



## Full wwPDB EM Validation Report ⓘ

Mar 24, 2025 – 03:38 PM EDT

PDB ID : 9DVN  
EMDB ID : EMD-47212  
Title : Structure of the phosphate exporter XPR1/SLC53A1, InsP8-bound, intracellular gate closed state  
Authors : Zhu, Q.; Diver, M.M.  
Deposited on : 2024-10-08  
Resolution : 2.75 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](mailto: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>.

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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

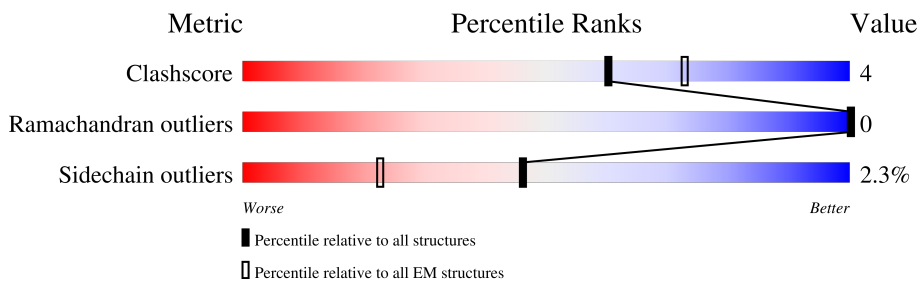
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*ELECTRON MICROSCOPY*

The reported resolution of this entry is 2.75 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  $\geq 3$ , 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>17%</div> <div>70%</div> <div>11%</div> <div>19%</div> </div>
1	B	702	<div> <div>12%</div> <div>71%</div> <div>10%</div> <div>18%</div> </div>

## 2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 19686 atoms, of which 9785 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	571	Total	C	H	N	O	S	0	0
			9499	3149	4746	782	801	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:

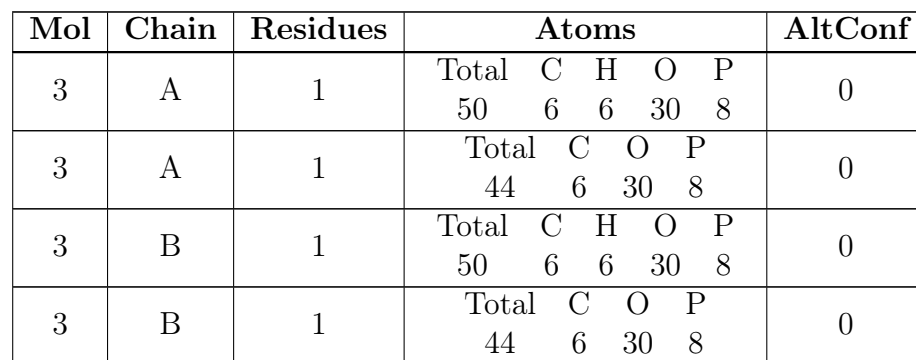
Chain	Residue	Modelled	Actual	Comment	Reference
A	697	LEU	-	expression tag	UNP Q9UBH6
A	698	GLU	-	expression tag	UNP Q9UBH6
A	699	VAL	-	expression tag	UNP Q9UBH6
A	700	LEU	-	expression tag	UNP Q9UBH6
A	701	PHE	-	expression tag	UNP Q9UBH6
A	702	GLN	-	expression tag	UNP Q9UBH6
B	697	LEU	-	expression tag	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: O<sub>4</sub>P) (labeled as "Ligand of Interest" by depositor).



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

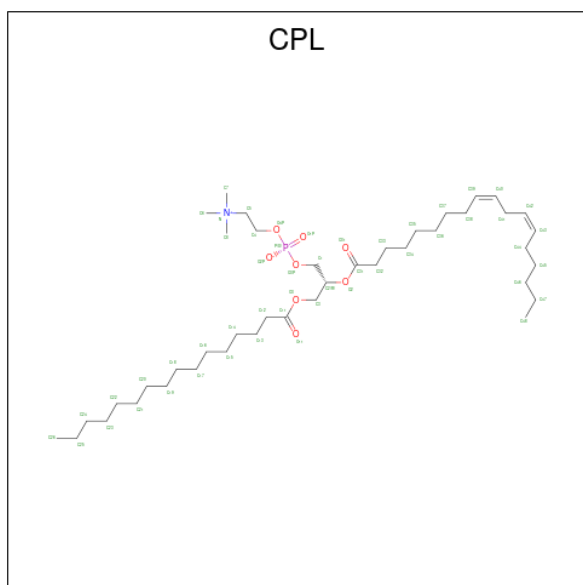
- Molecule 3 is (1R,3S,4R,5S,6R)-2,4,5,6-tetrakis(phosphonooxy)cyclohexane-1,3-diyl bis[trihydrogen (diphosphate)] (three-letter code: I8P) (formula: C<sub>6</sub>H<sub>20</sub>O<sub>30</sub>P<sub>8</sub>) (labeled as "Ligand of Interest" by depositor).



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- The chemical structure of CLR is a complex polycyclic molecule. It features a central bicyclic core with several fused rings. The stereochemistry is indicated by wedged and dashed bonds. Key features include a hydroxyl group (HO) attached to C1, a methyl group (C19) attached to C10, and a long side chain (C20-C27) attached to C17. The side chain is branched and includes a double bond between C20 and C21. The stereochemistry of the side chain is also indicated by wedged and dashed bonds. The structure is labeled with atom numbers (C1-C27) and stereochemical labels (R, S, H).

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

- Molecule 5 is 1-PALMITOYL-2-LINOLEOYL-SN-GLYCERO-3-PHOSPHOCHOLINE (three-letter code: CPL) (formula: C<sub>42</sub>H<sub>80</sub>NO<sub>8</sub>P).



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	

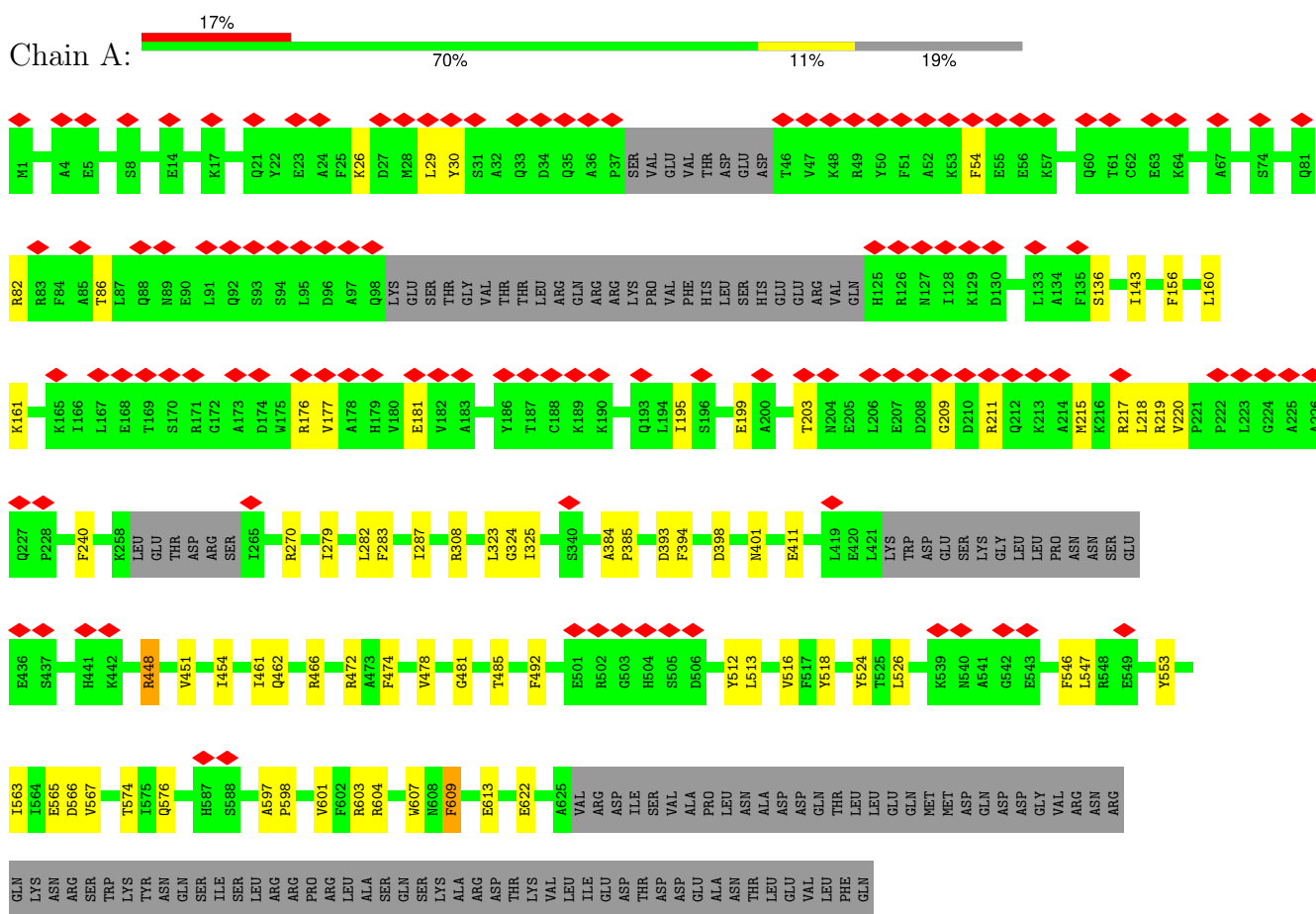
- Molecule 6 is water.

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

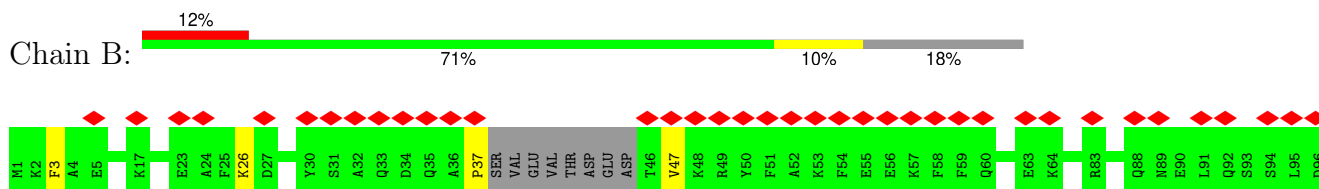
### 3 Residue-property plots

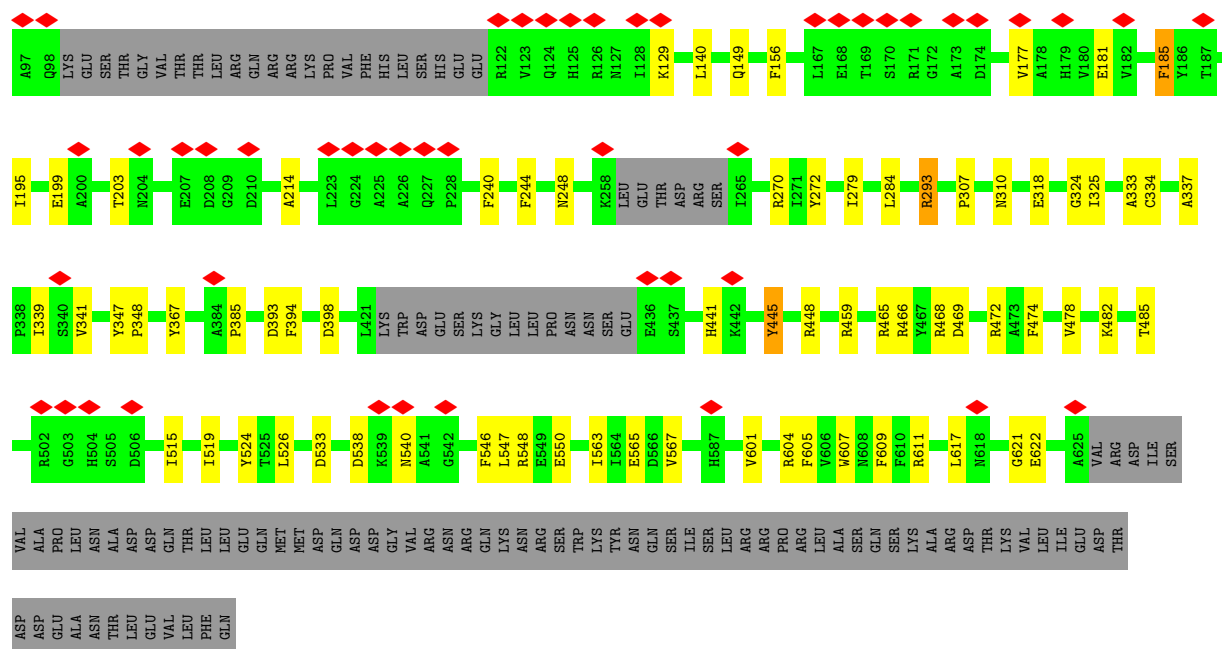
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion 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	295448	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	0.753	Depositor
Minimum map value	-0.518	Depositor
Average map value	-0.000	Depositor
Map value standard deviation	0.012	Depositor
Recommended contour level	0.07	Depositor
Map size (Å)	278.40002, 278.40002, 278.40002	wwPDB
Map dimensions	384, 384, 384	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	0.7250001, 0.7250001, 0.7250001	Depositor

## 5 Model quality

### 5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: PO4, CPL, I8P, CLR

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with  $|Z| > 5$  is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z  > 5$	RMSZ	$\# Z  > 5$
1	A	0.25	0/4892	0.44	0/6628
1	B	0.25	0/4919	0.45	0/6664
All	All	0.25	0/9811	0.44	0/13292

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

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	4753	4746	4746	40	0
1	B	4780	4775	4776	43	0
2	A	15	0	0	2	0
2	B	15	0	0	2	0
3	A	88	6	12	3	0
3	B	88	6	12	7	0
4	A	28	46	46	0	0
4	B	28	46	46	0	0
5	A	52	80	80	0	0
5	B	52	80	80	0	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	0	0
All	All	9901	9785	9798	85	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 4.

All (85) 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:293:ARG:NH2	1:B:310:ASN:OD1	2.22	0.73
1:B:149:GLN:NE2	1:B:185:PHE:O	2.22	0.72
1:B:129:LYS:NZ	3:B:805:I8P:O22	2.23	0.71
1:A:136:SER:OG	1:A:308:ARG:NH1	2.24	0.70
1:A:451:VAL:HA	1:A:454:ILE:HD12	1.77	0.66
1:A:211:ARG:NH1	3:B:804:I8P:O32	2.30	0.64
1:A:466:ARG:NH1	2:A:801:PO4:O3	2.32	0.63
1:B:240:PHE:HA	1:B:325:ILE:HD11	1.80	0.62
1:A:160:LEU:HD13	1:A:176:ARG:HB2	1.82	0.62
1:A:219:ARG:NH2	3:B:804:I8P:O33	2.32	0.62
1:B:3:PHE:N	3:B:804:I8P:O65	2.33	0.61
1:B:459:ARG:NH2	2:B:801:PO4:O2	2.33	0.61
1:B:515:ILE:O	1:B:519:ILE:HD12	2.00	0.61
3:B:805:I8P:H3	3:B:805:I8P:O24	2.00	0.61
1:A:240:PHE:HA	1:A:325:ILE:HD11	1.81	0.60
1:A:29:LEU:HD23	1:A:54:PHE:HZ	1.68	0.59
1:B:284:LEU:HD12	1:B:601:VAL:HG12	1.85	0.59
1:B:199:GLU:O	1:B:203:THR:HG23	2.04	0.57
1:B:140:LEU:HD22	1:B:307:PRO:HG2	1.89	0.55
1:B:177:VAL:HA	1:B:181:GLU:OE1	2.07	0.55
1:B:482:LYS:O	1:B:485:THR:OG1	2.25	0.55
1:A:29:LEU:HD23	1:A:54:PHE:CZ	2.42	0.54
1:B:474:PHE:O	1:B:478:VAL:HG23	2.07	0.54
1:B:270:ARG:NH2	2:B:803:PO4:O3	2.40	0.54
1:A:546:PHE:O	1:A:547:LEU:HD23	2.07	0.54
1:B:177:VAL:HA	1:B:181:GLU:CD	2.28	0.54
1:B:272:TYR:OH	1:B:334:CYS:SG	2.66	0.54
1:A:411:GLU:OE1	1:A:448:ARG:NH1	2.41	0.53
1:B:385:PRO:O	1:B:465:ARG:NH1	2.41	0.52
1:A:270:ARG:NH2	2:A:803:PO4:O4	2.42	0.52
1:B:533:ASP:OD1	1:B:611:ARG:NH1	2.41	0.51
1:B:244:PHE:O	1:B:248:ASN:ND2	2.43	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:474:PHE:O	1:A:478:VAL:HG23	2.11	0.50
1:A:472:ARG:NH1	1:A:622:GLU:OE1	2.44	0.50
1:B:26:LYS:NZ	3:B:804:I8P:O75	2.42	0.50
1:B:318:GLU:OE1	1:B:367:TYR:OH	2.30	0.50
1:B:333:ALA:O	1:B:337:ALA:N	2.40	0.50
1:B:195:ILE:HG22	1:B:199:GLU:OE2	2.13	0.49
1:A:177:VAL:HG13	1:A:181:GLU:OE1	2.13	0.49
1:A:481:GLY:O	1:A:485:THR:HG23	2.12	0.48
1:A:566:ASP:OD1	1:A:603:ARG:NH1	2.41	0.48
1:B:466:ARG:NH2	1:B:621:GLY:O	2.46	0.48
1:B:604:ARG:NH1	1:B:607:TRP:CE3	2.82	0.48
1:A:161:LYS:NZ	3:A:804:I8P:O75	2.47	0.48
1:B:398:ASP:HB3	1:B:604:ARG:NH1	2.29	0.47
1:A:143:ILE:HG21	1:A:220:VAL:HG11	1.95	0.47
1:B:279:ILE:HD13	1:B:324:GLY:HA2	1.95	0.47
1:A:217:ARG:NH1	3:A:805:I8P:O23	2.48	0.47
1:A:82:ARG:O	1:A:86:THR:HG23	2.15	0.46
1:A:492:PHE:CZ	1:A:513:LEU:HD13	2.50	0.46
1:B:203:THR:HG22	1:B:214:ALA:HB3	1.98	0.46
1:A:283:PHE:CE2	1:A:287:ILE:HD11	2.51	0.46
1:A:512:TYR:O	1:A:516:VAL:HG13	2.15	0.46
1:A:553:TYR:HH	1:A:609:PHE:HD1	1.61	0.45
1:A:195:ILE:O	1:A:199:GLU:HG3	2.16	0.45
1:A:26:LYS:NZ	1:A:30:TYR:OH	2.49	0.45
1:B:26:LYS:NZ	3:B:804:I8P:O55	2.50	0.45
1:A:384:ALA:HB1	1:A:462:GLN:HG3	1.99	0.44
1:A:282:LEU:CD1	1:A:323:LEU:HD12	2.47	0.44
1:A:526:LEU:HD21	1:A:567:VAL:HG22	2.00	0.44
1:B:538:ASP:OD2	1:B:540:ASN:ND2	2.51	0.43
1:B:468:ARG:NH1	1:B:469:ASP:OD1	2.51	0.43
1:A:279:ILE:HD13	1:A:324:GLY:HA2	1.99	0.43
1:B:445:TYR:OH	1:B:448:ARG:NH2	2.51	0.43
1:A:597:ALA:HB3	1:A:598:PRO:HD3	2.01	0.43
1:B:546:PHE:O	1:B:547:LEU:HD23	2.19	0.43
1:B:550:GLU:CD	1:B:617:LEU:HD22	2.38	0.43
1:B:526:LEU:HD11	1:B:567:VAL:HG22	2.00	0.43
1:A:597:ALA:O	1:A:601:VAL:HG23	2.19	0.42
1:B:526:LEU:HD21	1:B:567:VAL:HG22	2.02	0.41
1:B:339:ILE:HG22	1:B:341:VAL:HG22	2.02	0.41
1:A:563:ILE:O	1:A:567:VAL:HG23	2.20	0.41
1:B:563:ILE:O	1:B:567:VAL:HG23	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:347:TYR:HB2	1:B:348:PRO:HD3	2.02	0.41
1:A:604:ARG:NH1	1:A:607:TRP:CE3	2.88	0.41
1:A:143:ILE:CG2	1:A:220:VAL:HG11	2.50	0.41
1:A:215:MET:CE	1:A:218:LEU:HD23	2.51	0.41
1:A:385:PRO:HD3	1:A:461:ILE:HG21	2.03	0.41
1:B:3:PHE:O	1:B:3:PHE:CG	2.73	0.41
1:B:37:PRO:HG2	1:B:47:VAL:HG22	2.03	0.41
1:A:518:TYR:CD2	1:A:574:THR:HG22	2.56	0.41
1:B:472:ARG:NH1	1:B:622:GLU:OE1	2.54	0.41
3:A:805:I8P:O46	3:A:805:I8P:H5	2.21	0.40
1:B:203:THR:HG22	1:B:214:ALA:CB	2.51	0.40
1:A:203:THR:O	1:A:209:GLY:N	2.42	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	561/702 (80%)	547 (98%)	14 (2%)	0	100	100
1	B	564/702 (80%)	553 (98%)	11 (2%)	0	100	100
All	All	1125/1404 (80%)	1100 (98%)	25 (2%)	0	100	100

There are no Ramachandran outliers to report.

### 5.3.2 Protein sidechains [i](#)

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

The Analysed column shows the number of residues for which the sidechain conformation was

analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	504/627 (80%)	493 (98%)	11 (2%)	47	68
1	B	507/627 (81%)	495 (98%)	12 (2%)	44	65
All	All	1011/1254 (81%)	988 (98%)	23 (2%)	46	67

All (23) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	156	PHE
1	A	393	ASP
1	A	394	PHE
1	A	398	ASP
1	A	401	ASN
1	A	448	ARG
1	A	524	TYR
1	A	565	GLU
1	A	576	GLN
1	A	609	PHE
1	A	613	GLU
1	B	156	PHE
1	B	185	PHE
1	B	293	ARG
1	B	393	ASP
1	B	394	PHE
1	B	441	HIS
1	B	445	TYR
1	B	524	TYR
1	B	548	ARG
1	B	565	GLU
1	B	605	PHE
1	B	609	PHE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

## 5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

## 5.6 Ligand geometry [i](#)

14 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	B	803	-	4,4,4	1.56	1 (25%)	6,6,6	0.45	0
2	PO4	A	801	-	4,4,4	1.55	1 (25%)	6,6,6	0.48	0
5	CPL	B	807	-	51,51,51	1.04	3 (5%)	57,59,59	0.98	3 (5%)
2	PO4	B	802	-	4,4,4	1.56	1 (25%)	6,6,6	0.49	0
4	CLR	B	806	-	31,31,31	1.08	2 (6%)	48,48,48	1.34	8 (16%)
3	I8P	A	804	-	42,44,44	2.49	9 (21%)	68,74,74	1.40	10 (14%)
4	CLR	A	806	-	31,31,31	1.08	2 (6%)	48,48,48	1.36	7 (14%)
2	PO4	A	802	-	4,4,4	1.56	1 (25%)	6,6,6	0.50	0
3	I8P	B	805	-	42,44,44	2.46	9 (21%)	68,74,74	1.42	10 (14%)
5	CPL	A	807	-	51,51,51	1.04	3 (5%)	57,59,59	0.98	3 (5%)
2	PO4	A	803	-	4,4,4	1.53	1 (25%)	6,6,6	0.50	0
3	I8P	B	804	-	42,44,44	2.47	10 (23%)	68,74,74	1.38	11 (16%)
2	PO4	B	801	-	4,4,4	1.55	1 (25%)	6,6,6	0.48	0
3	I8P	A	805	-	42,44,44	2.42	11 (26%)	68,74,74	1.38	11 (16%)

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
5	CPL	B	807	-	-	23/55/55/55	-
4	CLR	B	806	-	-	4/10/68/68	0/4/4/4
4	CLR	A	806	-	-	1/10/68/68	0/4/4/4
3	I8P	A	804	-	-	9/42/66/66	0/1/1/1
3	I8P	B	805	-	-	17/42/66/66	0/1/1/1
5	CPL	A	807	-	-	22/55/55/55	-
3	I8P	B	804	-	-	3/42/66/66	0/1/1/1
3	I8P	A	805	-	-	17/42/66/66	0/1/1/1

All (55) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	805	I8P	PA4-O14	7.62	1.72	1.59
3	A	805	I8P	PA4-O14	7.32	1.72	1.59
3	B	804	I8P	PA4-O14	7.25	1.72	1.59
3	A	804	I8P	PA6-O16	7.25	1.72	1.59
3	A	804	I8P	PA4-O14	7.23	1.72	1.59
3	B	804	I8P	PA6-O16	7.09	1.71	1.59
3	B	805	I8P	PA6-O16	6.64	1.71	1.59
3	A	805	I8P	PA6-O16	6.63	1.71	1.59
3	B	804	I8P	PA3-O13	6.53	1.71	1.59
3	B	805	I8P	PA2-O12	6.50	1.70	1.59
3	A	805	I8P	PA2-O12	6.42	1.70	1.59
3	B	804	I8P	PA2-O12	6.41	1.70	1.59
3	A	804	I8P	PA2-O12	6.40	1.70	1.59
3	B	805	I8P	PA3-O13	6.38	1.70	1.59
3	A	804	I8P	PA3-O13	6.31	1.70	1.59
3	A	805	I8P	PA3-O13	6.23	1.70	1.59
5	B	807	CPL	P-O3P	3.84	1.74	1.59
5	A	807	CPL	P-O3P	3.84	1.74	1.59
3	A	804	I8P	C3-C2	3.82	1.60	1.52
3	B	805	I8P	C5-C4	3.24	1.58	1.52
5	A	807	CPL	P-O4P	3.16	1.71	1.59
5	B	807	CPL	P-O4P	3.14	1.71	1.59
3	A	804	I8P	C4-C3	3.11	1.58	1.52
2	A	802	PO4	P-O1	2.73	1.57	1.50
2	B	802	PO4	P-O1	2.72	1.56	1.50
2	B	803	PO4	P-O1	2.71	1.56	1.50
2	A	801	PO4	P-O1	2.69	1.56	1.50
2	B	801	PO4	P-O1	2.68	1.56	1.50
3	B	804	I8P	C2-C1	2.65	1.57	1.52
2	A	803	PO4	P-O1	2.63	1.56	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	804	I8P	C5-C4	2.62	1.57	1.52
3	B	805	I8P	C6-C5	2.60	1.57	1.52
3	B	804	I8P	C3-C2	2.50	1.57	1.52
3	A	804	I8P	C5-C4	2.44	1.57	1.52
3	A	804	I8P	C2-C1	2.43	1.57	1.52
3	A	805	I8P	C5-C4	2.36	1.57	1.52
3	A	805	I8P	C2-C1	2.29	1.57	1.52
3	B	805	I8P	C4-C3	2.27	1.56	1.52
3	A	805	I8P	C6-C1	2.25	1.56	1.52
3	A	805	I8P	C3-C2	2.25	1.56	1.52
3	B	804	I8P	C4-C3	2.20	1.56	1.52
3	A	805	I8P	C6-C5	2.14	1.56	1.52
3	A	804	I8P	PA2-O32	2.13	1.57	1.50
3	B	805	I8P	PA2-O32	2.13	1.57	1.50
3	B	804	I8P	PA2-O32	2.12	1.57	1.50
3	A	805	I8P	PA2-O32	2.12	1.57	1.50
3	B	804	I8P	PA1-O41	2.11	1.61	1.59
4	A	806	CLR	C16-C17	2.09	1.58	1.54
3	B	805	I8P	PA1-O41	2.09	1.61	1.59
5	A	807	CPL	O3P-C1	-2.04	1.36	1.44
4	B	806	CLR	C18-C13	-2.04	1.50	1.54
3	A	805	I8P	PA1-O41	2.04	1.61	1.59
4	B	806	CLR	C7-C6	2.03	1.54	1.50
5	B	807	CPL	O3P-C1	-2.03	1.36	1.44
4	A	806	CLR	C7-C6	2.01	1.54	1.50

All (63) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	B	807	CPL	O2P-P-O1P	4.80	134.76	112.44
5	A	807	CPL	O2P-P-O1P	4.80	134.75	112.44
3	A	804	I8P	O35-PA5-O45	-3.57	97.62	107.27
3	A	805	I8P	O35-PA5-O45	-3.53	97.74	107.27
3	B	804	I8P	O35-PA5-O45	-3.50	97.81	107.27
3	B	805	I8P	C6-C5-C4	3.50	118.11	110.43
3	B	805	I8P	O35-PA5-O45	-3.48	97.87	107.27
4	A	806	CLR	C22-C20-C17	-3.09	103.93	110.33
4	B	806	CLR	C22-C20-C17	-3.04	104.03	110.33
3	A	804	I8P	O71-PB1-O41	2.84	114.15	104.64
3	B	804	I8P	O71-PB1-O41	2.84	114.14	104.64
3	A	805	I8P	O71-PB1-O41	2.82	114.11	104.64
3	B	805	I8P	O71-PB1-O41	2.82	114.10	104.64

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	806	CLR	C18-C13-C12	2.70	114.58	110.61
3	A	804	I8P	O11-PA1-O21	2.68	118.36	109.81
3	A	805	I8P	C6-C5-C4	2.65	116.23	110.43
3	B	805	I8P	O11-PA1-O21	2.64	118.23	109.81
3	A	805	I8P	O11-PA1-O21	2.62	118.17	109.81
3	B	805	I8P	O24-PA4-O14	2.62	116.04	105.85
3	B	804	I8P	O24-PA4-O14	2.61	116.02	105.85
3	B	804	I8P	O11-PA1-O21	2.58	118.06	109.81
3	A	805	I8P	O24-PA4-O14	2.53	115.71	105.85
4	B	806	CLR	C18-C13-C12	2.53	114.33	110.61
3	B	805	I8P	O42-PA2-O12	2.52	115.68	105.85
3	A	805	I8P	O42-PA2-O12	2.52	115.67	105.85
3	B	804	I8P	C6-C5-C4	2.52	115.95	110.43
3	A	804	I8P	C6-C5-C4	2.52	115.95	110.43
3	A	804	I8P	O24-PA4-O14	2.51	115.63	105.85
3	A	804	I8P	O42-PA2-O12	2.51	115.62	105.85
3	B	804	I8P	O42-PA2-O12	2.51	115.62	105.85
5	A	807	CPL	C4-C5-N	-2.43	108.02	115.82
4	A	806	CLR	C21-C20-C22	-2.41	106.61	110.34
5	B	807	CPL	C4-C5-N	-2.40	108.13	115.82
3	B	805	I8P	O36-PA6-O26	2.38	116.71	107.80
3	A	805	I8P	O36-PA6-O26	2.37	116.68	107.80
3	B	804	I8P	O36-PA6-O26	2.35	116.61	107.80
4	A	806	CLR	C12-C13-C14	-2.32	103.77	107.25
3	A	804	I8P	O36-PA6-O26	2.27	116.32	107.80
5	A	807	CPL	O2-C31-C32	2.26	116.37	111.48
3	B	804	I8P	O23-PA3-O13	2.22	114.52	105.85
3	A	805	I8P	O23-PA3-O13	2.21	114.47	105.85
4	B	806	CLR	C12-C13-C14	-2.20	103.95	107.25
4	B	806	CLR	C10-C5-C6	2.20	126.14	122.93
5	B	807	CPL	O2-C31-C32	2.20	116.24	111.48
3	A	804	I8P	O23-PA3-O13	2.19	114.40	105.85
3	B	805	I8P	O23-PA3-O13	2.19	114.39	105.85
3	B	804	I8P	O12-C2-C1	2.19	113.41	108.76
4	B	806	CLR	C21-C20-C22	-2.18	106.97	110.34
4	A	806	CLR	C10-C5-C6	2.18	126.11	122.93
4	B	806	CLR	C7-C8-C14	-2.16	107.88	110.93
4	A	806	CLR	C24-C23-C22	-2.14	103.69	113.28
3	A	804	I8P	O75-PB5-O65	-2.14	99.79	107.80
3	B	804	I8P	O75-PB5-O65	-2.13	99.80	107.80
3	A	805	I8P	O75-PB5-O65	-2.12	99.86	107.80
3	B	805	I8P	O75-PB5-O65	-2.12	99.86	107.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	804	I8P	O15-PA5-O25	2.11	116.57	109.81
4	A	806	CLR	C7-C8-C14	-2.09	107.97	110.93
3	A	805	I8P	O12-C2-C1	2.09	113.20	108.76
3	A	805	I8P	O15-PA5-O25	2.08	116.45	109.81
4	B	806	CLR	C16-C17-C20	-2.07	109.05	112.18
4	B	806	CLR	C13-C17-C20	-2.05	116.33	119.50
3	A	804	I8P	O15-PA5-O25	2.04	116.33	109.81
3	B	805	I8P	O15-PA5-O25	2.02	116.25	109.81

There are no chirality outliers.

All (96) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	804	I8P	C6-C1-O11-PA1
3	A	804	I8P	C1-C6-O16-PA6
3	A	804	I8P	C5-O15-PA5-O45
3	A	805	I8P	C5-C6-O16-PA6
3	A	805	I8P	C1-O11-PA1-O41
3	A	805	I8P	C5-O15-PA5-O45
3	A	805	I8P	PA1-O41-PB1-O51
3	A	805	I8P	PA5-O45-PB5-O75
3	B	804	I8P	C5-O15-PA5-O25
3	B	804	I8P	C5-O15-PA5-O45
3	B	805	I8P	C2-C1-O11-PA1
3	B	805	I8P	C1-C2-O12-PA2
3	B	805	I8P	C3-C2-O12-PA2
3	B	805	I8P	C3-C4-O14-PA4
3	B	805	I8P	C5-C4-O14-PA4
3	B	805	I8P	C1-O11-PA1-O41
3	B	805	I8P	C5-O15-PA5-O45
3	B	805	I8P	PA1-O41-PB1-O51
5	A	807	CPL	C1-O3P-P-O2P
5	A	807	CPL	C1-O3P-P-O4P
5	A	807	CPL	C4-O4P-P-O1P
5	A	807	CPL	C4-O4P-P-O3P
5	B	807	CPL	C1-O3P-P-O2P
5	B	807	CPL	C4-O4P-P-O3P
5	A	807	CPL	C12-C11-O3-C3
5	A	807	CPL	O11-C11-O3-C3
4	B	806	CLR	C17-C20-C22-C23
4	B	806	CLR	C21-C20-C22-C23
5	B	807	CPL	C11-C12-C13-C14

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Mol	Chain	Res	Type	Atoms
5	A	807	CPL	C32-C31-O2-C2
5	A	807	CPL	O31-C31-O2-C2
5	B	807	CPL	C34-C35-C36-C37
5	A	807	CPL	C22-C23-C24-C25
5	B	807	CPL	C22-C23-C24-C25
5	A	807	CPL	C14-C15-C16-C17
5	B	807	CPL	C14-C15-C16-C17
5	B	807	CPL	C19-C20-C21-C22
5	B	807	CPL	C1-C2-C3-O3
3	A	804	I8P	PB1-O41-PA1-O21
5	A	807	CPL	C23-C24-C25-C26
5	A	807	CPL	C18-C19-C20-C21
5	B	807	CPL	O2-C2-C3-O3
5	A	807	CPL	C40-C41-C42-C43
3	A	804	I8P	PB1-O41-PA1-O11
3	B	804	I8P	PB1-O41-PA1-O11
3	B	805	I8P	PB1-O41-PA1-O11
5	B	807	CPL	C23-C24-C25-C26
4	B	806	CLR	C22-C23-C24-C25
5	A	807	CPL	O3-C11-C12-C13
3	A	805	I8P	C1-C6-O16-PA6
3	B	805	I8P	C4-C5-O15-PA5
5	A	807	CPL	C5-C4-O4P-P
3	A	805	I8P	C1-O11-PA1-O21
5	A	807	CPL	O4P-C4-C5-N
5	B	807	CPL	O4P-C4-C5-N
3	B	805	I8P	C4-O14-PA4-O34
5	B	807	CPL	C31-C32-C33-C34
5	B	807	CPL	C1-O3P-P-O4P
5	B	807	CPL	C4-O4P-P-O1P
4	A	806	CLR	C16-C17-C20-C22
5	B	807	CPL	C44-C45-C46-C47
3	A	805	I8P	C6-O16-PA6-O26
3	B	805	I8P	C3-O13-PA3-O23
3	A	805	I8P	PA5-O45-PB5-O55
5	B	807	CPL	C4-C5-N-C6
5	B	807	CPL	C45-C46-C47-C48
3	A	804	I8P	C5-C6-O16-PA6
3	A	805	I8P	C4-C5-O15-PA5
3	B	805	I8P	C2-O12-PA2-O32
3	B	805	I8P	C6-O16-PA6-O46
4	B	806	CLR	C20-C22-C23-C24

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Mol	Chain	Res	Type	Atoms
5	B	807	CPL	C32-C33-C34-C35
5	A	807	CPL	C43-C44-C45-C46
5	A	807	CPL	C12-C13-C14-C15
5	B	807	CPL	C42-C43-C44-C45
3	A	805	I8P	PA1-O41-PB1-O61
3	B	805	I8P	PA1-O41-PB1-O61
5	A	807	CPL	C32-C33-C34-C35
3	A	804	I8P	PA5-O45-PB5-O75
3	A	805	I8P	PA5-O45-PB5-O65
5	B	807	CPL	C37-C38-C39-C40
5	B	807	CPL	C21-C22-C23-C24
5	A	807	CPL	C45-C46-C47-C48
3	A	804	I8P	C1-O11-PA1-O21
3	A	804	I8P	C5-O15-PA5-O35
3	A	805	I8P	C1-O11-PA1-O31
3	A	805	I8P	C5-O15-PA5-O25
3	A	805	I8P	C5-O15-PA5-O35
3	A	805	I8P	PB5-O45-PA5-O25
3	B	805	I8P	C1-O11-PA1-O31
5	A	807	CPL	O11-C11-C12-C13
3	A	805	I8P	C2-O12-PA2-O22
5	A	807	CPL	C20-C21-C22-C23
5	B	807	CPL	O3-C11-C12-C13
3	B	805	I8P	C6-C5-O15-PA5
5	B	807	CPL	C4-C5-N-C7

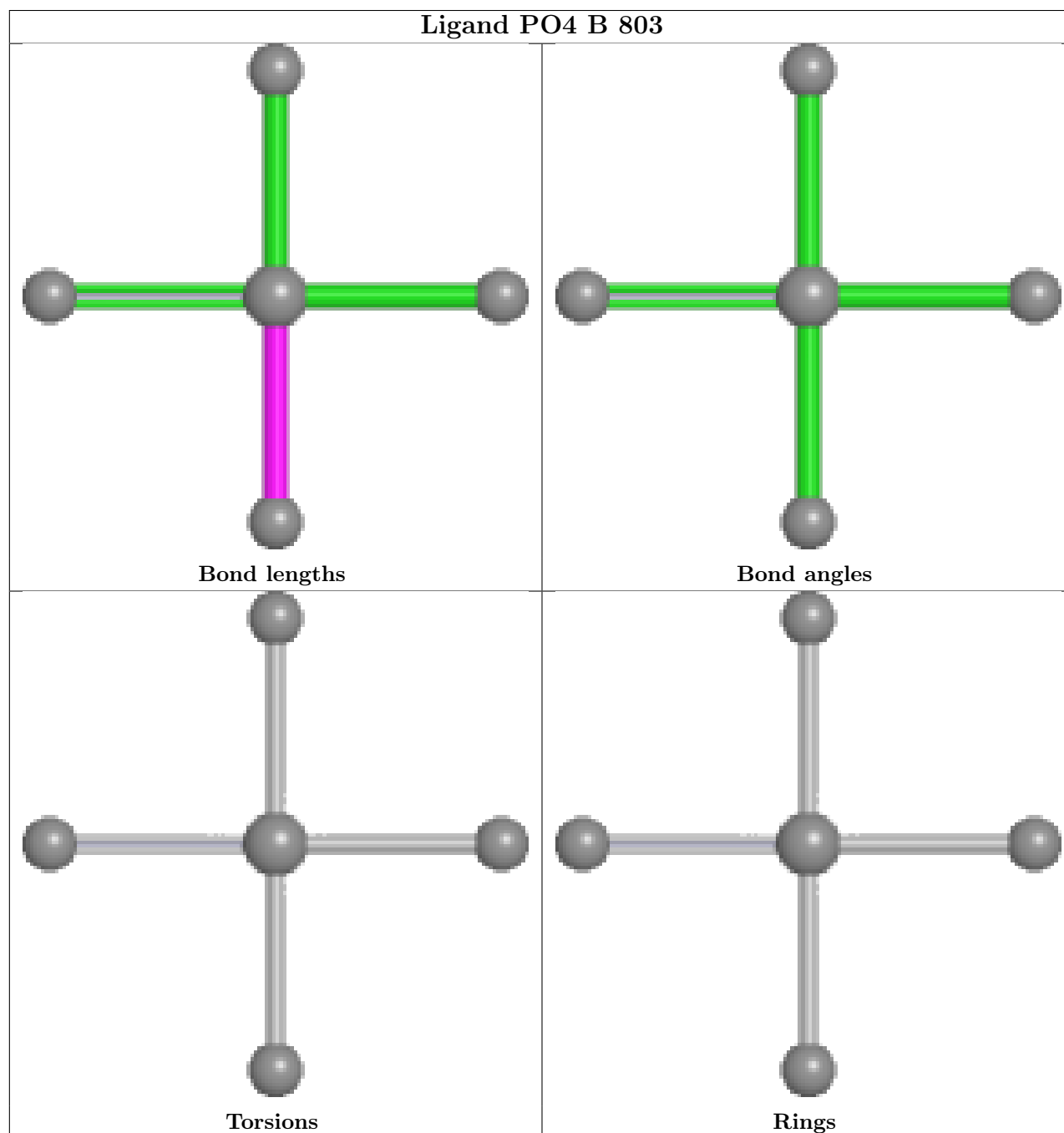
There are no ring outliers.

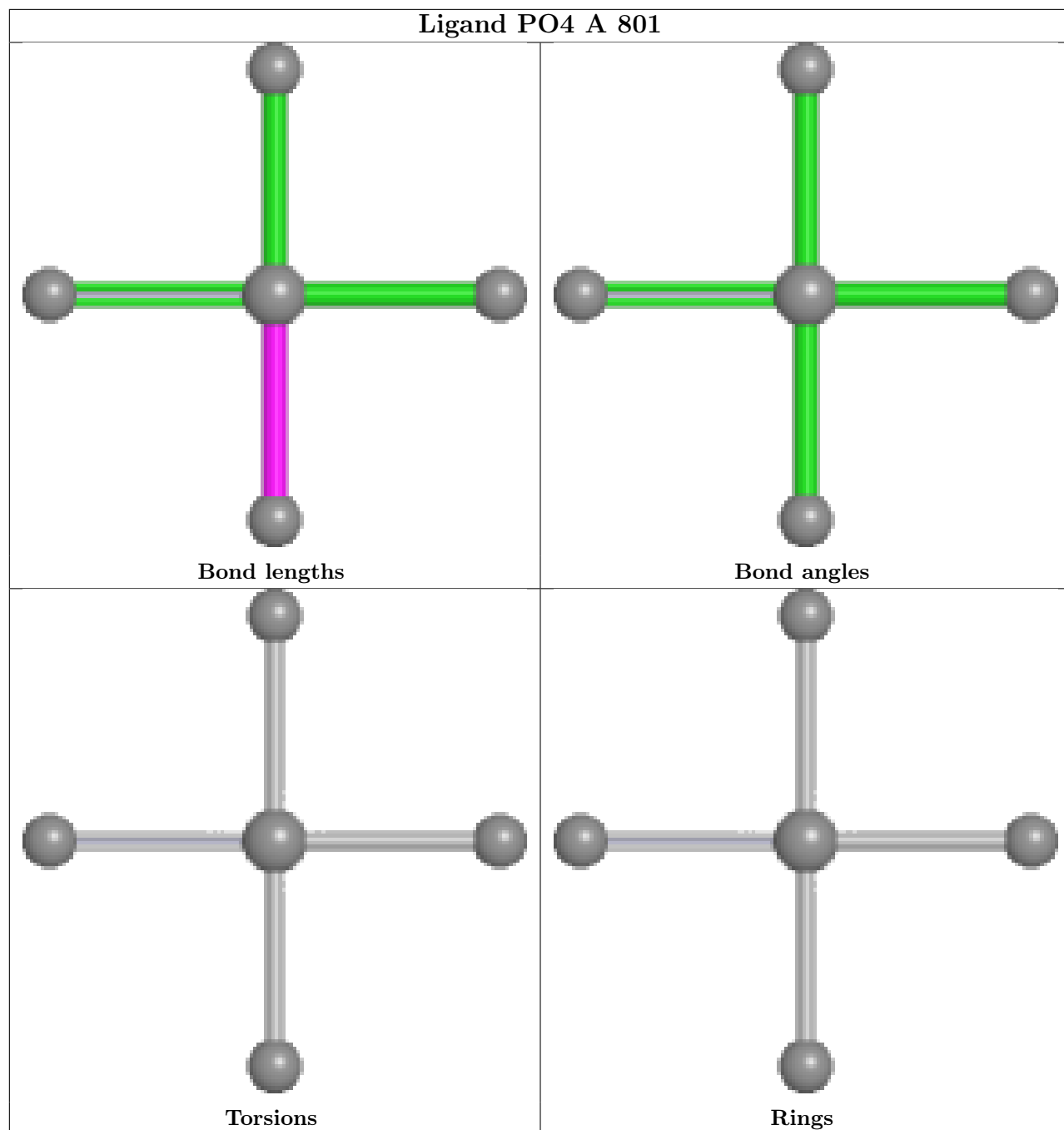
8 monomers are involved in 14 short contacts:

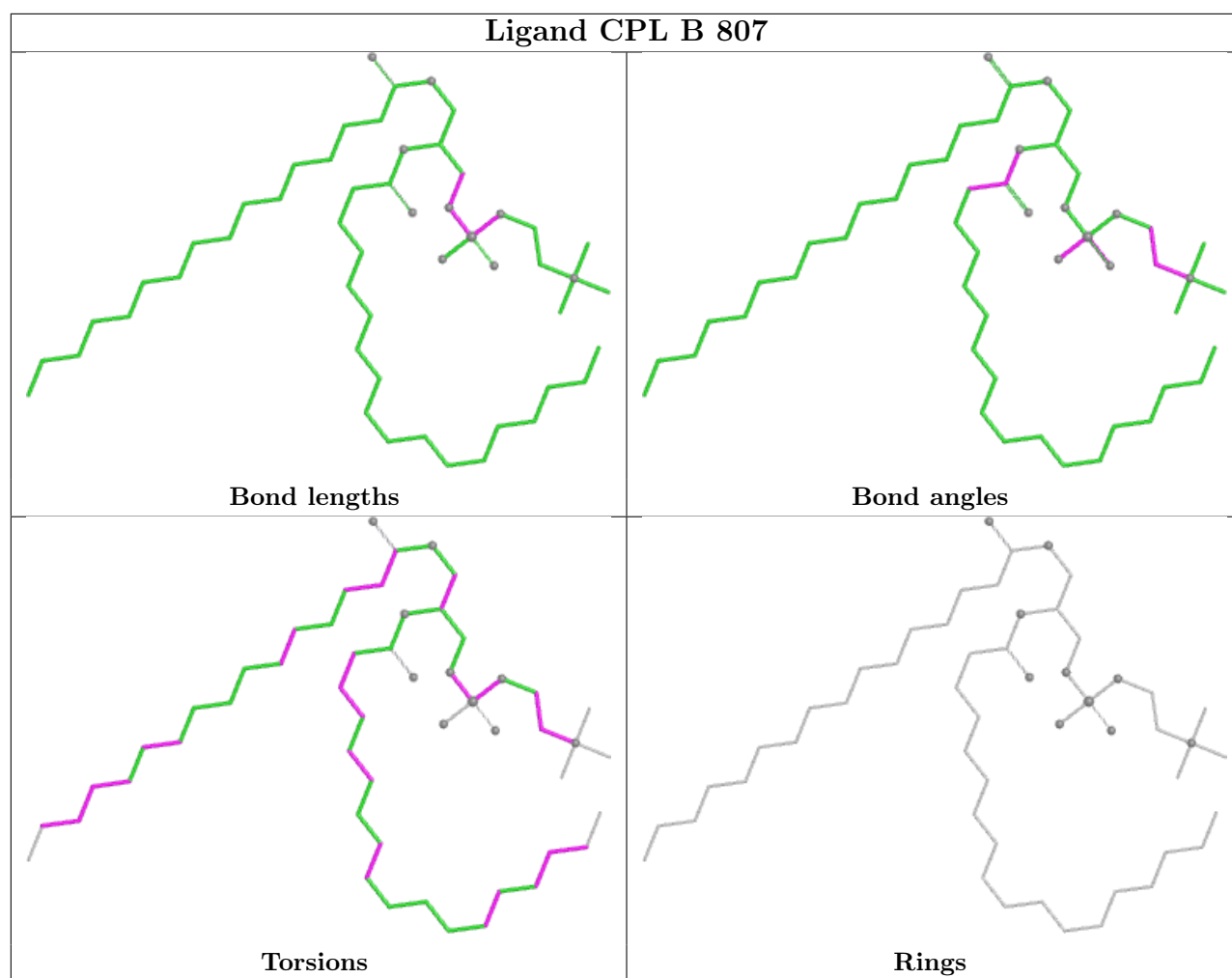
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	803	PO4	1	0
2	A	801	PO4	1	0
3	A	804	I8P	1	0
3	B	805	I8P	2	0
2	A	803	PO4	1	0
3	B	804	I8P	5	0
2	B	801	PO4	1	0
3	A	805	I8P	2	0

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

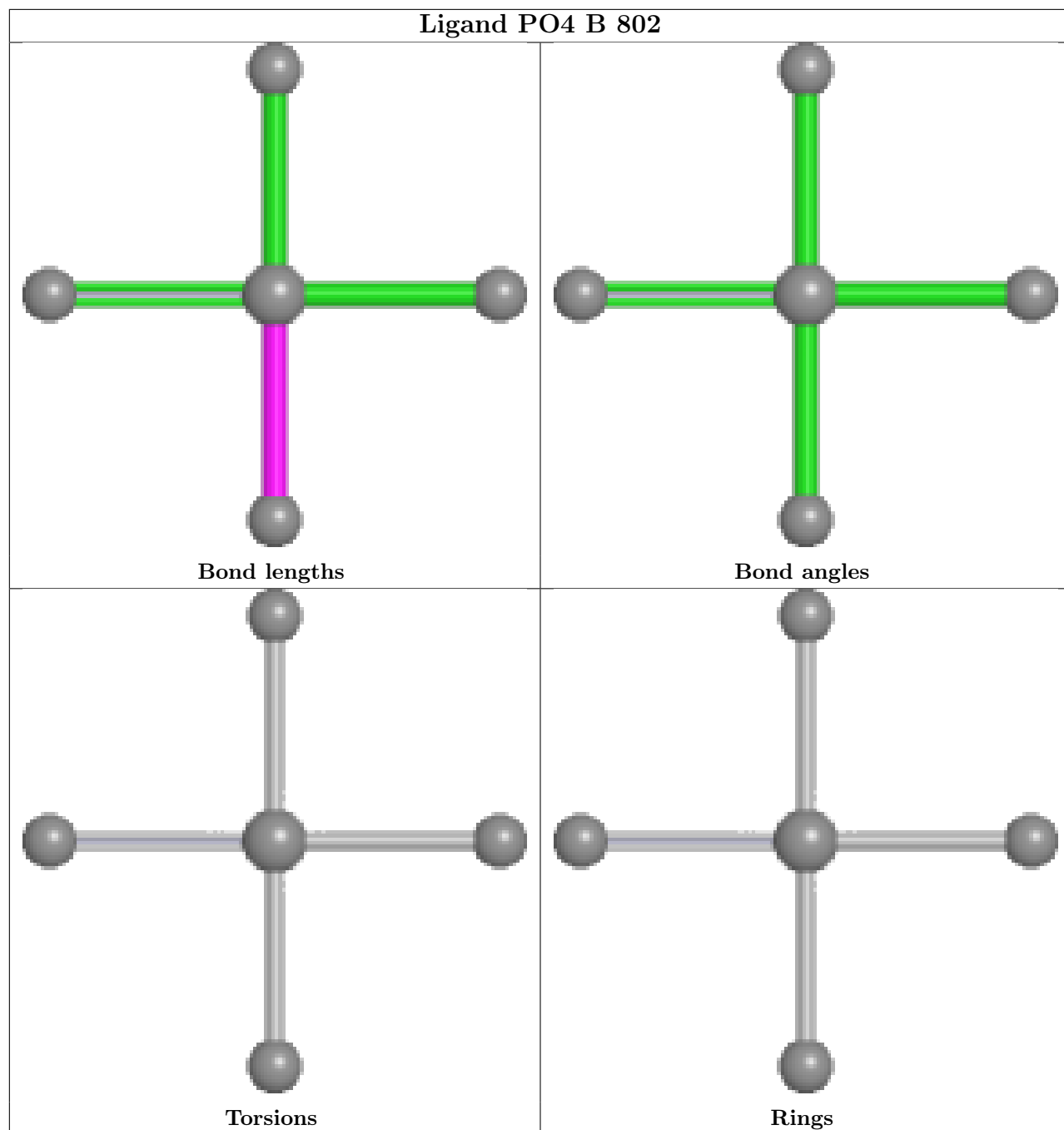
also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted 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.



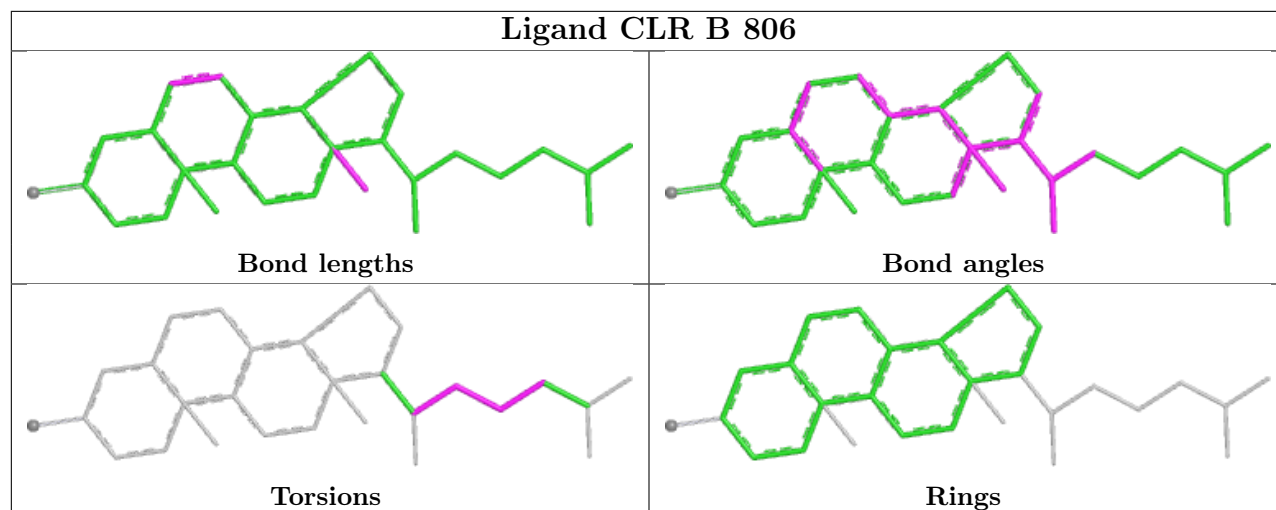




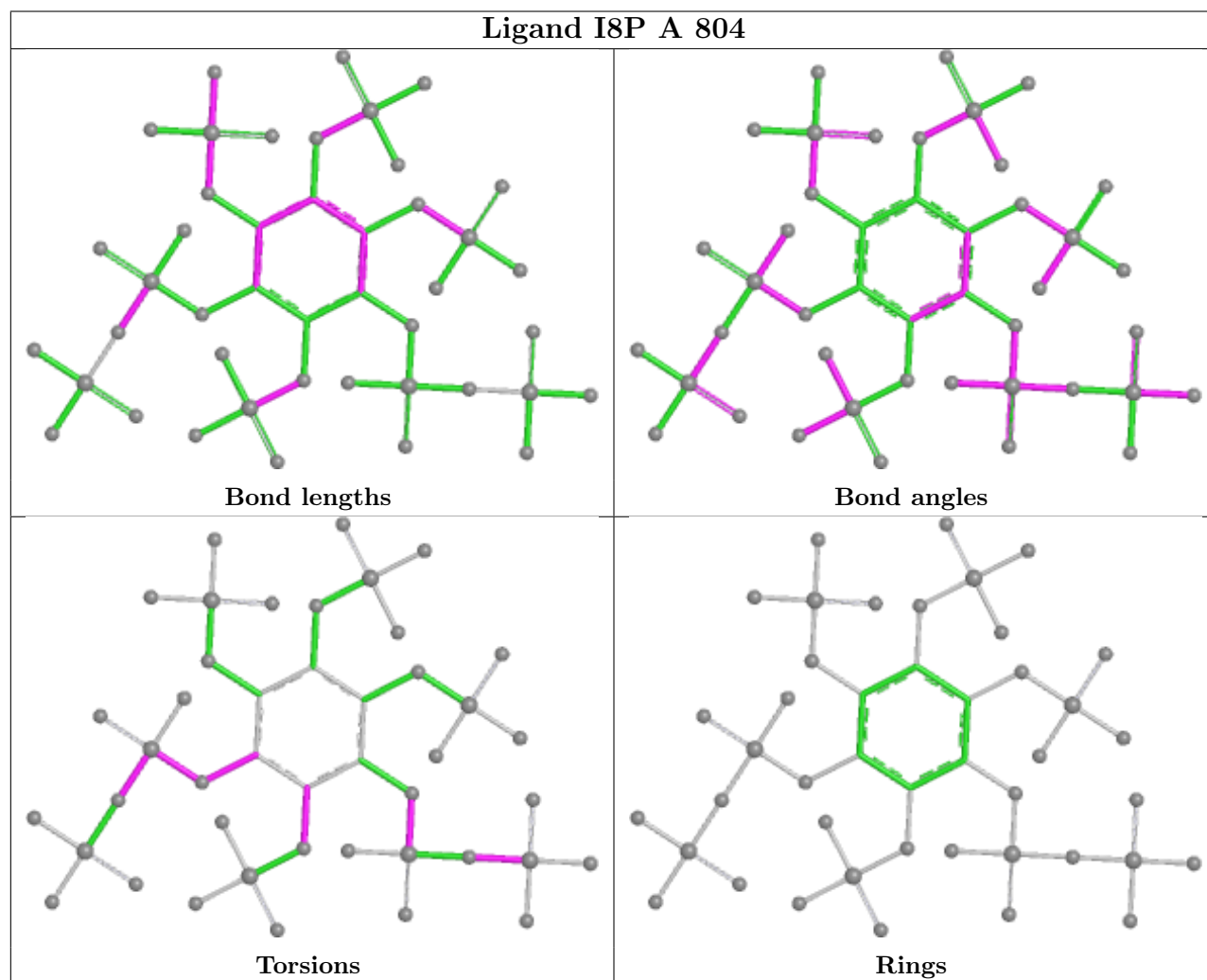


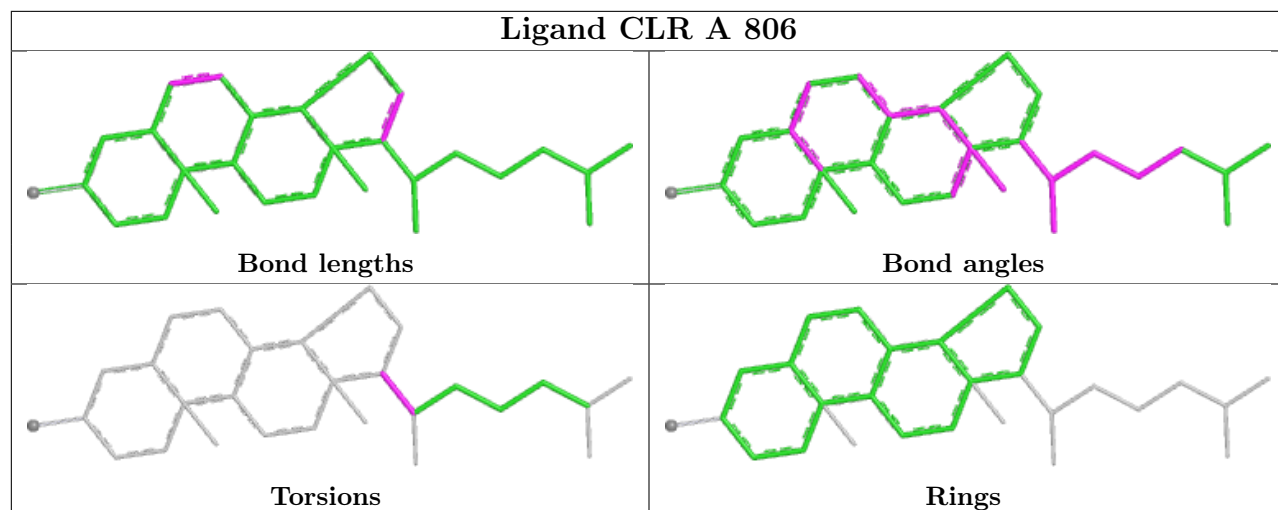


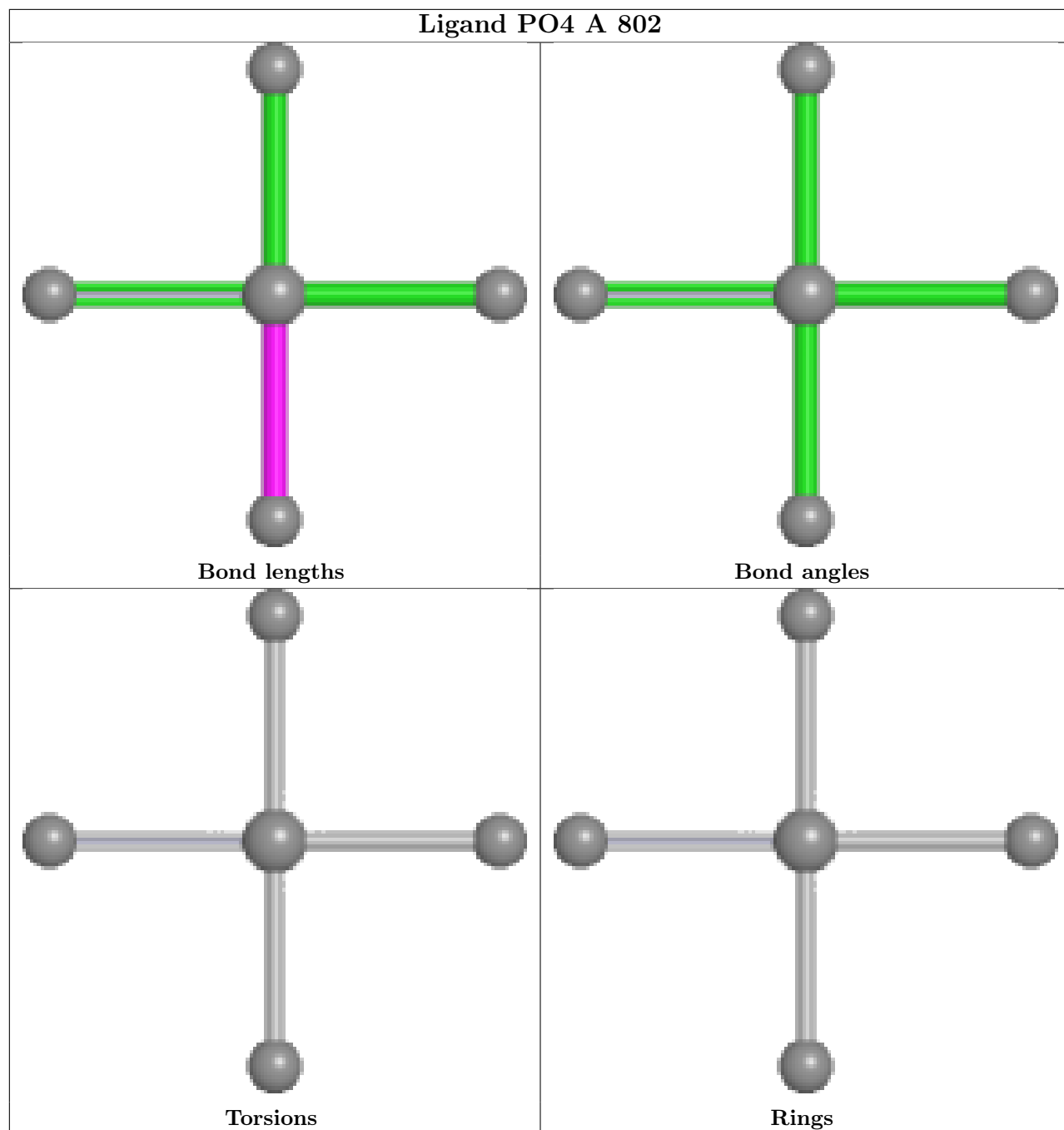
## Ligand CLR B 806



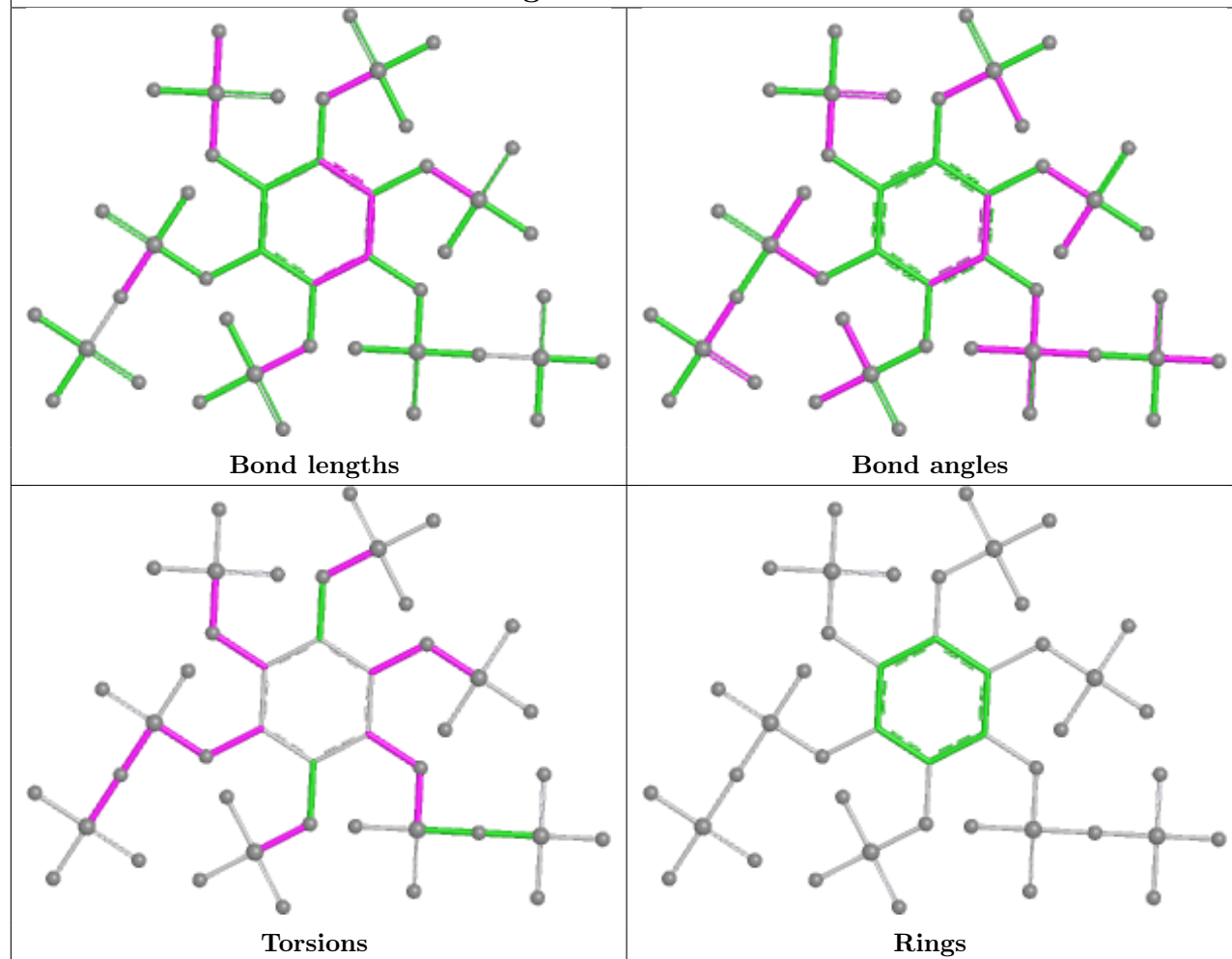
## Ligand I8P A 804

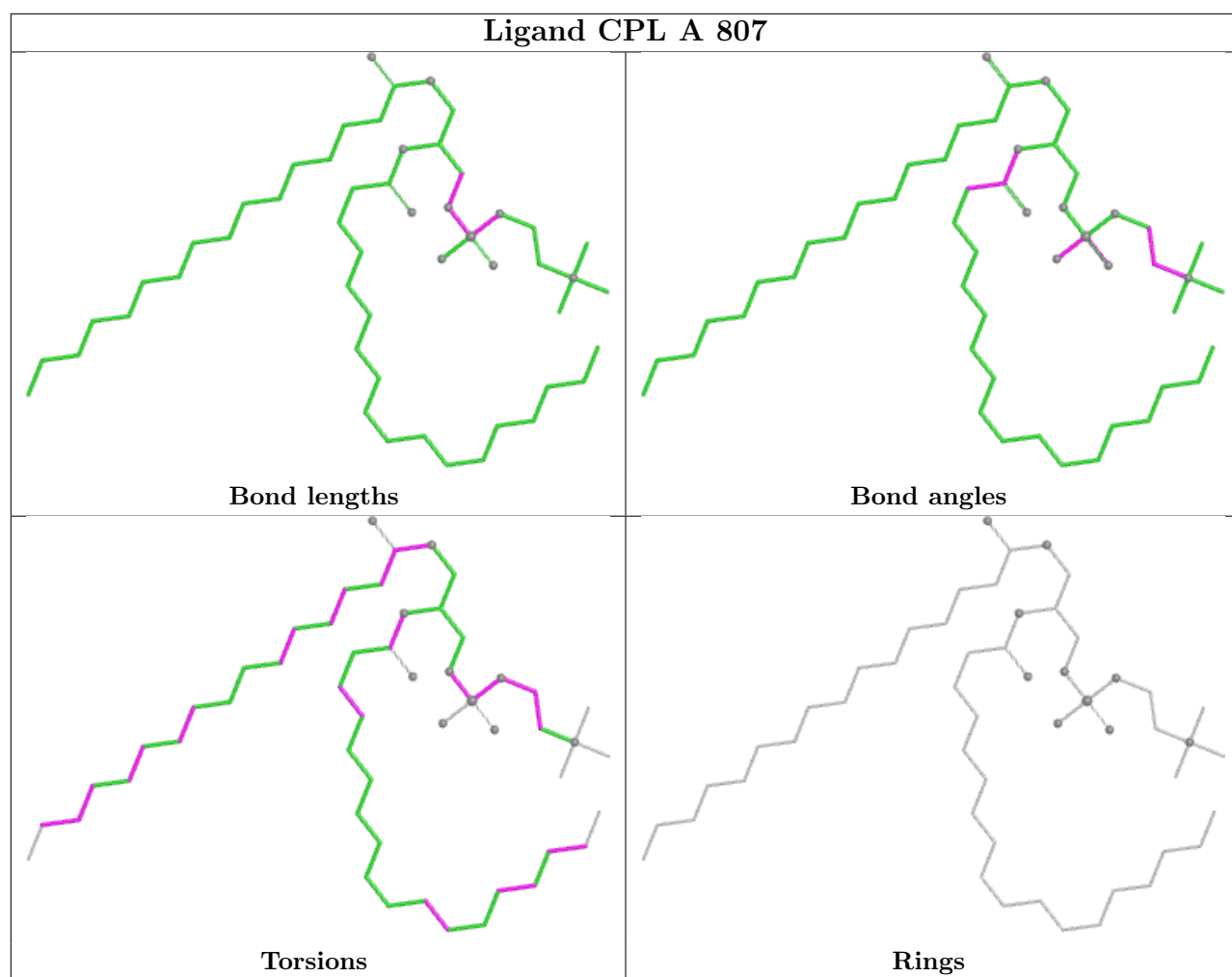


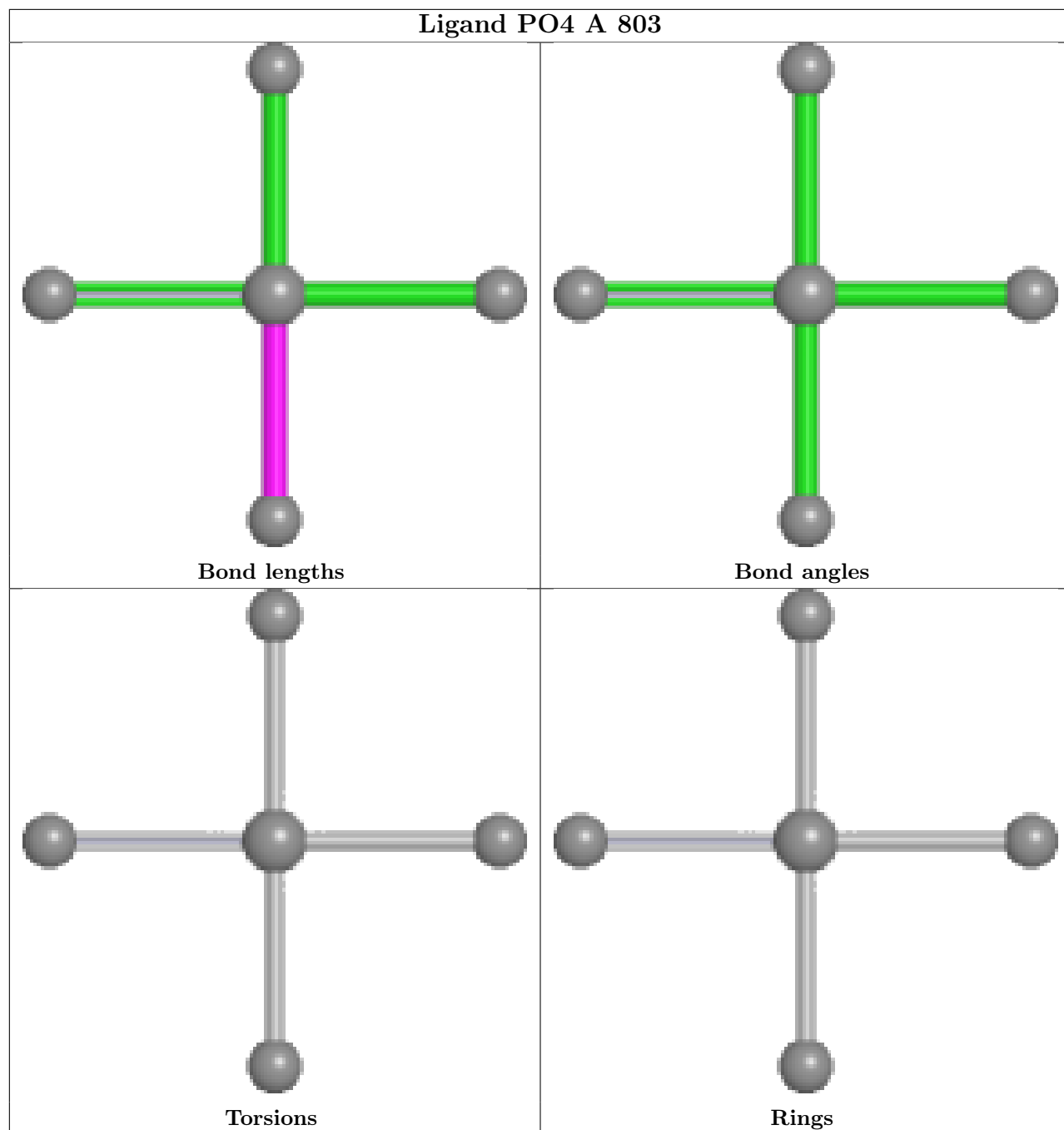




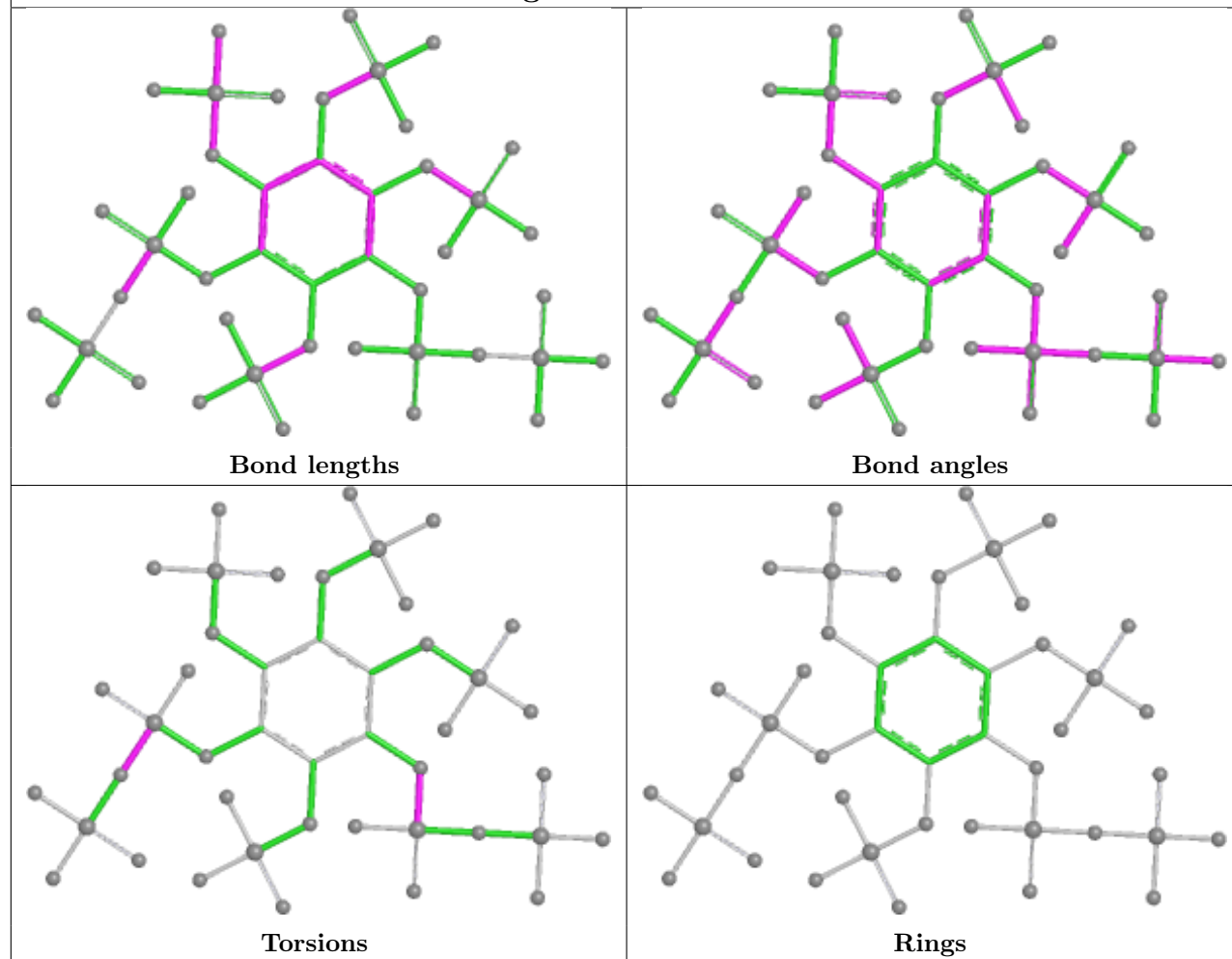
## Ligand I8P B 805



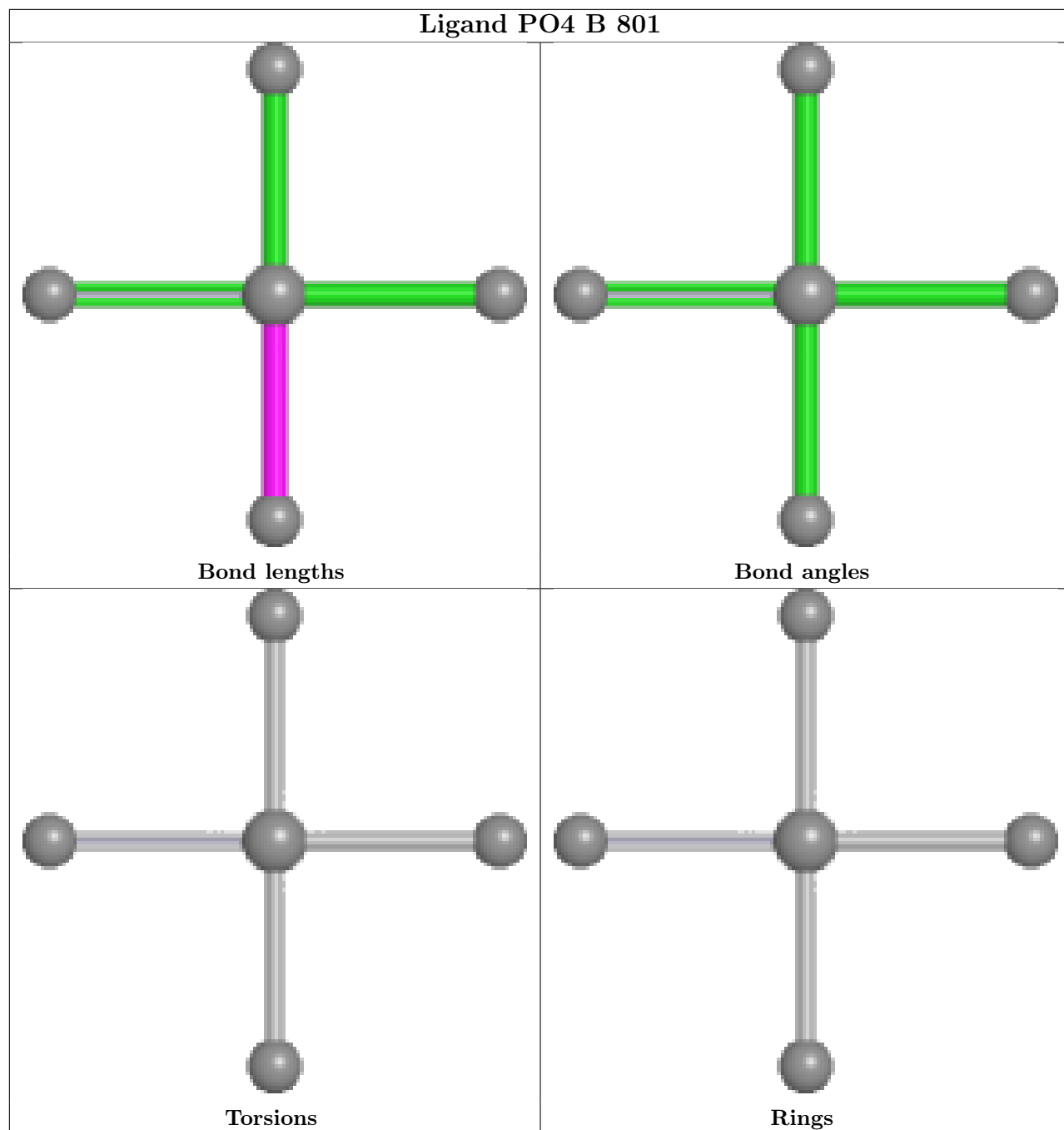


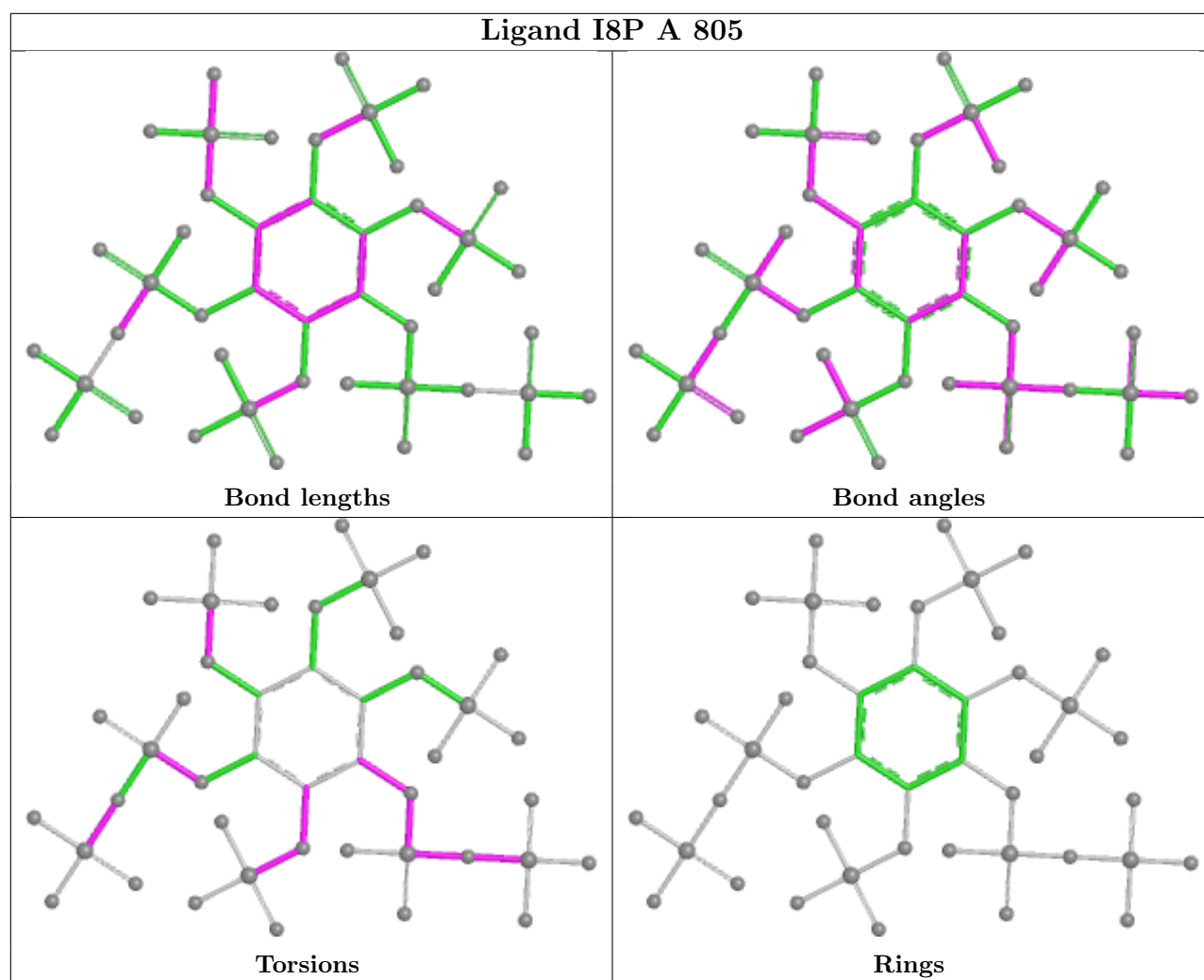


## Ligand I8P B 804









## 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.

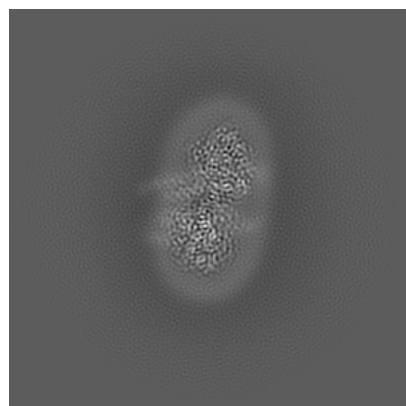
## 6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-47212. These allow visual inspection of the internal detail of the map and identification of artifacts.

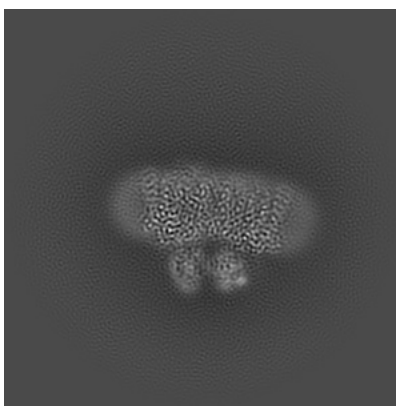
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

### 6.1 Orthogonal projections [i](#)

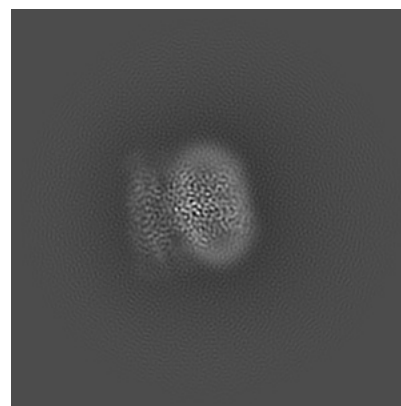
#### 6.1.1 Primary map



X

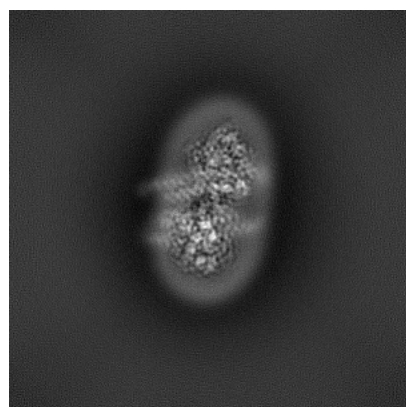


Y

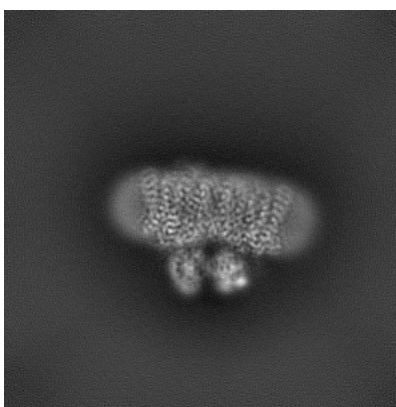


Z

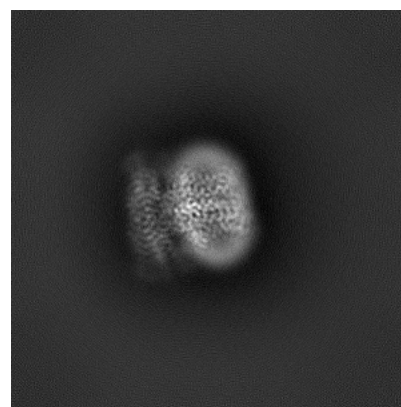
#### 6.1.2 Raw map



X



Y

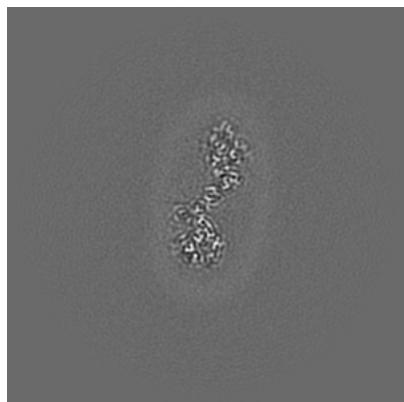


Z

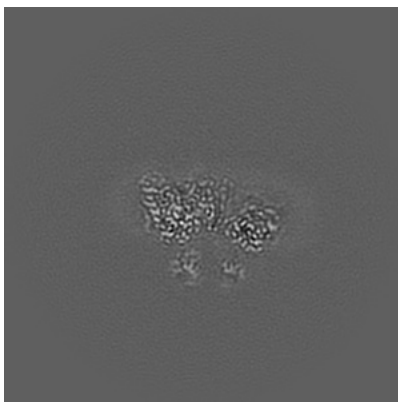
The images above show the map projected in three orthogonal directions.

## 6.2 Central slices [i](#)

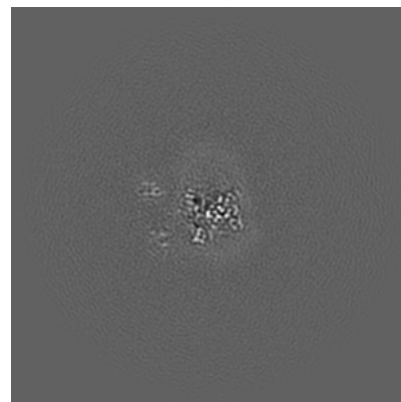
### 6.2.1 Primary map



X Index: 192

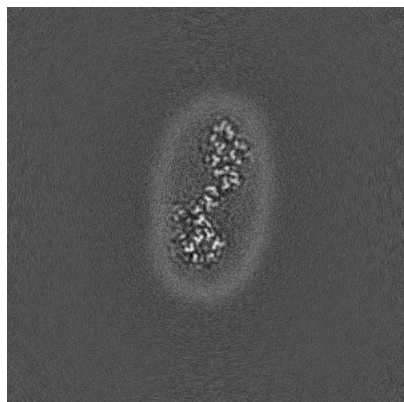


Y Index: 192

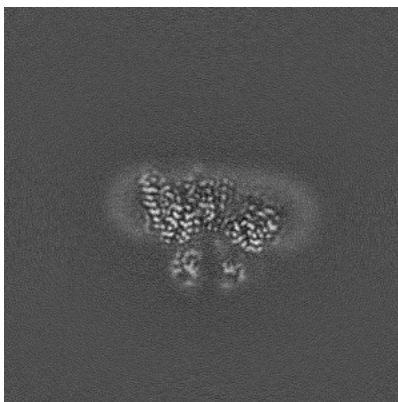


Z Index: 192

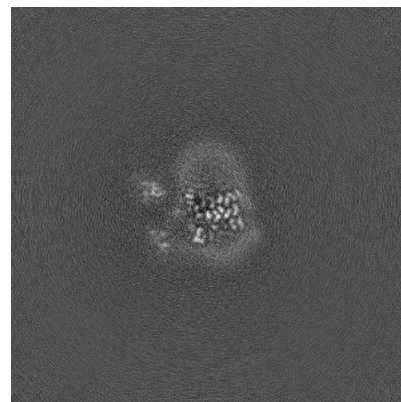
### 6.2.2 Raw map



X Index: 192



Y Index: 192

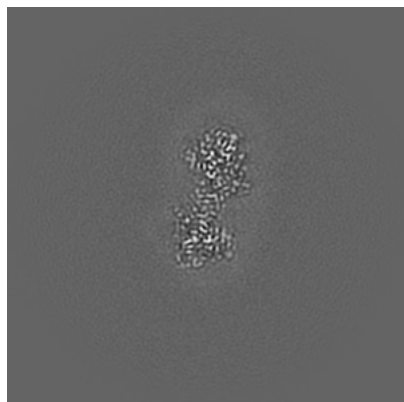


Z Index: 192

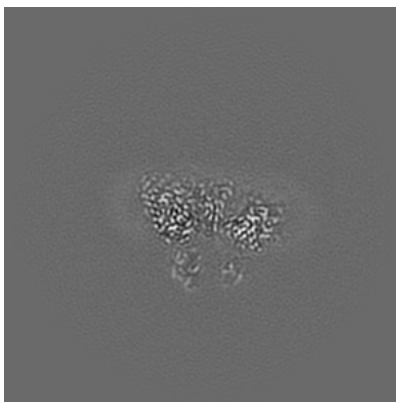
The images above show central slices of the map in three orthogonal directions.

## 6.3 Largest variance slices [i](#)

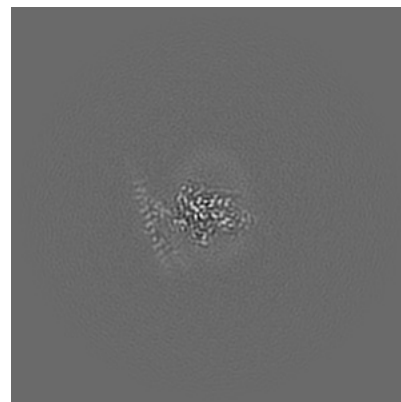
### 6.3.1 Primary map



X Index: 171

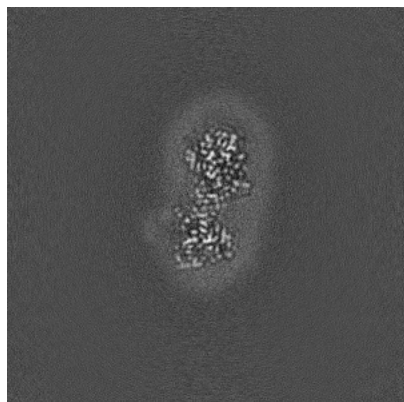


Y Index: 194

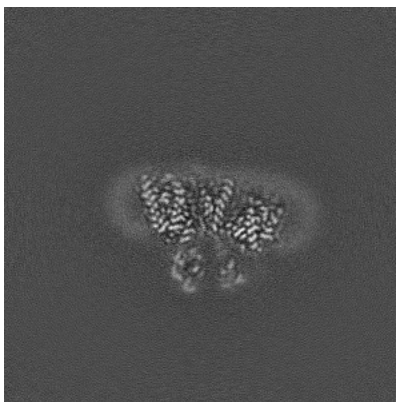


Z Index: 165

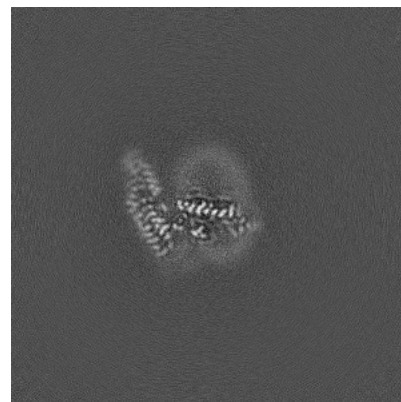
### 6.3.2 Raw map



X Index: 171



Y Index: 195

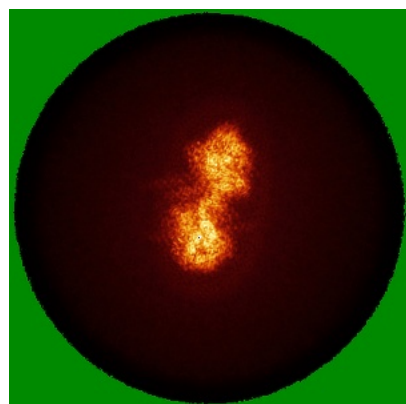


Z Index: 175

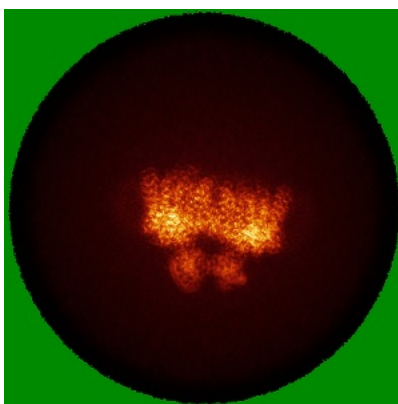
The images above show the largest variance slices of the map in three orthogonal directions.

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

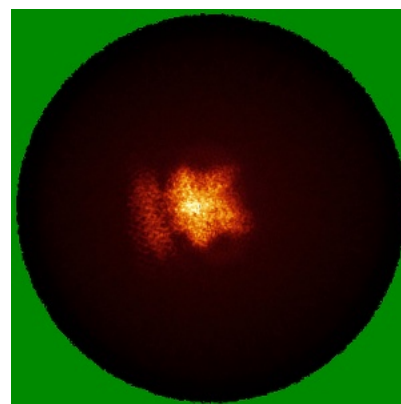
### 6.4.1 Primary map



X

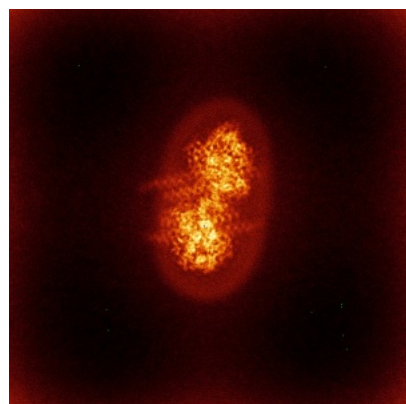


Y

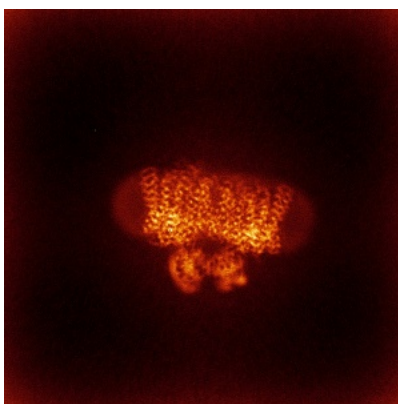


Z

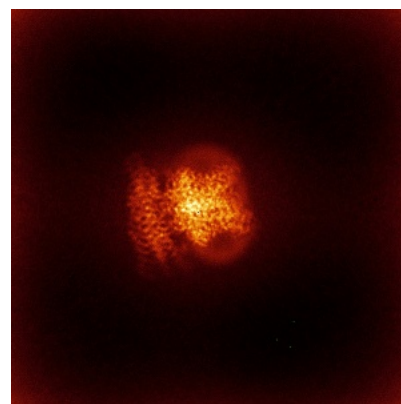
### 6.4.2 Raw map



X



Y



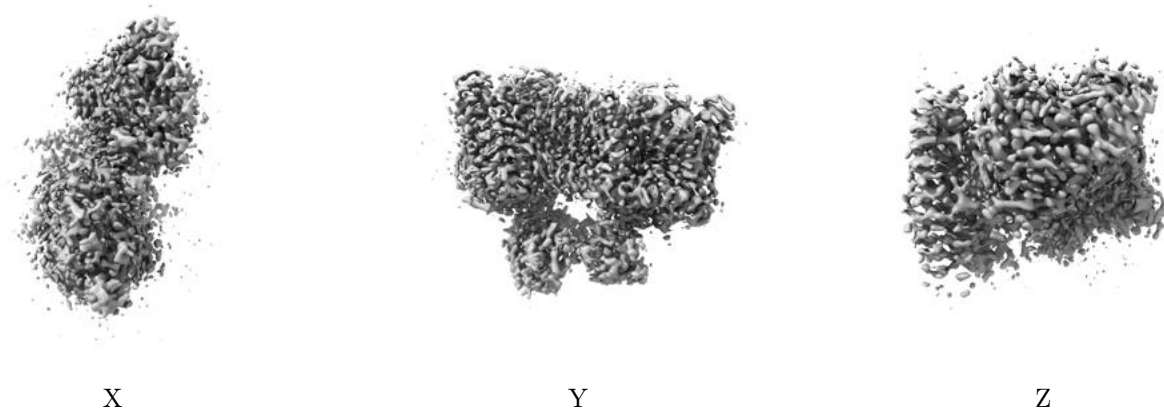
Z

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.



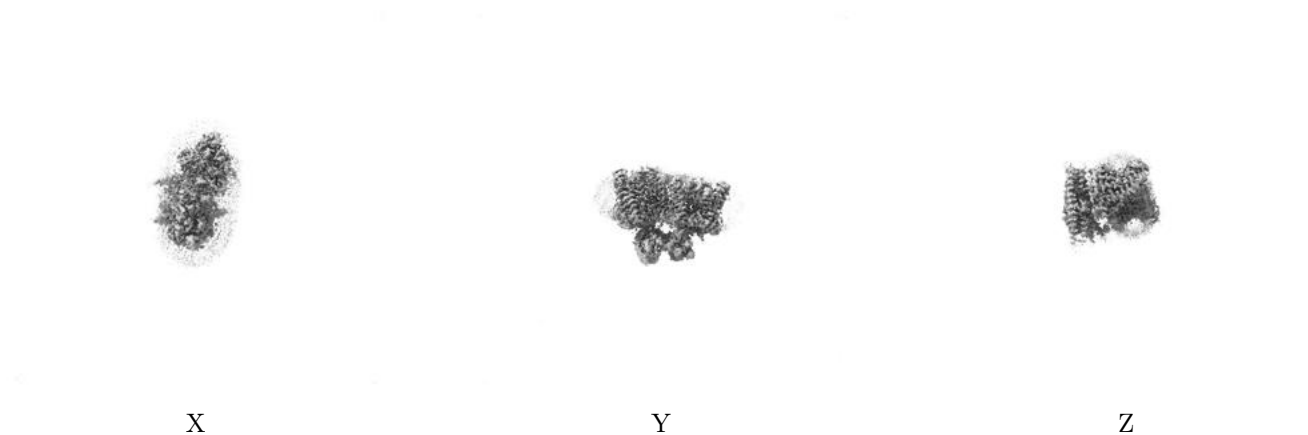
## 6.5 Orthogonal surface views [i](#)

### 6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.07. 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.

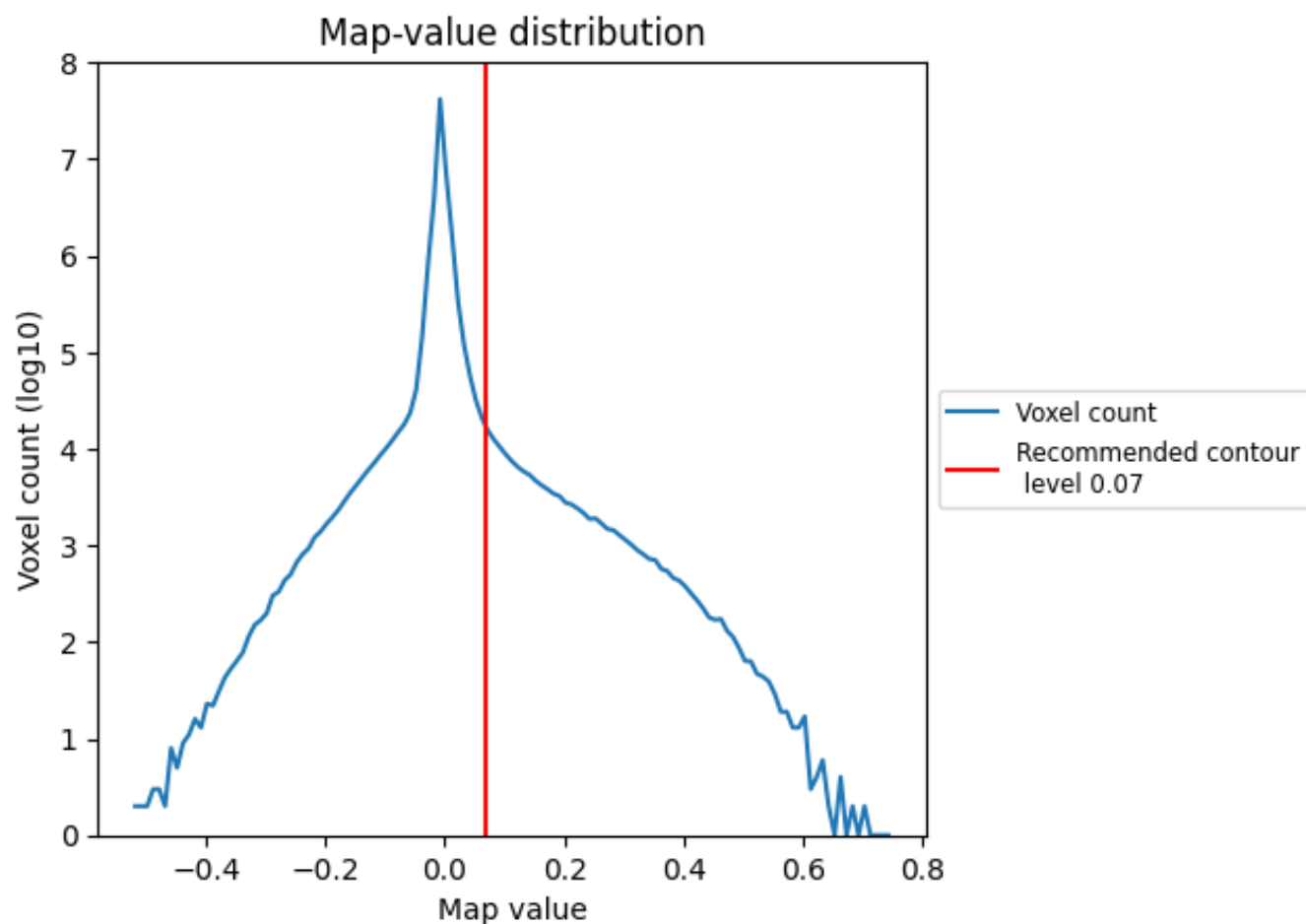
## 6.6 Mask visualisation [i](#)

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.

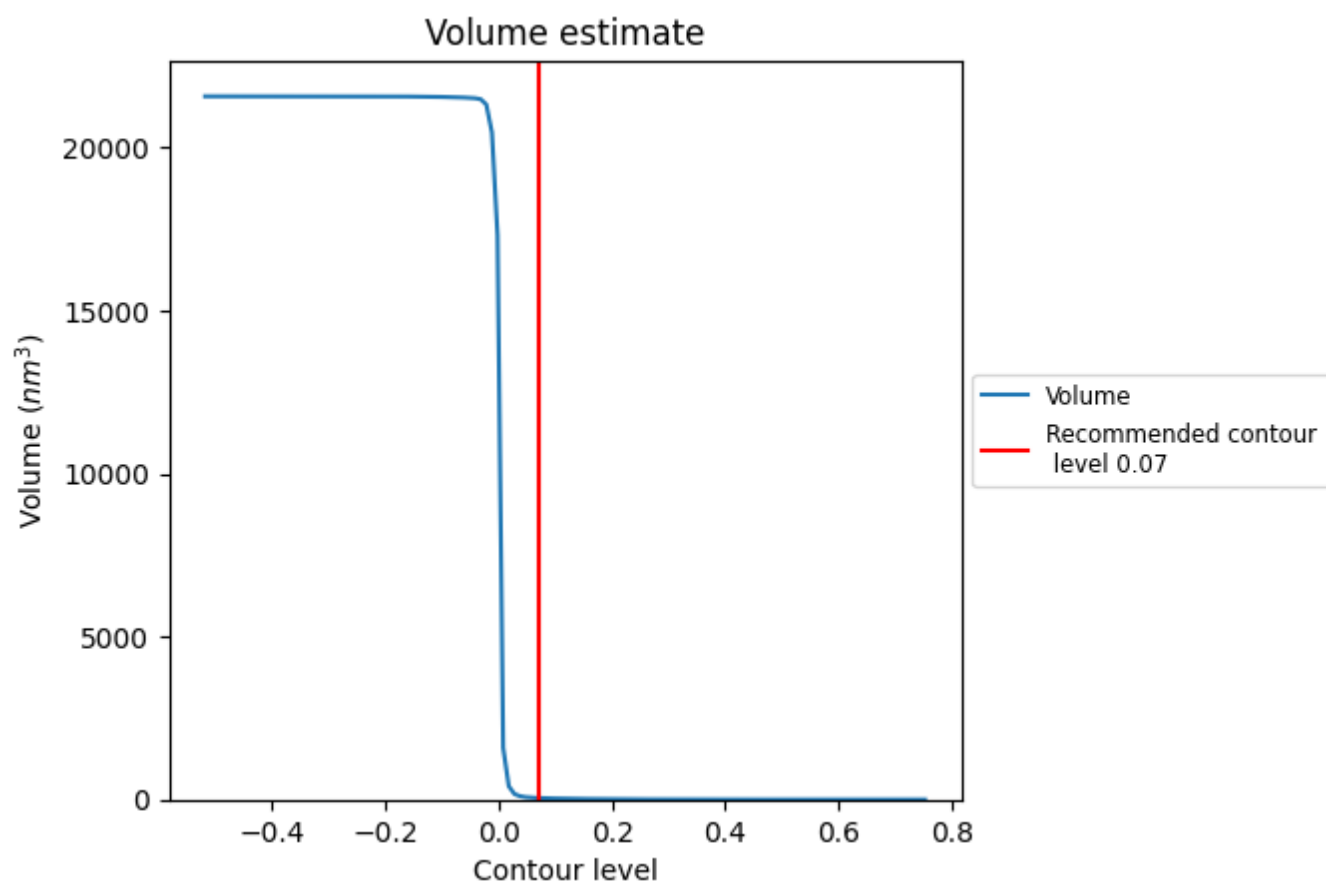
### 7.1 Map-value distribution [i](#)



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.



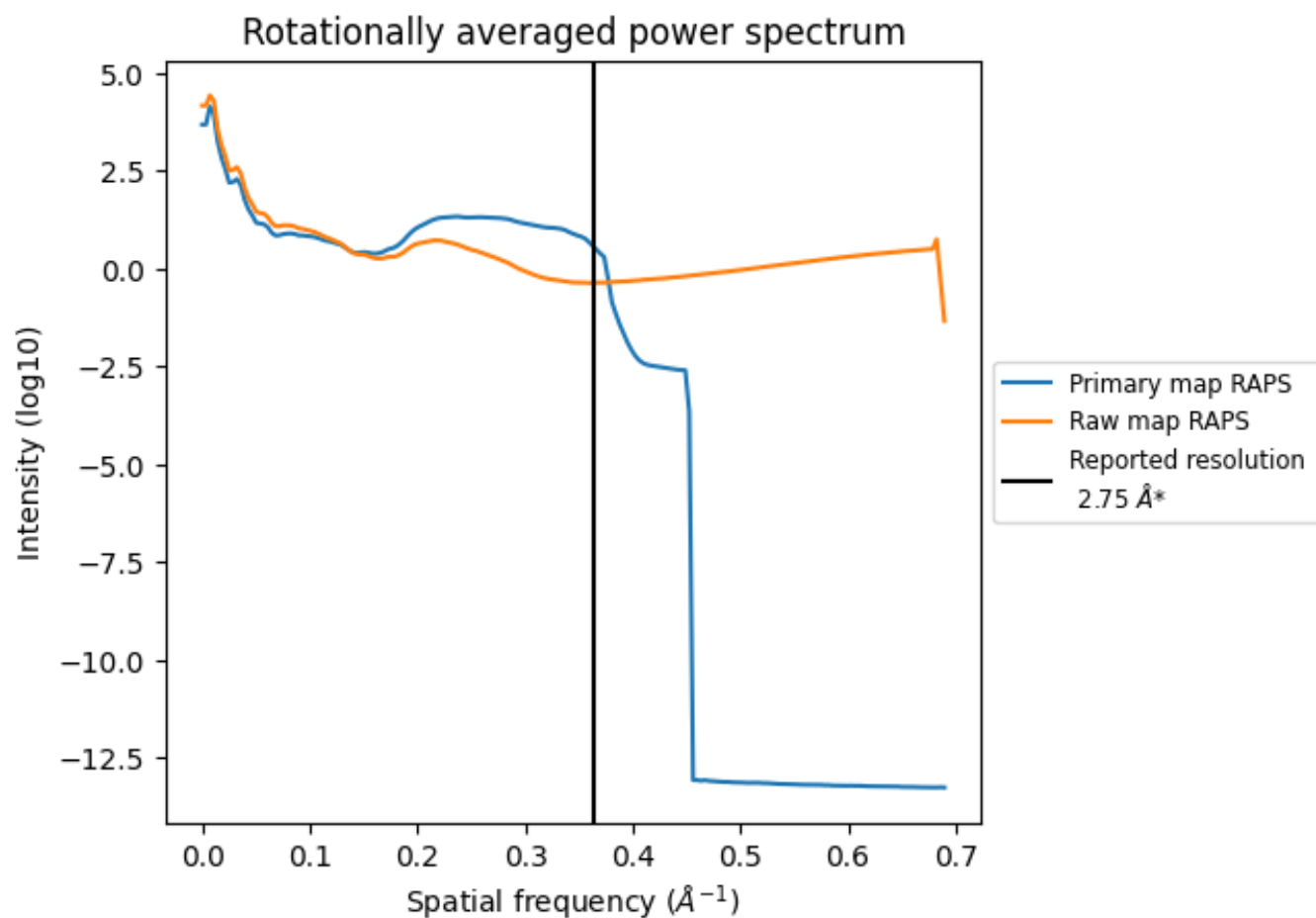
## 7.2 Volume estimate [i](#)



The volume at the recommended contour level is 48 nm<sup>3</sup>; this corresponds to an approximate mass of 43 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 ⓘ

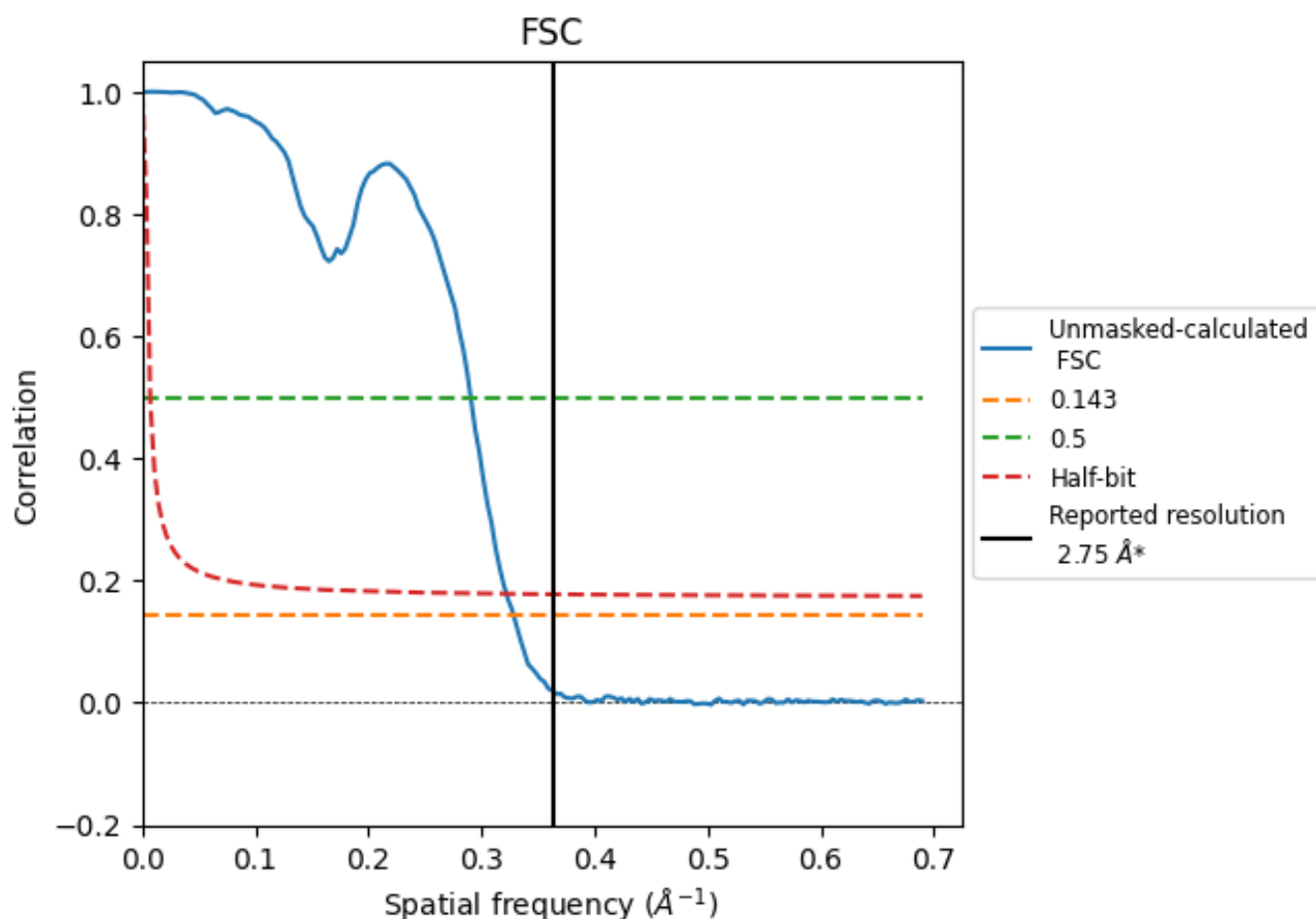


\*Reported resolution corresponds to spatial frequency of 0.364  $\text{\AA}^{-1}$

## 8 Fourier-Shell correlation [i](#)

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

### 8.1 FSC [i](#)



\*Reported resolution corresponds to spatial frequency of  $0.364 \text{ \AA}^{-1}$

## 8.2 Resolution estimates [i](#)

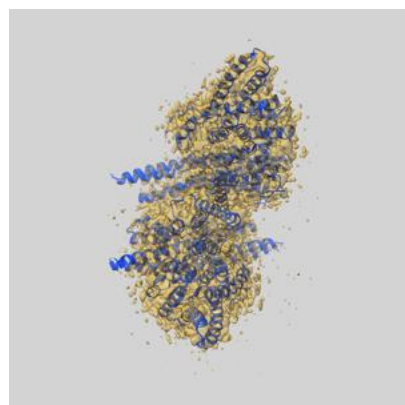
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	2.75	-	-
Author-provided FSC curve	-	-	-
Unmasked-calculated*	3.05	3.44	3.11

\*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 3.05 differs from the reported value 2.75 by more than 10 %

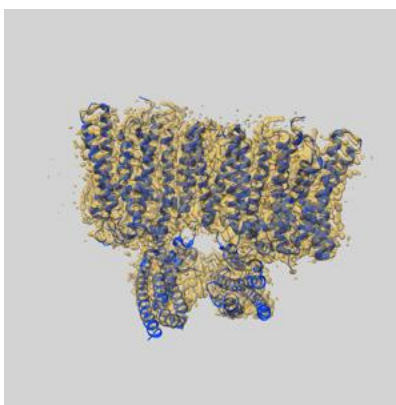
## 9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-47212 and PDB model 9DVN. Per-residue inclusion information can be found in section [3](#) on page [7](#).

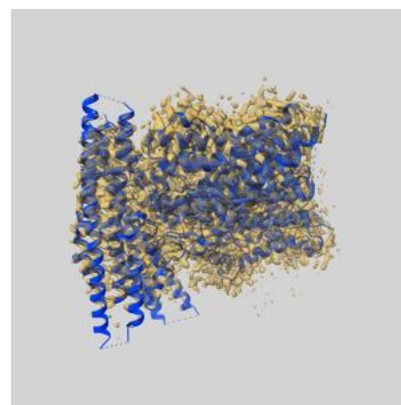
### 9.1 Map-model overlay [i](#)



X



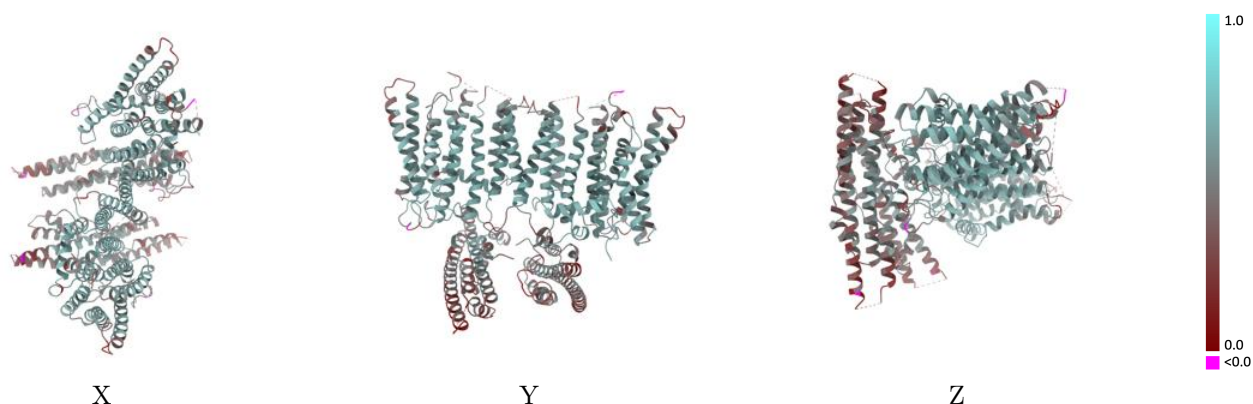
Y



Z

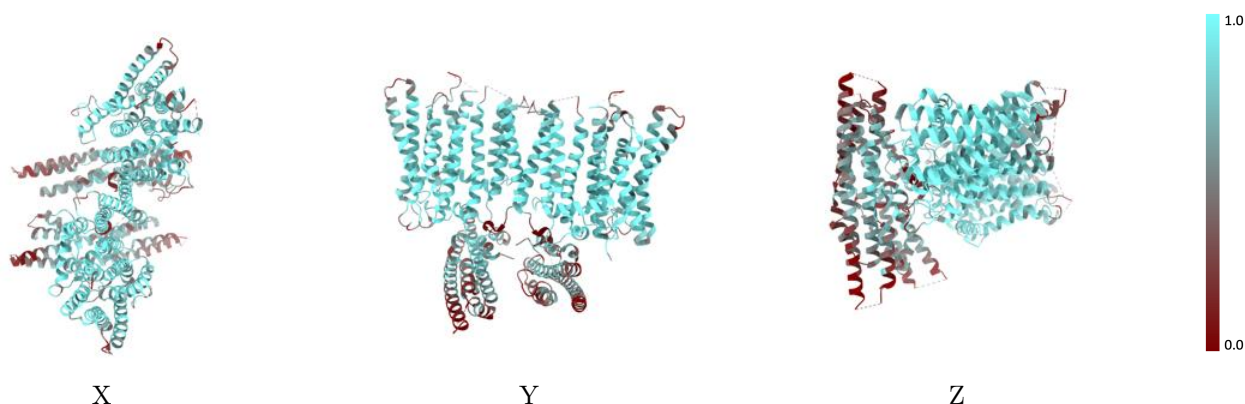
The images above show the 3D surface view of the map at the recommended contour level 0.07 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



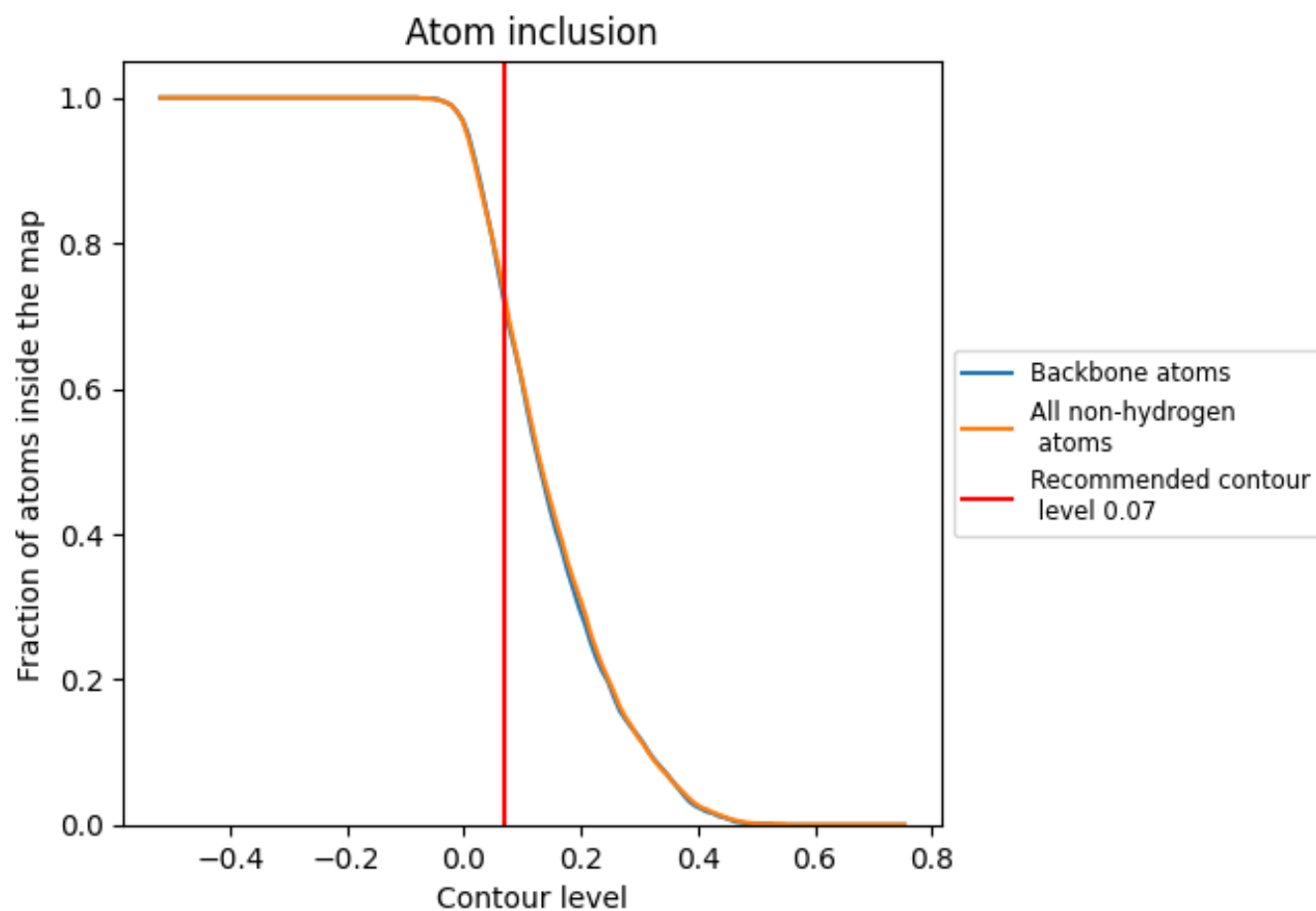
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.07).

## 9.4 Atom inclusion [i](#)



At the recommended contour level, 72% of all backbone atoms, 73% 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 (0.07) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	<div></div> 0.7260	<div></div> 0.5090
A	<div></div> 0.7010	<div></div> 0.5060
B	<div></div> 0.7410	<div></div> 0.5130

