



## Full wwPDB EM Validation Report ⓘ

May 15, 2023 – 04:57 pm BST

PDB ID : 8AYO  
EMDB ID : EMD-15718  
Title : Open state GluA1/A2 AMPA receptor in complex with TARP gamma 8 and ligand JNJ-61432059  
Authors : Zhang, D.; Lape, R.; Shaikh, S.; Kohegyi, B.; Watson, J.F.; Cais, O.; Nakagawa, T.; Greger, I.H.  
Deposited on : 2022-09-02  
Resolution : 3.30 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:

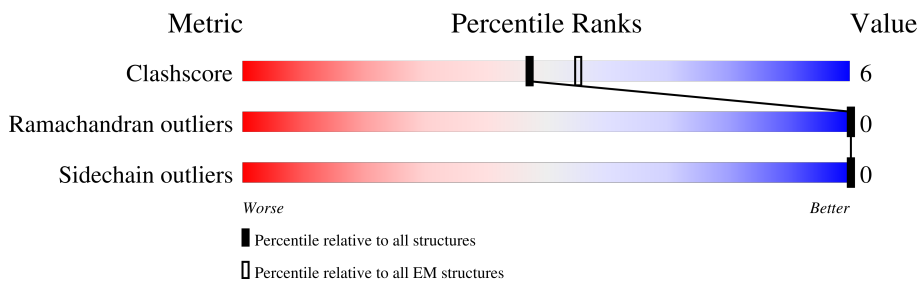
EMDB validation analysis : 0.0.1.dev50  
Mogul : 1.8.4, CSD as541be (2020)  
MolProbity : 4.02b-467  
buster-report : 1.1.7 (2018)  
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)  
MapQ : 1.9.9  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.32.2

# 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 3.30 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  $\geq 3$ , 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	915	
1	C	915	
2	B	860	
2	D	860	
3	I	423	
3	J	423	

## 2 Entry composition i

There are 9 unique types of molecules in this entry. The entry contains 14512 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called Isoform Flip of Glutamate receptor 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
1	A	399	2836	1851	455	515	15	0	0
1	C	399	2836	1851	455	515	15	0	0

There are 16 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-6	ASP	-	insertion	UNP P19490
A	-5	TYR	-	insertion	UNP P19490
A	-4	LYS	-	insertion	UNP P19490
A	-3	ASP	-	insertion	UNP P19490
A	-2	ASP	-	insertion	UNP P19490
A	-1	ASP	-	insertion	UNP P19490
A	0	ASP	-	insertion	UNP P19490
A	1	LYS	-	insertion	UNP P19490
C	-6	ASP	-	insertion	UNP P19490
C	-5	TYR	-	insertion	UNP P19490
C	-4	LYS	-	insertion	UNP P19490
C	-3	ASP	-	insertion	UNP P19490
C	-2	ASP	-	insertion	UNP P19490
C	-1	ASP	-	insertion	UNP P19490
C	0	ASP	-	insertion	UNP P19490
C	1	LYS	-	insertion	UNP P19490

- Molecule 2 is a protein called Isoform Flip of Glutamate receptor 2.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
2	D	398	2865	1868	464	514	19	0	0
2	B	398	2865	1868	464	514	19	0	0

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
D	586	ARG	GLN	variant	UNP P19491
B	586	ARG	GLN	variant	UNP P19491

- Molecule 3 is a protein called Voltage-dependent calcium channel gamma-8 subunit.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
3	I	182	1278	836	213	223	6	0	0
3	J	182	1278	836	213	223	6	0	0

There are 14 discrepancies between the modelled and reference sequences:

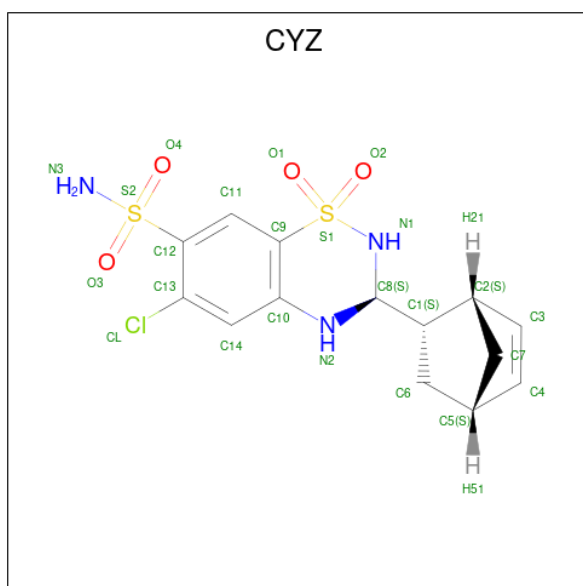
Chain	Residue	Modelled	Actual	Comment	Reference
I	1	GLY	-	expression tag	UNP Q8VHW5
I	418	LEU	-	expression tag	UNP Q8VHW5
I	419	GLU	-	expression tag	UNP Q8VHW5
I	420	VAL	-	expression tag	UNP Q8VHW5
I	421	LEU	-	expression tag	UNP Q8VHW5
I	422	PHE	-	expression tag	UNP Q8VHW5
I	423	GLN	-	expression tag	UNP Q8VHW5
J	1	GLY	-	expression tag	UNP Q8VHW5
J	418	LEU	-	expression tag	UNP Q8VHW5
J	419	GLU	-	expression tag	UNP Q8VHW5
J	420	VAL	-	expression tag	UNP Q8VHW5
J	421	LEU	-	expression tag	UNP Q8VHW5
J	422	PHE	-	expression tag	UNP Q8VHW5
J	423	GLN	-	expression tag	UNP Q8VHW5

- Molecule 4 is GLUTAMIC ACID (three-letter code: GLU) (formula: C<sub>5</sub>H<sub>9</sub>NO<sub>4</sub>) (labeled as "Ligand of Interest" by depositor).



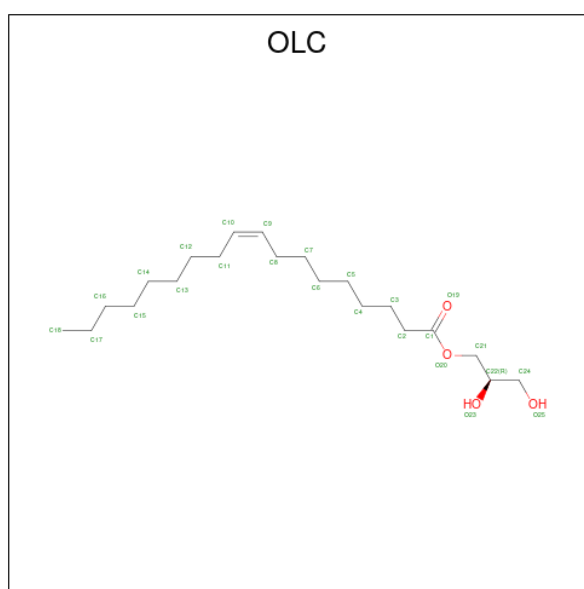
Mol	Chain	Residues	Atoms				AltConf
			Total	C	N	O	
4	A	1	Total 10	C 5	N 1	O 4	0
4	D	1	Total 10	C 5	N 1	O 4	0
4	C	1	Total 10	C 5	N 1	O 4	0
4	B	1	Total 10	C 5	N 1	O 4	0

- Molecule 5 is CYCLOTHIAZIDE (three-letter code: CYZ) (formula:  $C_{14}H_{16}ClN_3O_4S_2$ ) (labeled as "Ligand of Interest" by depositor).



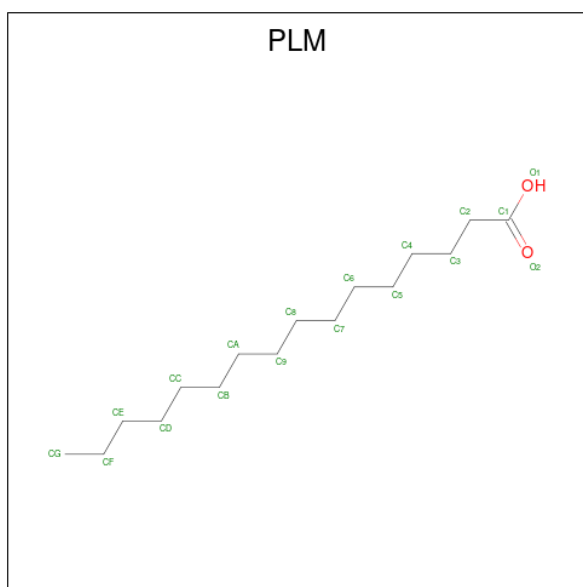
Mol	Chain	Residues	Atoms					AltConf	
5	A	1	Total	C	Cl	N	O	S	0
			24	14	1	3	4	2	
5	D	1	Total	C	Cl	N	O	S	0
			24	14	1	3	4	2	
5	C	1	Total	C	Cl	N	O	S	0
			24	14	1	3	4	2	
5	B	1	Total	C	Cl	N	O	S	0
			24	14	1	3	4	2	

- Molecule 6 is (2R)-2,3-dihydroxypropyl (9Z)-octadec-9-enoate (three-letter code: OLC) (formula: C<sub>21</sub>H<sub>40</sub>O<sub>4</sub>) (labeled as "Ligand of Interest" by depositor).



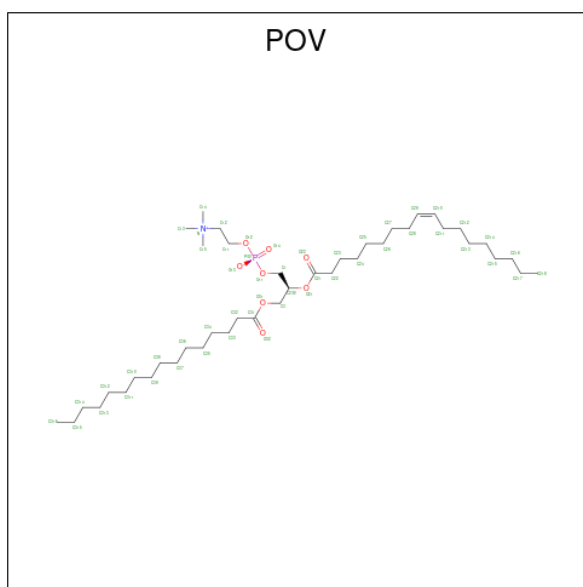
Mol	Chain	Residues	Atoms			AltConf
6	A	1	Total	C	O	0
			25	21	4	
6	D	1	Total	C	O	0
			25	21	4	
6	C	1	Total	C	O	0
			25	21	4	
6	B	1	Total	C	O	0
			25	21	4	

- Molecule 7 is PALMITIC ACID (three-letter code: PLM) (formula: C<sub>16</sub>H<sub>32</sub>O<sub>2</sub>) (labeled as "Ligand of Interest" by depositor).



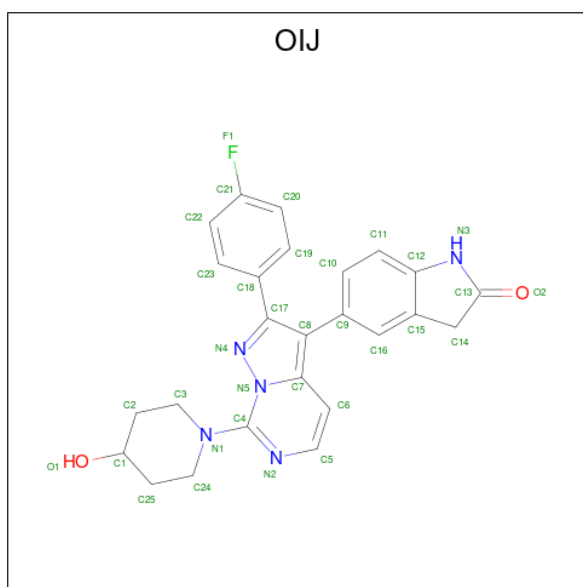
Mol	Chain	Residues	Atoms			AltConf
7	A	1	Total	C	O	0
			18	16	2	
7	A	1	Total	C	O	0
			18	16	2	
7	C	1	Total	C	O	0
			18	16	2	
7	C	1	Total	C	O	0
			18	16	2	
7	I	1	Total	C	O	0
			18	16	2	
7	I	1	Total	C	O	0
			18	16	2	
7	I	1	Total	C	O	0
			18	16	2	
7	J	1	Total	C	O	0
			18	16	2	
7	J	1	Total	C	O	0
			18	16	2	
7	J	1	Total	C	O	0
			18	16	2	

- Molecule 8 is (2S)-3-(hexadecanoyloxy)-2-[(9Z)-octadec-9-enoyloxy]propyl 2-(trimethylamm onio)ethyl phosphate (three-letter code: POV) (formula: C<sub>42</sub>H<sub>82</sub>NO<sub>8</sub>P) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms				AltConf
			Total	C	O	P	
8	A	1	36	27	8	1	0
8	C	1	36	27	8	1	0

- Molecule 9 is 5-[2-(4-fluorophenyl)-7-(4-oxidanylpiperidin-1-yl)pyrazolo[1,5-c]pyrimidin-3-yl]-1,3-dihydroindol-2-one (three-letter code: OIJ) (formula:  $C_{25}H_{22}FN_5O_2$ ) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms					AltConf
			Total	C	F	N	O	
9	I	1	33	25	1	5	2	0

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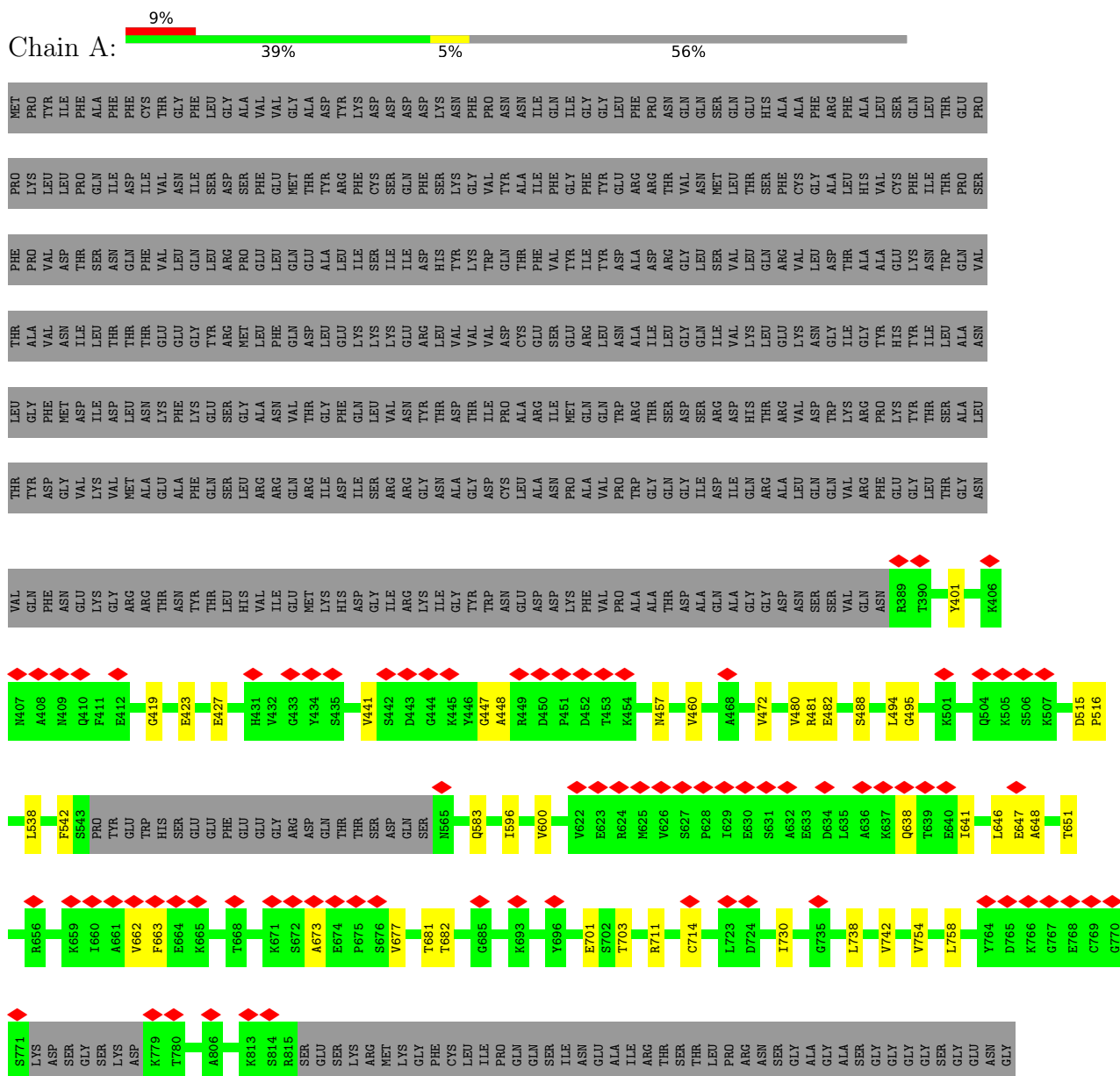
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Mol	Chain	Residues	Atoms					AltConf
			Total	C	F	N	O	
9	J	1	33	25	1	5	2	0

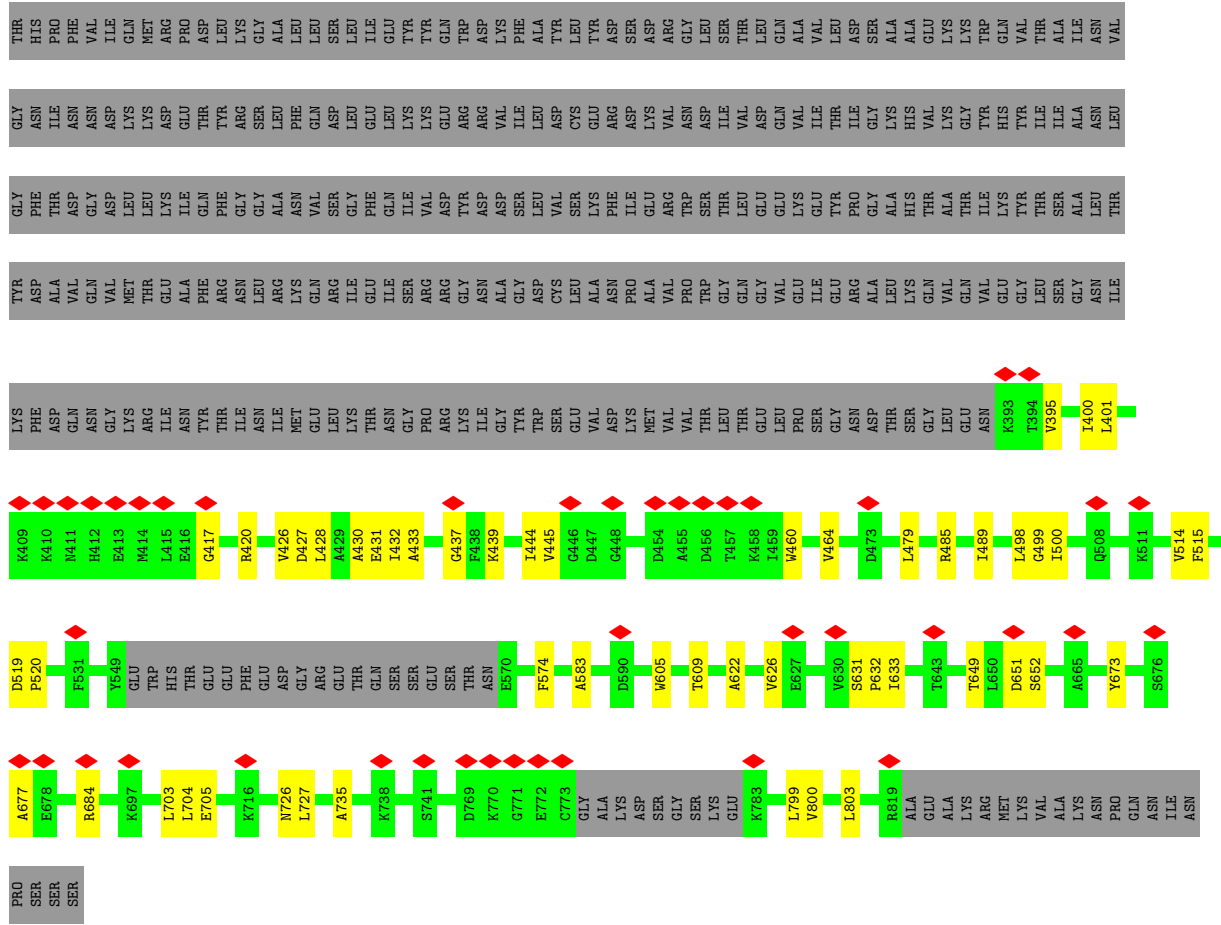
### 3 Residue-property plots

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.

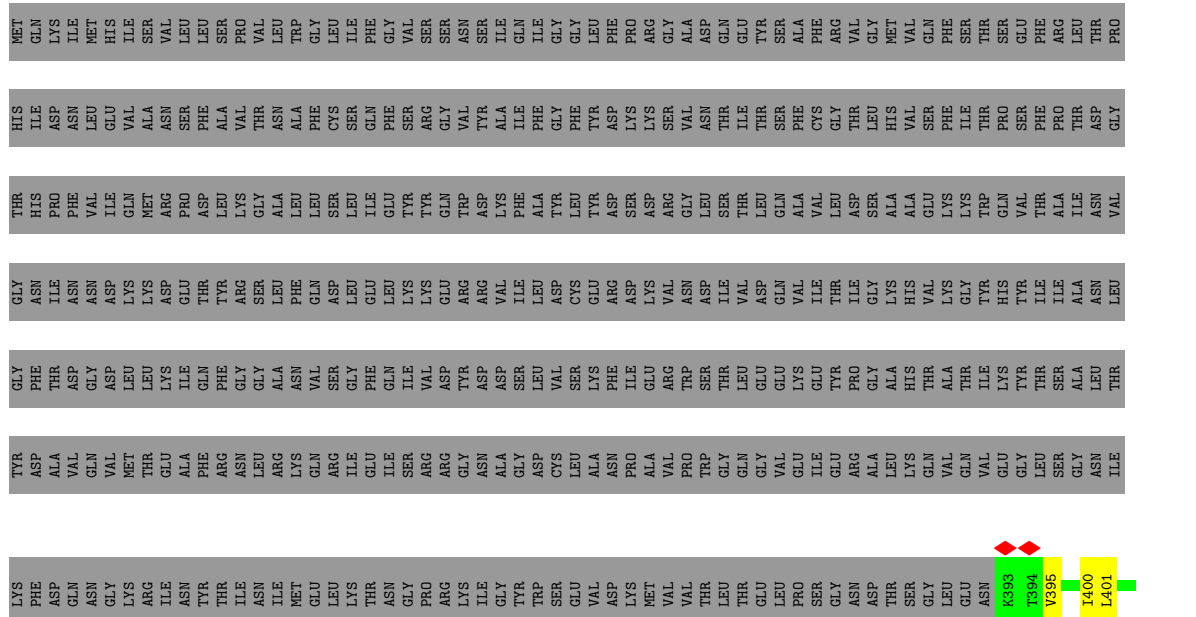
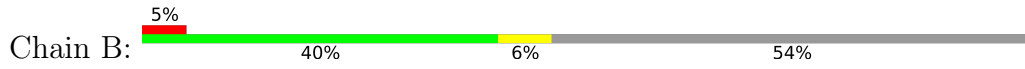
- Molecule 1: Isoform Flip of Glutamate receptor 1

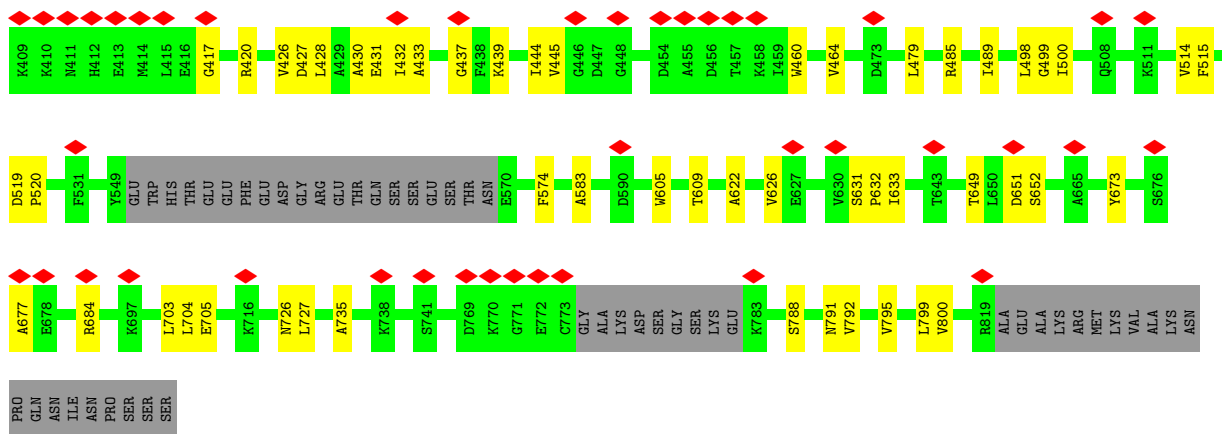




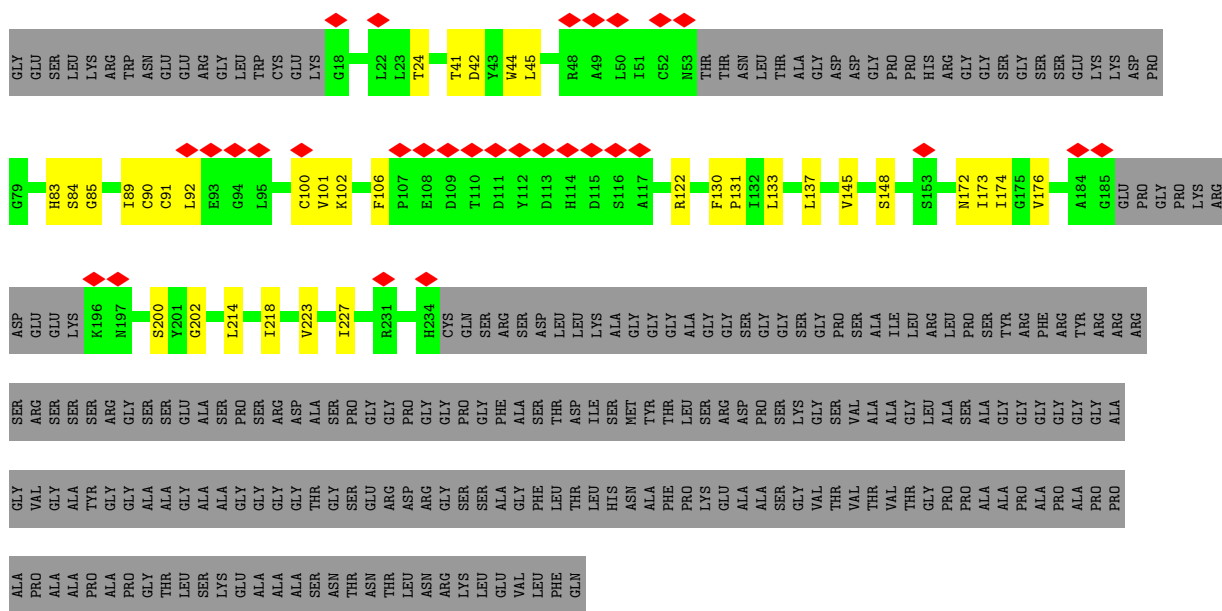
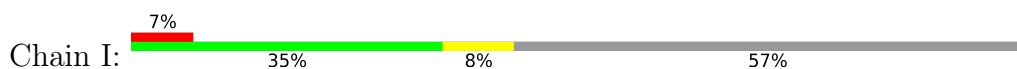


• Molecule 2: Isoform Flip of Glutamate receptor 2

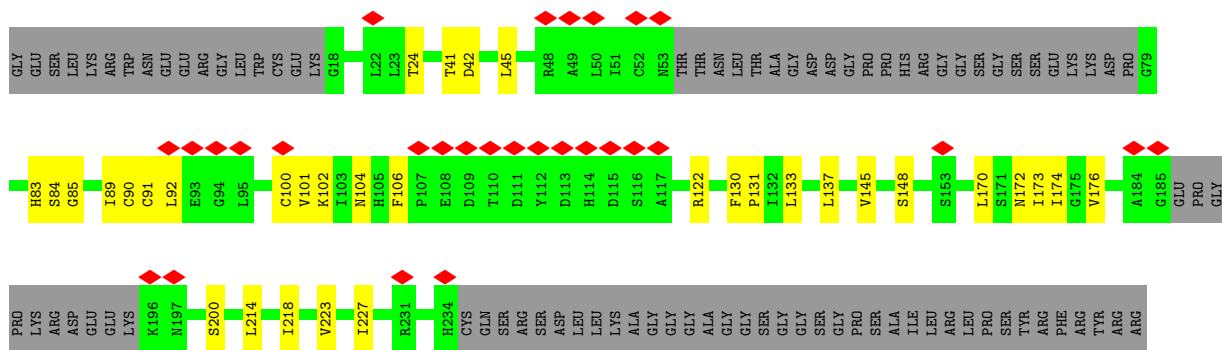
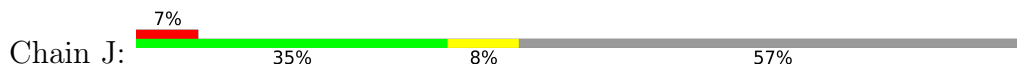




• Molecule 3: Voltage-dependent calcium channel gamma-8 subunit



• Molecule 3: Voltage-dependent calcium channel gamma-8 subunit





## 4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	281537	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ( $e^-/\text{\AA}^2$ )	50	Depositor
Minimum defocus (nm)	1200	Depositor
Maximum defocus (nm)	3000	Depositor
Magnification	Not provided	
Image detector	GATAN K3 (6k x 4k)	Depositor
Maximum map value	0.149	Depositor
Minimum map value	-0.083	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.002	Depositor
Recommended contour level	0.023	Depositor
Map size ( $\text{\AA}$ )	342.40002, 342.40002, 342.40002	wwPDB
Map dimensions	320, 320, 320	wwPDB
Map angles ( $^\circ$ )	90.0, 90.0, 90.0	wwPDB
Pixel spacing ( $\text{\AA}$ )	1.07, 1.07, 1.07	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: OLC, PLM, POV, OIJ, CYZ

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	0.37	0/2901	0.44	0/3967
1	C	0.38	0/2901	0.44	0/3967
2	B	0.37	0/2929	0.44	0/3993
2	D	0.37	0/2929	0.44	0/3993
3	I	0.37	0/1301	0.44	0/1778
3	J	0.36	0/1301	0.44	0/1778
All	All	0.37	0/14262	0.44	0/19476

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	2836	0	2600	29	0
1	C	2836	0	2600	27	0
2	B	2865	0	2703	38	0
2	D	2865	0	2703	39	0
3	I	1278	0	1227	26	0
3	J	1278	0	1227	27	0
4	A	10	0	5	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	B	10	0	5	0	0
4	C	10	0	5	1	0
4	D	10	0	5	0	0
5	A	24	0	10	0	0
5	B	24	0	10	1	0
5	C	24	0	10	0	0
5	D	24	0	10	1	0
6	A	25	0	40	0	0
6	B	25	0	40	1	0
6	C	25	0	40	0	0
6	D	25	0	40	2	0
7	A	36	0	62	0	0
7	C	36	0	62	0	0
7	I	54	0	93	0	0
7	J	54	0	93	0	0
8	A	36	0	43	1	0
8	C	36	0	43	1	0
9	I	33	0	0	1	0
9	J	33	0	0	1	0
All	All	14512	0	13676	179	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 (179) 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)
5:B:902:CYZ:N3	5:B:902:CYZ:CL	2.49	0.83
5:D:902:CYZ:N3	5:D:902:CYZ:CL	2.49	0.82
2:B:631:SER:OG	2:B:633:ILE:O	1.99	0.79
1:C:538:LEU:HD23	1:C:542:PHE:HE1	1.51	0.75
2:D:631:SER:OG	2:D:633:ILE:O	2.05	0.73
2:B:395:VAL:N	2:B:439:LYS:O	2.25	0.70
3:J:45:LEU:HD12	3:J:200:SER:O	1.92	0.69
2:D:395:VAL:N	2:D:439:LYS:O	2.24	0.69
3:I:45:LEU:HD12	3:I:200:SER:O	1.93	0.69
2:D:800:VAL:HG11	3:J:174:ILE:HD11	1.74	0.69
3:I:174:ILE:HD11	2:B:800:VAL:HG11	1.75	0.68
2:D:427:ASP:O	2:D:431:GLU:OE1	2.15	0.64
2:B:427:ASP:O	2:B:431:GLU:OE1	2.15	0.63
2:D:622:ALA:O	2:D:626:VAL:HG13	1.98	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:622:ALA:O	2:B:626:VAL:HG13	1.97	0.63
1:C:651:THR:HG22	4:C:901:GLU:OE2	2.00	0.61
1:A:651:THR:HG22	4:A:901:GLU:OE2	2.00	0.60
3:I:90:CYS:HA	3:I:100:CYS:CB	2.32	0.59
3:J:90:CYS:HA	3:J:100:CYS:CB	2.32	0.59
2:D:605:TRP:O	2:D:609:THR:HG23	2.03	0.59
2:D:498:LEU:HD13	2:D:705:GLU:HG3	1.85	0.59
1:A:472:VAL:HG12	1:A:472:VAL:O	2.03	0.58
1:C:494:LEU:HD12	1:C:495:GLY:N	2.19	0.58
1:C:538:LEU:HD23	1:C:542:PHE:CE1	2.37	0.58
2:B:605:TRP:O	2:B:609:THR:HG23	2.03	0.58
1:A:494:LEU:HD12	1:A:495:GLY:N	2.19	0.58
2:B:433:ALA:O	2:B:437:GLY:N	2.37	0.57
2:B:498:LEU:HD13	2:B:705:GLU:HG3	1.86	0.57
1:C:472:VAL:HG12	1:C:472:VAL:O	2.04	0.56
1:C:738:LEU:O	1:C:742:VAL:HG23	2.06	0.56
1:A:427:GLU:OE1	1:A:754:VAL:HG11	2.05	0.56
1:A:738:LEU:O	1:A:742:VAL:HG23	2.06	0.55
2:D:433:ALA:O	2:D:437:GLY:N	2.37	0.55
3:I:90:CYS:HA	3:I:100:CYS:HB3	1.88	0.55
3:I:101:VAL:HG22	3:I:102:LYS:N	2.23	0.54
1:C:711:ARG:O	1:C:714:CYS:N	2.40	0.53
3:J:90:CYS:HA	3:J:100:CYS:HB3	1.88	0.53
1:A:711:ARG:O	1:A:714:CYS:N	2.41	0.53
3:J:101:VAL:HG22	3:J:102:LYS:N	2.23	0.52
2:B:651:ASP:OD1	2:B:652:SER:N	2.41	0.52
1:C:596:ILE:O	1:C:600:VAL:HG23	2.10	0.52
1:A:583:GLN:NE2	2:B:583:ALA:O	2.38	0.51
3:I:145:VAL:O	3:I:148:SER:OG	2.20	0.51
3:J:145:VAL:O	3:J:148:SER:OG	2.20	0.51
1:C:638:GLN:NE2	1:C:641:ILE:O	2.38	0.51
2:D:651:ASP:OD1	2:D:652:SER:N	2.41	0.51
3:I:174:ILE:CD1	2:B:800:VAL:HG11	2.39	0.51
3:I:214:LEU:O	3:I:218:ILE:HG12	2.11	0.51
1:A:646:LEU:HD23	1:A:647:GLU:O	2.10	0.51
3:J:214:LEU:O	3:J:218:ILE:HG12	2.11	0.51
1:C:646:LEU:HD23	1:C:647:GLU:O	2.11	0.50
3:I:172:ASN:OD1	9:I:1802:OIJ:O2	2.30	0.50
2:D:583:ALA:O	1:C:583:GLN:NE2	2.39	0.50
3:J:172:ASN:OD1	9:J:1804:OIJ:O2	2.30	0.50
3:J:106:PHE:O	3:J:122:ARG:NH2	2.44	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:574:PHE:HE2	6:D:903:OLC:H18A	1.76	0.50
2:D:673:TYR:O	2:D:677:ALA:N	2.45	0.49
3:I:106:PHE:O	3:I:122:ARG:NH2	2.44	0.49
2:D:800:VAL:HG11	3:J:174:ILE:CD1	2.41	0.49
2:B:574:PHE:HE2	6:B:903:OLC:H18A	1.76	0.49
1:A:494:LEU:HD13	1:A:701:GLU:HG2	1.93	0.49
1:C:494:LEU:HD13	1:C:701:GLU:HG2	1.95	0.49
1:A:401:TYR:OH	1:A:703:THR:OG1	2.28	0.48
2:D:498:LEU:C	2:D:498:LEU:HD12	2.33	0.48
2:B:444:ILE:HG22	2:B:445:VAL:N	2.28	0.48
2:D:444:ILE:HG22	2:D:445:VAL:N	2.28	0.48
3:I:24:THR:HG23	3:I:218:ILE:HG23	1.95	0.48
2:B:498:LEU:C	2:B:498:LEU:HD12	2.33	0.48
1:A:482:GLU:HA	1:A:482:GLU:OE1	2.14	0.47
3:J:101:VAL:HG22	3:J:102:LYS:H	1.79	0.47
1:A:638:GLN:NE2	1:A:641:ILE:O	2.38	0.47
1:C:673:ALA:HB1	1:C:677:VAL:HG13	1.96	0.47
2:D:417:GLY:O	2:D:420:ARG:HG2	2.15	0.47
3:I:101:VAL:HG22	3:I:102:LYS:H	1.79	0.47
3:J:24:THR:HG23	3:J:218:ILE:HG23	1.95	0.47
2:D:428:LEU:O	2:D:432:ILE:HG12	2.15	0.47
2:B:673:TYR:O	2:B:677:ALA:N	2.46	0.47
1:C:482:GLU:HA	1:C:482:GLU:OE1	2.14	0.47
1:A:673:ALA:HB1	1:A:677:VAL:HG13	1.97	0.46
3:I:174:ILE:HD11	2:B:800:VAL:CG1	2.45	0.46
2:B:417:GLY:O	2:B:420:ARG:HG2	2.15	0.46
1:C:448:ALA:N	1:C:457:ASN:OD1	2.49	0.46
2:B:428:LEU:O	2:B:432:ILE:HG12	2.14	0.46
2:D:489:ILE:HD12	2:D:735:ALA:HB1	1.97	0.46
2:B:705:GLU:N	2:B:705:GLU:OE2	2.49	0.46
1:A:596:ILE:O	1:A:600:VAL:HG23	2.16	0.46
2:D:705:GLU:N	2:D:705:GLU:OE2	2.49	0.46
3:I:41:THR:HG22	3:I:42:ASP:N	2.31	0.46
1:C:401:TYR:OH	1:C:703:THR:OG1	2.31	0.46
2:B:489:ILE:HD12	2:B:735:ALA:HB1	1.97	0.46
2:D:632:PRO:HG2	2:D:633:ILE:HD12	1.99	0.45
1:C:754:VAL:O	1:C:758:LEU:HD13	2.16	0.45
3:I:89:ILE:HG23	3:I:89:ILE:O	2.16	0.45
3:J:41:THR:HG22	3:J:42:ASP:N	2.31	0.45
3:I:83:HIS:O	3:I:83:HIS:CG	2.70	0.45
3:I:90:CYS:HA	3:I:100:CYS:HB2	1.99	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:J:90:CYS:HA	3:J:100:CYS:HB2	1.99	0.45
3:J:83:HIS:CG	3:J:83:HIS:O	2.70	0.45
3:J:122:ARG:HG3	3:J:122:ARG:NH1	2.32	0.44
1:C:600:VAL:CG1	2:B:799:LEU:HA	2.48	0.44
8:C:906:POV:H36A	8:C:906:POV:H39A	1.64	0.44
3:I:122:ARG:HG3	3:I:122:ARG:NH1	2.32	0.44
3:J:89:ILE:O	3:J:89:ILE:HG23	2.16	0.44
1:A:600:VAL:CG1	2:D:799:LEU:HA	2.47	0.44
2:B:632:PRO:HG2	2:B:633:ILE:HD12	1.99	0.44
1:A:662:VAL:HG23	1:A:663:PHE:N	2.33	0.44
1:C:441:VAL:HG13	1:C:441:VAL:O	2.17	0.44
2:B:727:LEU:HD12	2:B:727:LEU:N	2.33	0.44
1:A:441:VAL:O	1:A:441:VAL:HG13	2.18	0.44
2:B:479:LEU:HD11	2:B:485:ARG:HH11	1.83	0.43
3:I:223:VAL:O	3:I:227:ILE:HG12	2.19	0.43
2:D:649:THR:HG22	2:D:703:LEU:HB2	2.01	0.43
2:B:788:SER:N	2:B:791:ASN:OD1	2.41	0.43
1:C:662:VAL:HG23	1:C:663:PHE:N	2.33	0.43
2:D:479:LEU:HD11	2:D:485:ARG:HH11	1.83	0.43
2:B:704:LEU:N	2:B:704:LEU:HD23	2.34	0.43
3:J:84:SER:OG	3:J:85:GLY:N	2.52	0.43
3:J:223:VAL:O	3:J:227:ILE:HG12	2.19	0.43
2:D:426:VAL:HG23	2:D:427:ASP:N	2.33	0.43
2:D:727:LEU:HD12	2:D:727:LEU:N	2.33	0.43
1:C:473:ALA:HB1	1:C:474:PRO:HD2	2.01	0.43
3:J:133:LEU:O	3:J:137:LEU:HG	2.19	0.43
2:B:426:VAL:HG23	2:B:427:ASP:N	2.33	0.43
2:B:519:ASP:N	2:B:520:PRO:HD2	2.34	0.43
2:D:704:LEU:HD23	2:D:704:LEU:N	2.34	0.42
2:D:519:ASP:N	2:D:520:PRO:HD2	2.34	0.42
1:C:538:LEU:O	1:C:542:PHE:CD1	2.72	0.42
2:D:800:VAL:CG1	3:J:174:ILE:HD11	2.46	0.42
3:I:84:SER:OG	3:I:85:GLY:N	2.52	0.42
3:I:133:LEU:O	3:I:137:LEU:HG	2.19	0.42
1:A:538:LEU:HD23	1:A:542:PHE:CE1	2.55	0.42
2:B:514:VAL:O	2:B:515:PHE:HB2	2.20	0.42
8:A:906:POV:H36A	8:A:906:POV:H39A	1.64	0.42
2:D:400:ILE:HG22	2:D:401:LEU:N	2.35	0.42
3:J:122:ARG:HG3	3:J:122:ARG:HH11	1.84	0.42
2:D:427:ASP:O	2:D:430:ALA:HB3	2.20	0.42
2:D:460:TRP:CE3	2:D:464:VAL:HG11	2.55	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:400:ILE:HG22	2:B:401:LEU:N	2.34	0.42
2:B:649:THR:HG22	2:B:703:LEU:HB2	2.01	0.42
1:A:538:LEU:HD23	1:A:542:PHE:HE1	1.85	0.42
1:C:681:THR:HG22	1:C:682:THR:N	2.34	0.42
1:A:647:GLU:O	1:A:648:ALA:HB3	2.20	0.41
2:D:514:VAL:O	2:D:515:PHE:HB2	2.20	0.41
1:C:515:ASP:N	1:C:516:PRO:CD	2.83	0.41
3:I:122:ARG:HG3	3:I:122:ARG:HH11	1.84	0.41
1:A:419:GLY:O	1:A:423:GLU:OE1	2.39	0.41
1:A:681:THR:HG22	1:A:682:THR:N	2.35	0.41
1:C:405:LYS:NZ	1:C:415:ASP:O	2.42	0.41
2:B:684:ARG:CZ	2:B:684:ARG:HB2	2.51	0.41
2:D:500:ILE:O	2:D:726:ASN:HA	2.20	0.41
2:D:684:ARG:HB2	2:D:684:ARG:CZ	2.51	0.41
1:C:647:GLU:O	1:C:648:ALA:HB3	2.21	0.41
3:J:91:CYS:SG	3:J:92:LEU:N	2.94	0.41
3:I:44:TRP:O	3:I:202:GLY:N	2.43	0.41
3:I:130:PHE:HB2	3:I:131:PRO:HD3	2.02	0.41
3:J:130:PHE:HB2	3:J:131:PRO:HD3	2.02	0.41
2:B:500:ILE:O	2:B:726:ASN:HA	2.20	0.41
1:A:488:SER:N	1:A:730:ILE:O	2.54	0.41
2:B:427:ASP:O	2:B:430:ALA:HB3	2.21	0.41
1:C:419:GLY:O	1:C:423:GLU:OE1	2.39	0.40
3:I:91:CYS:SG	3:I:92:LEU:N	2.94	0.40
2:B:479:LEU:HD11	2:B:485:ARG:NH1	2.37	0.40
1:A:600:VAL:HG11	2:D:799:LEU:HA	2.03	0.40
2:D:498:LEU:HD12	2:D:499:GLY:N	2.36	0.40
2:B:498:LEU:HD12	2:B:499:GLY:N	2.37	0.40
1:A:515:ASP:N	1:A:516:PRO:CD	2.84	0.40
3:J:104:ASN:OD1	3:J:104:ASN:O	2.39	0.40
3:J:173:ILE:O	3:J:176:VAL:HG12	2.21	0.40
2:B:460:TRP:CE3	2:B:464:VAL:HG11	2.56	0.40
1:A:447:GLY:HA3	1:A:460:VAL:HG12	2.04	0.40
1:A:480:VAL:HG23	1:A:481:ARG:N	2.37	0.40
1:A:754:VAL:O	1:A:758:LEU:HD13	2.22	0.40
2:D:574:PHE:CE2	6:D:903:OLC:H18A	2.55	0.40
3:I:173:ILE:O	3:I:176:VAL:HG12	2.21	0.40
3:J:170:LEU:O	3:J:173:ILE:HG22	2.22	0.40
1:A:448:ALA:O	1:A:457:ASN:OD1	2.40	0.40
2:D:479:LEU:HD11	2:D:485:ARG:NH1	2.36	0.40
2:D:799:LEU:O	2:D:803:LEU:HG	2.22	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:792:VAL:O	2:B:795:VAL:HG12	2.22	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	393/915 (43%)	383 (98%)	10 (2%)	0	100	100
1	C	393/915 (43%)	382 (97%)	11 (3%)	0	100	100
2	B	392/860 (46%)	386 (98%)	6 (2%)	0	100	100
2	D	392/860 (46%)	385 (98%)	7 (2%)	0	100	100
3	I	176/423 (42%)	172 (98%)	4 (2%)	0	100	100
3	J	176/423 (42%)	172 (98%)	4 (2%)	0	100	100
All	All	1922/4396 (44%)	1880 (98%)	42 (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	258/778 (33%)	258 (100%)	0	100	100
1	C	258/778 (33%)	258 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	B	272/737 (37%)	272 (100%)	0	100	100
2	D	272/737 (37%)	272 (100%)	0	100	100
3	I	118/309 (38%)	118 (100%)	0	100	100
3	J	118/309 (38%)	118 (100%)	0	100	100
All	All	1296/3648 (36%)	1296 (100%)	0	100	100

There are no protein residues with a non-rotameric sidechain to report.

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

### 5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

## 5.5 Carbohydrates [i](#)

There are no monosaccharides in this entry.

## 5.6 Ligand geometry [i](#)

26 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	$\# Z  > 2$
9	OIJ	J	1804	-	36,38,38	4.56	15 (41%)	43,56,56	1.79	9 (20%)
6	OLC	C	903	-	24,24,24	0.80	2 (8%)	25,25,25	0.95	1 (4%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
7	PLM	A	905	-	17,17,17	0.56	0	17,17,17	1.07	0
4	GLU	A	901	-	8,9,9	1.07	1 (12%)	10,11,11	1.30	2 (20%)
7	PLM	C	905	-	17,17,17	0.57	0	17,17,17	1.07	0
9	OIJ	I	1802	-	36,38,38	4.57	15 (41%)	43,56,56	1.79	9 (20%)
6	OLC	D	903	-	24,24,24	0.80	2 (8%)	25,25,25	0.97	1 (4%)
8	POV	A	906	-	35,35,51	1.28	4 (11%)	39,40,59	1.32	3 (7%)
6	OLC	B	903	-	24,24,24	0.80	2 (8%)	25,25,25	0.97	1 (4%)
5	CYZ	B	902	-	26,27,27	7.62	19 (73%)	38,44,44	3.19	13 (34%)
7	PLM	J	1801	-	17,17,17	0.59	0	17,17,17	1.08	0
7	PLM	C	904	-	17,17,17	0.55	0	17,17,17	1.08	0
7	PLM	I	1804	-	17,17,17	0.55	0	17,17,17	1.01	1 (5%)
4	GLU	C	901	-	8,9,9	1.06	1 (12%)	10,11,11	1.30	2 (20%)
7	PLM	A	904	-	17,17,17	0.55	0	17,17,17	1.08	0
7	PLM	I	1801	-	17,17,17	0.58	0	17,17,17	1.07	0
6	OLC	A	903	-	24,24,24	0.79	2 (8%)	25,25,25	0.94	1 (4%)
7	PLM	J	1802	-	17,17,17	0.56	0	17,17,17	1.06	0
5	CYZ	D	902	-	26,27,27	7.61	19 (73%)	38,44,44	3.19	13 (34%)
5	CYZ	C	902	-	26,27,27	7.57	18 (69%)	38,44,44	3.42	13 (34%)
7	PLM	J	1803	-	17,17,17	0.55	0	17,17,17	1.01	1 (5%)
4	GLU	D	901	-	8,9,9	1.10	1 (12%)	10,11,11	1.37	2 (20%)
5	CYZ	A	902	-	26,27,27	7.57	18 (69%)	38,44,44	3.40	12 (31%)
4	GLU	B	901	-	8,9,9	1.10	1 (12%)	10,11,11	1.36	2 (20%)
7	PLM	I	1803	-	17,17,17	0.57	0	17,17,17	1.05	0
8	POV	C	906	-	35,35,51	1.28	4 (11%)	39,40,59	1.32	3 (7%)

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
9	OIJ	J	1804	-	-	4/12/30/30	0/6/6/6
6	OLC	C	903	-	-	10/24/24/24	-
7	PLM	A	905	-	-	6/15/15/15	-
4	GLU	A	901	-	-	3/9/9/9	-
7	PLM	C	905	-	-	6/15/15/15	-
9	OIJ	I	1802	-	-	4/12/30/30	0/6/6/6

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
6	OLC	D	903	-	-	9/24/24/24	-
8	POV	A	906	-	-	18/37/37/55	-
6	OLC	B	903	-	-	9/24/24/24	-
5	CYZ	B	902	-	-	6/6/42/42	0/5/4/4
7	PLM	J	1801	-	-	7/15/15/15	-
7	PLM	C	904	-	-	8/15/15/15	-
7	PLM	I	1804	-	-	9/15/15/15	-
4	GLU	C	901	-	-	3/9/9/9	-
7	PLM	A	904	-	-	8/15/15/15	-
7	PLM	I	1801	-	-	7/15/15/15	-
6	OLC	A	903	-	-	10/24/24/24	-
7	PLM	J	1802	-	-	7/15/15/15	-
5	CYZ	D	902	-	-	6/6/42/42	0/5/4/4
5	CYZ	C	902	-	-	2/6/42/42	0/5/4/4
7	PLM	J	1803	-	-	9/15/15/15	-
4	GLU	D	901	-	-	2/9/9/9	-
5	CYZ	A	902	-	-	2/6/42/42	0/5/4/4
4	GLU	B	901	-	-	2/9/9/9	-
7	PLM	I	1803	-	-	7/15/15/15	-
8	POV	C	906	-	-	18/37/37/55	-

All (124) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	C	902	CYZ	C2-C3	-18.88	0.99	1.51
5	D	902	CYZ	C2-C3	-18.83	0.99	1.51
5	B	902	CYZ	C2-C3	-18.83	0.99	1.51
5	A	902	CYZ	C2-C3	-18.81	0.99	1.51
9	I	1802	OIJ	C14-C13	-18.42	1.38	1.52
9	J	1804	OIJ	C14-C13	-18.35	1.38	1.52
5	B	902	CYZ	C2-C1	-15.77	1.21	1.55
5	D	902	CYZ	C2-C1	-15.77	1.21	1.55
5	C	902	CYZ	C2-C1	-15.62	1.21	1.55
5	A	902	CYZ	C2-C1	-15.60	1.21	1.55
5	B	902	CYZ	C7-C2	-11.73	1.27	1.54
5	D	902	CYZ	C7-C2	-11.72	1.27	1.54
5	C	902	CYZ	C7-C2	-11.64	1.27	1.54
5	A	902	CYZ	C7-C2	-11.59	1.27	1.54

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	B	902	CYZ	C10-N2	10.67	1.58	1.39
5	D	902	CYZ	C10-N2	10.60	1.58	1.39
5	A	902	CYZ	C10-N2	10.48	1.58	1.39
5	C	902	CYZ	C10-N2	10.41	1.58	1.39
5	B	902	CYZ	O1-S1	10.21	1.55	1.43
5	C	902	CYZ	O1-S1	10.14	1.55	1.43
5	D	902	CYZ	O1-S1	10.12	1.55	1.43
5	A	902	CYZ	O1-S1	10.09	1.55	1.43
5	B	902	CYZ	C9-S1	-9.91	1.67	1.75
5	D	902	CYZ	C9-S1	-9.74	1.67	1.75
5	A	902	CYZ	C9-S1	-9.53	1.67	1.75
5	C	902	CYZ	C9-S1	-9.47	1.67	1.75
5	D	902	CYZ	C5-C4	-9.05	1.07	1.50
5	B	902	CYZ	C5-C4	-9.02	1.07	1.50
5	C	902	CYZ	C5-C4	-9.02	1.07	1.50
5	A	902	CYZ	C5-C4	-8.97	1.08	1.50
5	D	902	CYZ	C6-C1	-8.59	1.30	1.53
5	A	902	CYZ	C6-C1	-8.55	1.30	1.53
5	C	902	CYZ	C6-C1	-8.54	1.30	1.53
5	B	902	CYZ	C6-C1	-8.54	1.30	1.53
5	C	902	CYZ	C4-C3	8.52	1.57	1.32
5	A	902	CYZ	C4-C3	8.50	1.57	1.32
9	I	1802	OIJ	O2-C13	8.44	1.40	1.23
5	B	902	CYZ	C4-C3	8.43	1.57	1.32
9	J	1804	OIJ	O2-C13	8.42	1.40	1.23
5	D	902	CYZ	C4-C3	8.41	1.57	1.32
9	I	1802	OIJ	C6-C5	7.78	1.47	1.36
9	J	1804	OIJ	C6-C5	7.73	1.47	1.36
9	I	1802	OIJ	C4-N2	7.24	1.46	1.32
9	J	1804	OIJ	C4-N2	7.20	1.46	1.32
5	A	902	CYZ	S2-N3	7.12	1.74	1.60
5	C	902	CYZ	S2-N3	7.11	1.74	1.60
5	D	902	CYZ	S2-N3	7.05	1.74	1.60
5	B	902	CYZ	S2-N3	7.03	1.74	1.60
9	J	1804	OIJ	C4-N1	6.98	1.45	1.35
9	I	1802	OIJ	C4-N1	6.97	1.45	1.35
5	D	902	CYZ	C6-C5	-6.95	1.12	1.51
5	B	902	CYZ	C6-C5	-6.95	1.12	1.51
5	A	902	CYZ	C6-C5	-6.94	1.12	1.51
5	C	902	CYZ	C6-C5	-6.91	1.12	1.51
5	B	902	CYZ	C8-N2	6.71	1.54	1.46
5	D	902	CYZ	C8-N2	6.68	1.54	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	A	902	CYZ	C8-N2	6.54	1.54	1.46
5	C	902	CYZ	C8-N2	6.41	1.54	1.46
9	I	1802	OIJ	C6-C7	5.86	1.52	1.41
9	J	1804	OIJ	C6-C7	5.86	1.52	1.41
9	J	1804	OIJ	C14-C15	-5.13	1.42	1.50
9	I	1802	OIJ	C14-C15	-5.09	1.42	1.50
9	J	1804	OIJ	C7-N5	-4.77	1.34	1.40
9	I	1802	OIJ	C7-N5	-4.72	1.34	1.40
9	I	1802	OIJ	C3-N1	4.69	1.54	1.46
9	J	1804	OIJ	C3-N1	4.68	1.54	1.46
5	B	902	CYZ	C12-S2	4.65	1.83	1.77
5	D	902	CYZ	C12-S2	4.65	1.83	1.77
5	C	902	CYZ	C12-S2	4.61	1.83	1.77
5	A	902	CYZ	C12-S2	4.61	1.83	1.77
5	A	902	CYZ	C10-C9	-4.51	1.33	1.40
5	D	902	CYZ	C10-C9	-4.42	1.34	1.40
5	C	902	CYZ	C10-C9	-4.42	1.34	1.40
5	B	902	CYZ	C10-C9	-4.38	1.34	1.40
9	I	1802	OIJ	C24-N1	3.91	1.52	1.46
9	J	1804	OIJ	C24-N1	3.85	1.52	1.46
5	A	902	CYZ	C8-N1	-3.62	1.42	1.46
5	C	902	CYZ	C8-N1	-3.61	1.42	1.46
5	B	902	CYZ	C8-N1	-3.43	1.42	1.46
5	D	902	CYZ	C8-N1	-3.41	1.42	1.46
9	I	1802	OIJ	C18-C17	3.34	1.52	1.49
9	J	1804	OIJ	C5-N2	3.32	1.41	1.34
9	J	1804	OIJ	C18-C17	3.28	1.52	1.49
9	I	1802	OIJ	C5-N2	3.25	1.41	1.34
8	C	906	POV	P-O12	3.11	1.66	1.54
8	A	906	POV	P-O12	3.09	1.66	1.54
5	B	902	CYZ	O3-S2	3.05	1.49	1.43
9	J	1804	OIJ	C12-C15	-3.04	1.36	1.39
5	A	902	CYZ	O3-S2	3.04	1.49	1.43
5	D	902	CYZ	O3-S2	3.02	1.49	1.43
5	C	902	CYZ	O3-S2	3.02	1.49	1.43
9	I	1802	OIJ	C12-C15	-2.94	1.36	1.39
8	A	906	POV	O31-C31	2.83	1.41	1.33
8	C	906	POV	O31-C31	2.82	1.41	1.33
8	C	906	POV	O21-C21	2.71	1.42	1.34
8	A	906	POV	O21-C21	2.65	1.41	1.34
5	C	902	CYZ	C14-C13	-2.55	1.34	1.38
9	I	1802	OIJ	C2-C1	-2.45	1.45	1.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	B	902	CYZ	C14-C13	-2.44	1.34	1.38
5	D	902	CYZ	C14-C13	-2.41	1.34	1.38
9	J	1804	OIJ	C2-C1	-2.40	1.45	1.51
6	B	903	OLC	O20-C1	2.38	1.40	1.33
6	D	903	OLC	O20-C1	2.37	1.40	1.33
6	C	903	OLC	O20-C1	2.36	1.40	1.33
6	A	903	OLC	O20-C1	2.35	1.40	1.33
5	A	902	CYZ	C14-C13	-2.35	1.34	1.38
9	J	1804	OIJ	C8-C9	2.31	1.52	1.49
9	I	1802	OIJ	C8-C9	2.24	1.52	1.49
4	B	901	GLU	OXT-C	-2.23	1.23	1.30
4	D	901	GLU	OXT-C	-2.23	1.23	1.30
6	D	903	OLC	O20-C21	-2.19	1.40	1.45
8	C	906	POV	O21-C2	-2.19	1.41	1.46
8	A	906	POV	O21-C2	-2.16	1.41	1.46
6	B	903	OLC	O20-C21	-2.14	1.40	1.45
5	D	902	CYZ	C7-C5	2.13	1.64	1.51
4	A	901	GLU	OXT-C	-2.12	1.23	1.30
5	B	902	CYZ	C7-C5	2.12	1.64	1.51
5	A	902	CYZ	C7-C5	2.10	1.63	1.51
5	C	902	CYZ	C7-C5	2.09	1.63	1.51
4	C	901	GLU	OXT-C	-2.09	1.23	1.30
5	D	902	CYZ	O2-S1	-2.07	1.41	1.43
5	B	902	CYZ	O2-S1	-2.07	1.41	1.43
6	A	903	OLC	O20-C21	-2.06	1.40	1.45
6	C	903	OLC	O20-C21	-2.06	1.40	1.45

All (89) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	C	902	CYZ	C9-S1-N1	11.86	118.57	103.43
5	A	902	CYZ	C9-S1-N1	11.82	118.51	103.43
5	A	902	CYZ	O4-S2-O3	-10.66	101.24	118.76
5	C	902	CYZ	O4-S2-O3	-10.64	101.27	118.76
5	D	902	CYZ	O4-S2-O3	-10.46	101.57	118.76
5	B	902	CYZ	O4-S2-O3	-10.44	101.60	118.76
5	B	902	CYZ	C9-S1-N1	10.28	116.55	103.43
5	D	902	CYZ	C9-S1-N1	10.27	116.53	103.43
5	A	902	CYZ	O2-S1-O1	-8.10	110.19	118.46
5	C	902	CYZ	O2-S1-O1	-8.10	110.19	118.46
5	B	902	CYZ	O2-S1-O1	-7.43	110.87	118.46
5	D	902	CYZ	O2-S1-O1	-7.39	110.92	118.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
9	I	1802	OIJ	C15-C14-C13	4.74	105.56	103.15
9	J	1804	OIJ	C15-C14-C13	4.74	105.56	103.15
9	J	1804	OIJ	C6-C5-N2	-4.38	119.50	123.81
9	I	1802	OIJ	C6-C5-N2	-4.36	119.52	123.81
8	C	906	POV	O21-C21-C22	4.23	120.62	111.50
8	A	906	POV	O21-C21-C22	4.21	120.58	111.50
5	C	902	CYZ	C1-C2-C3	4.03	113.44	106.92
5	A	902	CYZ	C1-C2-C3	3.99	113.37	106.92
5	B	902	CYZ	C1-C2-C3	3.64	112.81	106.92
5	D	902	CYZ	C1-C2-C3	3.63	112.80	106.92
9	I	1802	OIJ	C5-N2-C4	3.49	120.07	115.37
9	J	1804	OIJ	C5-N2-C4	3.47	120.04	115.37
8	C	906	POV	C37-C36-C35	3.34	131.40	114.42
8	A	906	POV	C37-C36-C35	3.34	131.39	114.42
5	D	902	CYZ	C6-C1-C2	3.24	109.96	104.22
9	J	1804	OIJ	O2-C13-C14	-3.23	125.24	127.00
5	B	902	CYZ	C6-C1-C2	3.20	109.90	104.22
5	A	902	CYZ	C6-C1-C2	3.18	109.87	104.22
9	I	1802	OIJ	O2-C13-C14	-3.17	125.28	127.00
5	C	902	CYZ	C6-C1-C2	3.16	109.82	104.22
5	C	902	CYZ	O3-S2-C12	3.13	111.87	107.29
9	J	1804	OIJ	C12-N3-C13	-3.13	110.24	111.65
5	D	902	CYZ	O3-S2-C12	3.12	111.86	107.29
5	B	902	CYZ	O3-S2-C12	3.12	111.86	107.29
5	A	902	CYZ	O3-S2-C12	3.11	111.85	107.29
5	C	902	CYZ	O3-S2-N3	3.11	111.97	107.36
9	I	1802	OIJ	C12-N3-C13	-3.08	110.27	111.65
4	D	901	GLU	OXT-C-O	-3.06	117.13	124.09
4	B	901	GLU	OXT-C-O	-3.05	117.17	124.09
5	D	902	CYZ	C2-C1-C8	-3.04	110.49	114.81
5	B	902	CYZ	C2-C1-C8	-3.03	110.50	114.81
5	B	902	CYZ	O3-S2-N3	3.02	111.84	107.36
5	D	902	CYZ	O3-S2-N3	3.01	111.83	107.36
5	A	902	CYZ	O3-S2-N3	3.01	111.83	107.36
5	C	902	CYZ	C13-C12-S2	-2.99	119.69	123.49
5	D	902	CYZ	C13-C12-S2	-2.87	119.85	123.49
6	C	903	OLC	O20-C1-C2	2.86	120.87	111.91
5	A	902	CYZ	C13-C12-S2	-2.86	119.87	123.49
5	B	902	CYZ	C13-C12-S2	-2.85	119.87	123.49
6	A	903	OLC	O20-C1-C2	2.84	120.82	111.91
5	C	902	CYZ	O4-S2-N3	2.80	111.51	107.36
5	A	902	CYZ	O4-S2-N3	2.77	111.46	107.36

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	901	GLU	OXT-C-O	-2.71	117.93	124.09
4	C	901	GLU	OXT-C-O	-2.71	117.93	124.09
5	B	902	CYZ	O4-S2-N3	2.68	111.33	107.36
5	D	902	CYZ	O4-S2-N3	2.67	111.32	107.36
9	J	1804	OIJ	C18-C17-N4	2.67	125.35	120.78
6	B	903	OLC	O20-C1-C2	2.66	120.26	111.91
6	D	903	OLC	O20-C1-C2	2.65	120.22	111.91
9	I	1802	OIJ	C18-C17-N4	2.65	125.32	120.78
5	A	902	CYZ	C2-C1-C8	-2.54	111.20	114.81
9	I	1802	OIJ	C14-C13-N3	2.52	109.05	107.80
5	C	902	CYZ	O4-S2-C12	2.51	110.97	107.29
5	A	902	CYZ	O4-S2-C12	2.51	110.96	107.29
8	A	906	POV	O31-C31-C32	2.47	119.67	111.91
5	C	902	CYZ	C2-C1-C8	-2.47	111.30	114.81
5	D	902	CYZ	O4-S2-C12	2.47	110.90	107.29
5	B	902	CYZ	O4-S2-C12	2.46	110.89	107.29
8	C	906	POV	O31-C31-C32	2.46	119.62	111.91
9	J	1804	OIJ	C14-C13-N3	2.44	109.01	107.80
5	B	902	CYZ	C12-C13-CL	-2.29	119.82	121.49
5	D	902	CYZ	C12-C13-CL	-2.28	119.82	121.49
5	C	902	CYZ	C12-C13-CL	-2.27	119.83	121.49
4	A	901	GLU	OXT-C-CA	2.26	121.10	113.38
5	D	902	CYZ	C6-C1-C8	-2.26	108.62	114.40
5	B	902	CYZ	C6-C1-C8	-2.26	108.63	114.40
4	C	901	GLU	OXT-C-CA	2.24	121.01	113.38
4	D	901	GLU	OXT-C-CA	2.23	120.97	113.38
9	J	1804	OIJ	C14-C15-C16	2.23	133.18	129.81
4	B	901	GLU	OXT-C-CA	2.21	120.91	113.38
9	I	1802	OIJ	C14-C15-C16	2.17	133.10	129.81
5	A	902	CYZ	C12-C13-CL	-2.16	119.91	121.49
9	I	1802	OIJ	C20-C21-C22	-2.08	120.06	122.83
5	C	902	CYZ	C11-C9-S1	2.08	121.52	119.82
7	J	1803	PLM	C3-C2-C1	-2.07	109.26	114.47
7	I	1804	PLM	C3-C2-C1	-2.05	109.31	114.47
9	J	1804	OIJ	C20-C21-C22	-2.04	120.12	122.83

There are no chirality outliers.

All (182) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	D	902	CYZ	C11-C12-S2-O4
5	D	902	CYZ	C11-C12-S2-N3

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Mol	Chain	Res	Type	Atoms
5	D	902	CYZ	C13-C12-S2-O3
5	D	902	CYZ	C13-C12-S2-O4
5	D	902	CYZ	C13-C12-S2-N3
5	B	902	CYZ	C11-C12-S2-O4
5	B	902	CYZ	C11-C12-S2-N3
5	B	902	CYZ	C13-C12-S2-O3
5	B	902	CYZ	C13-C12-S2-O4
5	B	902	CYZ	C13-C12-S2-N3
8	A	906	POV	C1-O11-P-O12
8	A	906	POV	C1-O11-P-O13
8	A	906	POV	C22-C21-O21-C2
8	C	906	POV	C1-O11-P-O13
8	C	906	POV	C22-C21-O21-C2
9	I	1802	OIJ	C7-C8-C9-C10
9	I	1802	OIJ	C7-C8-C9-C16
9	J	1804	OIJ	C7-C8-C9-C10
9	J	1804	OIJ	C7-C8-C9-C16
8	A	906	POV	O22-C21-O21-C2
8	C	906	POV	O22-C21-O21-C2
5	D	902	CYZ	C11-C12-S2-O3
5	B	902	CYZ	C11-C12-S2-O3
6	A	903	OLC	C2-C1-O20-C21
6	C	903	OLC	C2-C1-O20-C21
6	C	903	OLC	O19-C1-O20-C21
6	A	903	OLC	O19-C1-O20-C21
8	A	906	POV	C32-C31-O31-C3
8	C	906	POV	C32-C31-O31-C3
6	A	903	OLC	C1-C2-C3-C4
6	C	903	OLC	C1-C2-C3-C4
8	A	906	POV	O32-C31-O31-C3
8	C	906	POV	O32-C31-O31-C3
6	A	903	OLC	O20-C21-C22-O23
6	C	903	OLC	O20-C21-C22-O23
8	C	906	POV	C31-C32-C33-C34
6	A	903	OLC	O20-C21-C22-C24
6	C	903	OLC	O20-C21-C22-C24
6	B	903	OLC	C2-C3-C4-C5
6	D	903	OLC	C2-C3-C4-C5
8	A	906	POV	C31-C32-C33-C34
7	A	904	PLM	C4-C5-C6-C7
7	C	904	PLM	C4-C5-C6-C7
7	A	905	PLM	C7-C8-C9-CA

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Mol	Chain	Res	Type	Atoms
7	C	905	PLM	C7-C8-C9-CA
7	I	1803	PLM	CB-CC-CD-CE
7	J	1802	PLM	CB-CC-CD-CE
7	C	904	PLM	CC-CD-CE-CF
7	A	904	PLM	CC-CD-CE-CF
7	I	1804	PLM	C8-C9-CA-CB
7	J	1803	PLM	C8-C9-CA-CB
7	I	1804	PLM	C9-CA-CB-CC
6	D	903	OLC	C10-C11-C12-C13
7	J	1803	PLM	C9-CA-CB-CC
7	A	905	PLM	CC-CD-CE-CF
7	C	905	PLM	CC-CD-CE-CF
8	A	906	POV	C35-C36-C37-C38
8	C	906	POV	C35-C36-C37-C38
7	I	1801	PLM	C6-C7-C8-C9
7	J	1801	PLM	C6-C7-C8-C9
7	J	1803	PLM	C6-C7-C8-C9
6	B	903	OLC	C10-C11-C12-C13
7	I	1804	PLM	C4-C5-C6-C7
7	I	1804	PLM	C6-C7-C8-C9
7	J	1803	PLM	C4-C5-C6-C7
7	I	1803	PLM	C5-C6-C7-C8
6	D	903	OLC	C12-C13-C14-C15
7	J	1802	PLM	C5-C6-C7-C8
6	B	903	OLC	C12-C13-C14-C15
6	A	903	OLC	C2-C3-C4-C5
6	C	903	OLC	C2-C3-C4-C5
7	I	1801	PLM	CD-CE-CF-CG
7	J	1801	PLM	CD-CE-CF-CG
8	A	906	POV	C3-C2-O21-C21
8	C	906	POV	C3-C2-O21-C21
7	C	904	PLM	CA-CB-CC-CD
7	A	904	PLM	CA-CB-CC-CD
8	A	906	POV	C1-O11-P-O14
8	C	906	POV	C1-O11-P-O14
7	A	904	PLM	C6-C7-C8-C9
7	C	904	PLM	C6-C7-C8-C9
6	B	903	OLC	C4-C5-C6-C7
6	D	903	OLC	C4-C5-C6-C7
7	I	1803	PLM	C3-C4-C5-C6
7	J	1802	PLM	C3-C4-C5-C6
8	C	906	POV	C1-O11-P-O12

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Mol	Chain	Res	Type	Atoms
8	A	906	POV	C33-C34-C35-C36
5	C	902	CYZ	C13-C12-S2-N3
7	A	905	PLM	CA-CB-CC-CD
7	C	905	PLM	CA-CB-CC-CD
8	C	906	POV	C33-C34-C35-C36
7	I	1801	PLM	C9-CA-CB-CC
7	J	1801	PLM	C9-CA-CB-CC
7	I	1801	PLM	C3-C4-C5-C6
7	A	904	PLM	C9-CA-CB-CC
7	J	1801	PLM	C3-C4-C5-C6
7	J	1802	PLM	CC-CD-CE-CF
7	C	904	PLM	C9-CA-CB-CC
7	I	1803	PLM	CC-CD-CE-CF
6	C	903	OLC	C3-C4-C5-C6
6	A	903	OLC	C3-C4-C5-C6
4	A	901	GLU	OXT-C-CA-CB
4	C	901	GLU	OXT-C-CA-CB
7	I	1804	PLM	CA-CB-CC-CD
7	J	1802	PLM	CD-CE-CF-CG
7	J	1803	PLM	CA-CB-CC-CD
7	I	1803	PLM	CD-CE-CF-CG
8	A	906	POV	C25-C26-C27-C28
8	C	906	POV	C25-C26-C27-C28
6	D	903	OLC	C7-C8-C9-C10
6	B	903	OLC	C7-C8-C9-C10
8	A	906	POV	C24-C25-C26-C27
8	C	906	POV	C24-C25-C26-C27
7	A	904	PLM	O1-C1-C2-C3
7	C	904	PLM	O1-C1-C2-C3
4	A	901	GLU	CA-CB-CG-CD
4	C	901	GLU	CA-CB-CG-CD
8	C	906	POV	O31-C31-C32-C33
7	A	904	PLM	O2-C1-C2-C3
7	J	1802	PLM	C2-C3-C4-C5
4	C	901	GLU	O-C-CA-CB
8	A	906	POV	O31-C31-C32-C33
7	J	1801	PLM	O2-C1-C2-C3
7	I	1801	PLM	O2-C1-C2-C3
6	A	903	OLC	C7-C8-C9-C10
6	C	903	OLC	C7-C8-C9-C10
7	C	904	PLM	O2-C1-C2-C3
8	A	906	POV	C36-C37-C38-C39

*Continued on next page...*

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Mol	Chain	Res	Type	Atoms
7	I	1801	PLM	O1-C1-C2-C3
7	I	1801	PLM	C5-C6-C7-C8
8	C	906	POV	C36-C37-C38-C39
7	J	1801	PLM	C5-C6-C7-C8
7	I	1803	PLM	C2-C3-C4-C5
8	A	906	POV	C26-C27-C28-C29
8	C	906	POV	C26-C27-C28-C29
7	J	1801	PLM	O1-C1-C2-C3
8	A	906	POV	C37-C38-C39-C310
4	A	901	GLU	O-C-CA-CB
8	C	906	POV	C37-C38-C39-C310
4	D	901	GLU	O-C-CA-N
4	B	901	GLU	O-C-CA-N
4	D	901	GLU	CA-CB-CG-CD
6	D	903	OLC	C15-C16-C17-C18
6	B	903	OLC	C15-C16-C17-C18
7	I	1804	PLM	O1-C1-C2-C3
5	C	902	CYZ	C11-C12-S2-O4
4	B	901	GLU	CA-CB-CG-CD
6	D	903	OLC	O20-C1-C2-C3
6	B	903	OLC	O20-C1-C2-C3
7	J	1802	PLM	C8-C9-CA-CB
7	I	1803	PLM	C8-C9-CA-CB
6	C	903	OLC	O20-C1-C2-C3
6	A	903	OLC	O20-C1-C2-C3
6	D	903	OLC	C9-C10-C11-C12
6	B	903	OLC	C9-C10-C11-C12
7	J	1803	PLM	C5-C6-C7-C8
7	J	1803	PLM	O1-C1-C2-C3
7	A	905	PLM	O1-C1-C2-C3
7	C	905	PLM	O2-C1-C2-C3
7	I	1804	PLM	O2-C1-C2-C3
5	A	902	CYZ	C13-C12-S2-N3
7	A	905	PLM	O2-C1-C2-C3
7	C	905	PLM	O1-C1-C2-C3
7	J	1803	PLM	O2-C1-C2-C3
8	A	906	POV	C27-C28-C29-C210
8	C	906	POV	C27-C28-C29-C210
7	J	1803	PLM	CC-CD-CE-CF
7	I	1804	PLM	CC-CD-CE-CF
6	A	903	OLC	O19-C1-C2-C3
6	D	903	OLC	O19-C1-C2-C3

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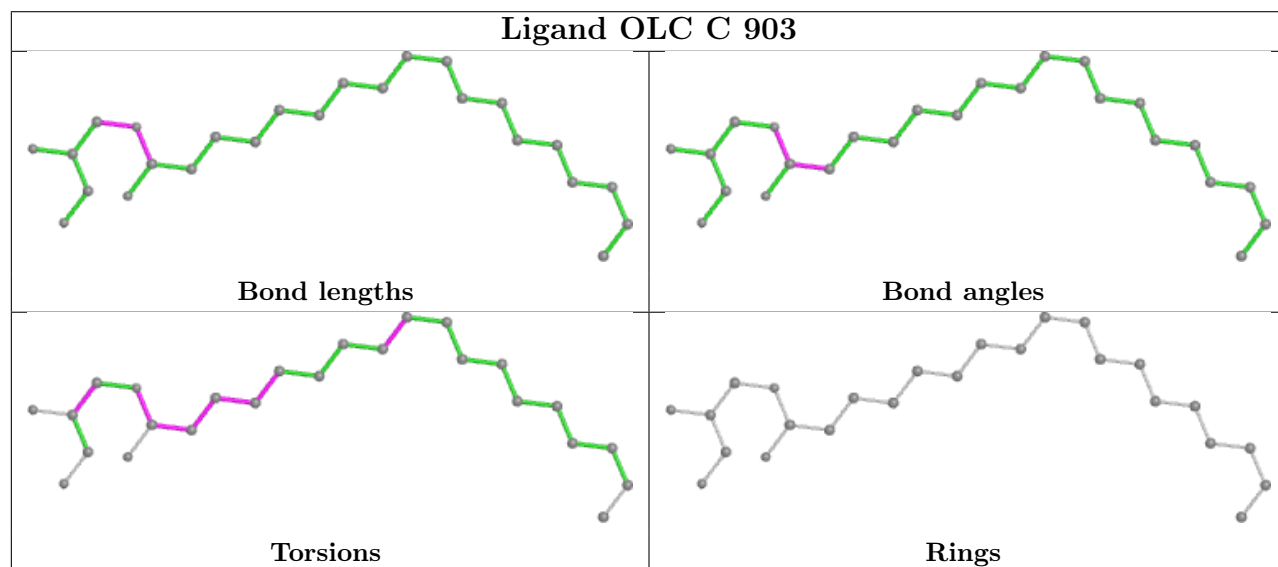
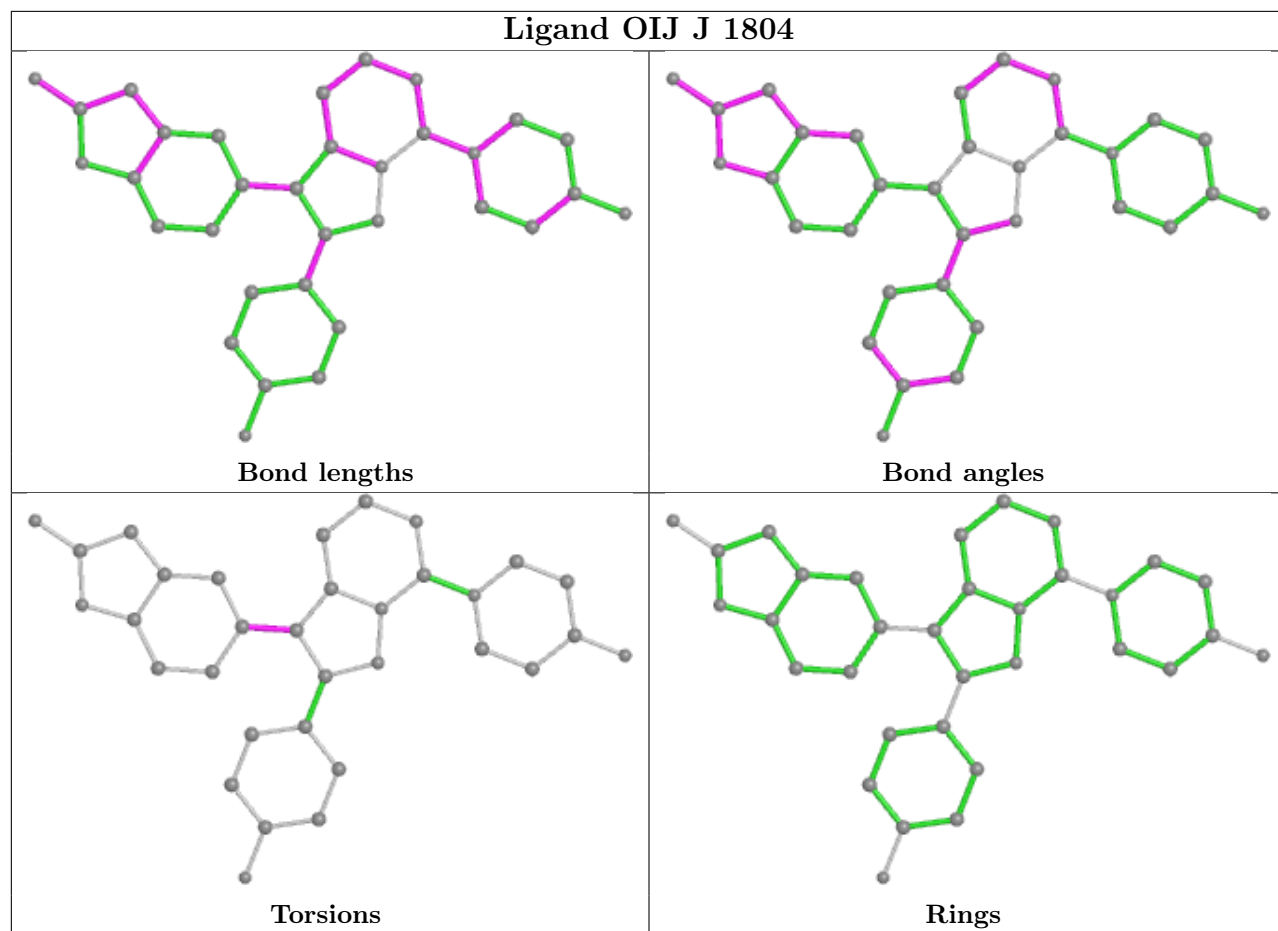
Mol	Chain	Res	Type	Atoms
6	C	903	OLC	O19-C1-C2-C3
5	A	902	CYZ	C11-C12-S2-O4
7	I	1804	PLM	C5-C6-C7-C8
6	B	903	OLC	O19-C1-C2-C3
7	C	904	PLM	C5-C6-C7-C8
7	A	904	PLM	C5-C6-C7-C8
7	A	905	PLM	C2-C3-C4-C5
7	C	905	PLM	C2-C3-C4-C5
9	I	1802	OIJ	C17-C8-C9-C10
9	I	1802	OIJ	C17-C8-C9-C16
9	J	1804	OIJ	C17-C8-C9-C10
9	J	1804	OIJ	C17-C8-C9-C16

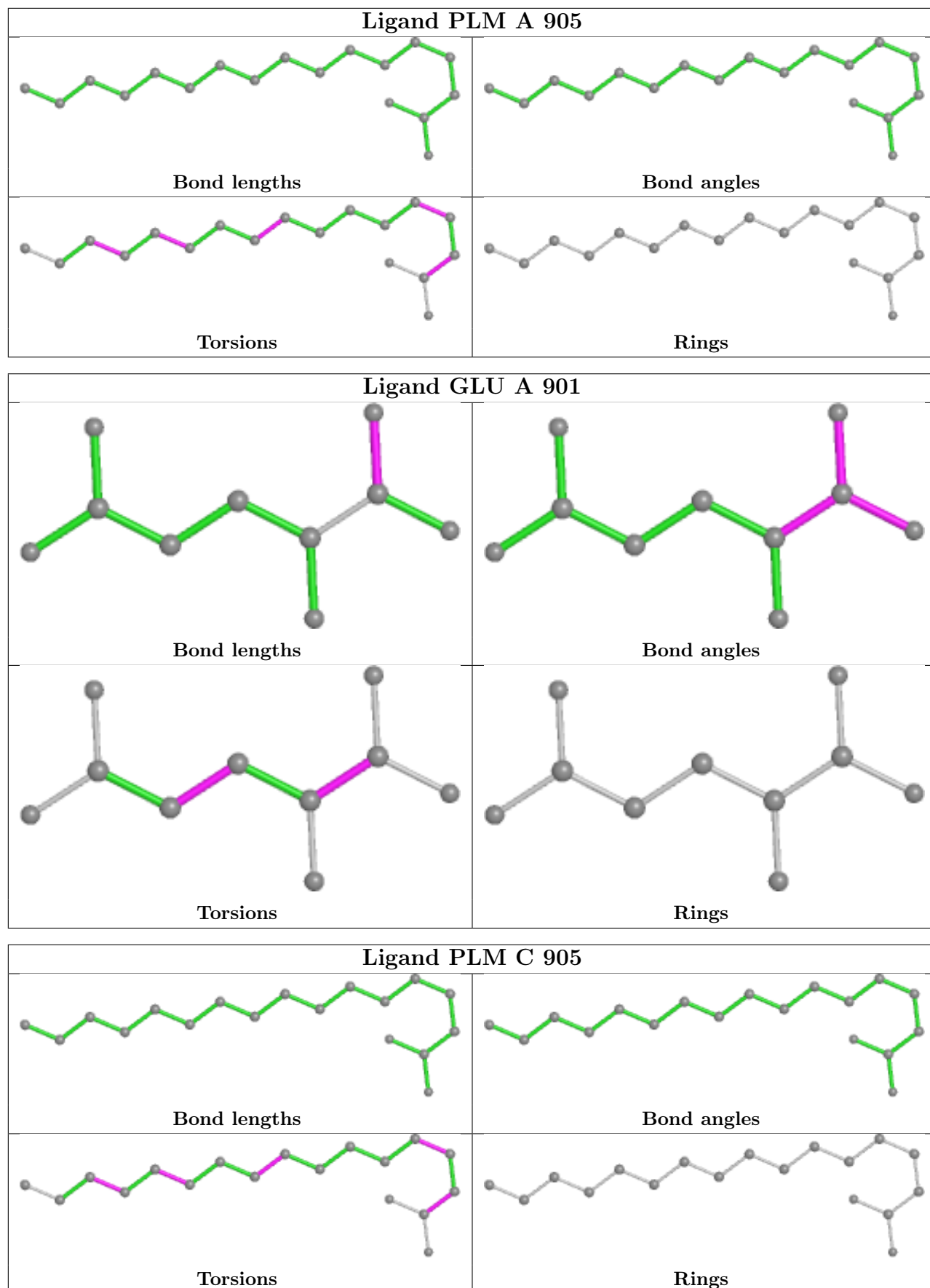
There are no ring outliers.

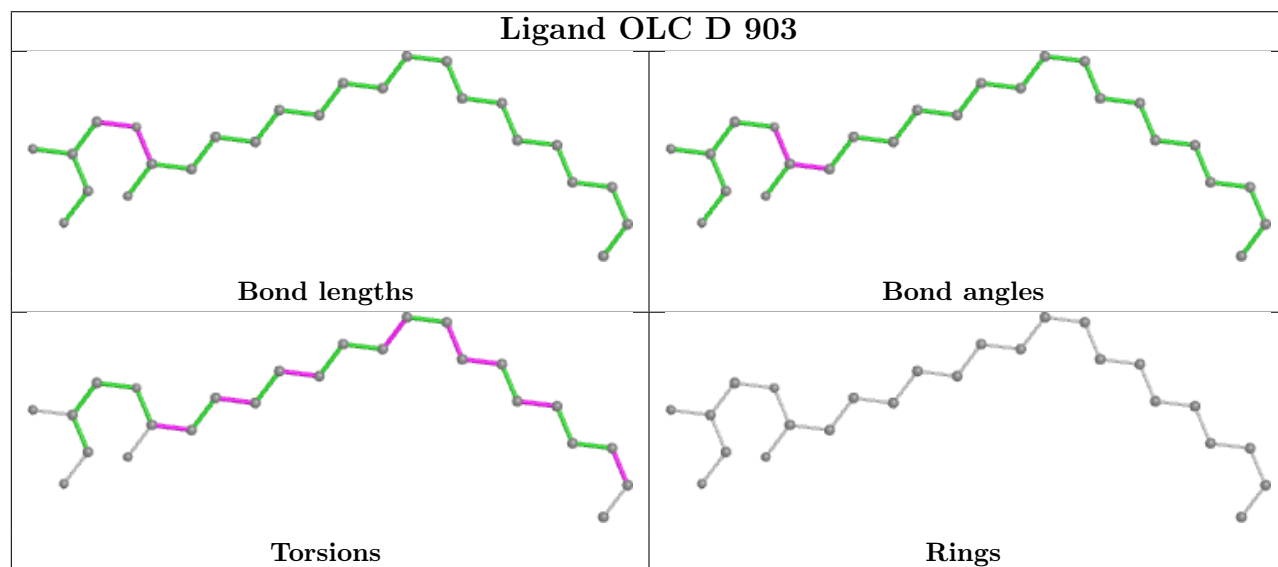
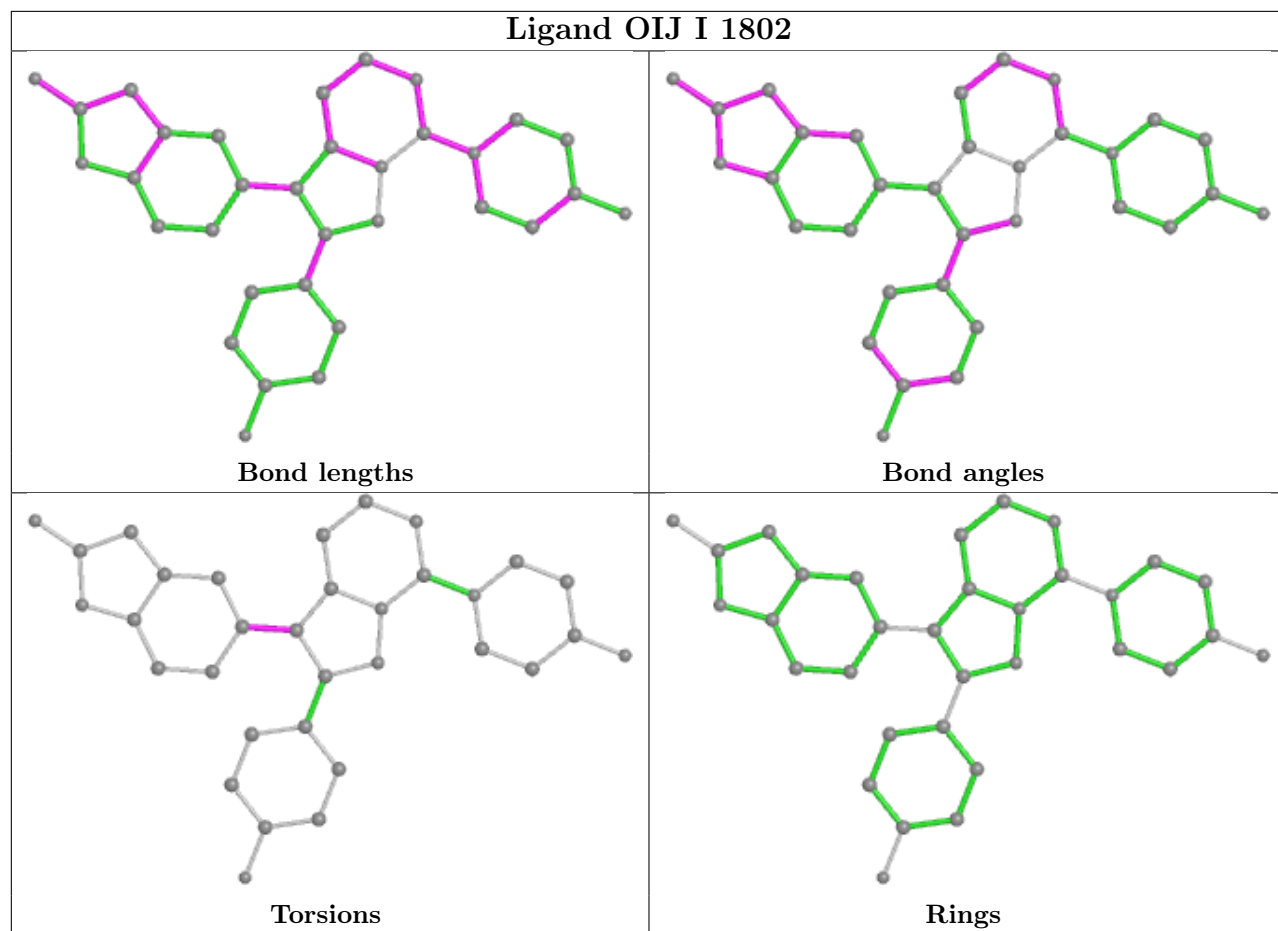
10 monomers are involved in 11 short contacts:

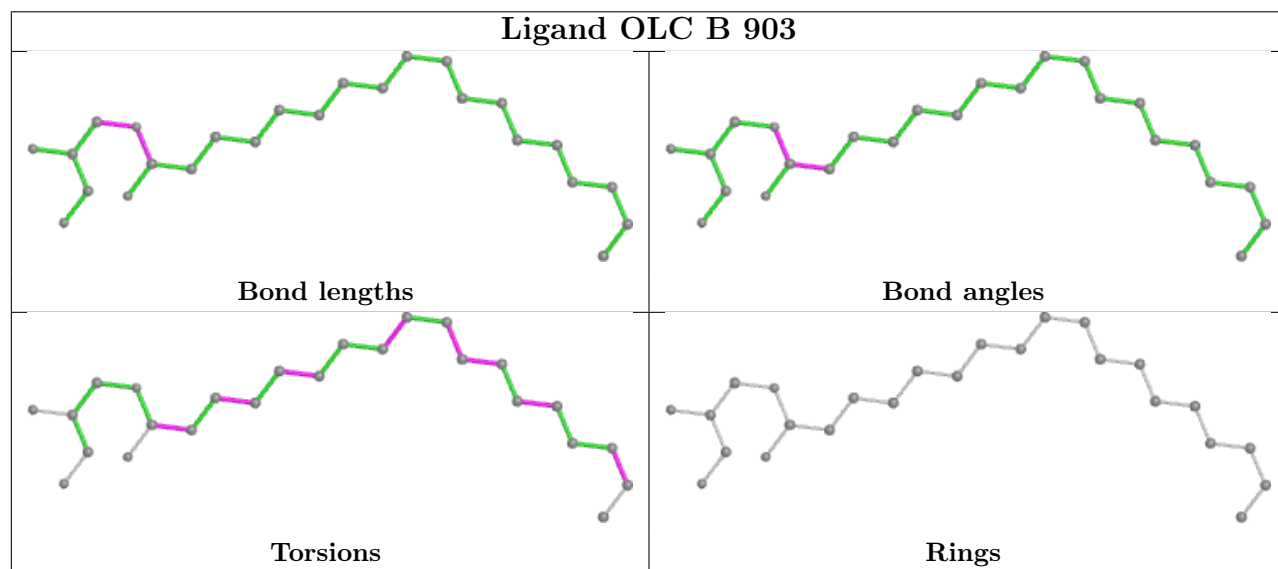
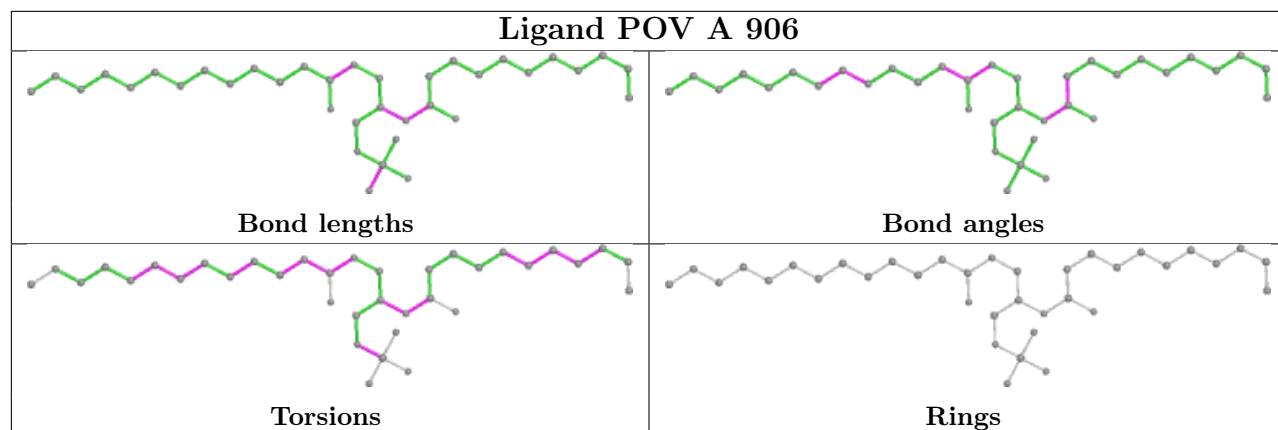
Mol	Chain	Res	Type	Clashes	Symm-Clashes
9	J	1804	OIJ	1	0
4	A	901	GLU	1	0
9	I	1802	OIJ	1	0
6	D	903	OLC	2	0
8	A	906	POV	1	0
6	B	903	OLC	1	0
5	B	902	CYZ	1	0
4	C	901	GLU	1	0
5	D	902	CYZ	1	0
8	C	906	POV	1	0

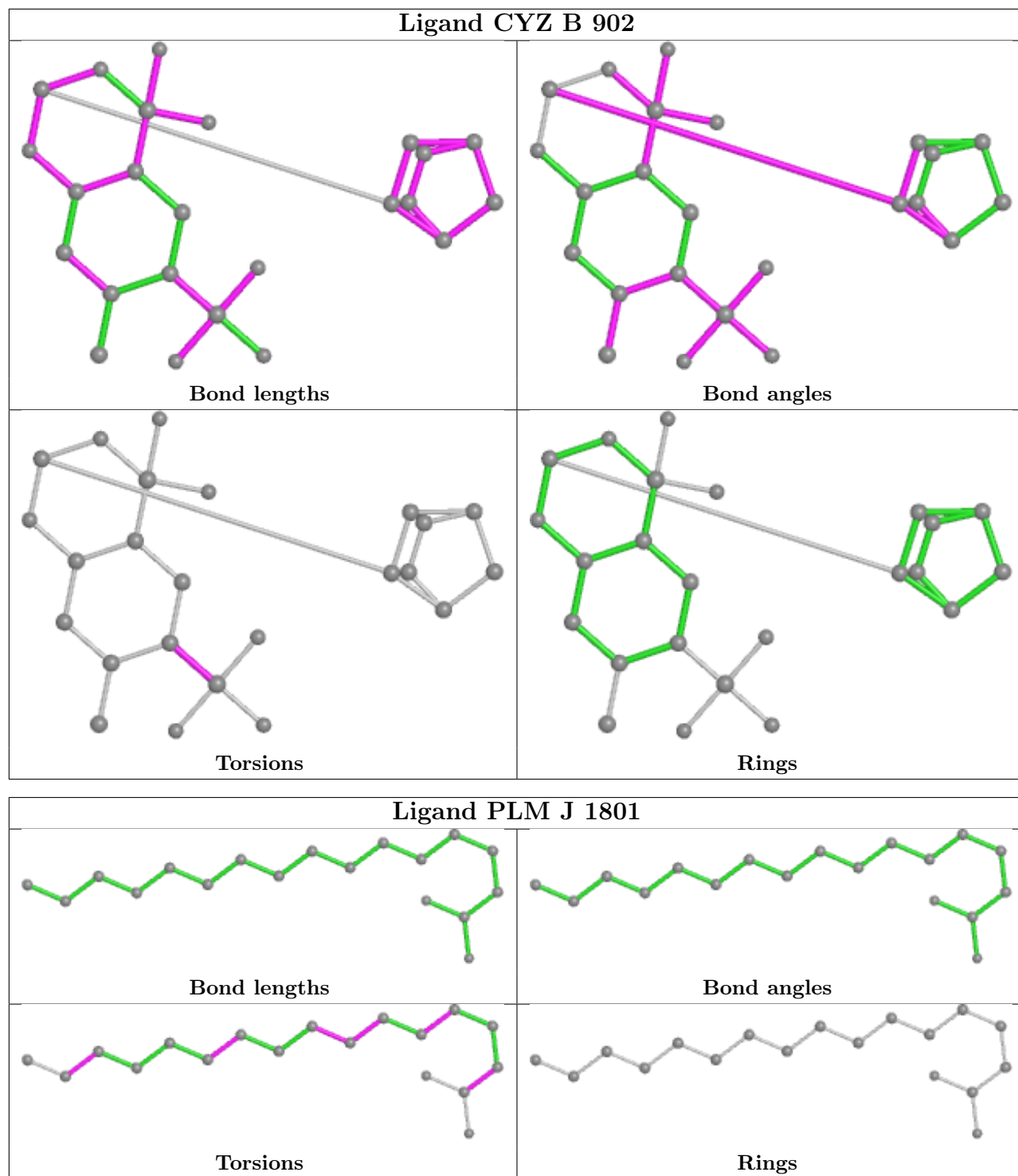
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.



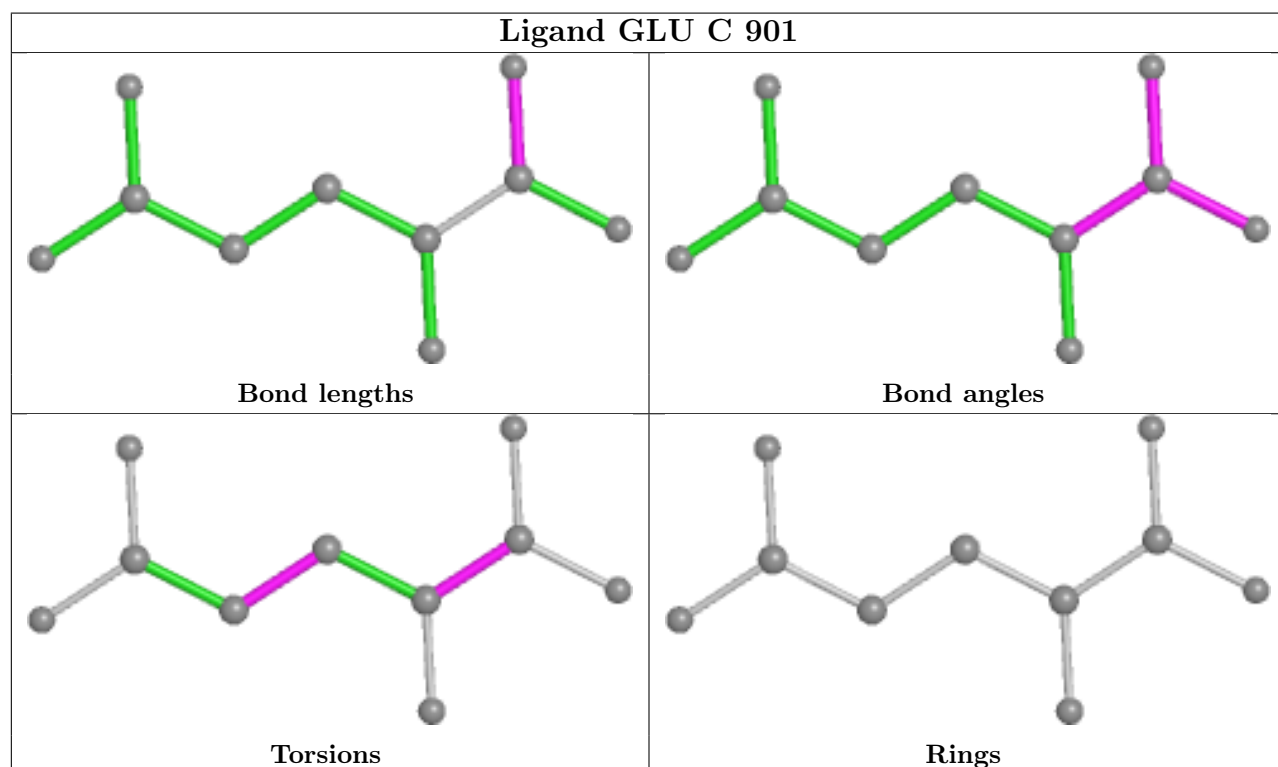
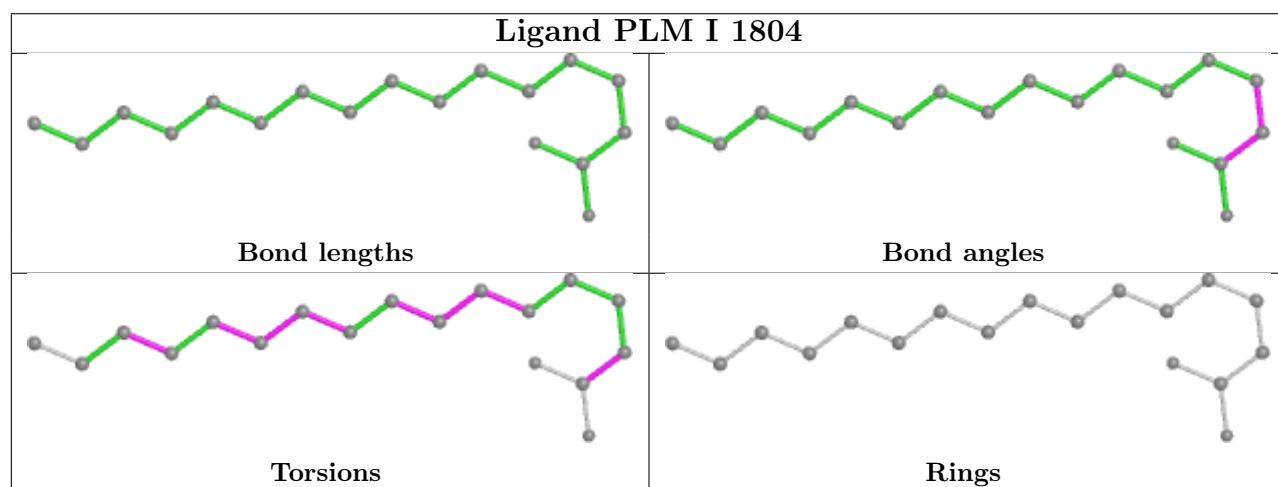
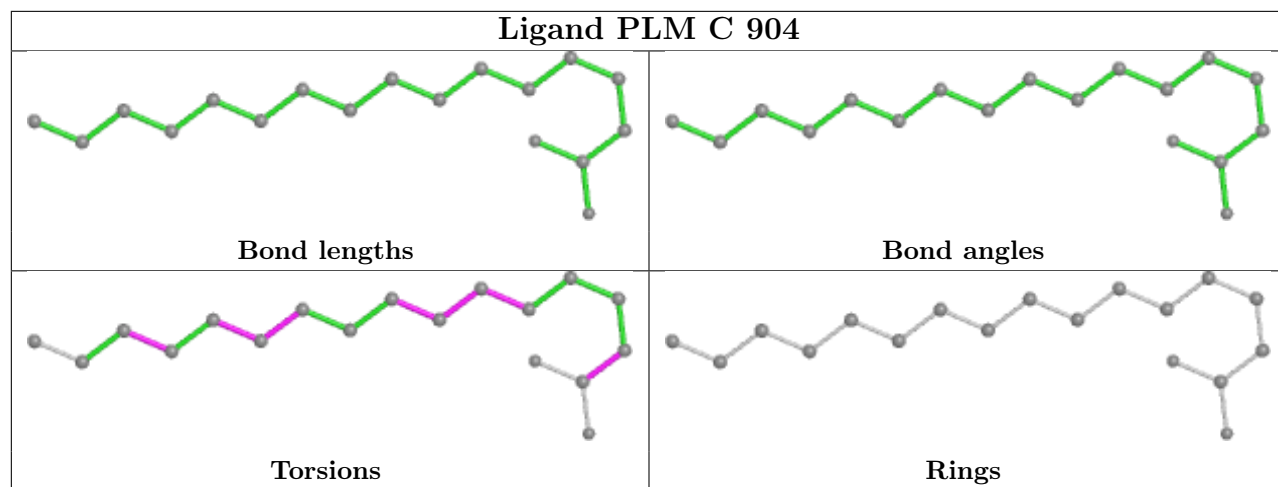


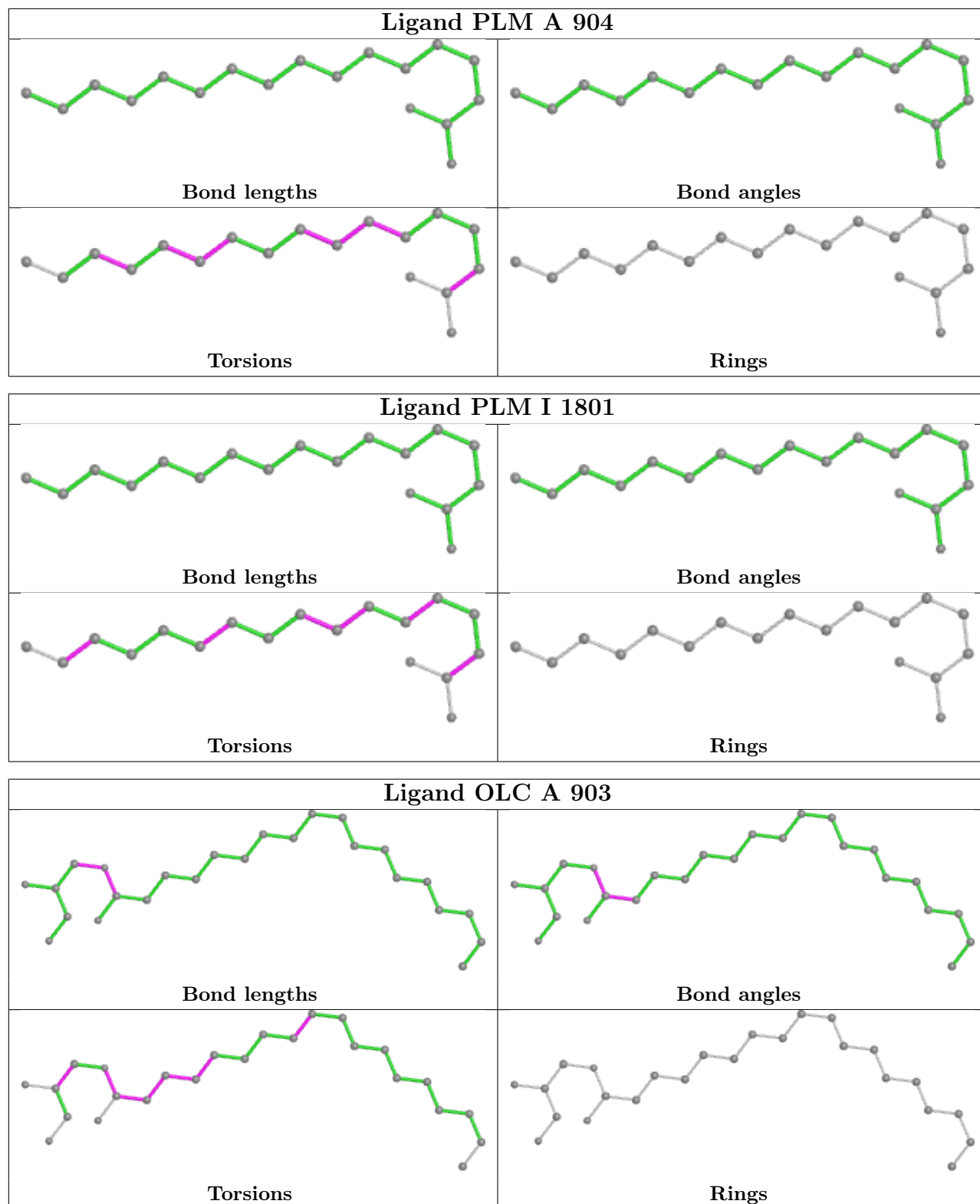


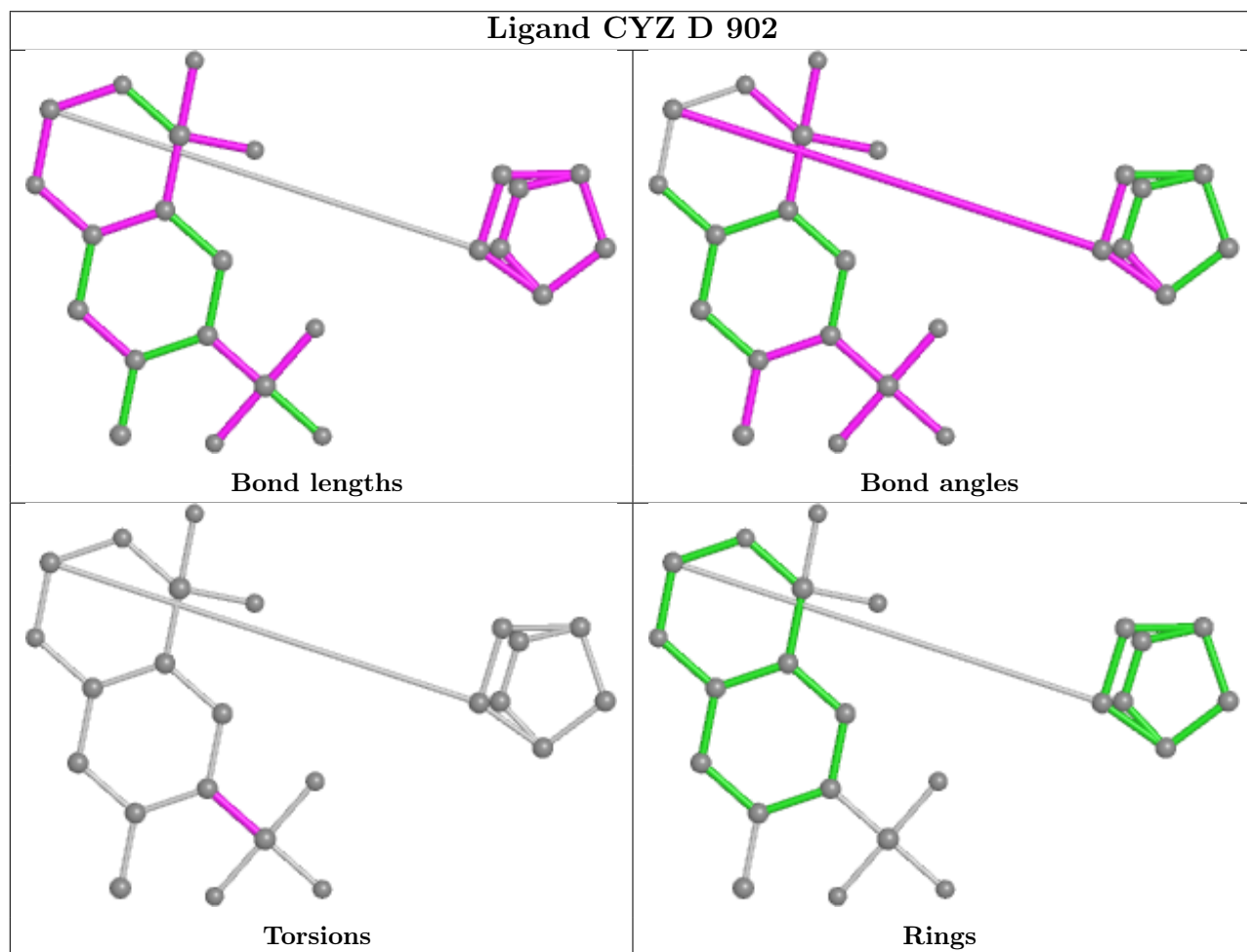
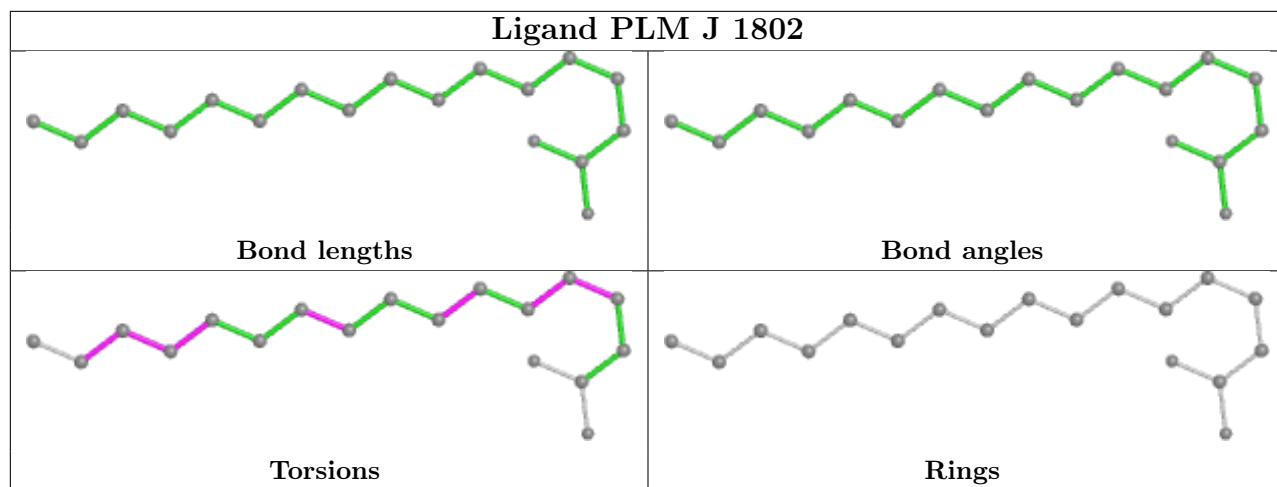


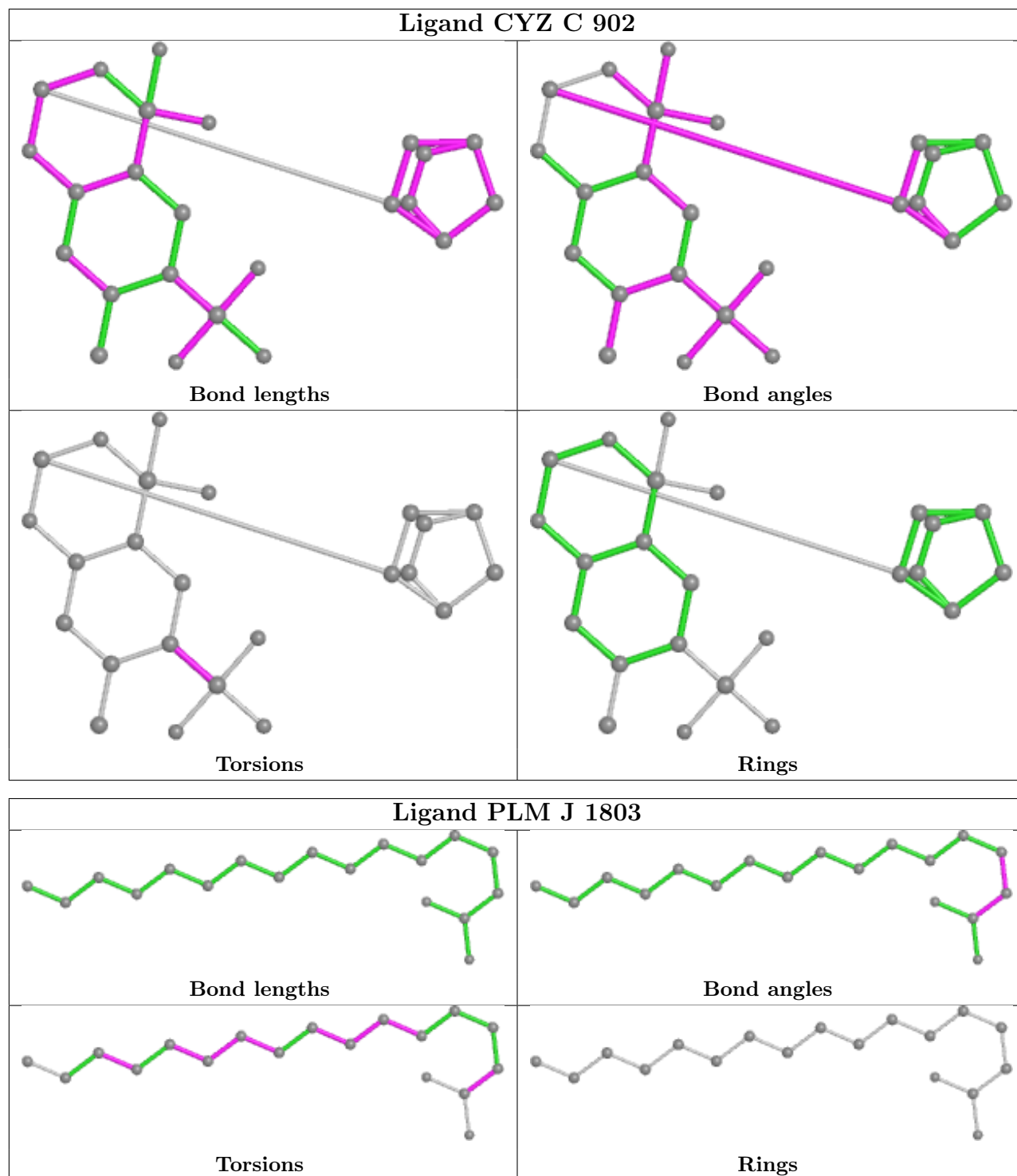


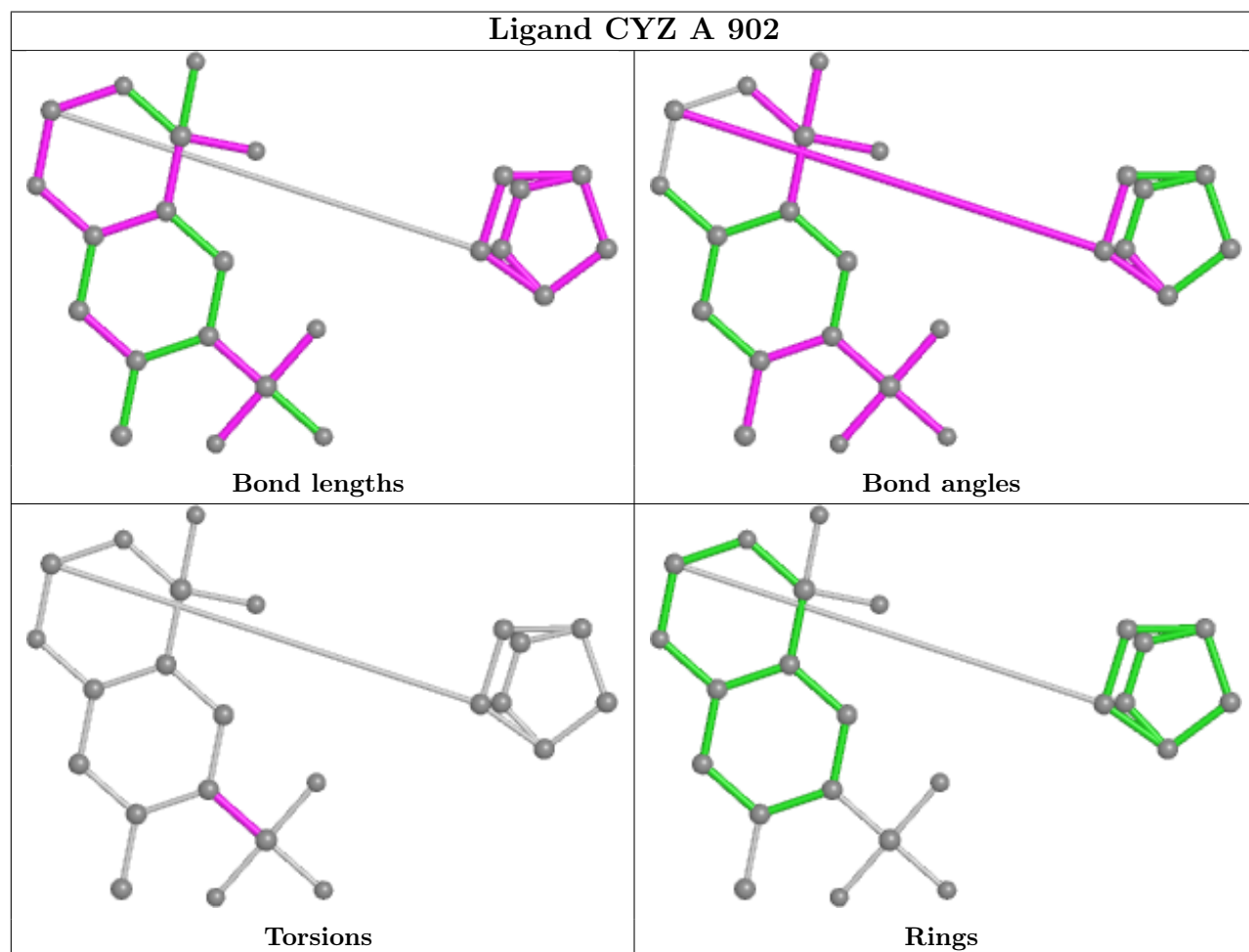
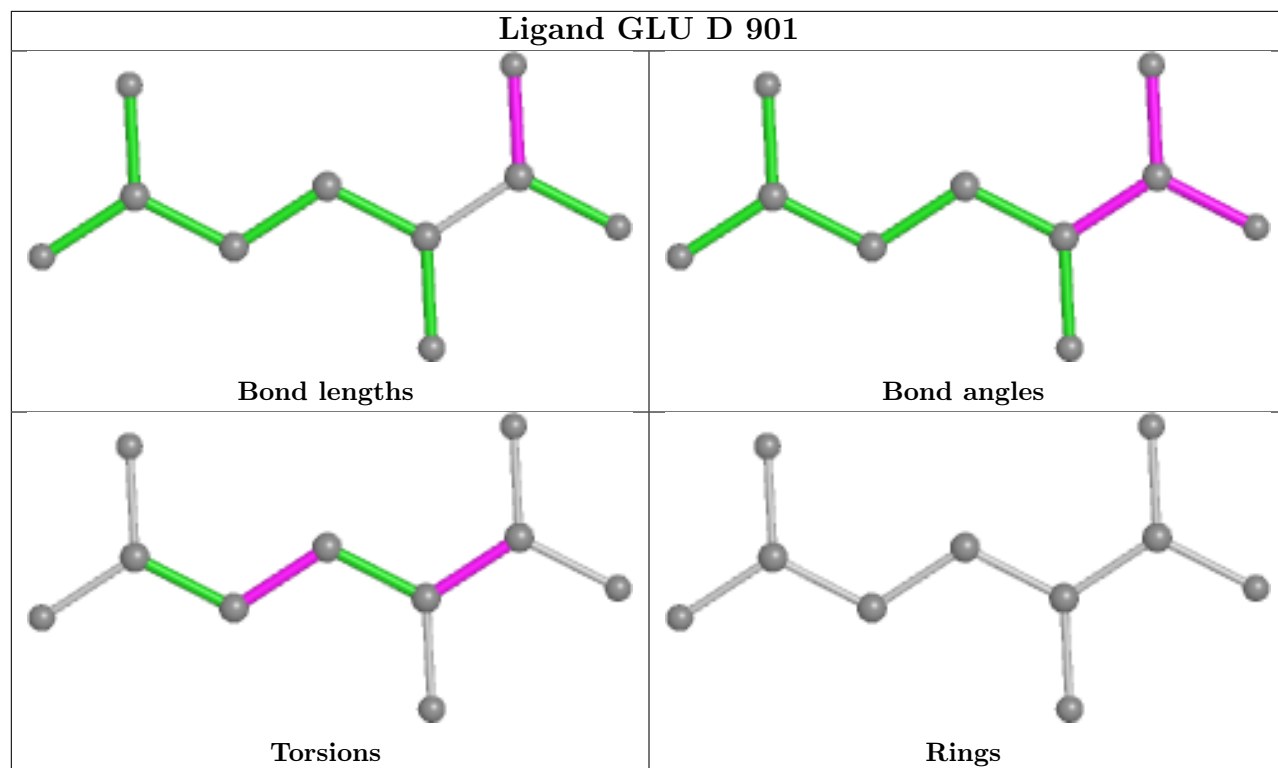


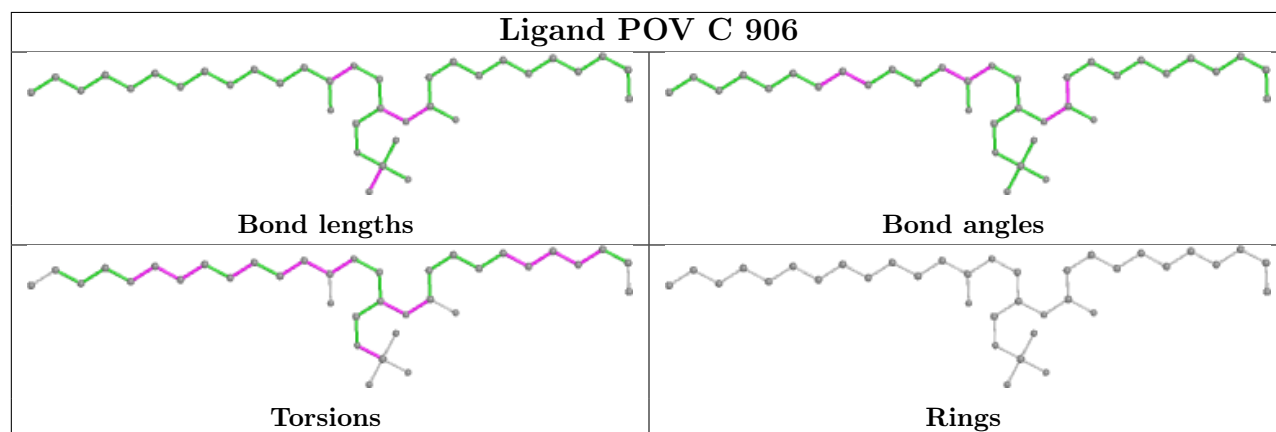
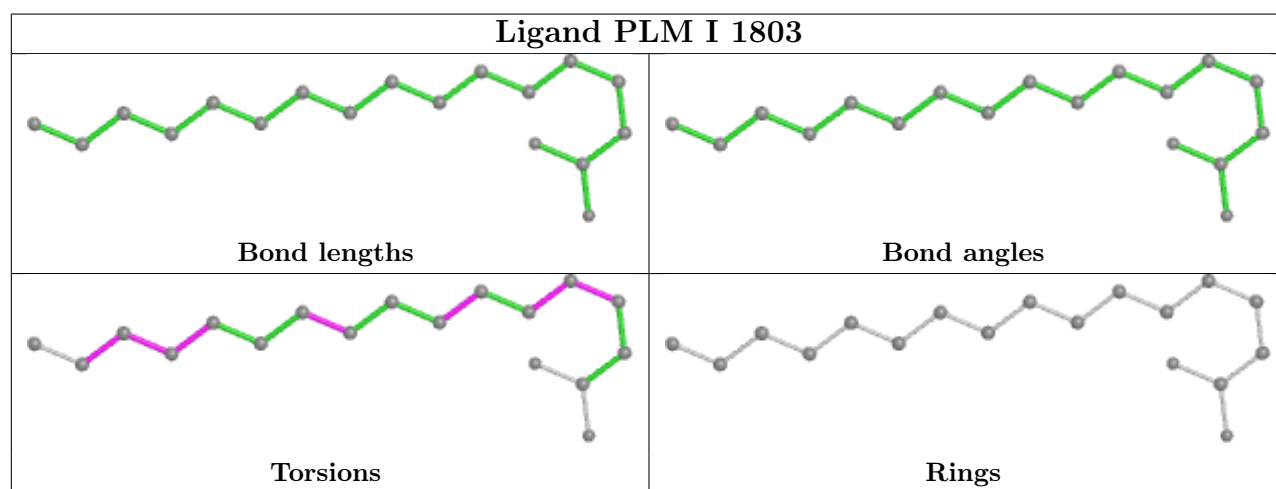
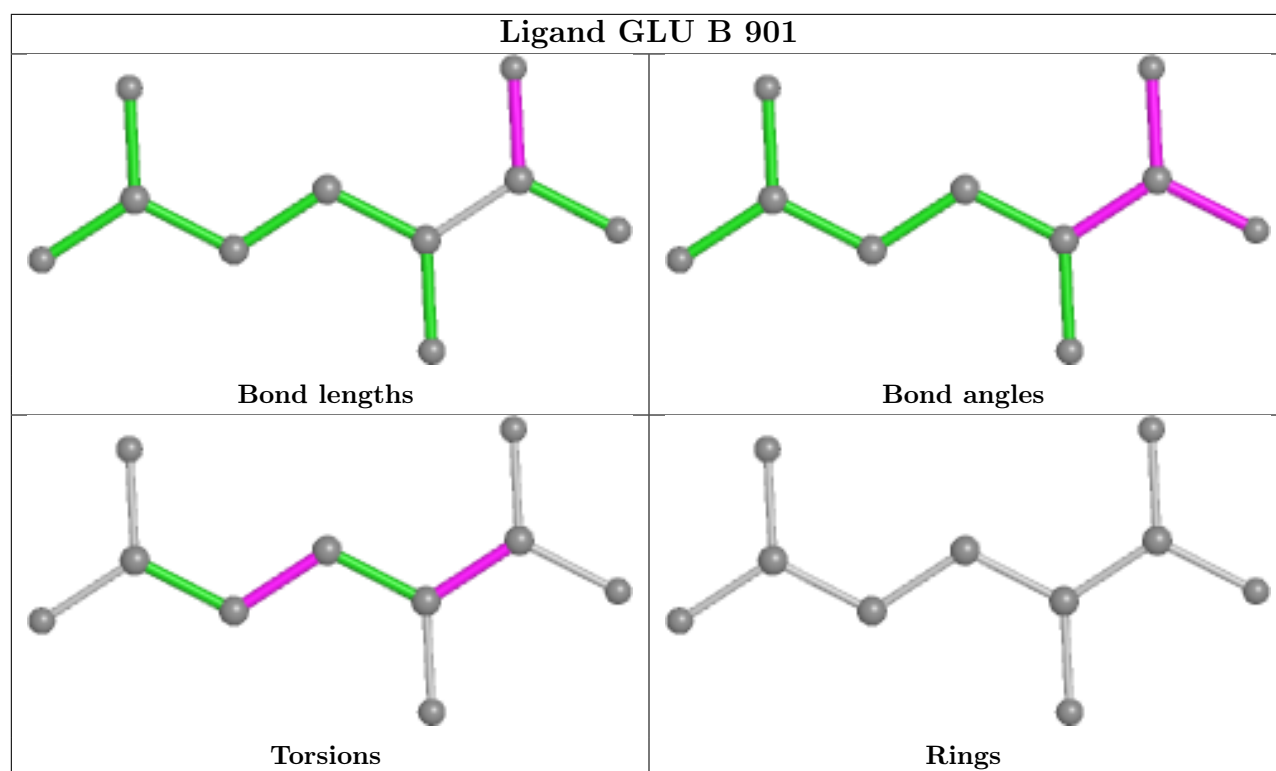












## 5.7 Other polymers [i](#)

There are no such residues in this entry.

## 5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

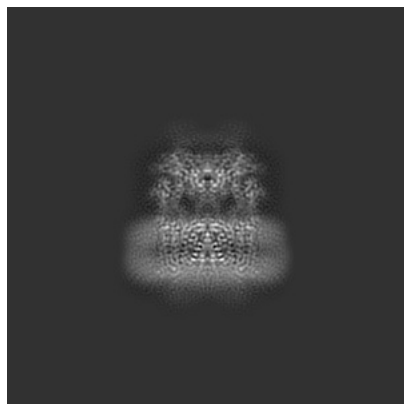
## 6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-15718. These allow visual inspection of the internal detail of the map and identification of artifacts.

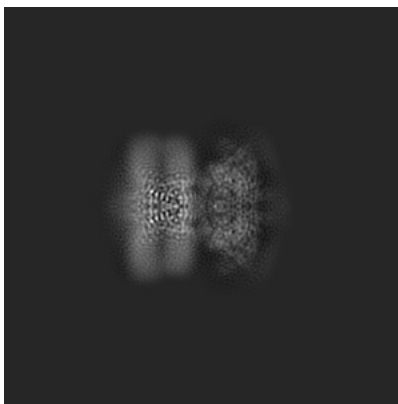
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

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

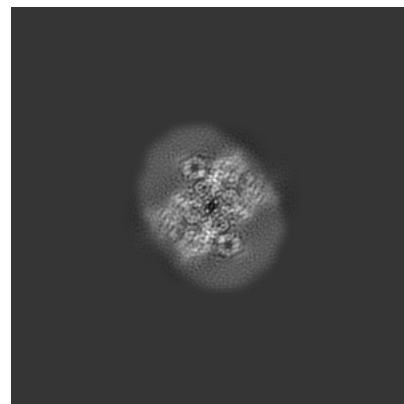
#### 6.1.1 Primary map



X

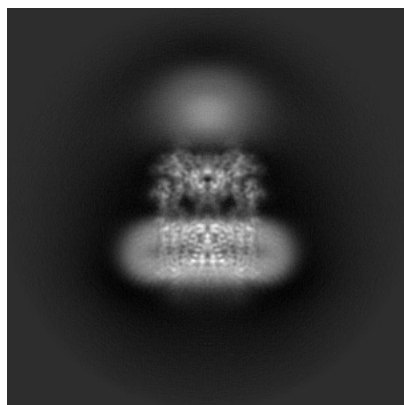


Y

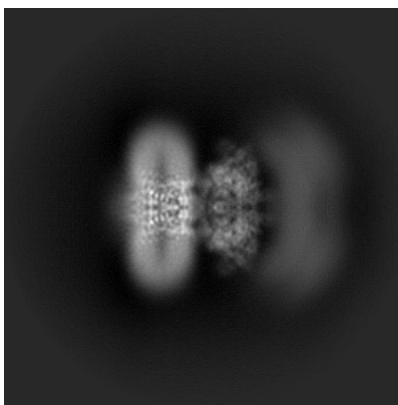


Z

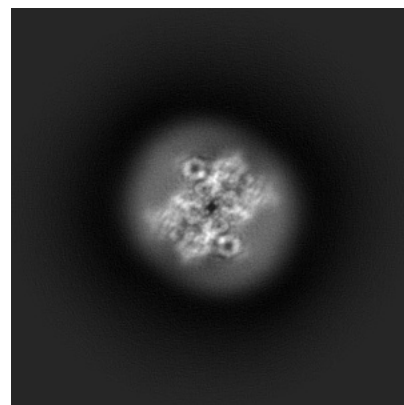
#### 6.1.2 Raw map



X



Y



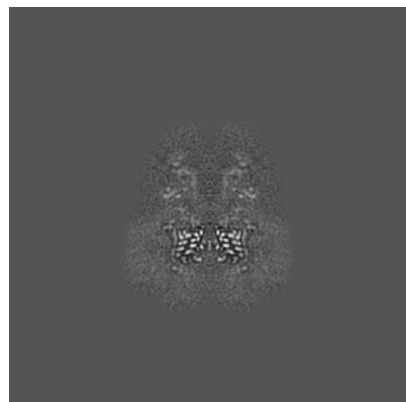
Z

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

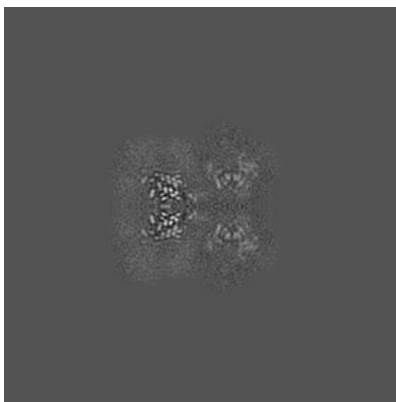


## 6.2 Central slices [i](#)

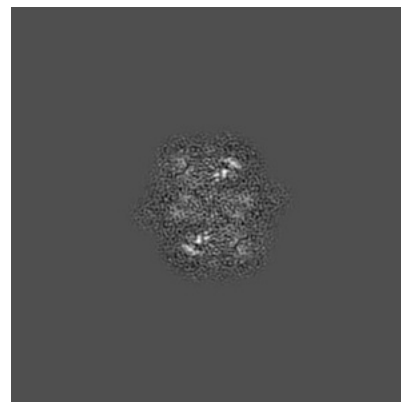
### 6.2.1 Primary map



X Index: 160

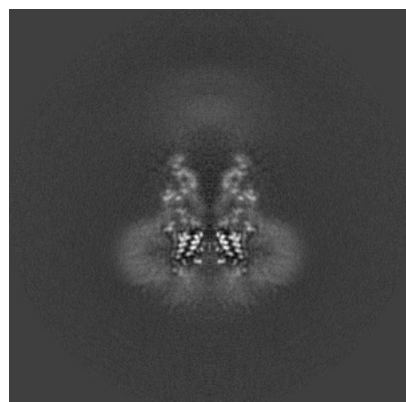


Y Index: 160

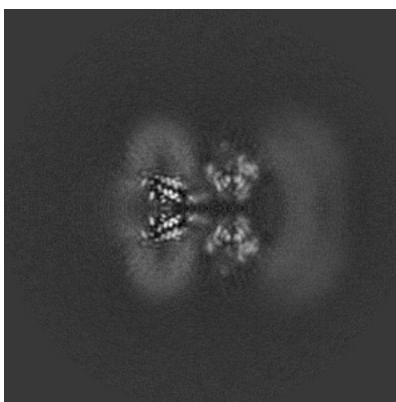


Z Index: 160

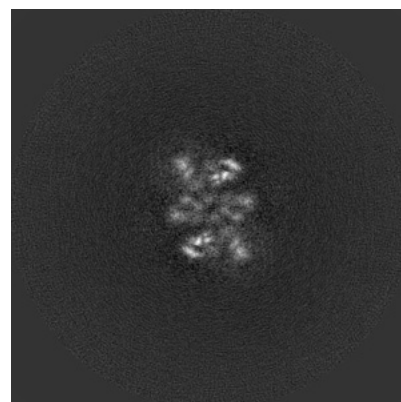
### 6.2.2 Raw map



X Index: 160



Y Index: 160

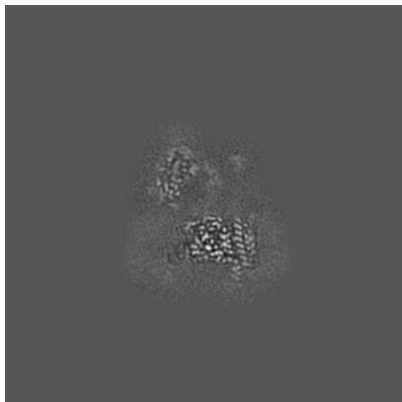


Z Index: 160

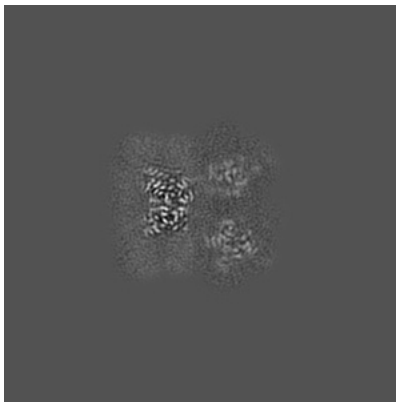
The images above show central slices of the map in three orthogonal directions.

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

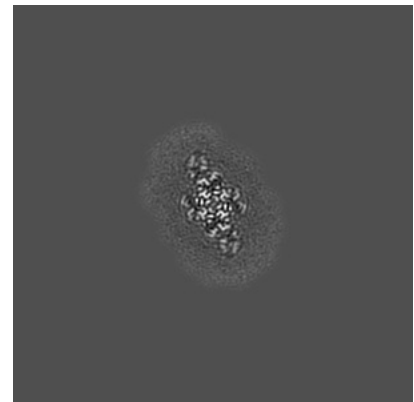
### 6.3.1 Primary map



X Index: 151

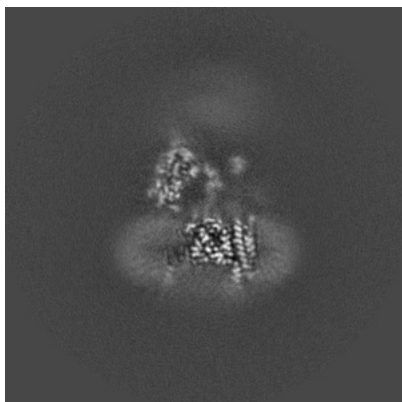


Y Index: 156

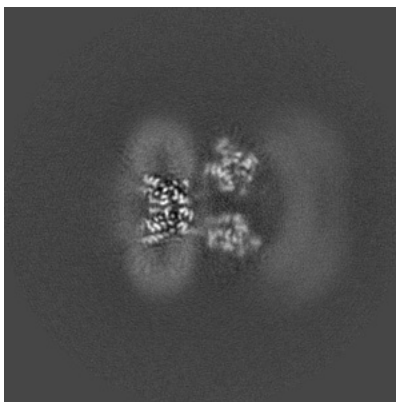


Z Index: 126

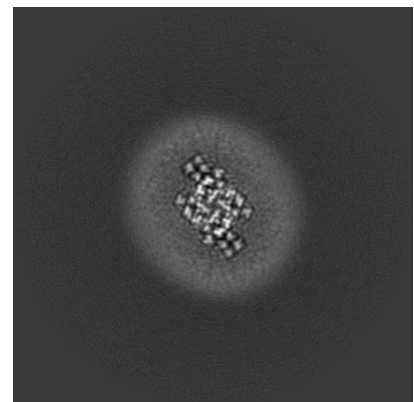
### 6.3.2 Raw map



X Index: 151



Y Index: 164

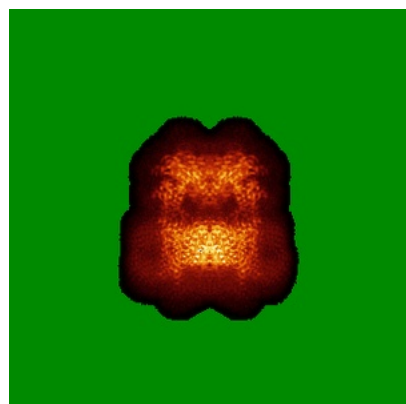


Z Index: 117

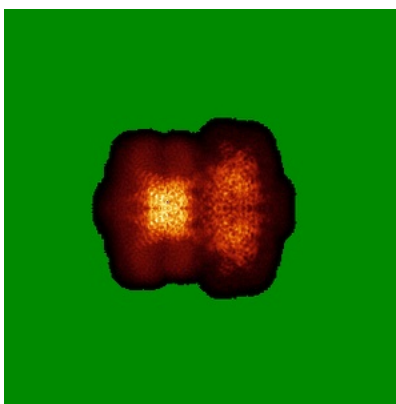
The images above show the largest variance slices of the map in three orthogonal directions.

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

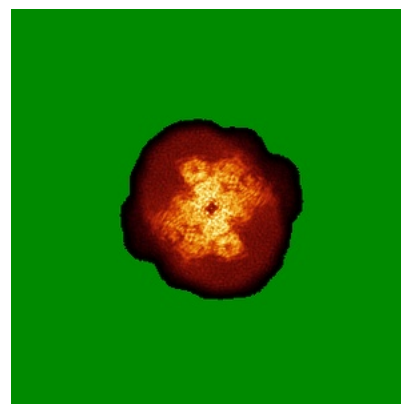
### 6.4.1 Primary map



X

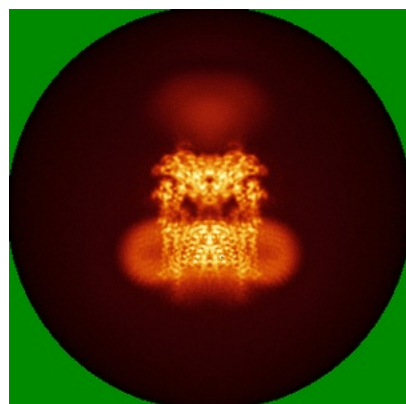


Y

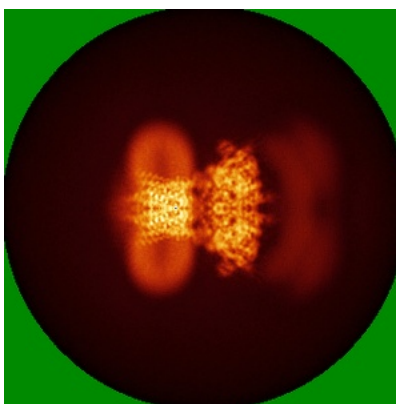


Z

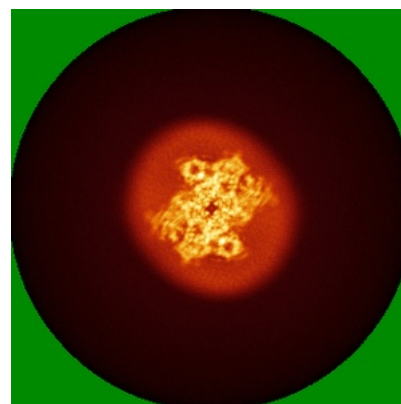
### 6.4.2 Raw map



X



Y

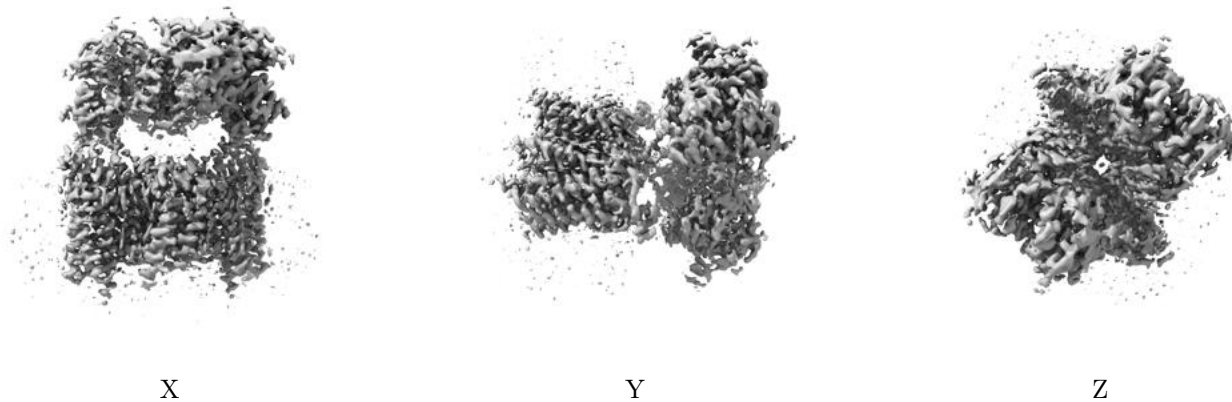


Z

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.

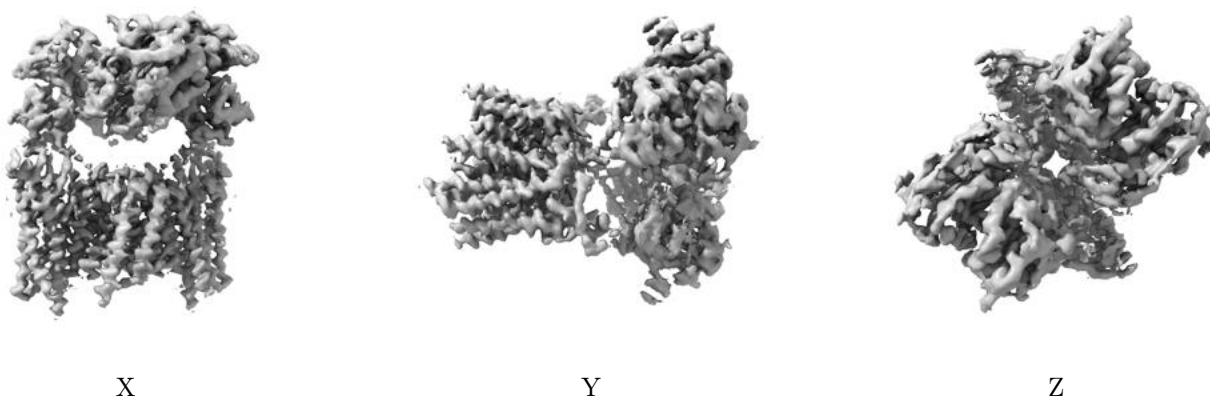
## 6.5 Orthogonal surface views [i](#)

### 6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.023. 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.

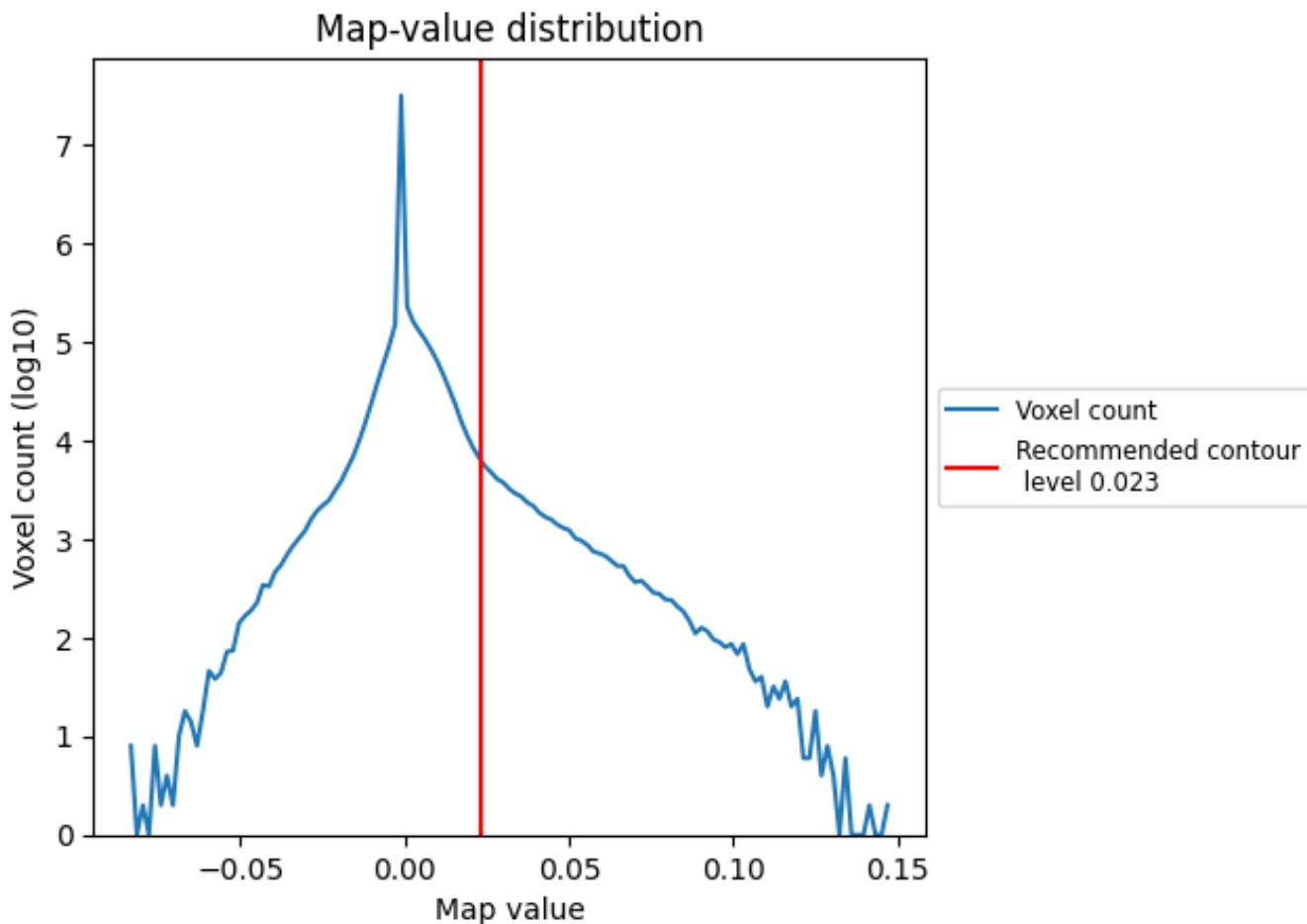
## 6.6 Mask visualisation [i](#)

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

## 7 Map analysis [i](#)

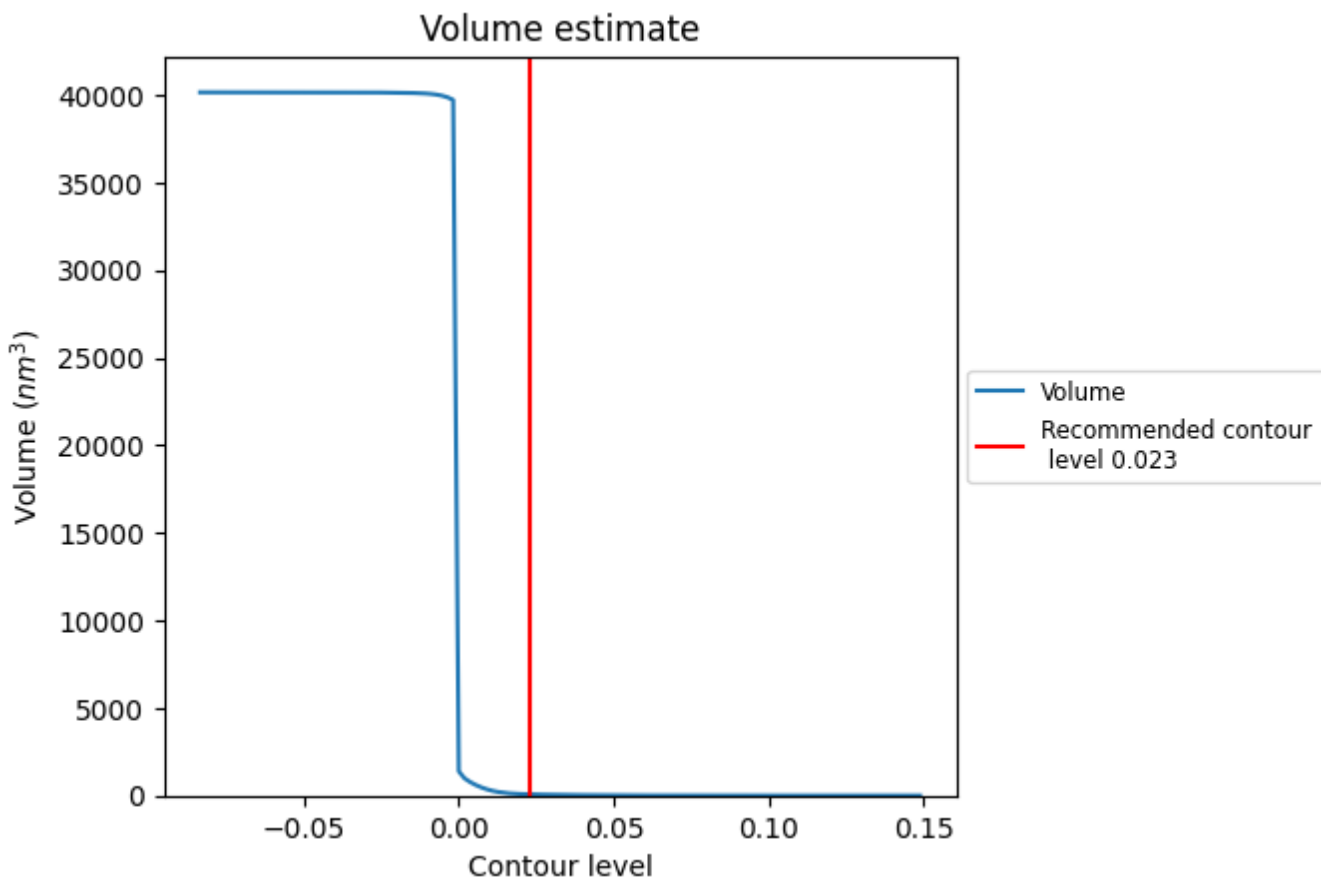
This section contains the results of statistical analysis of the map.

### 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.

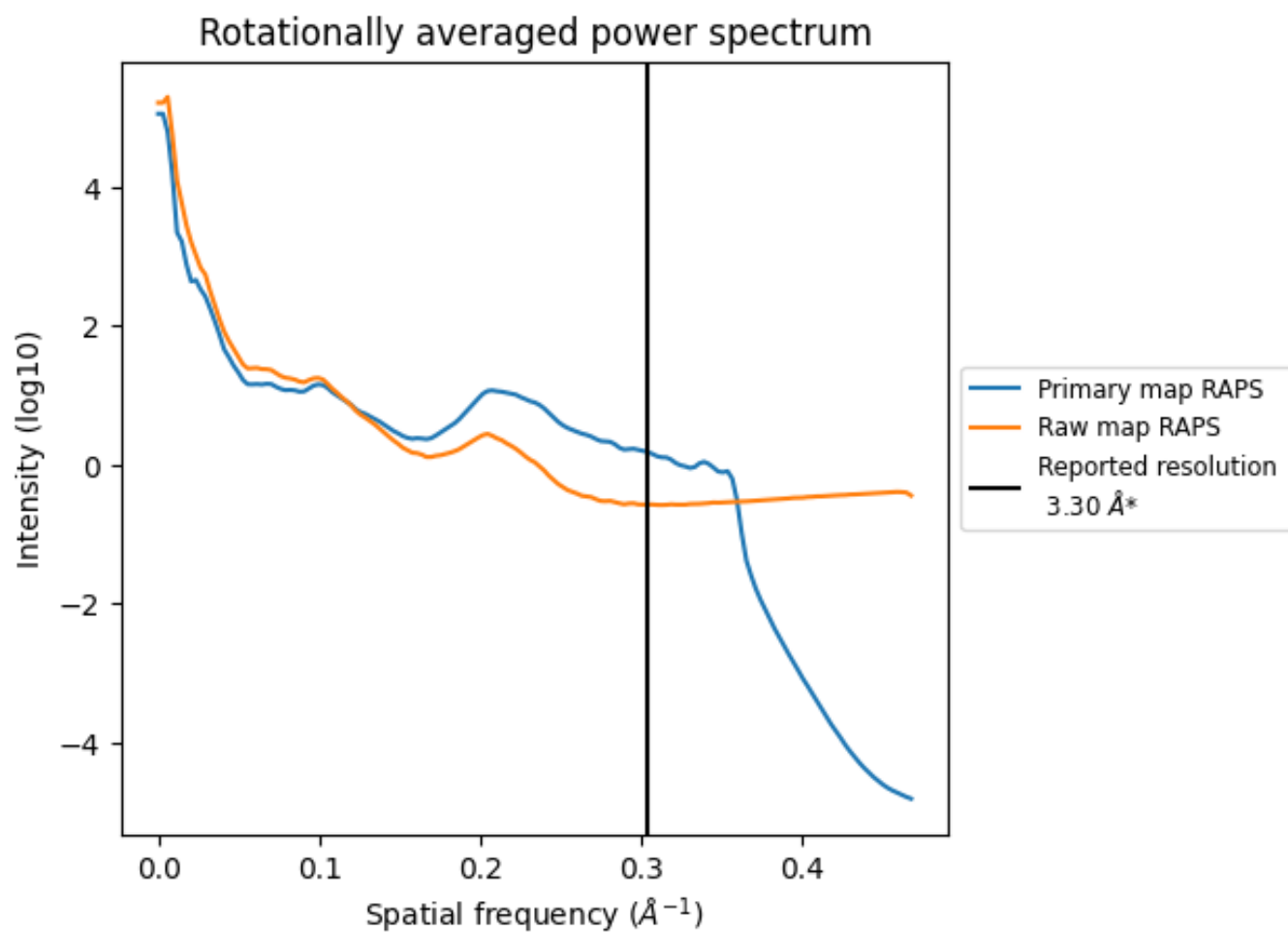
## 7.2 Volume estimate [\(i\)](#)



The volume at the recommended contour level is 69 nm<sup>3</sup>; this corresponds to an approximate mass of 63 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 i

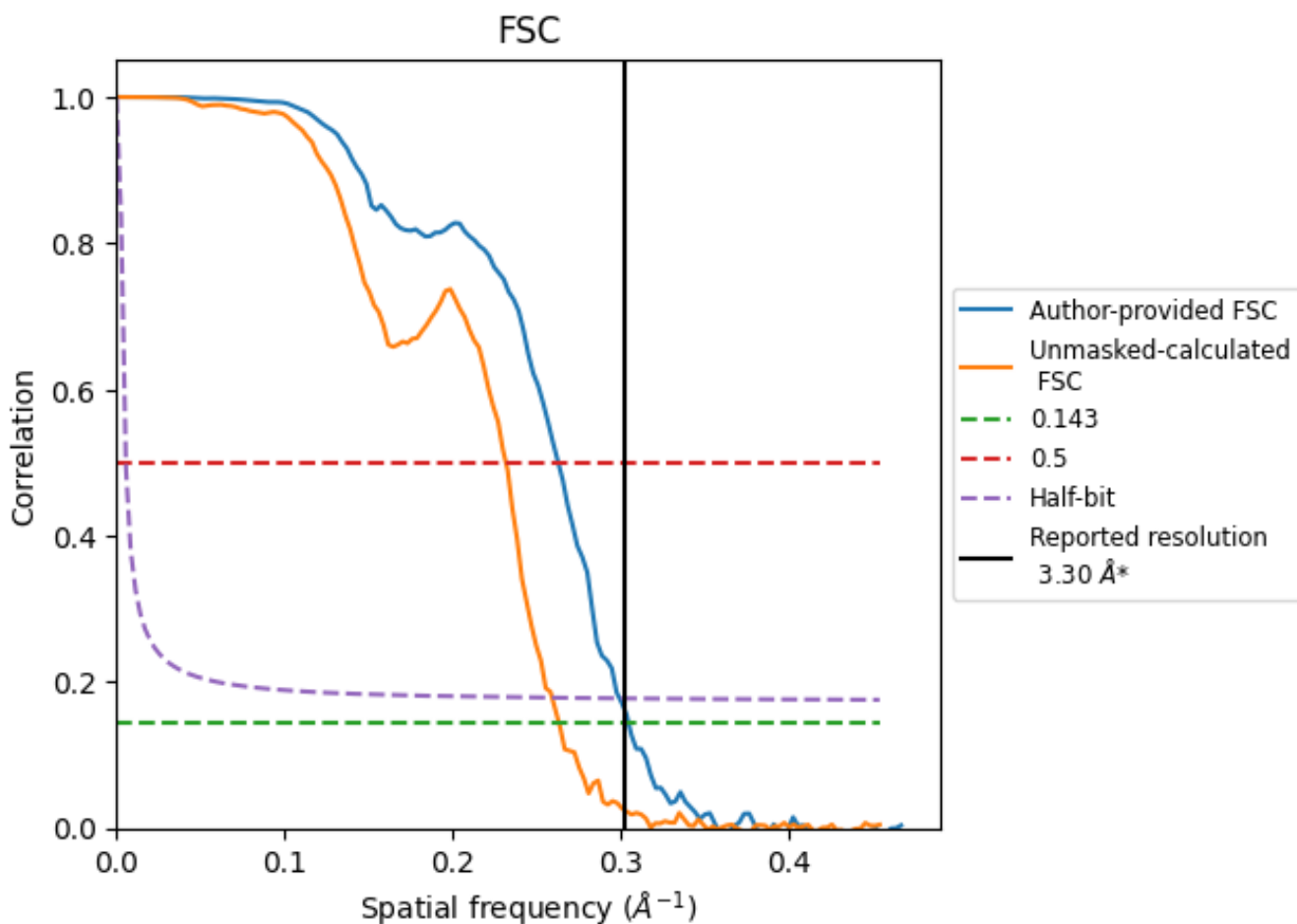


\*Reported resolution corresponds to spatial frequency of 0.303 Å<sup>-1</sup>

## 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  $0.303 \text{\AA}^{-1}$



## 8.2 Resolution estimates [i](#)

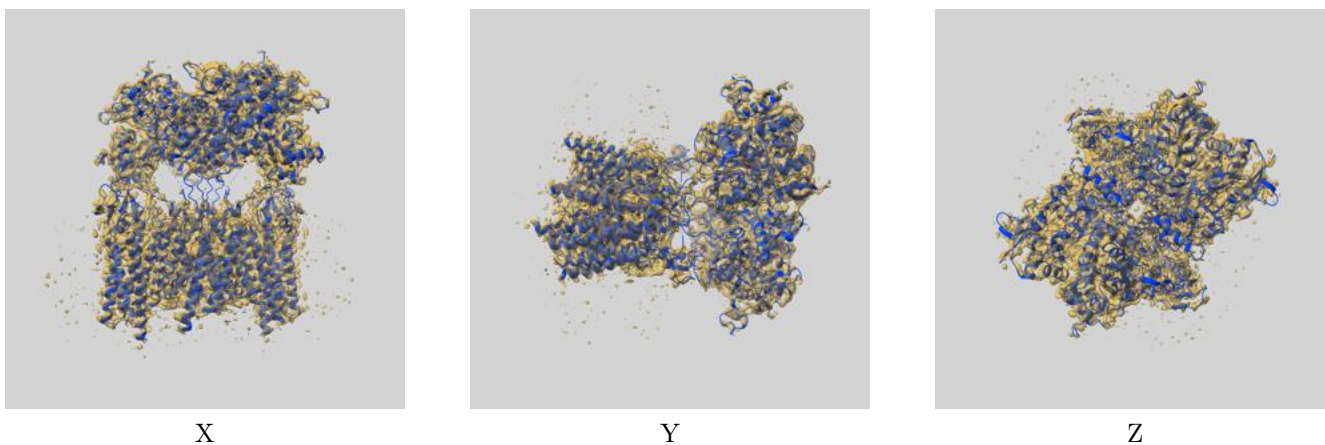
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.30	-	-
Author-provided FSC curve	3.28	3.80	3.34
Unmasked-calculated*	3.79	4.31	3.85

\*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 3.79 differs from the reported value 3.3 by more than 10 %

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

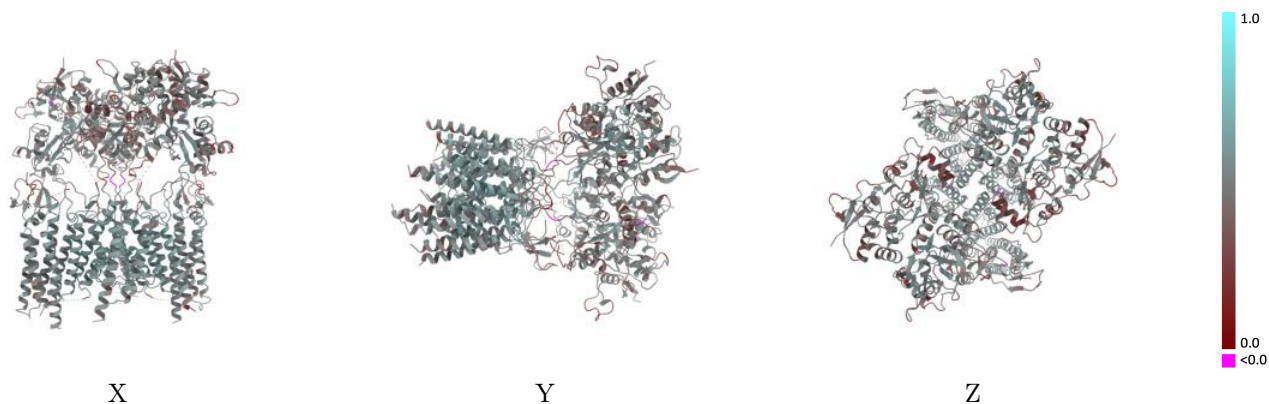
This section contains information regarding the fit between EMDB map EMD-15718 and PDB model 8AYO. Per-residue inclusion information can be found in section 3 on page 10.

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



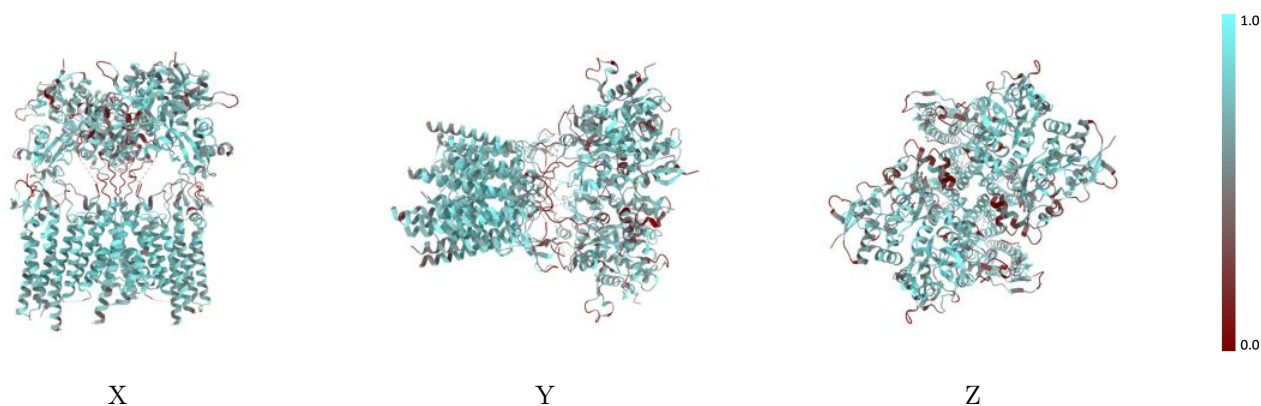
The images above show the 3D surface view of the map at the recommended contour level 0.023 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



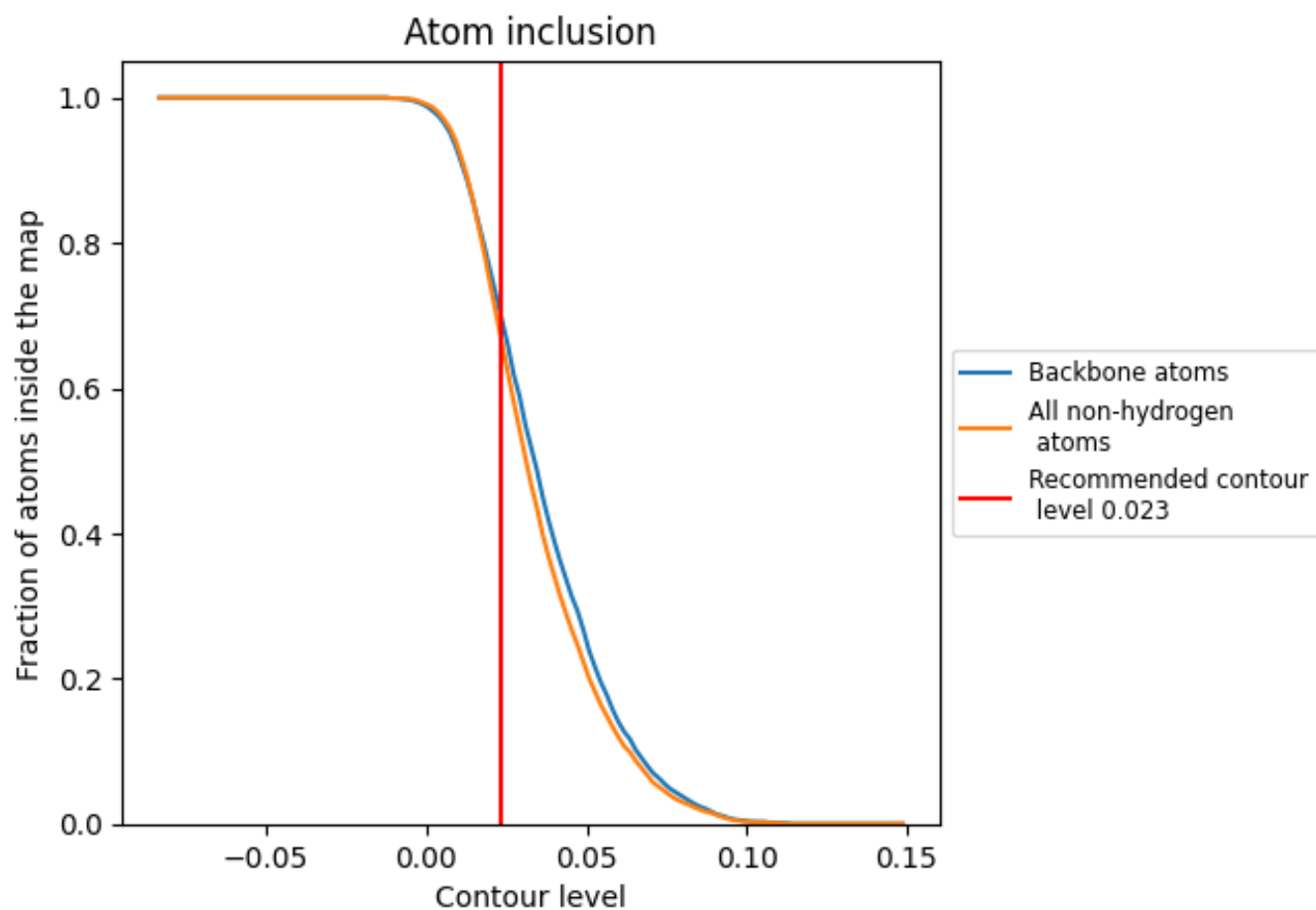
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.023).















## 9.4 Atom inclusion [i](#)



At the recommended contour level, 70% of all backbone atoms, 68% 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 (0.023) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.6750	 0.4980
A	 0.6470	 0.4850
B	 0.7120	 0.5100
C	 0.6460	 0.4860
D	 0.7140	 0.5120
I	 0.6580	 0.5000
J	 0.6550	 0.4990

