	O 4	P 1	0
2	A	1	Total 5	O 4	P 1	0
2	A	1	Total 5	O 4	P 1	0
2	B	1	Total 5	O 4	P 1	0

- Molecule 3 is (1R,3S,4R,5S,6R)-2,4,5,6-tetrakis(phosphonooxy)cyclohexane-1,3-diyl bis[trihydrogen (diphosphate)] (three-letter code: I8P) (formula: C₆H₂₀O₃₀P₈) (labeled as "Ligand of Interest" by depositor).



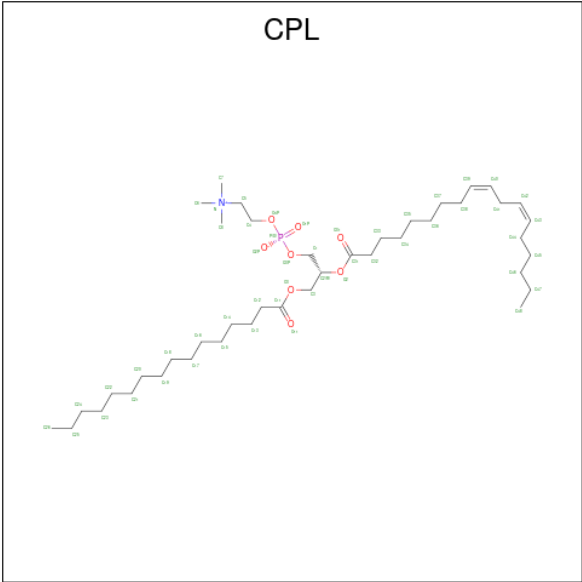
Mol	Chain	Residues	Atoms	AltConf
3	A	1	Total C H O P 50 6 6 30 8	0
3	A	1	Total C O P 44 6 30 8	0
3	B	1	Total C H O P 50 6 6 30 8	0
3	B	1	Total C O P 44 6 30 8	0

- Molecule 4 is CHOLESTEROL (three-letter code: CLR) (formula: $C_{27}H_{46}O$).



Mol	Chain	Residues	Atoms	AltConf
4	A	1	Total C H O 74 27 46 1	0
4	B	1	Total C H O 74 27 46 1	0

- Molecule 5 is 1-PALMITOYL-2-LINOLEOYL-SN-GLYCERO-3-PHOSPHOCHOLINE (three-letter code: CPL) (formula: $C_{42}H_{80}NO_8P$).



Mol	Chain	Residues	Atoms						AltConf
5	A	1	Total	C	H	N	O	P	0
			132	42	80	1	8	1	
5	B	1	Total	C	H	N	O	P	0
			132	42	80	1	8	1	

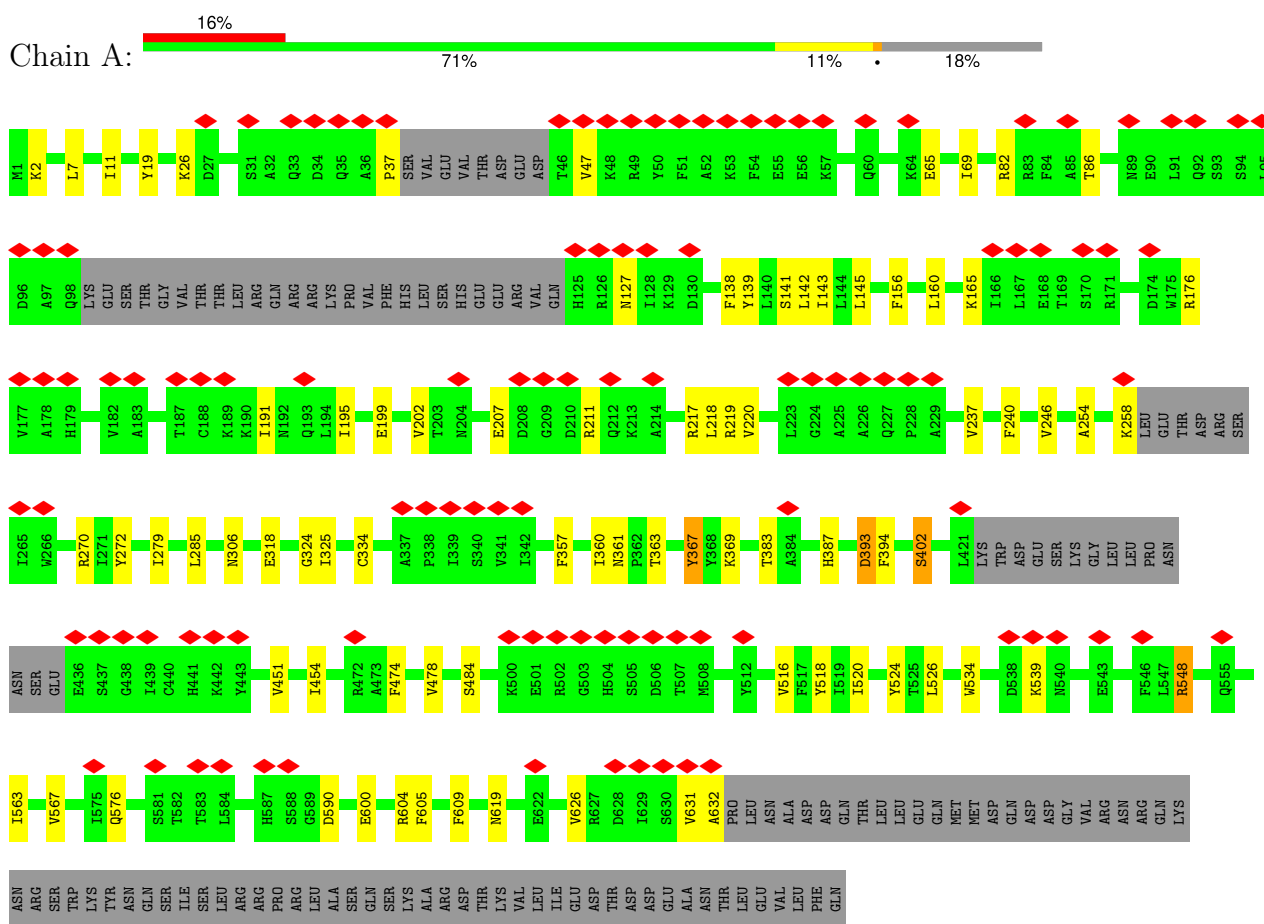
- Molecule 6 is water.

Mol	Chain	Residues	Atoms		AltConf
6	A	1	Total	O	0
			1	1	
6	B	1	Total	O	0
			1	1	

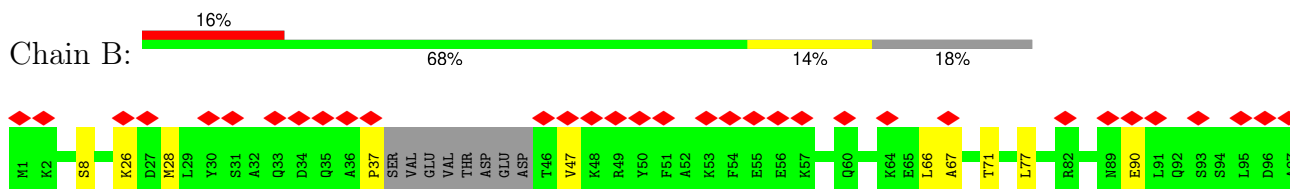
3 Residue-property plots

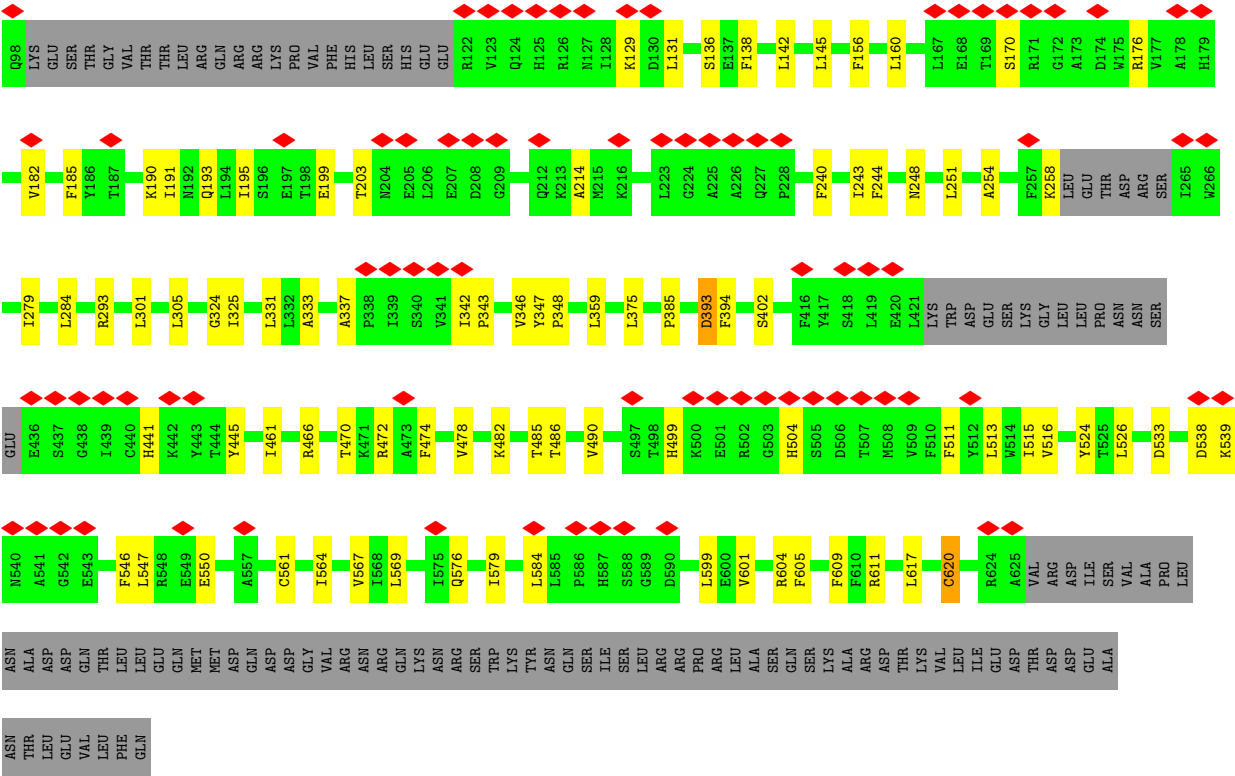
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion in map density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red diamond above a residue indicates a poor fit to the EM map for this residue (all-atom inclusion < 40%). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

• Molecule 1: Solute carrier family 53 member 1



• Molecule 1: Solute carrier family 53 member 1





4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	116612	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	TFS KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	60.45	Depositor
Minimum defocus (nm)	700	Depositor
Maximum defocus (nm)	1700	Depositor
Magnification	Not provided	
Image detector	TFS FALCON 4i (4k x 4k)	Depositor
Maximum map value	0.454	Depositor
Minimum map value	-0.274	Depositor
Average map value	-0.000	Depositor
Map value standard deviation	0.009	Depositor
Recommended contour level	0.065	Depositor
Map size (\AA)	278.40002, 278.40002, 278.40002	wwPDB
Map dimensions	384, 384, 384	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (\AA)	0.7250001, 0.7250001, 0.7250001	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: CLR, PO4, I8P, CPL

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	0.26	0/4944	0.45	0/6699
1	B	0.26	0/4919	0.46	0/6664
All	All	0.26	0/9863	0.45	0/13363

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	4805	4797	4802	52	0
1	B	4780	4775	4776	59	0
2	A	15	0	0	2	0
2	B	5	0	0	1	0
3	A	88	6	12	5	0
3	B	88	6	12	4	0
4	A	28	46	46	0	0
4	B	28	46	46	0	0
5	A	52	80	80	2	0
5	B	52	80	80	1	0
6	A	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
6	B	1	0	0	1	0
All	All	9943	9836	9854	113	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 6.

All (113) 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:251:LEU:HD21	1:B:331:LEU:HD23	1.29	1.13
1:A:7:LEU:O	1:A:11:ILE:HG13	1.62	0.98
1:A:7:LEU:HG	1:A:11:ILE:HD11	1.48	0.94
1:B:474:PHE:O	1:B:478:VAL:HG23	1.82	0.79
1:A:11:ILE:HG23	1:A:19:TYR:CD2	2.23	0.72
1:A:270:ARG:NH1	2:A:703:PO4:O2	2.23	0.71
1:A:160:LEU:HD13	1:A:176:ARG:HB2	1.74	0.70
1:B:182:VAL:HG12	1:B:182:VAL:O	1.91	0.70
1:A:604:ARG:NH2	2:A:702:PO4:O3	2.24	0.70
1:B:550:GLU:N	1:B:550:GLU:OE1	2.27	0.68
1:B:26:LYS:NZ	3:B:702:I8P:O55	2.22	0.67
1:B:190:LYS:O	1:B:193:GLN:NE2	2.31	0.64
1:B:254:ALA:O	1:B:258:LYS:N	2.31	0.64
1:B:579:ILE:HD13	1:B:584:LEU:HD23	1.79	0.63
1:A:145:LEU:HD23	1:A:191:ILE:HD11	1.80	0.62
1:B:343:PRO:O	1:B:346:VAL:HG22	1.99	0.62
1:A:240:PHE:HA	1:A:325:ILE:HD11	1.82	0.60
1:B:191:ILE:O	1:B:195:ILE:HG13	2.03	0.58
1:A:2:LYS:HA	3:A:704:I8P:O61	2.02	0.58
1:A:474:PHE:O	1:A:478:VAL:HG23	2.04	0.57
1:A:139:TYR:CD2	1:A:218:LEU:HD13	2.40	0.57
1:A:218:LEU:HD12	1:A:218:LEU:O	2.06	0.56
1:B:499:HIS:ND1	1:B:504:HIS:CD2	2.73	0.56
1:B:561:CYS:HA	1:B:564:ILE:HD12	1.87	0.56
1:B:546:PHE:O	1:B:547:LEU:HD23	2.06	0.56
1:A:199:GLU:OE1	1:A:211:ARG:NH2	2.39	0.56
1:A:65:GLU:OE2	1:A:69:ILE:HD11	2.07	0.55
1:B:129:LYS:NZ	3:B:703:I8P:O42	2.40	0.55
1:A:7:LEU:HG	1:A:11:ILE:CD1	2.27	0.54
1:B:160:LEU:HD13	1:B:176:ARG:HB2	1.89	0.54
1:A:285:LEU:HD21	5:A:707:CPL:H362	1.89	0.54
1:B:466:ARG:NH1	2:B:701:PO4:O4	2.41	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:611:ARG:NH1	1:B:620:CYS:SG	2.81	0.53
1:B:138:PHE:CE2	1:B:142:LEU:HD11	2.45	0.52
1:B:550:GLU:HG2	1:B:617:LEU:HD13	1.91	0.52
1:B:538:ASP:OD1	1:B:539:LYS:N	2.42	0.52
1:A:127:ASN:OD1	1:A:631:VAL:CG1	2.58	0.52
1:B:402:SER:HB2	1:B:604:ARG:HE	1.75	0.51
1:B:482:LYS:O	1:B:485:THR:OG1	2.28	0.51
1:B:244:PHE:O	1:B:248:ASN:ND2	2.44	0.51
1:A:11:ILE:HG23	1:A:19:TYR:CE2	2.45	0.51
1:B:199:GLU:O	1:B:203:THR:HG23	2.11	0.51
1:A:246:VAL:HG23	1:B:243:ILE:HD13	1.92	0.51
1:B:203:THR:HG22	1:B:214:ALA:HB3	1.93	0.51
1:B:511:PHE:CE2	1:B:515:ILE:HD11	2.47	0.50
1:B:579:ILE:CD1	1:B:584:LEU:HD23	2.41	0.50
1:B:182:VAL:O	1:B:182:VAL:CG1	2.60	0.50
1:A:383:THR:OG1	1:A:387:HIS:NE2	2.42	0.49
1:B:240:PHE:HA	1:B:325:ILE:HD11	1.95	0.49
1:B:333:ALA:O	1:B:337:ALA:N	2.40	0.49
1:B:342:ILE:HG23	1:B:346:VAL:HG21	1.93	0.49
1:B:284:LEU:HD12	1:B:601:VAL:HG12	1.95	0.48
1:B:67:ALA:O	1:B:71:THR:HG23	2.13	0.48
1:A:361:ASN:ND2	1:A:363:THR:OG1	2.46	0.48
1:B:145:LEU:HD23	1:B:191:ILE:CD1	2.43	0.48
1:A:357:PHE:O	1:A:361:ASN:N	2.46	0.48
1:B:569:LEU:HD22	1:B:599:LEU:HB3	1.96	0.48
1:A:369:LYS:NZ	3:A:705:I8P:O24	2.44	0.47
1:B:513:LEU:HA	1:B:516:VAL:HG12	1.95	0.47
1:A:563:ILE:O	1:A:567:VAL:HG23	2.15	0.47
1:B:195:ILE:O	1:B:199:GLU:HG3	2.15	0.47
1:A:138:PHE:CE2	1:A:142:LEU:HD11	2.50	0.47
1:B:90:GLU:HG2	1:B:131:LEU:HD21	1.97	0.46
1:A:318:GLU:OE2	1:A:367:TYR:OH	2.25	0.46
1:B:170:SER:O	1:B:170:SER:OG	2.29	0.46
1:A:37:PRO:HG2	1:A:47:VAL:HG22	1.98	0.46
1:B:359:LEU:HG	1:B:375:LEU:HD21	1.98	0.46
1:B:526:LEU:HD11	1:B:567:VAL:HG22	1.98	0.46
1:B:37:PRO:HG2	1:B:47:VAL:HG22	1.98	0.45
1:B:393:ASP:N	1:B:393:ASP:OD1	2.48	0.45
1:A:143:ILE:HG21	1:A:220:VAL:HG11	1.97	0.45
1:A:254:ALA:O	1:A:258:LYS:N	2.48	0.45
3:A:705:I8P:H1	3:A:705:I8P:O46	2.17	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:B:703:I8P:O24	3:B:703:I8P:H3	2.16	0.45
1:B:441:HIS:O	1:B:441:HIS:ND1	2.50	0.45
1:A:306:ASN:HB2	5:A:707:CPL:HC71	1.99	0.44
1:B:203:THR:HG22	1:B:214:ALA:CB	2.47	0.44
3:B:702:I8P:O42	6:B:801:HOH:O	2.21	0.44
1:B:77:LEU:O	1:B:77:LEU:HD13	2.16	0.44
1:A:82:ARG:O	1:A:86:THR:HG23	2.17	0.44
1:A:393:ASP:N	1:A:393:ASP:OD1	2.50	0.44
1:B:66:LEU:HD12	1:B:66:LEU:O	2.18	0.44
1:A:127:ASN:ND2	1:A:632:ALA:O	2.50	0.44
1:A:195:ILE:O	1:A:199:GLU:HG3	2.17	0.44
1:A:272:TYR:OH	1:A:334:CYS:SG	2.74	0.44
1:B:305:LEU:HD13	5:B:705:CPL:HC11	1.99	0.44
1:A:516:VAL:O	1:A:520:ILE:HG12	2.18	0.44
1:A:272:TYR:HH	1:A:334:CYS:HG	1.59	0.44
1:A:520:ILE:HD13	1:A:520:ILE:N	2.33	0.44
1:B:513:LEU:O	1:B:516:VAL:HG12	2.18	0.44
1:B:486:THR:O	1:B:490:VAL:HG23	2.17	0.43
1:A:451:VAL:HA	1:A:454:ILE:HD12	2.01	0.43
1:B:385:PRO:HD3	1:B:461:ILE:HG21	1.99	0.43
1:A:26:LYS:HD2	3:A:704:I8P:O51	2.19	0.43
1:A:237:VAL:HG22	1:A:318:GLU:HB3	2.00	0.43
1:B:145:LEU:HD23	1:B:191:ILE:HD11	2.01	0.42
1:B:347:TYR:HB2	1:B:348:PRO:HD3	2.01	0.42
1:A:141:SER:OG	1:A:626:VAL:HG21	2.19	0.42
1:A:202:VAL:HG11	1:A:218:LEU:HD21	2.01	0.42
1:B:301:LEU:C	1:B:301:LEU:HD23	2.40	0.42
1:B:546:PHE:C	1:B:547:LEU:HD23	2.40	0.42
1:A:143:ILE:CG2	1:A:220:VAL:HG11	2.50	0.41
1:A:279:ILE:HD13	1:A:324:GLY:HA2	2.01	0.41
1:A:402:SER:OG	1:A:600:GLU:OE2	2.34	0.41
1:A:165:LYS:HZ1	3:A:704:I8P:PA2	2.43	0.41
1:A:526:LEU:HD11	1:A:567:VAL:HG22	2.02	0.41
1:A:207:GLU:OE2	1:A:217:ARG:NH1	2.50	0.41
1:B:279:ILE:HD13	1:B:324:GLY:HA2	2.02	0.41
1:A:7:LEU:CG	1:A:11:ILE:HD11	2.35	0.41
1:B:533:ASP:OD1	1:B:611:ARG:NE	2.53	0.41
1:A:360:ILE:O	1:A:360:ILE:CG2	2.69	0.41
1:A:534:TRP:O	1:A:548:ARG:NH2	2.43	0.41
1:B:470:THR:HG22	1:B:472:ARG:HG3	2.03	0.41

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	568/702 (81%)	557 (98%)	11 (2%)	0	100	100
1	B	564/702 (80%)	553 (98%)	11 (2%)	0	100	100
All	All	1132/1404 (81%)	1110 (98%)	22 (2%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	510/627 (81%)	494 (97%)	16 (3%)	35	63
1	B	507/627 (81%)	493 (97%)	14 (3%)	38	66
All	All	1017/1254 (81%)	987 (97%)	30 (3%)	39	65

All (30) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	156	PHE
1	A	219	ARG
1	A	367	TYR
1	A	393	ASP
1	A	394	PHE
1	A	402	SER
1	A	484	SER
1	A	518	TYR

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Mol	Chain	Res	Type
1	A	524	TYR
1	A	539	LYS
1	A	548	ARG
1	A	576	GLN
1	A	590	ASP
1	A	605	PHE
1	A	609	PHE
1	A	619	ASN
1	B	8	SER
1	B	28	MET
1	B	136	SER
1	B	156	PHE
1	B	185	PHE
1	B	293	ARG
1	B	393	ASP
1	B	394	PHE
1	B	445	TYR
1	B	524	TYR
1	B	576	GLN
1	B	605	PHE
1	B	609	PHE
1	B	620	CYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (3) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	476	HIS
1	B	504	HIS
1	B	614	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

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

5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry ⓘ

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	PO4	A	702	-	4,4,4	1.57	1 (25%)	6,6,6	0.49	0
3	I8P	B	702	-	42,44,44	2.40	10 (23%)	68,74,74	1.36	11 (16%)
3	I8P	B	703	-	42,44,44	2.42	10 (23%)	68,74,74	1.39	10 (14%)
4	CLR	B	704	-	31,31,31	1.08	1 (3%)	48,48,48	1.34	7 (14%)
4	CLR	A	706	-	31,31,31	1.08	2 (6%)	48,48,48	1.35	7 (14%)
5	CPL	B	705	-	51,51,51	1.04	3 (5%)	57,59,59	0.98	3 (5%)
3	I8P	A	704	-	42,44,44	2.48	10 (23%)	68,74,74	1.39	11 (16%)
2	PO4	A	703	-	4,4,4	1.55	1 (25%)	6,6,6	0.46	0
5	CPL	A	707	-	51,51,51	1.04	3 (5%)	57,59,59	0.98	3 (5%)
2	PO4	B	701	-	4,4,4	1.56	1 (25%)	6,6,6	0.48	0
3	I8P	A	705	-	42,44,44	2.42	10 (23%)	68,74,74	1.39	10 (14%)
2	PO4	A	701	-	4,4,4	1.56	1 (25%)	6,6,6	0.48	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
3	I8P	B	702	-	-	7/42/66/66	0/1/1/1
3	I8P	B	703	-	-	15/42/66/66	0/1/1/1
4	CLR	B	704	-	-	4/10/68/68	0/4/4/4
4	CLR	A	706	-	-	1/10/68/68	0/4/4/4

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	CPL	B	705	-	-	21/55/55/55	-
3	I8P	A	704	-	-	11/42/66/66	0/1/1/1
5	CPL	A	707	-	-	24/55/55/55	-
3	I8P	A	705	-	-	20/42/66/66	0/1/1/1

All (53) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	703	I8P	PA4-O14	7.30	1.72	1.59
3	A	705	I8P	PA4-O14	7.28	1.72	1.59
3	B	702	I8P	PA4-O14	7.27	1.72	1.59
3	A	704	I8P	PA4-O14	7.21	1.72	1.59
3	A	704	I8P	PA6-O16	7.02	1.71	1.59
3	A	705	I8P	PA6-O16	6.70	1.71	1.59
3	B	703	I8P	PA6-O16	6.65	1.71	1.59
3	B	702	I8P	PA6-O16	6.57	1.71	1.59
3	B	703	I8P	PA2-O12	6.45	1.70	1.59
3	A	705	I8P	PA2-O12	6.43	1.70	1.59
3	B	703	I8P	PA3-O13	6.37	1.70	1.59
3	A	704	I8P	PA3-O13	6.35	1.70	1.59
3	B	702	I8P	PA2-O12	6.35	1.70	1.59
3	A	705	I8P	PA3-O13	6.33	1.70	1.59
3	A	704	I8P	PA2-O12	6.28	1.70	1.59
3	B	702	I8P	PA3-O13	6.19	1.70	1.59
3	A	704	I8P	C3-C2	3.85	1.60	1.52
5	A	707	CPL	P-O3P	3.83	1.74	1.59
5	B	705	CPL	P-O3P	3.82	1.74	1.59
3	A	704	I8P	C4-C3	3.14	1.58	1.52
5	A	707	CPL	P-O4P	3.14	1.71	1.59
5	B	705	CPL	P-O4P	3.13	1.71	1.59
3	B	702	I8P	C3-C2	2.85	1.58	1.52
3	A	704	I8P	C2-C1	2.75	1.57	1.52
2	A	702	PO4	P-O1	2.73	1.57	1.50
2	B	701	PO4	P-O1	2.72	1.56	1.50
2	A	703	PO4	P-O1	2.71	1.56	1.50
3	B	703	I8P	C5-C4	2.71	1.57	1.52
2	A	701	PO4	P-O1	2.70	1.56	1.50
3	A	705	I8P	C5-C4	2.65	1.57	1.52
3	B	702	I8P	C2-C1	2.50	1.57	1.52
3	A	705	I8P	C6-C5	2.31	1.57	1.52
3	A	704	I8P	C5-C4	2.29	1.57	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	702	I8P	C4-C3	2.23	1.56	1.52
3	A	704	I8P	PA1-O41	2.20	1.61	1.59
3	B	703	I8P	C4-C3	2.16	1.56	1.52
3	B	703	I8P	C6-C5	2.15	1.56	1.52
3	B	702	I8P	PA2-O32	2.15	1.57	1.50
3	A	704	I8P	PA2-O32	2.12	1.57	1.50
3	A	705	I8P	PA2-O32	2.11	1.57	1.50
3	B	703	I8P	C3-C2	2.11	1.56	1.52
3	A	705	I8P	PA1-O41	2.11	1.61	1.59
3	B	702	I8P	C5-C4	2.10	1.56	1.52
3	B	703	I8P	PA2-O32	2.09	1.57	1.50
3	B	703	I8P	PA1-O41	2.07	1.61	1.59
3	A	705	I8P	C6-C1	2.07	1.56	1.52
4	A	706	CLR	C16-C17	2.06	1.58	1.54
3	B	702	I8P	PA1-O41	2.05	1.61	1.59
4	A	706	CLR	C7-C6	2.04	1.54	1.50
3	A	705	I8P	C3-C2	2.03	1.56	1.52
5	B	705	CPL	O3P-C1	-2.03	1.36	1.44
5	A	707	CPL	O3P-C1	-2.02	1.36	1.44
4	B	704	CLR	C18-C13	-2.02	1.51	1.54

All (62) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	A	707	CPL	O2P-P-O1P	4.80	134.78	112.44
5	B	705	CPL	O2P-P-O1P	4.80	134.77	112.44
3	A	704	I8P	O35-PA5-O45	-3.59	97.57	107.27
3	A	705	I8P	O35-PA5-O45	-3.54	97.72	107.27
3	B	702	I8P	O35-PA5-O45	-3.53	97.73	107.27
3	B	703	I8P	O35-PA5-O45	-3.52	97.76	107.27
4	B	704	CLR	C22-C20-C17	-3.12	103.86	110.33
4	A	706	CLR	C22-C20-C17	-3.02	104.08	110.33
3	B	703	I8P	C6-C5-C4	2.92	116.83	110.43
3	A	705	I8P	C6-C5-C4	2.90	116.78	110.43
3	A	705	I8P	O71-PB1-O41	2.83	114.14	104.64
3	B	702	I8P	O71-PB1-O41	2.81	114.07	104.64
3	B	703	I8P	O71-PB1-O41	2.81	114.07	104.64
3	A	704	I8P	O71-PB1-O41	2.81	114.05	104.64
3	B	703	I8P	O11-PA1-O21	2.64	118.25	109.81
3	A	704	I8P	O11-PA1-O21	2.64	118.23	109.81
3	A	705	I8P	O11-PA1-O21	2.63	118.20	109.81
3	B	702	I8P	O11-PA1-O21	2.62	118.18	109.81

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	706	CLR	C18-C13-C12	2.58	114.40	110.61
4	B	704	CLR	C18-C13-C12	2.57	114.40	110.61
3	A	704	I8P	O24-PA4-O14	2.55	115.78	105.85
3	B	702	I8P	O24-PA4-O14	2.54	115.75	105.85
3	B	703	I8P	O24-PA4-O14	2.54	115.73	105.85
3	A	705	I8P	O42-PA2-O12	2.53	115.72	105.85
3	A	704	I8P	O42-PA2-O12	2.53	115.69	105.85
3	B	703	I8P	O42-PA2-O12	2.52	115.67	105.85
3	B	702	I8P	O42-PA2-O12	2.52	115.66	105.85
3	A	705	I8P	O24-PA4-O14	2.52	115.65	105.85
4	A	706	CLR	C21-C20-C22	-2.43	106.58	110.34
3	A	704	I8P	C6-C5-C4	2.42	115.74	110.43
5	B	705	CPL	C4-C5-N	-2.39	108.16	115.82
3	A	705	I8P	O36-PA6-O26	2.38	116.73	107.80
5	A	707	CPL	C4-C5-N	-2.38	108.19	115.82
3	B	702	I8P	O36-PA6-O26	2.38	116.72	107.80
3	B	703	I8P	O36-PA6-O26	2.37	116.69	107.80
4	B	704	CLR	C7-C8-C14	-2.34	107.62	110.93
4	A	706	CLR	C12-C13-C14	-2.30	103.80	107.25
3	A	704	I8P	O36-PA6-O26	2.30	116.42	107.80
4	B	704	CLR	C21-C20-C22	-2.30	106.78	110.34
3	B	702	I8P	C6-C5-C4	2.23	115.33	110.43
5	A	707	CPL	O2-C31-C32	2.23	116.30	111.48
4	A	706	CLR	C7-C8-C14	-2.21	107.80	110.93
4	B	704	CLR	C10-C5-C6	2.21	126.16	122.93
5	B	705	CPL	O2-C31-C32	2.21	116.26	111.48
3	A	704	I8P	O23-PA3-O13	2.20	114.43	105.85
3	B	703	I8P	O23-PA3-O13	2.20	114.41	105.85
3	A	705	I8P	O23-PA3-O13	2.19	114.36	105.85
3	B	702	I8P	O23-PA3-O13	2.17	114.32	105.85
3	A	704	I8P	O75-PB5-O65	-2.13	99.81	107.80
3	A	705	I8P	O75-PB5-O65	-2.13	99.83	107.80
3	B	703	I8P	O75-PB5-O65	-2.12	99.87	107.80
3	B	702	I8P	O75-PB5-O65	-2.11	99.88	107.80
3	A	705	I8P	O15-PA5-O25	2.08	116.47	109.81
4	A	706	CLR	C24-C23-C22	-2.08	103.95	113.28
3	B	702	I8P	O15-PA5-O25	2.07	116.42	109.81
4	A	706	CLR	C10-C5-C6	2.07	125.94	122.93
3	A	704	I8P	C5-C6-C1	-2.06	105.90	110.43
4	B	704	CLR	C12-C13-C17	-2.06	113.57	116.60
3	B	703	I8P	O15-PA5-O25	2.05	116.36	109.81
3	B	702	I8P	O12-C2-C1	2.05	113.12	108.76

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	704	I8P	O15-PA5-O25	2.05	116.34	109.81
4	B	704	CLR	C16-C17-C20	-2.04	109.09	112.18

There are no chirality outliers.

All (103) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	704	I8P	C6-C1-O11-PA1
3	A	704	I8P	C1-C6-O16-PA6
3	A	704	I8P	C5-O15-PA5-O45
3	A	704	I8P	PA1-O41-PB1-O51
3	A	704	I8P	PA1-O41-PB1-O71
3	A	705	I8P	C2-C1-O11-PA1
3	A	705	I8P	C6-C1-O11-PA1
3	A	705	I8P	C1-C2-O12-PA2
3	A	705	I8P	C3-C2-O12-PA2
3	A	705	I8P	C5-C6-O16-PA6
3	A	705	I8P	C1-O11-PA1-O41
3	A	705	I8P	C5-O15-PA5-O45
3	A	705	I8P	PB1-O41-PA1-O11
3	B	702	I8P	C5-O15-PA5-O45
3	B	703	I8P	C3-C4-O14-PA4
3	B	703	I8P	C5-C4-O14-PA4
3	B	703	I8P	C1-O11-PA1-O41
3	B	703	I8P	C5-O15-PA5-O45
5	A	707	CPL	O4P-C4-C5-N
5	A	707	CPL	C4-O4P-P-O1P
5	A	707	CPL	C4-O4P-P-O3P
5	B	705	CPL	C1-O3P-P-O2P
5	B	705	CPL	C4-O4P-P-O3P
4	B	704	CLR	C21-C20-C22-C23
4	B	704	CLR	C17-C20-C22-C23
5	B	705	CPL	C11-C12-C13-C14
5	A	707	CPL	C11-C12-C13-C14
3	A	705	I8P	C4-C5-O15-PA5
5	A	707	CPL	C14-C15-C16-C17
5	B	705	CPL	C19-C20-C21-C22
5	A	707	CPL	C22-C23-C24-C25
5	B	705	CPL	C22-C23-C24-C25
5	B	705	CPL	C14-C15-C16-C17
5	A	707	CPL	C19-C20-C21-C22
5	A	707	CPL	C31-C32-C33-C34

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Mol	Chain	Res	Type	Atoms
5	A	707	CPL	C33-C34-C35-C36
3	B	702	I8P	C6-O16-PA6-O46
5	A	707	CPL	C43-C44-C45-C46
5	A	707	CPL	C36-C37-C38-C39
5	B	705	CPL	C34-C35-C36-C37
3	A	705	I8P	C1-C6-O16-PA6
4	B	704	CLR	C20-C22-C23-C24
5	A	707	CPL	C23-C24-C25-C26
5	B	705	CPL	C45-C46-C47-C48
5	B	705	CPL	C32-C33-C34-C35
5	B	705	CPL	C20-C21-C22-C23
5	A	707	CPL	C40-C41-C42-C43
5	A	707	CPL	C18-C19-C20-C21
3	A	705	I8P	PB5-O45-PA5-O15
3	B	703	I8P	PB1-O41-PA1-O11
5	A	707	CPL	C32-C33-C34-C35
3	A	705	I8P	C6-C5-O15-PA5
5	B	705	CPL	C1-C2-C3-O3
3	A	704	I8P	C5-O15-PA5-O25
3	A	705	I8P	C1-O11-PA1-O21
3	B	702	I8P	PB1-O41-PA1-O31
3	B	703	I8P	C1-O11-PA1-O21
3	B	703	I8P	C5-O15-PA5-O25
5	B	705	CPL	O4P-C4-C5-N
5	A	707	CPL	C12-C11-O3-C3
3	B	703	I8P	C2-O12-PA2-O32
5	A	707	CPL	O3P-C1-C2-O2
5	A	707	CPL	O11-C11-O3-C3
5	B	705	CPL	C23-C24-C25-C26
5	B	705	CPL	C4-O4P-P-O1P
3	A	705	I8P	PA1-O41-PB1-O61
5	B	705	CPL	C4-C5-N-C6
5	B	705	CPL	O2-C2-C3-O3
5	A	707	CPL	C34-C35-C36-C37
4	B	704	CLR	C22-C23-C24-C25
3	B	703	I8P	C2-C1-O11-PA1
3	A	705	I8P	C6-O16-PA6-O26
4	A	706	CLR	C16-C17-C20-C22
5	A	707	CPL	C13-C14-C15-C16
5	A	707	CPL	O3P-C1-C2-C3
3	A	705	I8P	C2-C3-O13-PA3
3	A	705	I8P	C4-C3-O13-PA3

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Mol	Chain	Res	Type	Atoms
3	B	703	I8P	C6-C1-O11-PA1
3	B	702	I8P	C2-O12-PA2-O32
3	B	703	I8P	C6-O16-PA6-O46
3	A	704	I8P	PB1-O41-PA1-O21
3	A	704	I8P	PA1-O41-PB1-O61
5	B	705	CPL	C42-C43-C44-C45
5	A	707	CPL	C5-C4-O4P-P
3	A	704	I8P	C1-O11-PA1-O21
3	A	704	I8P	C5-O15-PA5-O35
3	A	705	I8P	C1-O11-PA1-O31
3	A	705	I8P	C5-O15-PA5-O25
3	B	702	I8P	C5-O15-PA5-O25
3	B	702	I8P	C5-O15-PA5-O35
3	B	702	I8P	PB1-O41-PA1-O21
3	B	703	I8P	C1-O11-PA1-O31
5	B	705	CPL	C37-C38-C39-C40
3	A	705	I8P	C4-O14-PA4-O24
3	B	703	I8P	C4-O14-PA4-O24
3	B	703	I8P	C6-O16-PA6-O26
5	B	705	CPL	C4-C5-N-C7
5	A	707	CPL	C45-C46-C47-C48
3	A	704	I8P	C2-O12-PA2-O32
3	B	703	I8P	C4-O14-PA4-O34
5	B	705	CPL	C44-C45-C46-C47
5	B	705	CPL	C31-C32-C33-C34
5	A	707	CPL	C42-C43-C44-C45

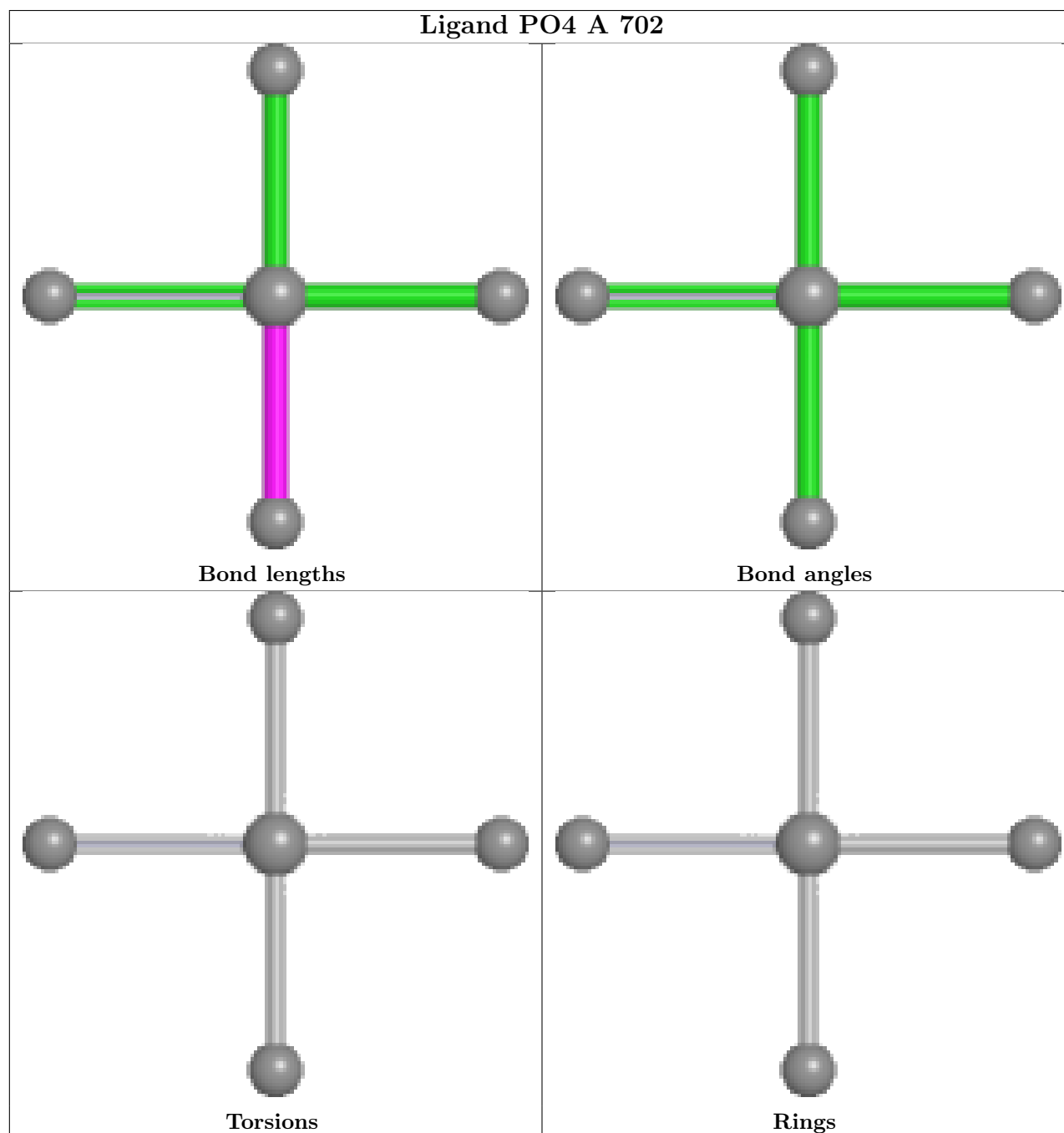
There are no ring outliers.

9 monomers are involved in 15 short contacts:

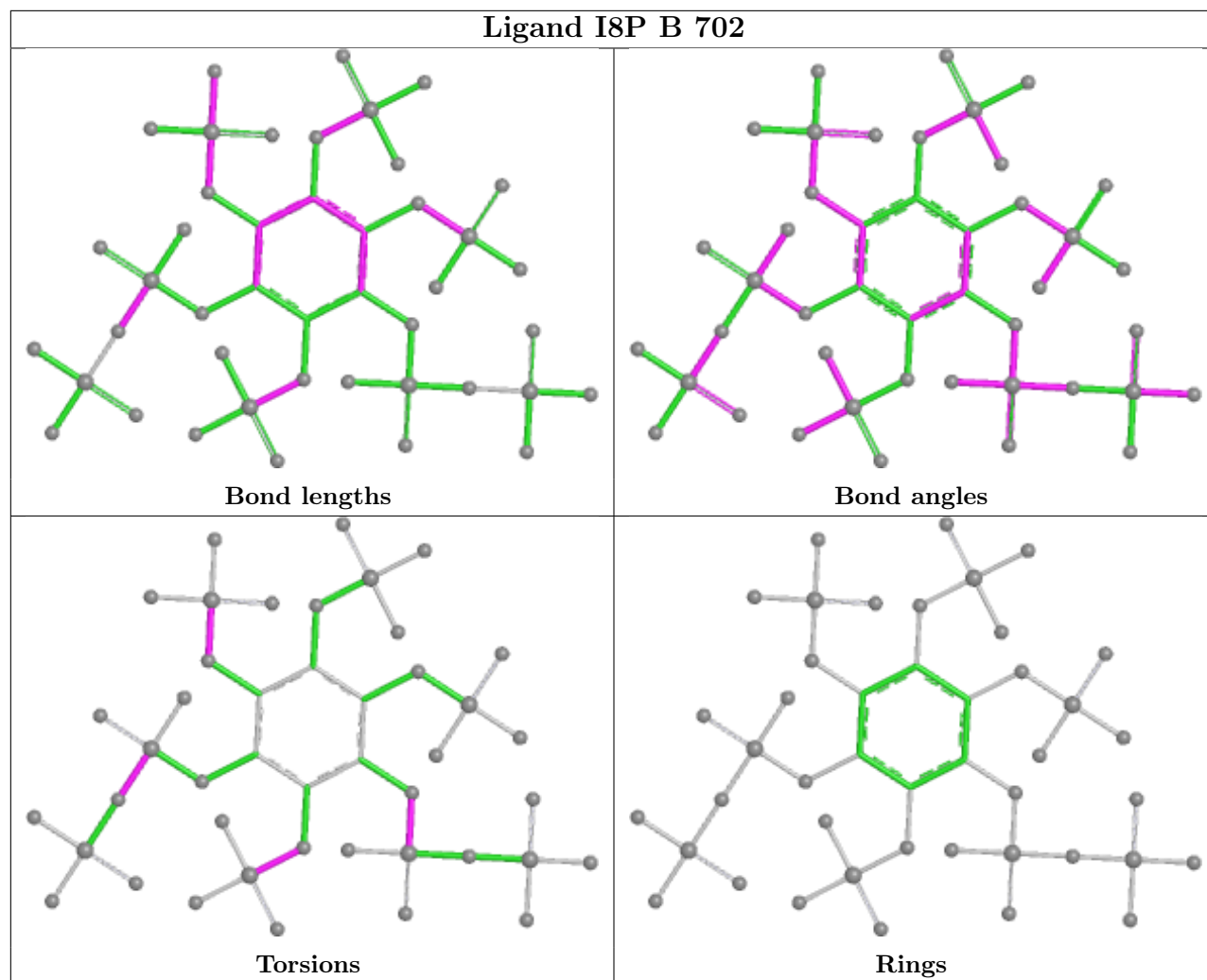
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	702	PO4	1	0
3	B	702	I8P	2	0
3	B	703	I8P	2	0
5	B	705	CPL	1	0
3	A	704	I8P	3	0
2	A	703	PO4	1	0
5	A	707	CPL	2	0
2	B	701	PO4	1	0
3	A	705	I8P	2	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths,

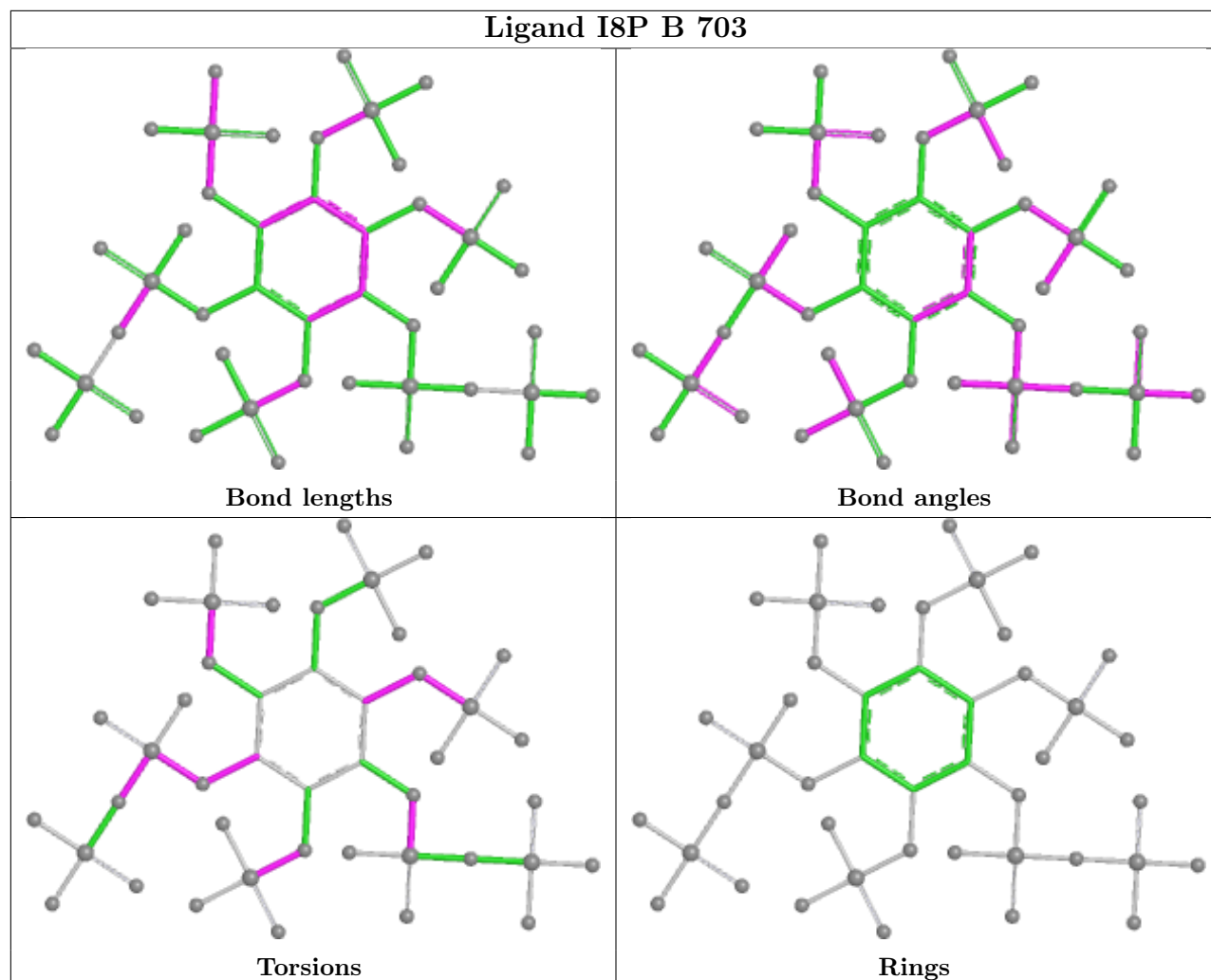
bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 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.



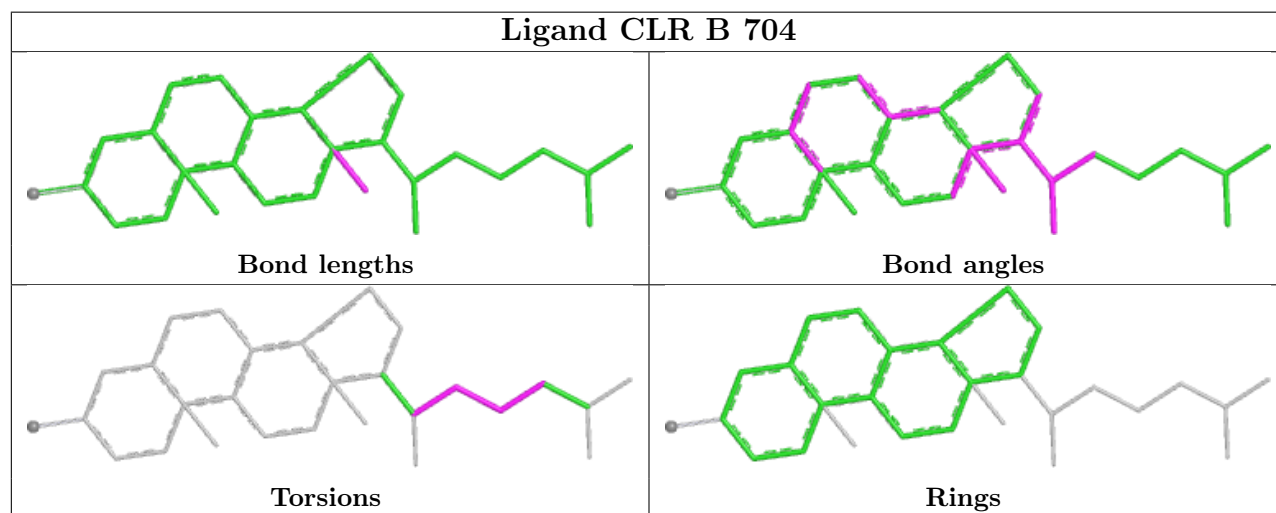
Ligand I8P B 702

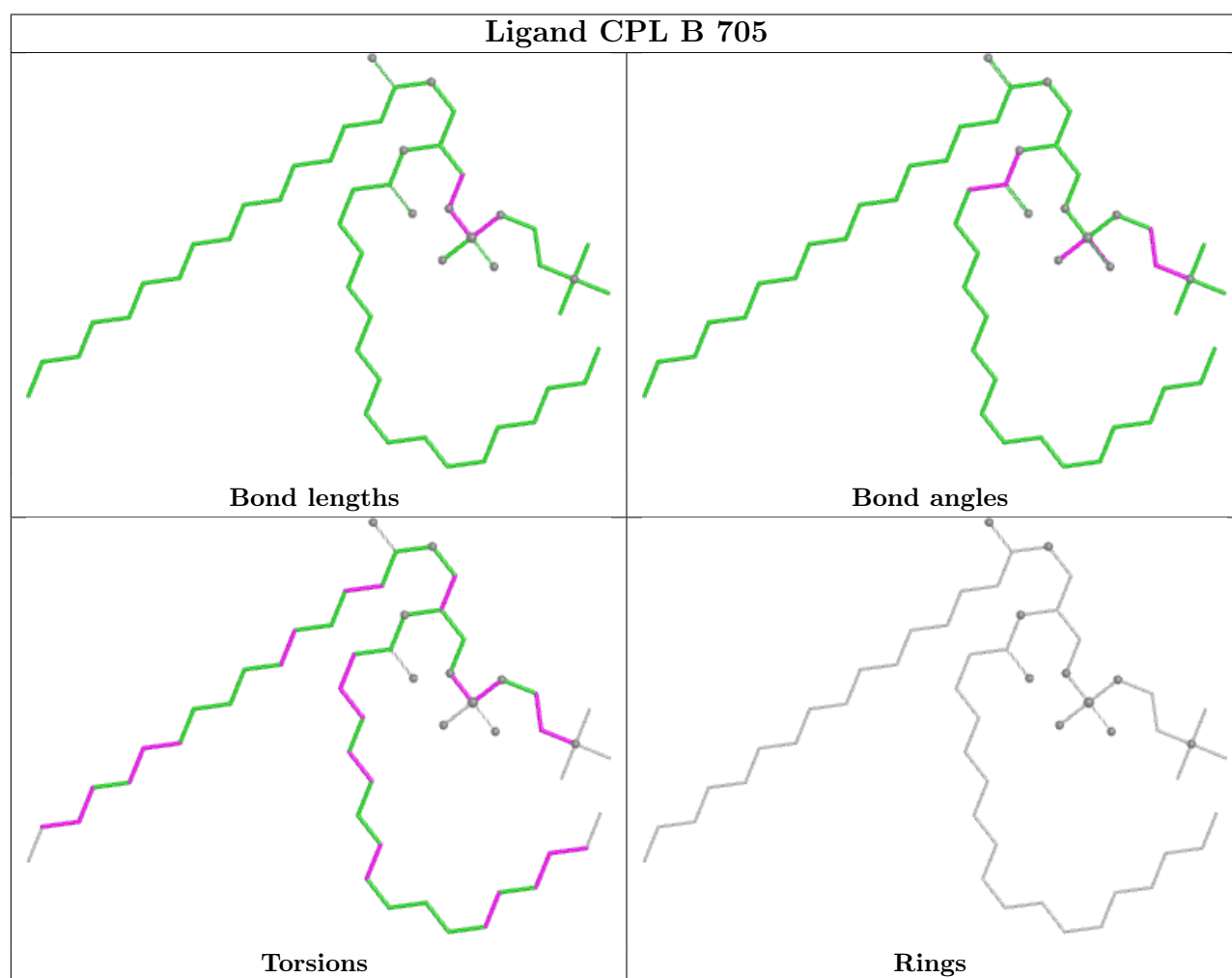
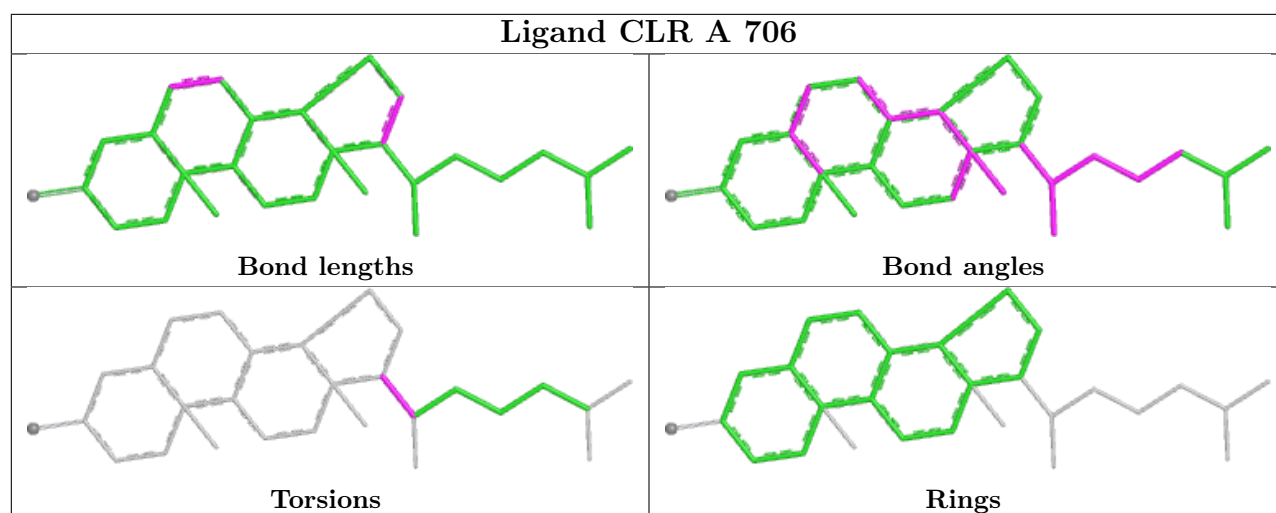


Ligand I8P B 703

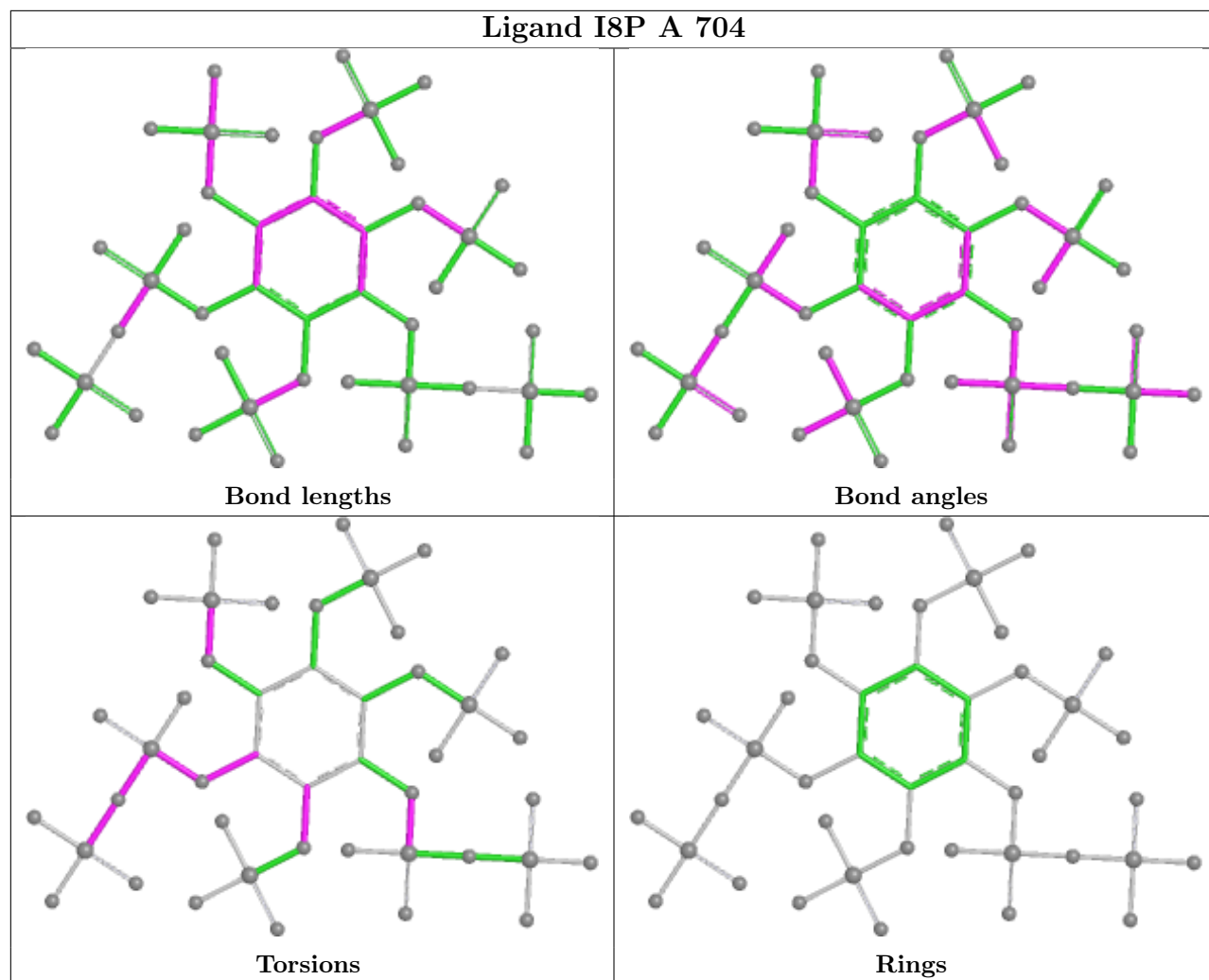


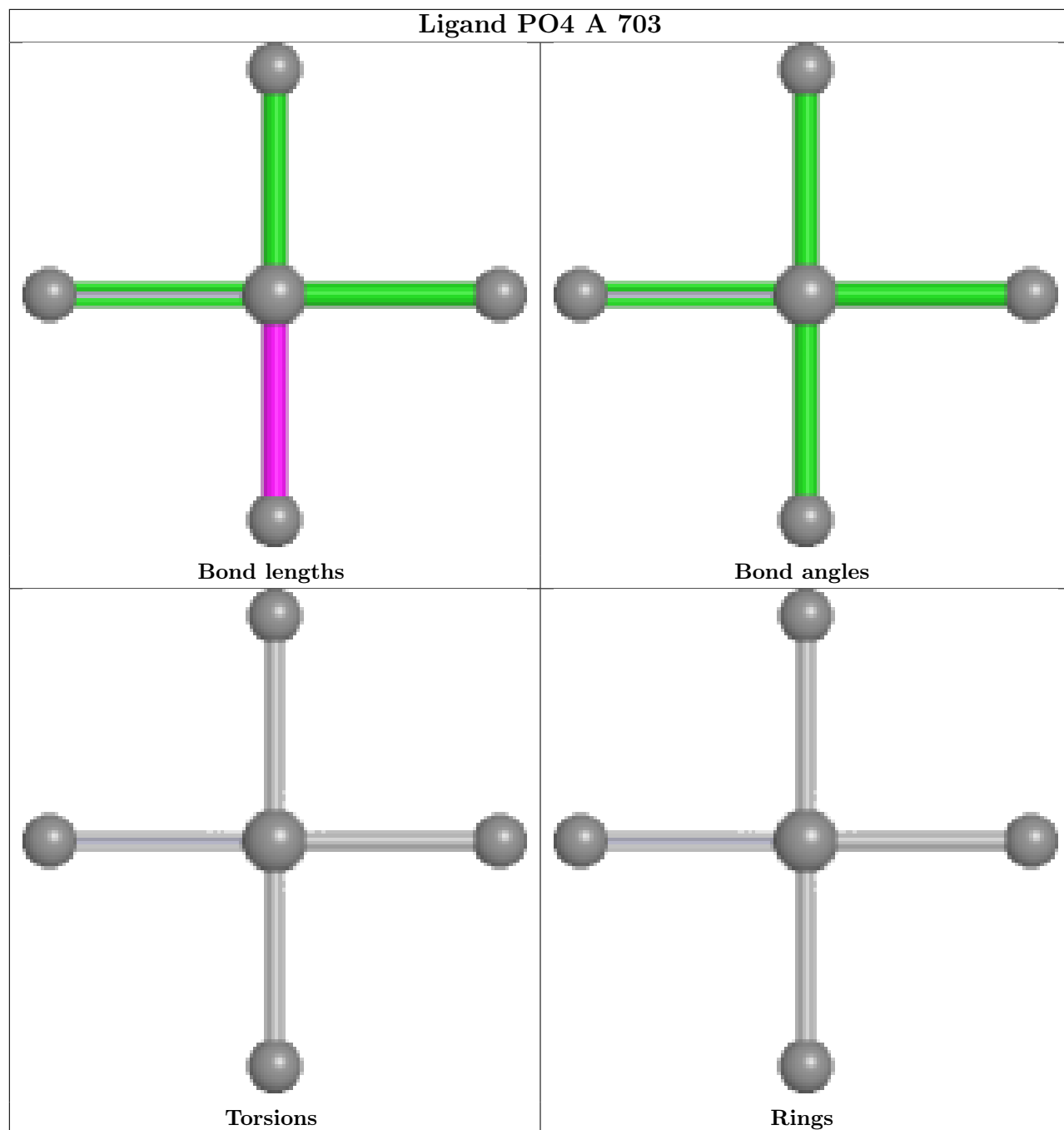
Ligand CLR B 704

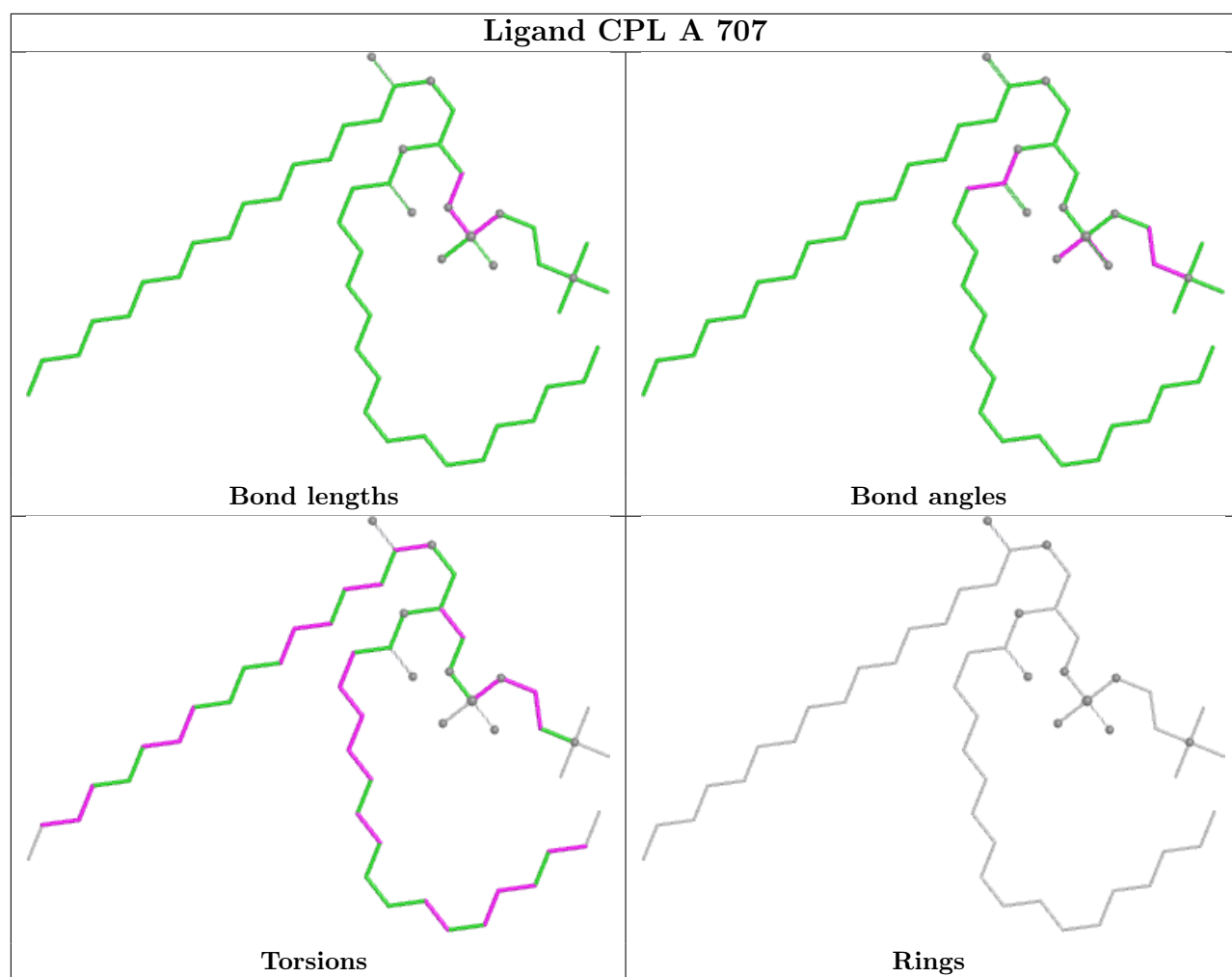


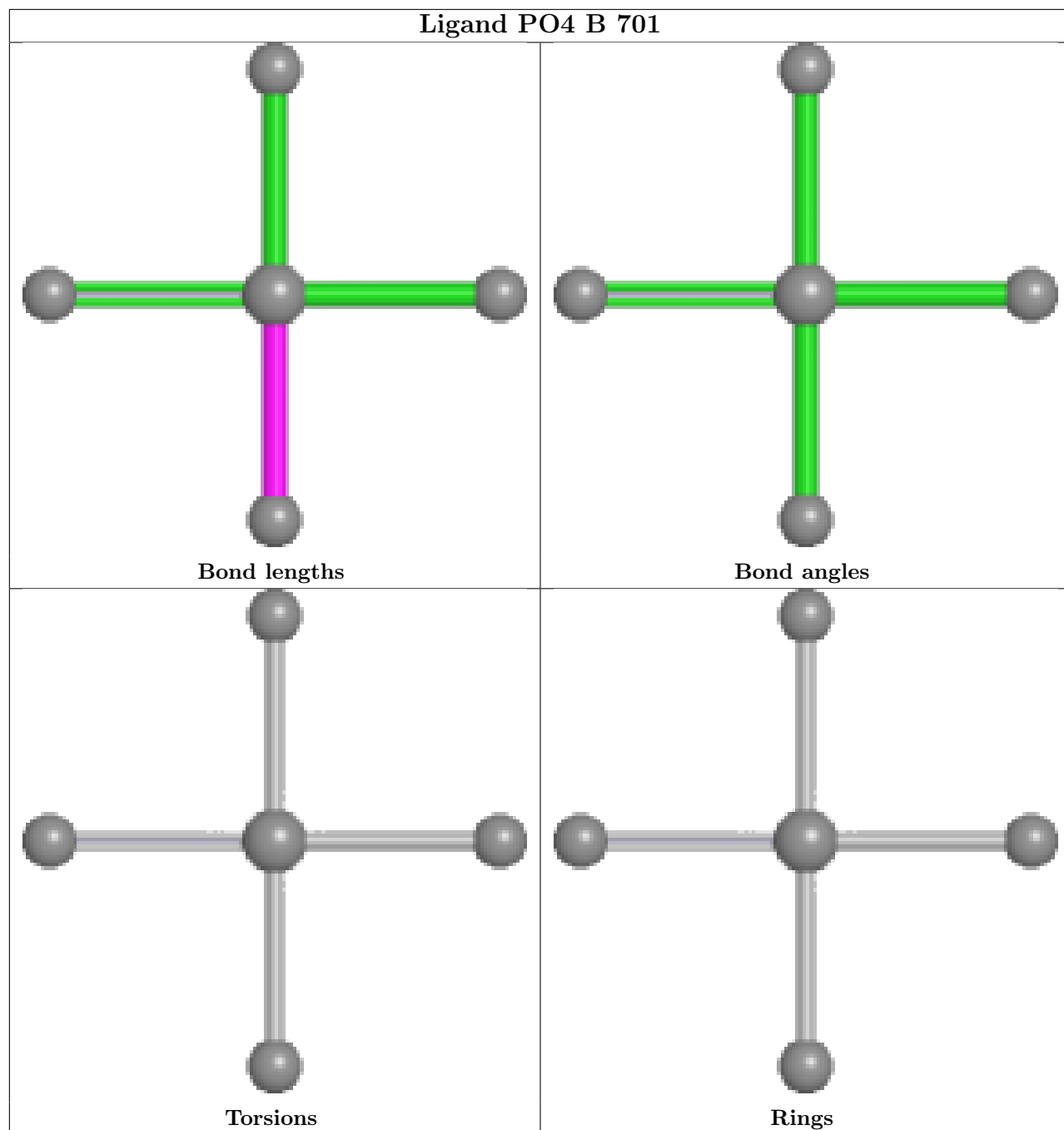


Ligand I8P A 704

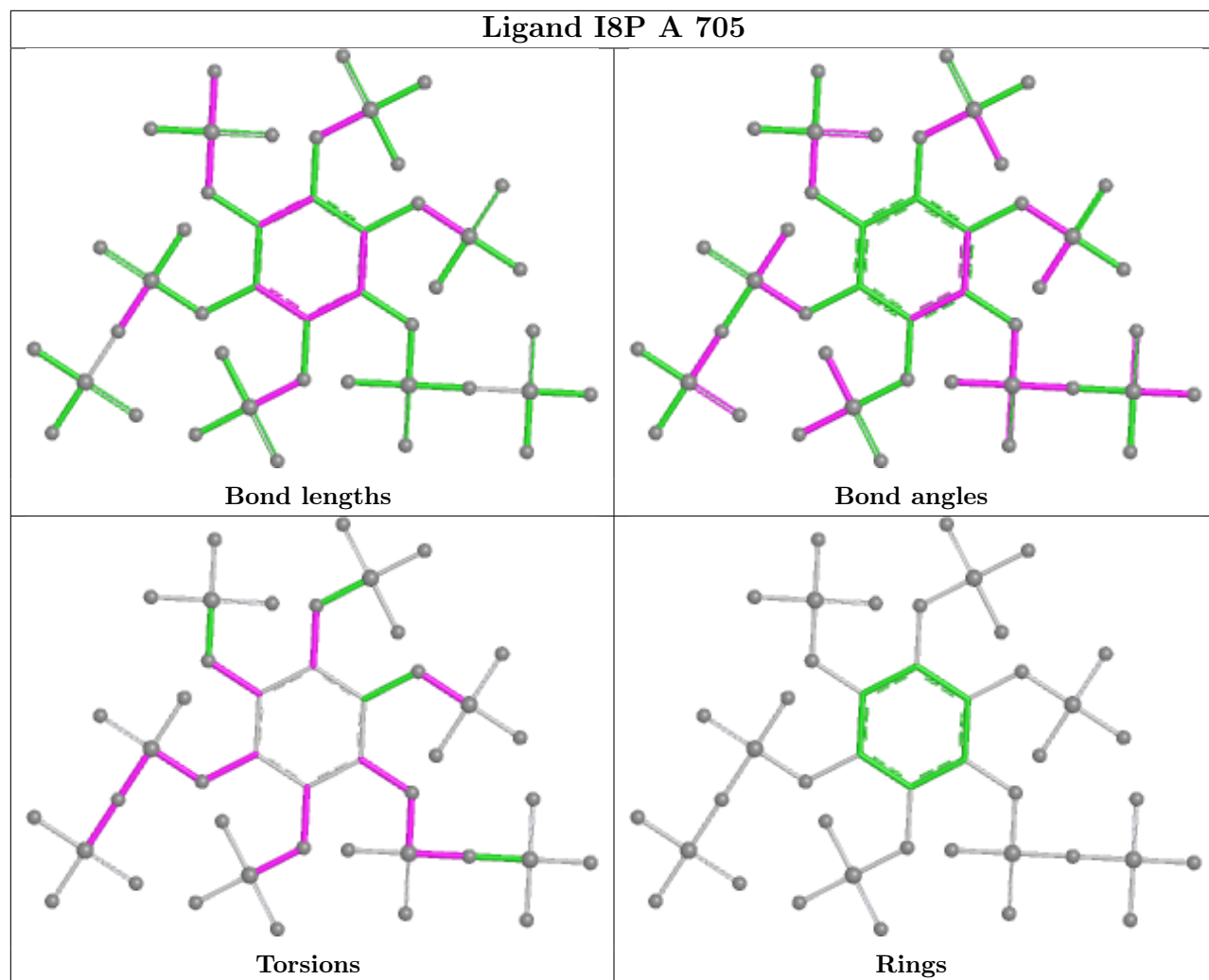


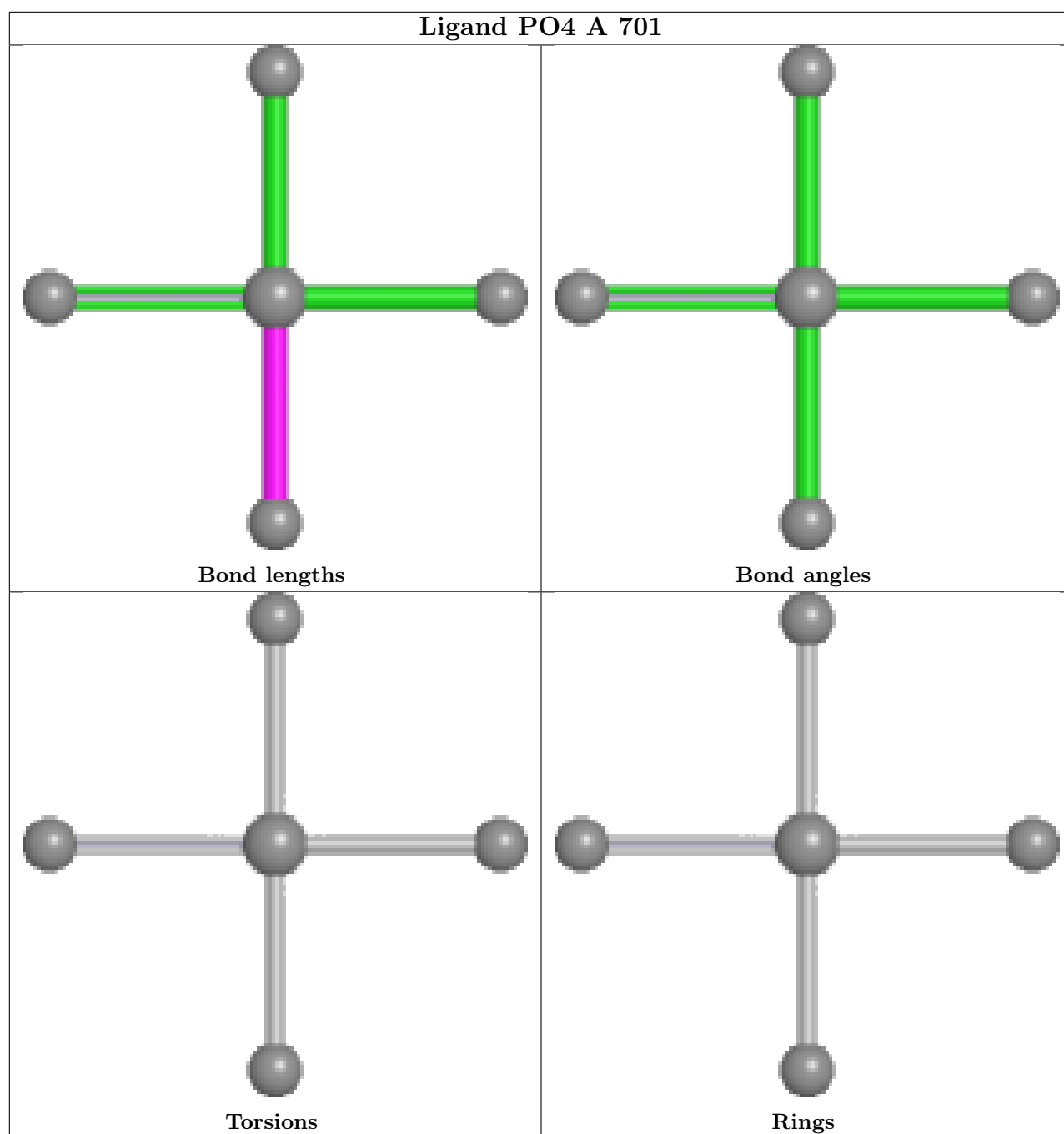






Ligand I8P A 705





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.

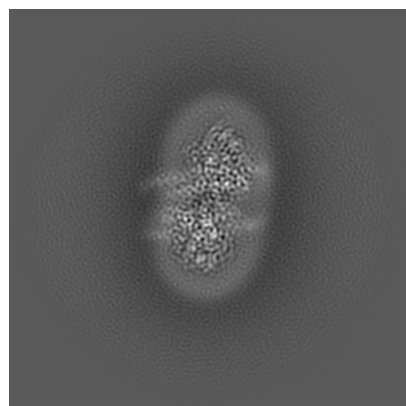
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-47213. These allow visual inspection of the internal detail of the map and identification of artifacts.

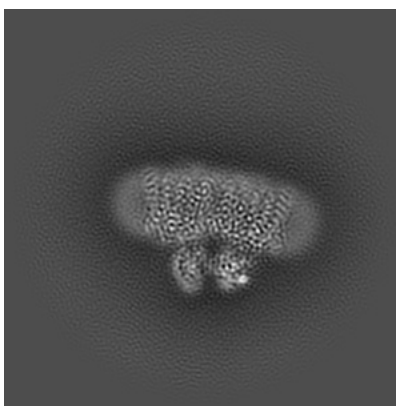
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

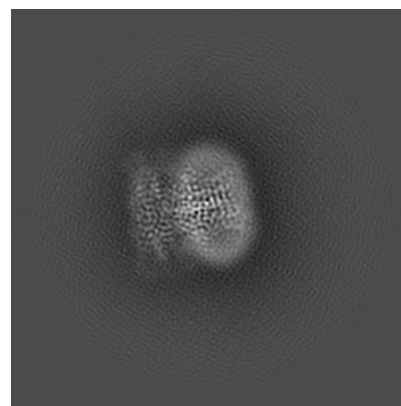
6.1.1 Primary map



X

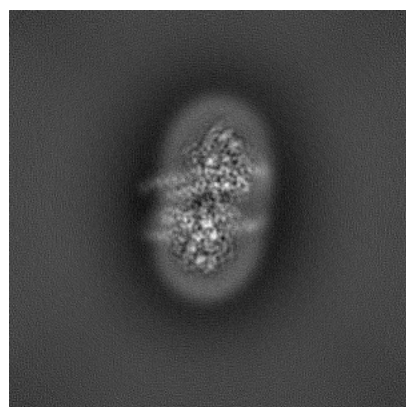


Y

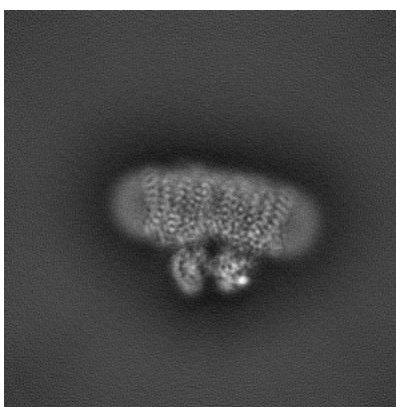


Z

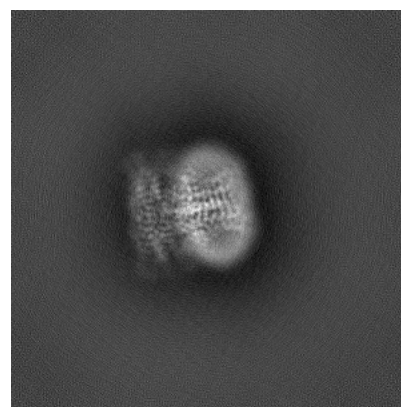
6.1.2 Raw map



X



Y

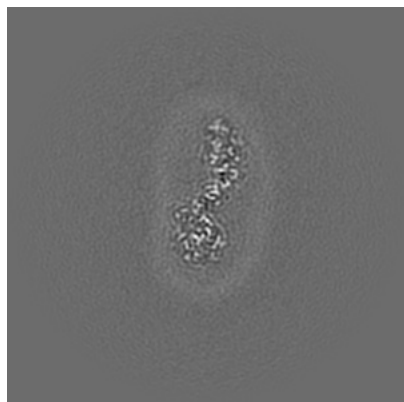


Z

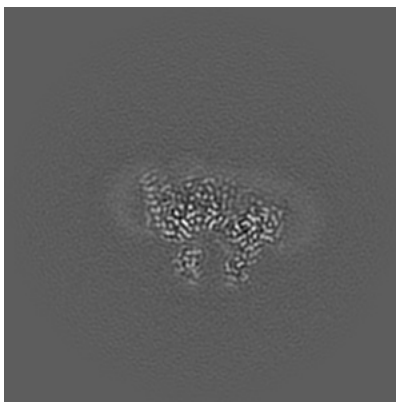
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

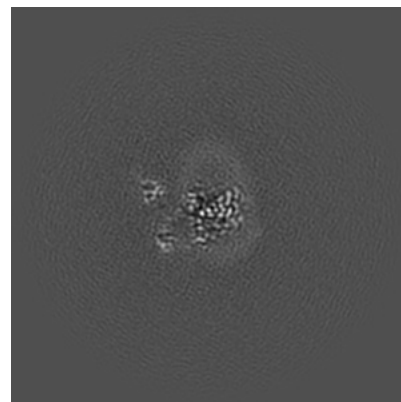
6.2.1 Primary map



X Index: 192

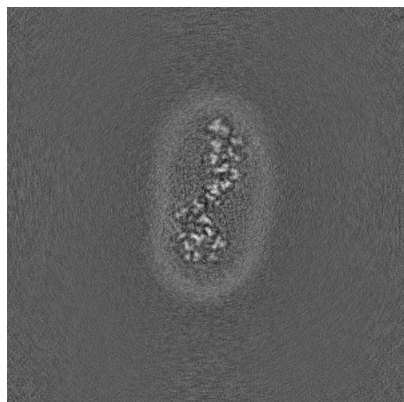


Y Index: 192

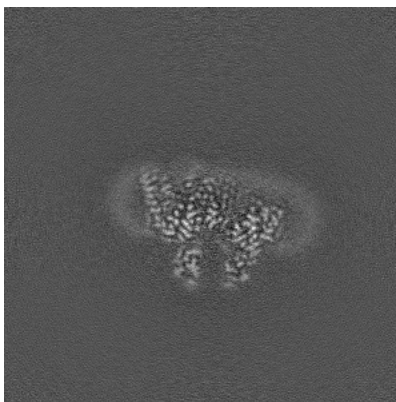


Z Index: 192

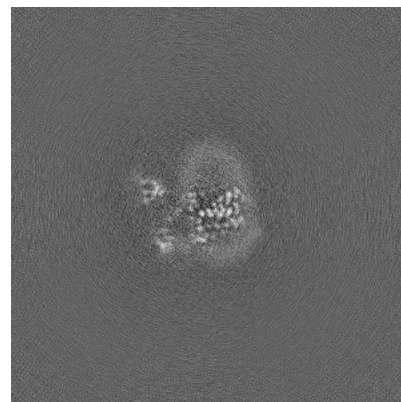
6.2.2 Raw map



X Index: 192



Y Index: 192

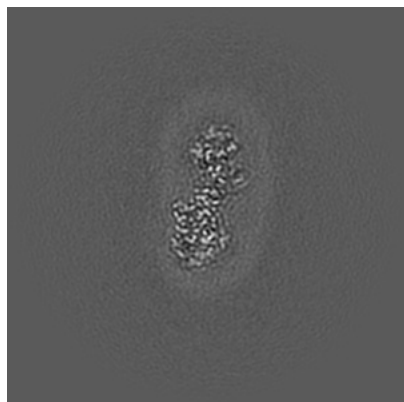


Z Index: 192

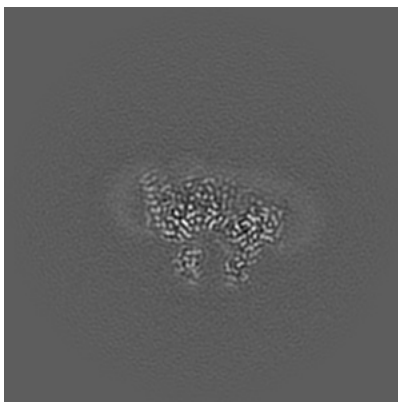
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

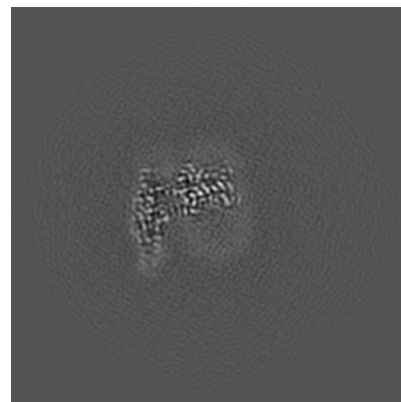
6.3.1 Primary map



X Index: 180

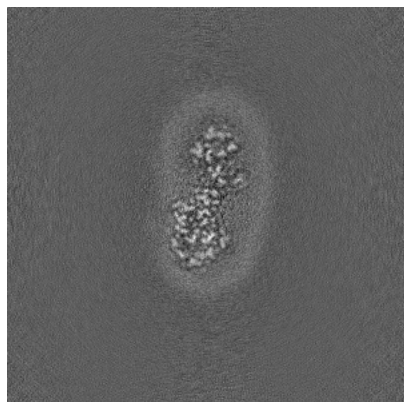


Y Index: 192

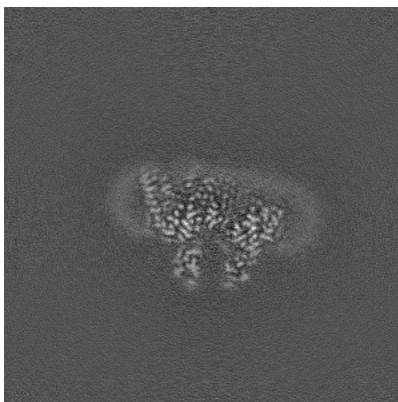


Z Index: 217

6.3.2 Raw map



X Index: 180



Y Index: 192

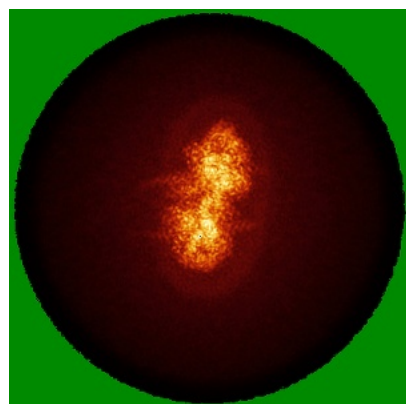


Z Index: 216

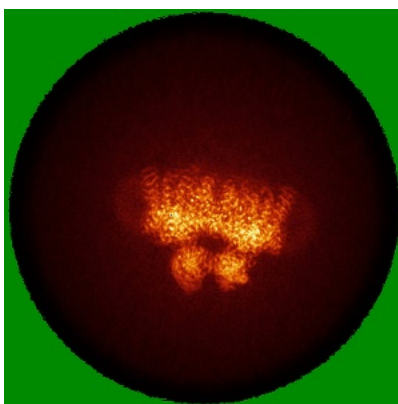
The images above show the largest variance slices of the map in three orthogonal directions.

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

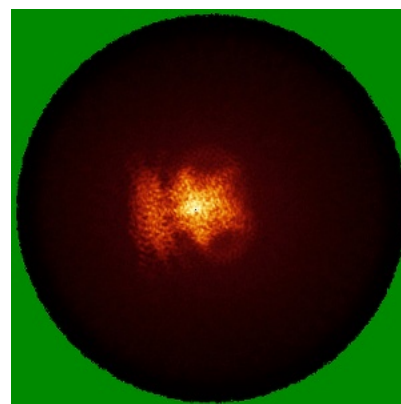
6.4.1 Primary map



X

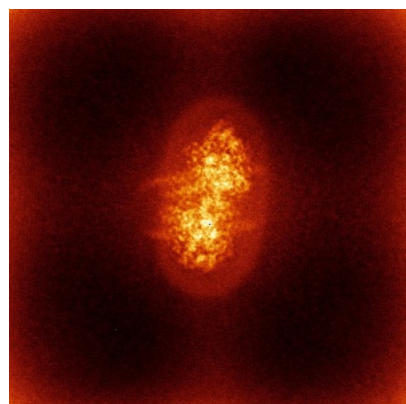


Y

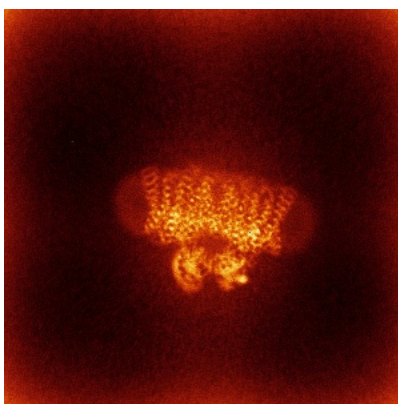


Z

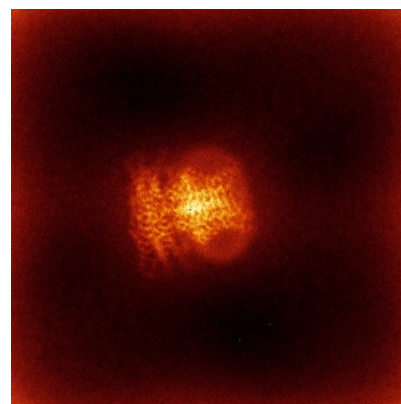
6.4.2 Raw map



X



Y

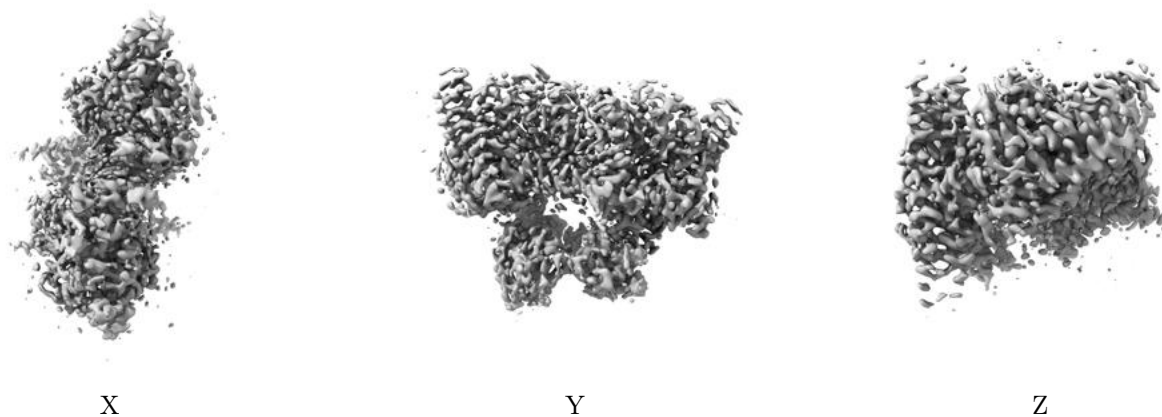


Z

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.

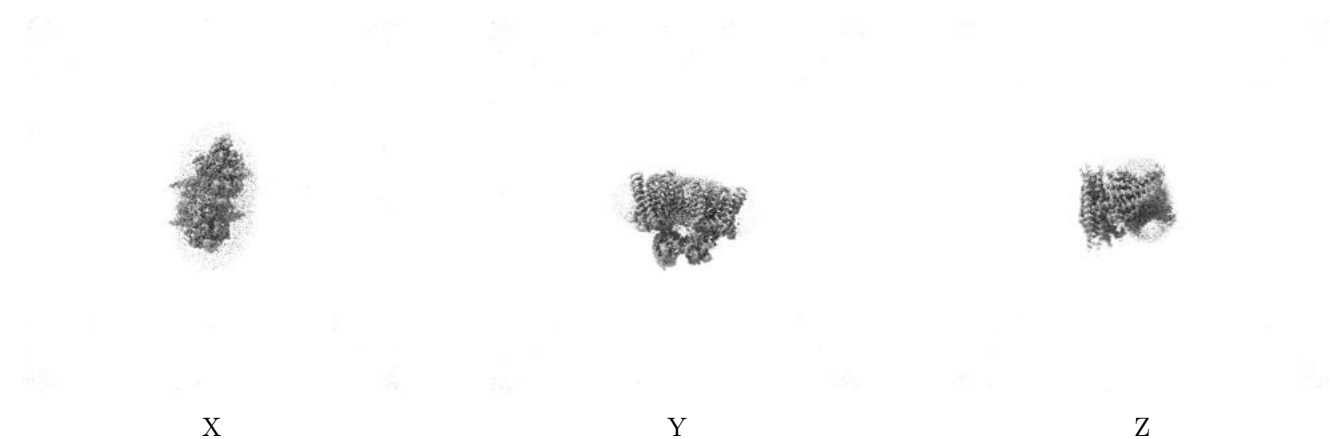
6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.065. 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.

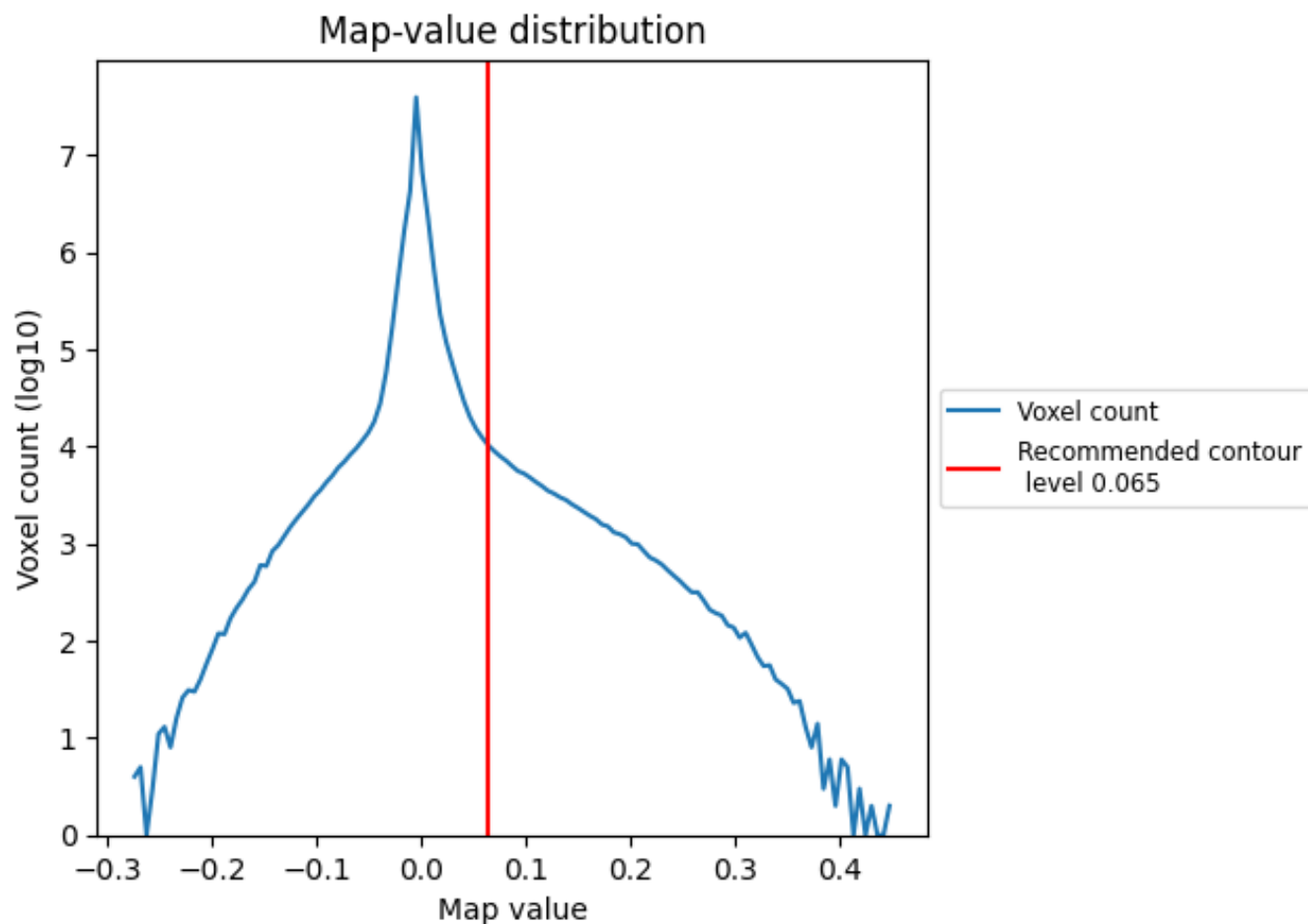
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

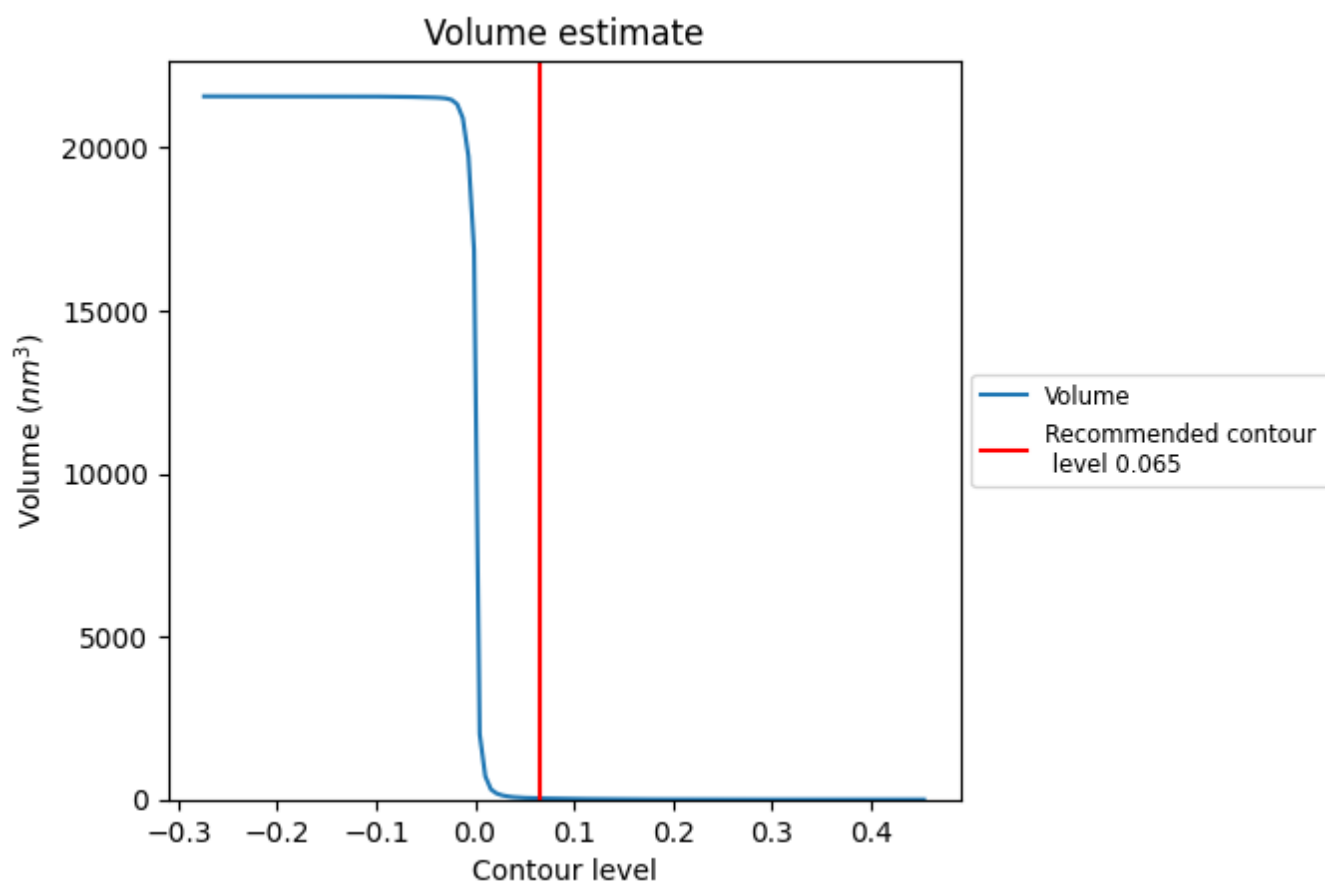
This section contains the results of statistical analysis of the map.

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.

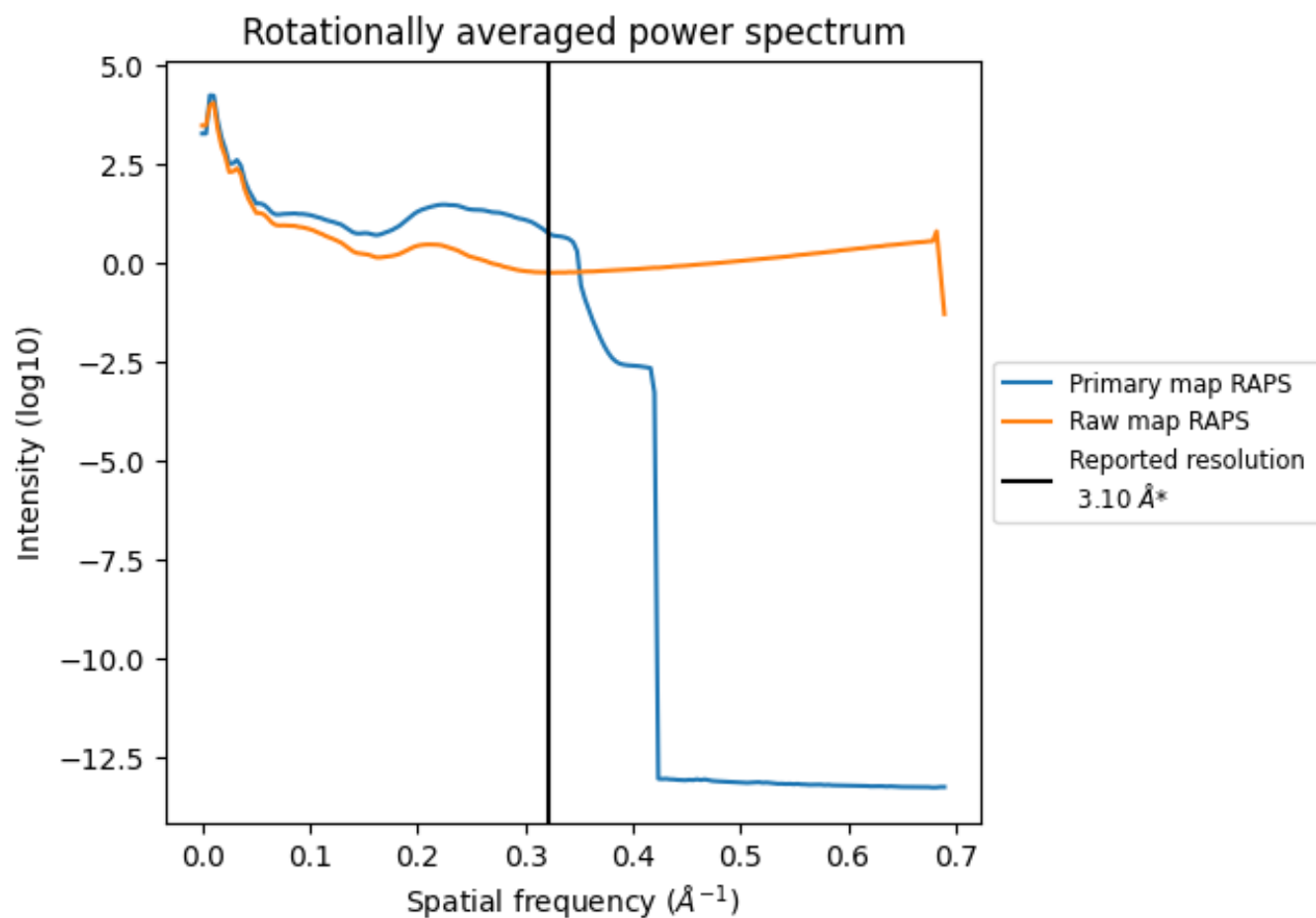
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 39 nm^3 ; this corresponds to an approximate mass of 35 kDa.

The volume estimate graph shows how the enclosed volume varies with the contour level. The recommended contour level is shown as a vertical line and the intersection between the line and the curve gives the volume of the enclosed surface at the given level.

7.3 Rotationally averaged power spectrum ⓘ

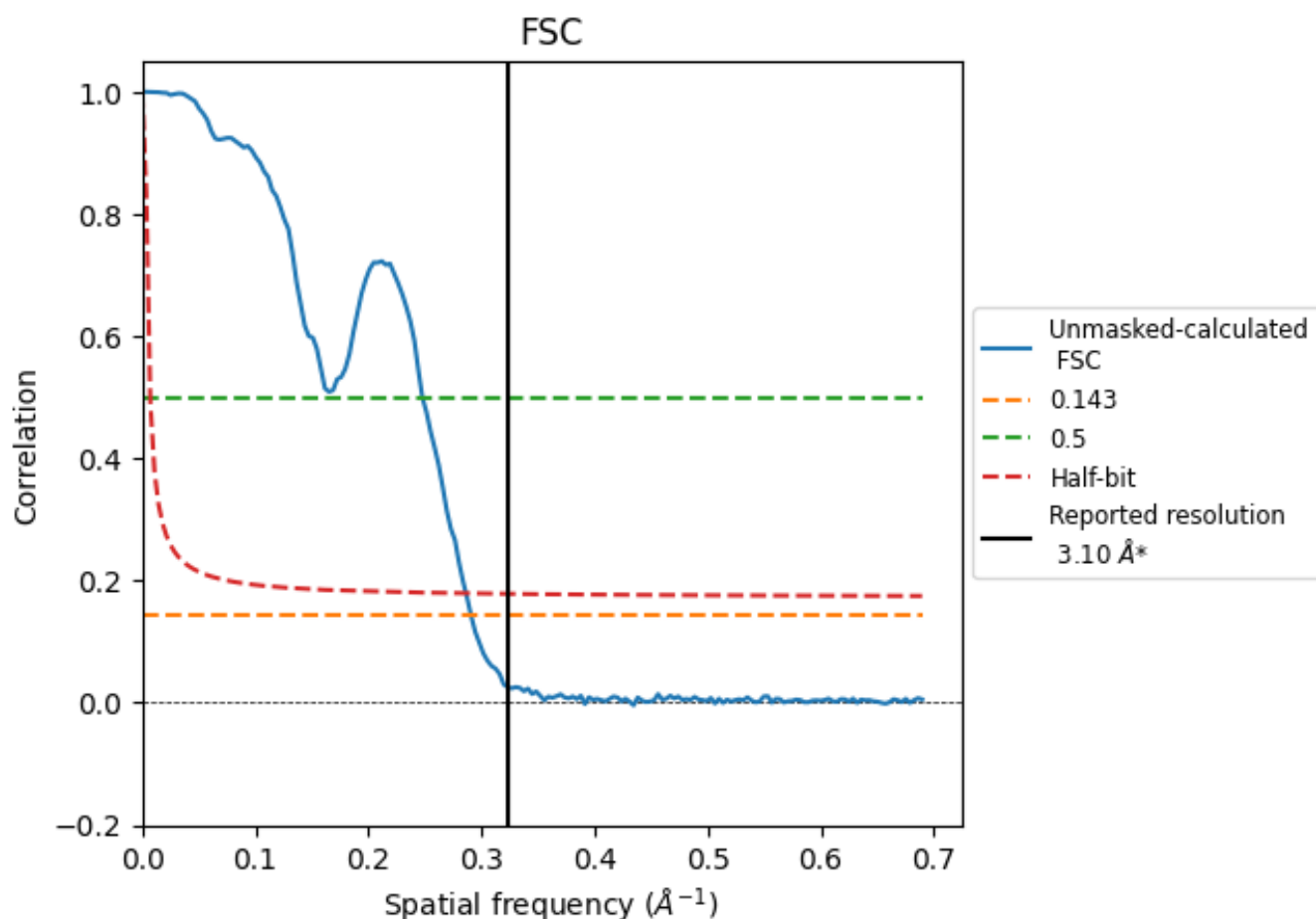


*Reported resolution corresponds to spatial frequency of 0.323 \AA^{-1}

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 0.323 \AA^{-1}

8.2 Resolution estimates [i](#)

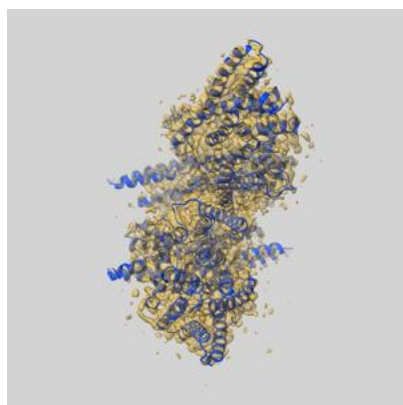
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.10	-	-
Author-provided FSC curve	-	-	-
Unmasked-calculated*	3.44	4.04	3.49

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 3.44 differs from the reported value 3.1 by more than 10 %

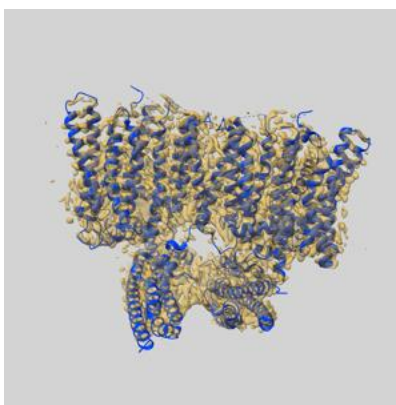
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-47213 and PDB model 9DVO. Per-residue inclusion information can be found in [section 3](#) on [page 7](#).

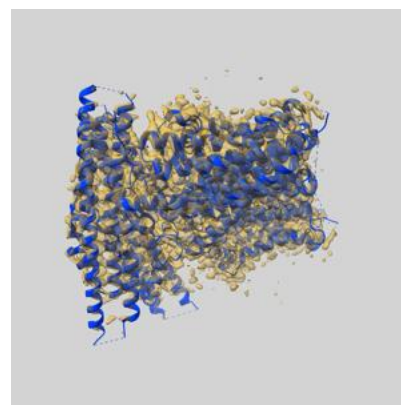
9.1 Map-model overlay [i](#)



X



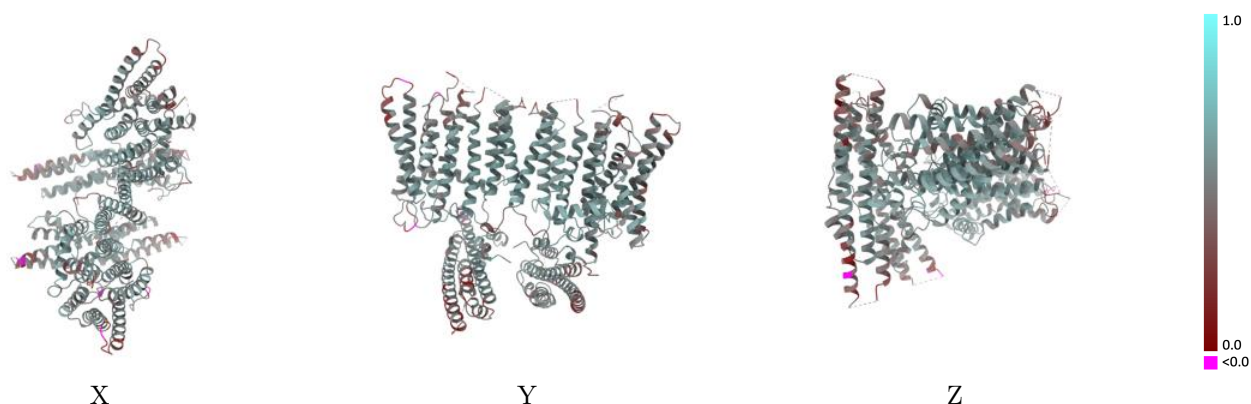
Y



Z

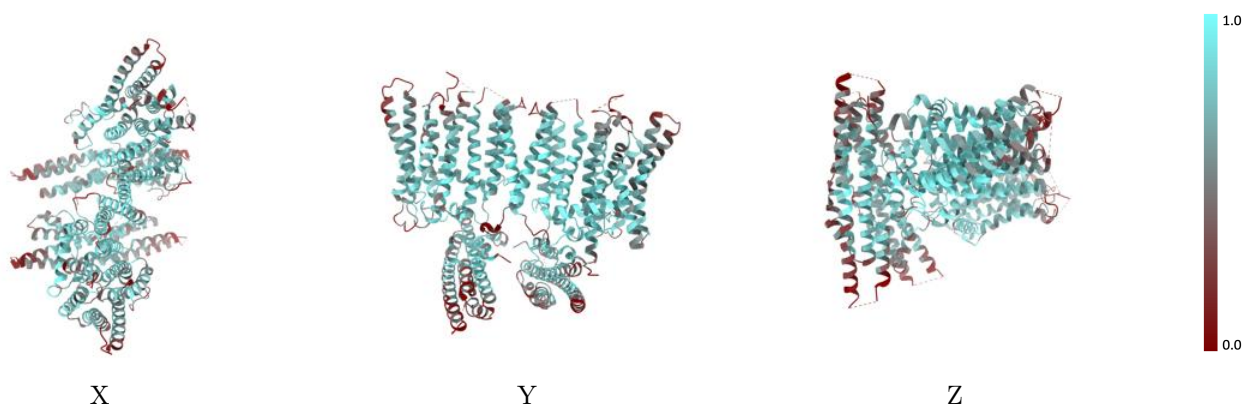
The images above show the 3D surface view of the map at the recommended contour level 0.065 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



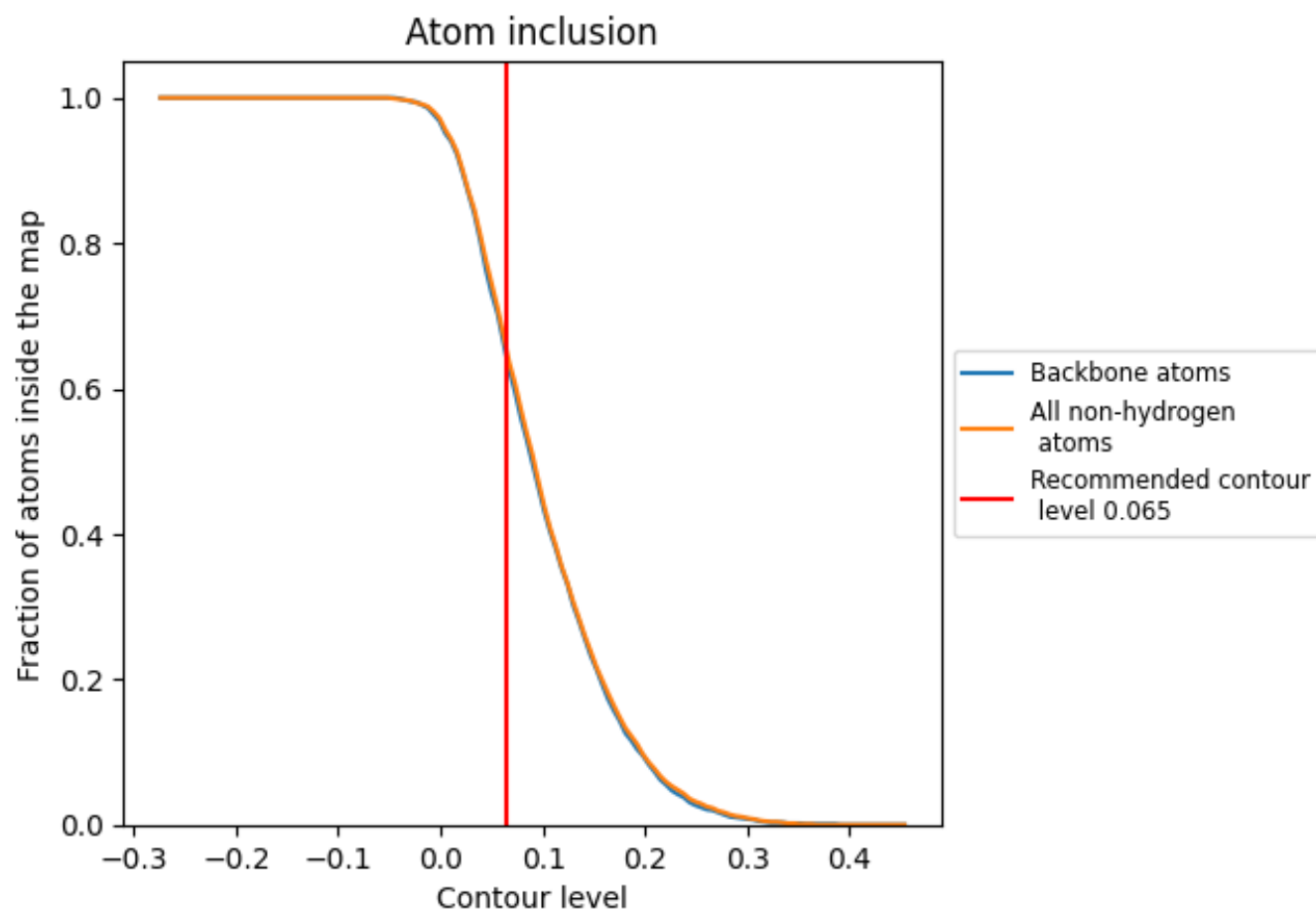
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.065).

9.4 Atom inclusion [i](#)



At the recommended contour level, 64% of all backbone atoms, 65% 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 (0.065) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	<div></div> 0.6500	<div></div> 0.5040
A	<div></div> 0.6570	<div></div> 0.5080
B	<div></div> 0.6430	<div></div> 0.4990

