



wwPDB EM Validation Summary Report ⓘ

Nov 14, 2022 – 07:56 AM EST

PDB ID : 7LHF
EMDB ID : EMD-23338
Title : Structure of full-length IP3R1 channel solubilized in LNMG & lipid in the apo-state
Authors : Baker, M.R.; Fan, G.; Baker, M.L.; Serysheva, I.I.
Deposited on : 2021-01-22
Resolution : 2.96 Å(reported)
Based on initial model : 6MU2

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

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

A user guide is available at

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

The types of validation reports are described at

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

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

EMDB validation analysis : 0.0.1.dev43
Mogul : 1.8.5 (274361), 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) : 2.31.2

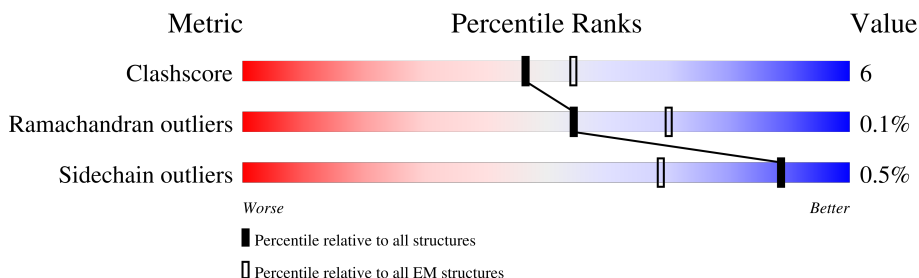
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 2.96 Å.

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



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

The table below summarises the geometric issues observed across the polymeric chains and their fit to the map. The red, orange, yellow and green segments of the bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the EM map (all-atom inclusion $< 40\%$). The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	2736	
1	B	2736	
1	C	2736	
1	D	2736	

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	PLX	A	2801	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	PLX	A	2802	X	-	-	-
2	PLX	A	2803	X	-	-	-
2	PLX	A	2804	X	-	-	-
2	PLX	A	2805	X	-	-	-
2	PLX	A	2806	X	-	-	-
2	PLX	A	2807	X	-	-	-
2	PLX	B	2801	X	-	-	-
2	PLX	B	2802	X	-	-	-
2	PLX	B	2803	X	-	-	-
2	PLX	B	2804	X	-	-	-
2	PLX	B	2805	X	-	-	-
2	PLX	B	2806	X	-	-	-
2	PLX	B	2807	X	-	-	-
2	PLX	C	5102	X	-	-	-
2	PLX	C	5103	X	-	-	-
2	PLX	C	5104	X	-	-	-
2	PLX	C	5105	X	-	-	-
2	PLX	C	5106	X	-	-	-
2	PLX	C	5107	X	-	-	-
2	PLX	C	5108	X	-	-	-
2	PLX	D	5102	X	-	-	-
2	PLX	D	5103	X	-	-	-
2	PLX	D	5104	X	-	-	-
2	PLX	D	5105	X	-	-	-
2	PLX	D	5106	X	-	-	-
2	PLX	D	5107	X	-	-	-
2	PLX	D	5108	X	-	-	-

2 Entry composition ⓘ

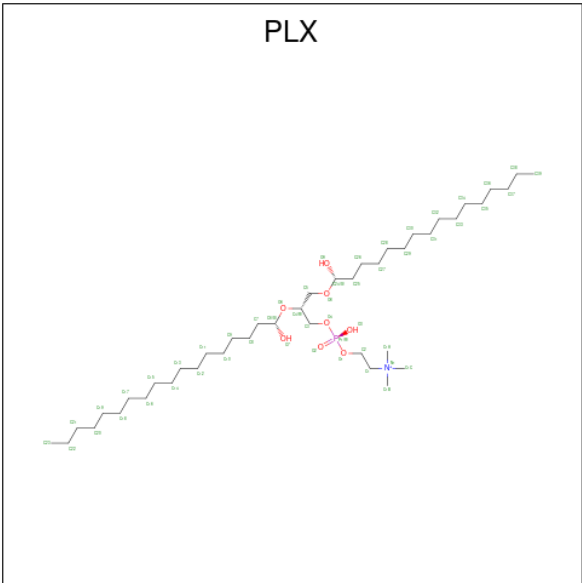
There are 3 unique types of molecules in this entry. The entry contains 72092 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 Inositol 1,4,5-trisphosphate receptor type 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	2300	Total	C	N	O	S	0	0
			17734	11338	3140	3156	100		
1	D	2300	Total	C	N	O	S	0	0
			17734	11338	3140	3156	100		
1	B	2300	Total	C	N	O	S	0	0
			17734	11338	3140	3156	100		
1	C	2300	Total	C	N	O	S	0	0
			17734	11338	3140	3156	100		

- Molecule 2 is (9R,11S)-9-({[(1S)-1-HYDROXYHEXADECYL]OXY}METHYL)-2,2-DIMETHYL-5,7,10-TRIOXA-2LAMBDA 5 -AZA-6LAMBDA 5 -PHOSPHAOCTACOSANE-6,6,11-TRIOL (three-letter code: PLX) (formula: C₄₂H₈₉NO₈P) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms					AltConf
2	A	1	Total	C	N	O	P	0
			288	218	7	56	7	

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Mol	Chain	Residues	Atoms					AltConf
2	A	1	Total 288	C 218	N 7	O 56	P 7	0
2	A	1	Total 288	C 218	N 7	O 56	P 7	0
2	A	1	Total 288	C 218	N 7	O 56	P 7	0
2	A	1	Total 288	C 218	N 7	O 56	P 7	0
2	A	1	Total 288	C 218	N 7	O 56	P 7	0
2	A	1	Total 288	C 218	N 7	O 56	P 7	0
2	D	1	Total 288	C 218	N 7	O 56	P 7	0
2	D	1	Total 288	C 218	N 7	O 56	P 7	0
2	D	1	Total 288	C 218	N 7	O 56	P 7	0
2	D	1	Total 288	C 218	N 7	O 56	P 7	0
2	D	1	Total 288	C 218	N 7	O 56	P 7	0
2	D	1	Total 288	C 218	N 7	O 56	P 7	0
2	D	1	Total 288	C 218	N 7	O 56	P 7	0
2	D	1	Total 288	C 218	N 7	O 56	P 7	0
2	B	1	Total 288	C 218	N 7	O 56	P 7	0
2	B	1	Total 288	C 218	N 7	O 56	P 7	0
2	B	1	Total 288	C 218	N 7	O 56	P 7	0
2	B	1	Total 288	C 218	N 7	O 56	P 7	0
2	B	1	Total 288	C 218	N 7	O 56	P 7	0
2	B	1	Total 288	C 218	N 7	O 56	P 7	0
2	B	1	Total 288	C 218	N 7	O 56	P 7	0
2	C	1	Total 288	C 218	N 7	O 56	P 7	0

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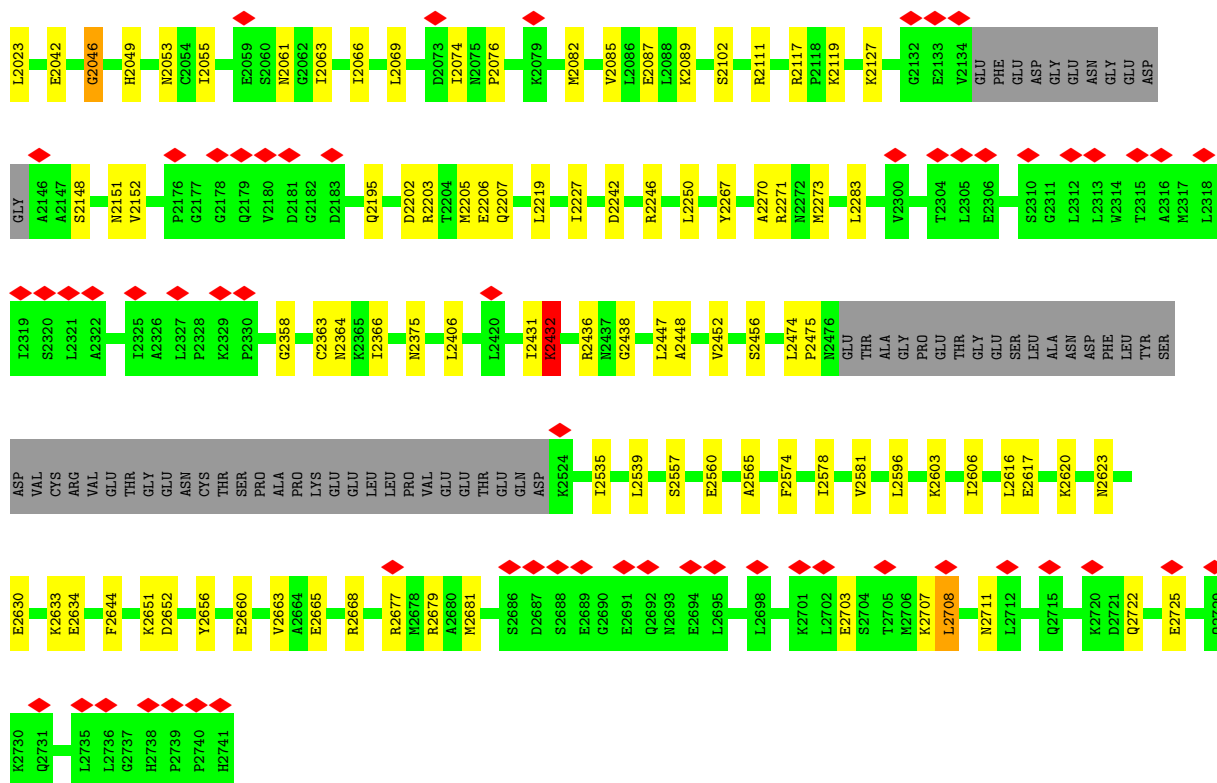
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Mol	Chain	Residues	Atoms					AltConf
2	C	1	Total	C	N	O	P	0
			288	218	7	56	7	
2	C	1	Total	C	N	O	P	0
			288	218	7	56	7	
2	C	1	Total	C	N	O	P	0
			288	218	7	56	7	
2	C	1	Total	C	N	O	P	0
			288	218	7	56	7	
2	C	1	Total	C	N	O	P	0
			288	218	7	56	7	

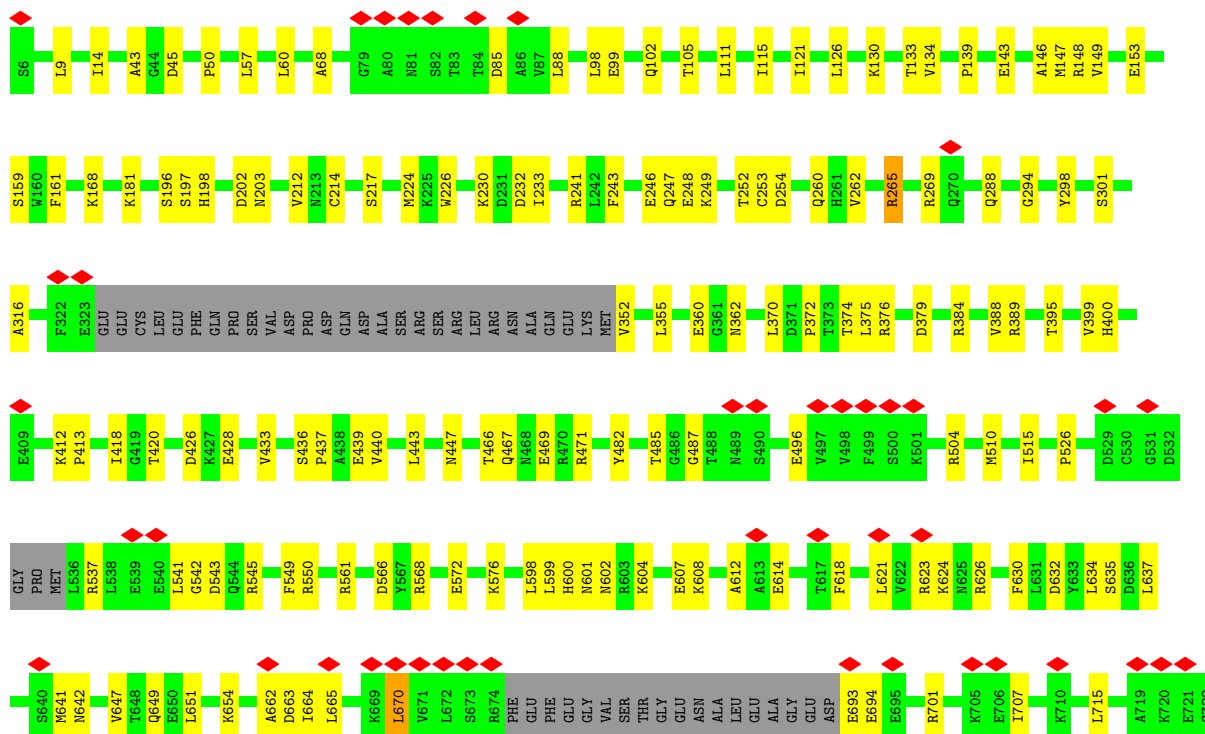
- Molecule 3 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		AltConf
3	A	1	Total	Zn	0
			1	1	
3	D	1	Total	Zn	0
			1	1	
3	B	1	Total	Zn	0
			1	1	
3	C	1	Total	Zn	0
			1	1	



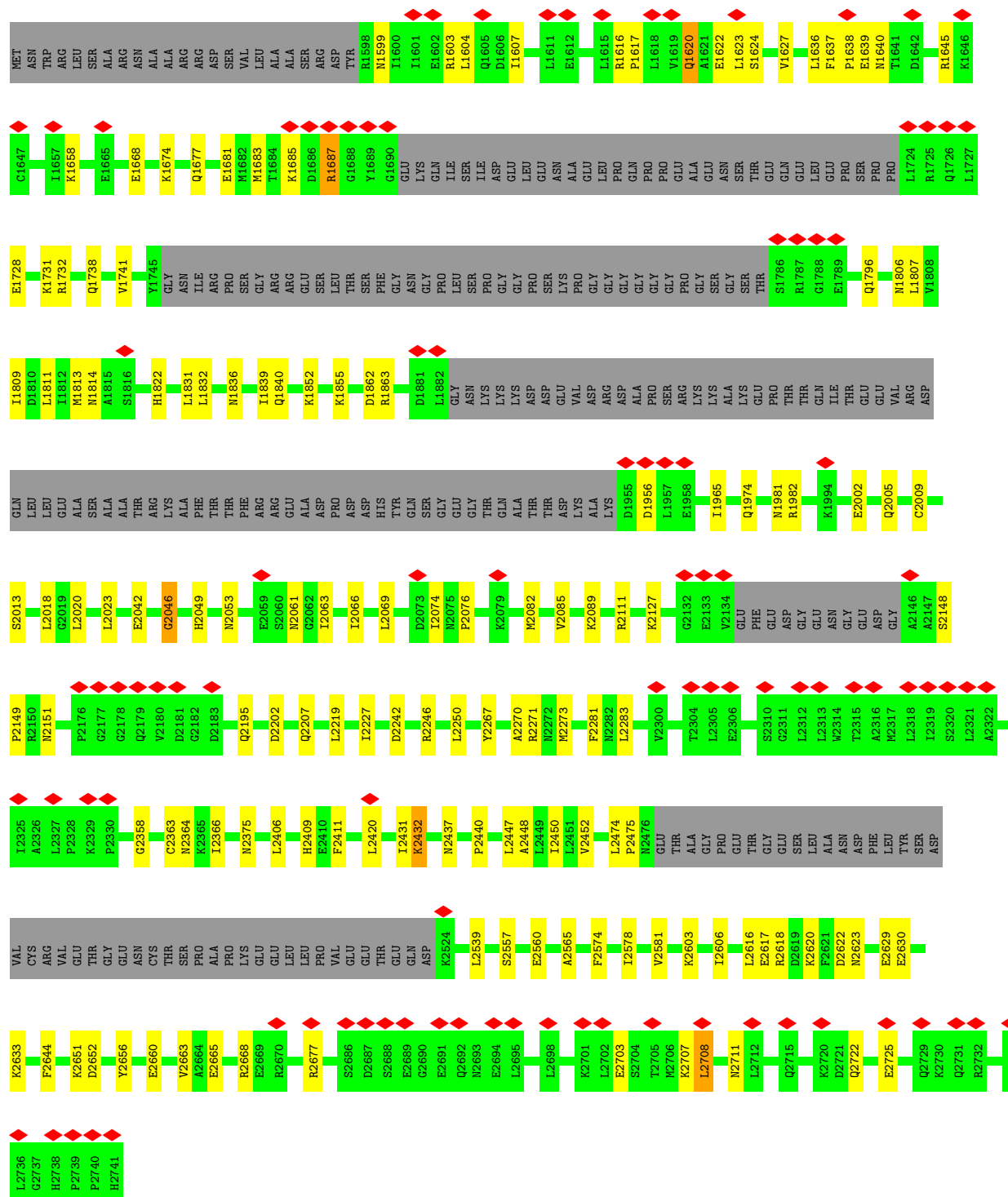


• Molecule 1: Inositol 1,4,5-trisphosphate receptor type 1

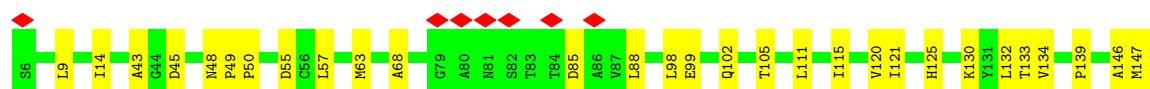


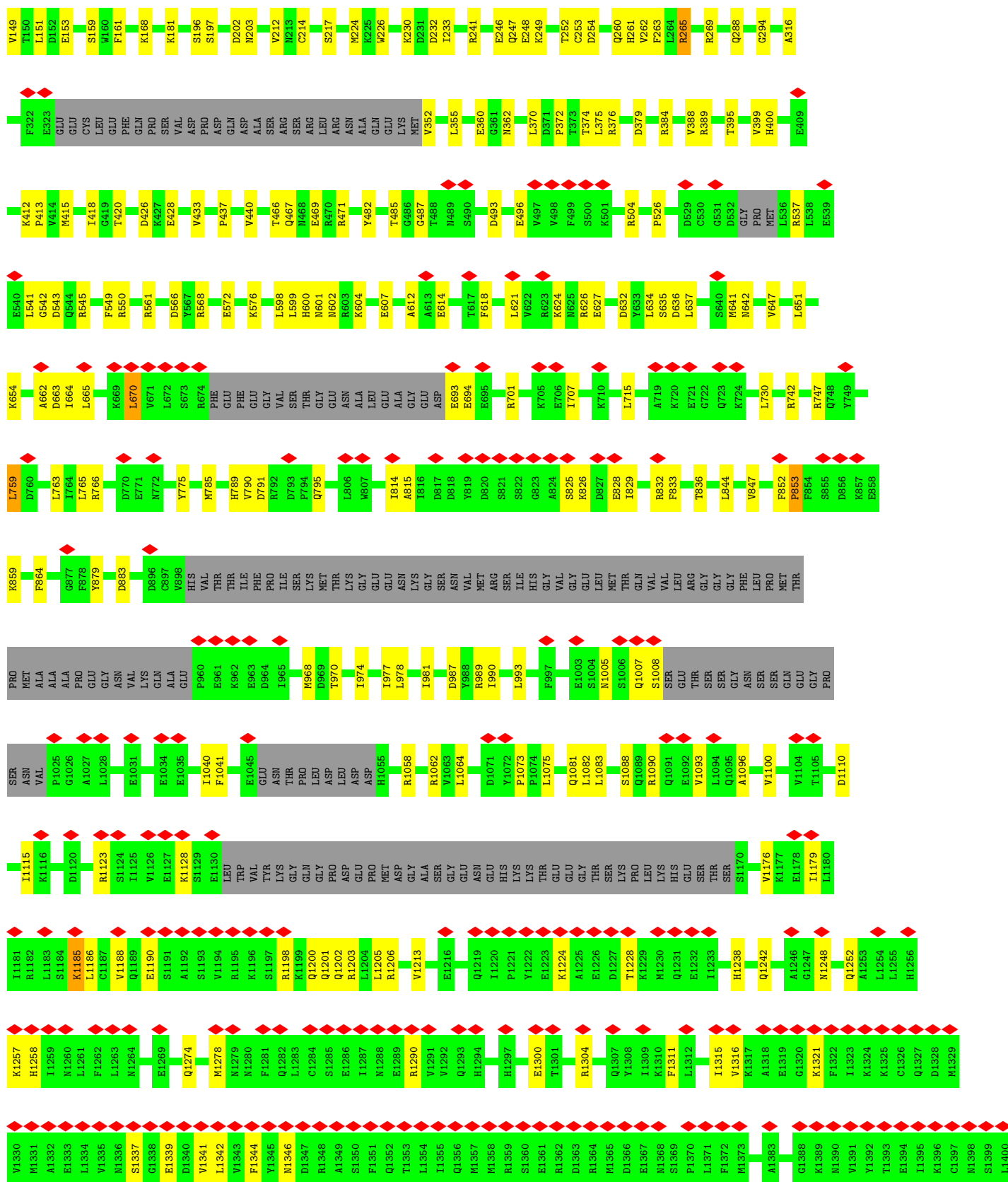






• Molecule 1: Inositol 1,4,5-trisphosphate receptor type 1







4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C4	Depositor
Number of particles used	303481	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	NONE	Depositor
Microscope	TFS KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	42	Depositor
Minimum defocus (nm)	800	Depositor
Maximum defocus (nm)	3500	Depositor
Magnification	46943	Depositor
Image detector	GATAN K2 QUANTUM (4k x 4k)	Depositor
Maximum map value	0.087	Depositor
Minimum map value	-0.046	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.002	Depositor
Recommended contour level	0.0112	Depositor
Map size (\AA)	470.80002, 470.80002, 470.80002	wwPDB
Map dimensions	440, 440, 440	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (\AA)	1.07, 1.07, 1.07	Depositor

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: PLX, ZN

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	0.28	0/18029	0.64	12/24246 (0.0%)
1	B	0.28	0/18029	0.64	10/24246 (0.0%)
1	C	0.28	0/18029	0.64	12/24246 (0.0%)
1	D	0.29	0/18029	0.64	9/24246 (0.0%)
All	All	0.28	0/72116	0.64	43/96984 (0.0%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	4
1	B	0	5
1	C	0	5
1	D	0	6
All	All	0	20

There are no bond length outliers.

The worst 5 of 43 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	2432	LYS	CB-CG-CD	-9.79	86.14	111.60
1	B	670	LEU	CA-CB-CG	7.65	132.90	115.30
1	C	670	LEU	CA-CB-CG	7.65	132.89	115.30
1	D	670	LEU	CA-CB-CG	7.63	132.84	115.30
1	A	2432	LYS	CD-CE-NZ	-7.57	94.29	111.70

There are no chirality outliers.

5 of 20 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	1346	ASN	Peptide
1	A	1637	PHE	Peptide
1	A	2046	GLY	Peptide
1	A	663	ASP	Peptide
1	D	663	ASP	Peptide

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	17734	0	17384	240	0
1	B	17734	0	17383	229	0
1	C	17734	0	17383	219	0
1	D	17734	0	17383	232	0
2	A	288	0	399	12	0
2	B	288	0	395	10	0
2	C	288	0	398	8	0
2	D	288	0	398	9	0
3	A	1	0	0	0	0
3	B	1	0	0	0	0
3	C	1	0	0	0	0
3	D	1	0	0	0	0
All	All	72092	0	71123	924	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.

The worst 5 of 924 close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1096:ALA:O	1:A:1100:VAL:HB	1.78	0.83
1:D:1096:ALA:O	1:D:1100:VAL:HB	1.79	0.82
1:B:1096:ALA:O	1:B:1100:VAL:HB	1.83	0.78
1:C:1096:ALA:O	1:C:1100:VAL:HB	1.87	0.73
1:D:288:GLN:HG3	1:D:294:GLY:HA2	1.69	0.73

There are no symmetry-related clashes.

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	2272/2736 (83%)	2038 (90%)	233 (10%)	1 (0%)	100	100
1	B	2272/2736 (83%)	2038 (90%)	232 (10%)	2 (0%)	51	83
1	C	2272/2736 (83%)	2034 (90%)	236 (10%)	2 (0%)	51	83
1	D	2272/2736 (83%)	2037 (90%)	233 (10%)	2 (0%)	51	83
All	All	9088/10944 (83%)	8147 (90%)	934 (10%)	7 (0%)	54	83

5 of 7 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	D	147	MET
1	B	147	MET
1	C	147	MET
1	D	853	PRO
1	A	853	PRO

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	1877/2446 (77%)	1866 (99%)	11 (1%)	86	94
1	B	1877/2446 (77%)	1867 (100%)	10 (0%)	88	95
1	C	1877/2446 (77%)	1867 (100%)	10 (0%)	88	95
1	D	1877/2446 (77%)	1867 (100%)	10 (0%)	88	95
All	All	7508/9784 (77%)	7467 (100%)	41 (0%)	89	95

5 of 41 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	1658	LYS
1	C	1185	LYS
1	B	1687	ARG
1	C	766	ARG
1	C	1620	GLN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 23 such sidechains are listed below:

Mol	Chain	Res	Type
1	B	1742	ASN
1	B	2409	HIS
1	B	2361	ASN
1	C	362	ASN
1	A	2195	GLN

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](#)

Of 32 ligands modelled in this entry, 4 are monoatomic - leaving 28 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	PLX	D	5107	-	38,38,51	1.95	4 (10%)	42,46,59	1.63	5 (11%)
2	PLX	A	2802	-	45,45,51	1.80	5 (11%)	49,53,59	1.52	5 (10%)
2	PLX	A	2801	-	45,45,51	1.80	4 (8%)	49,53,59	1.49	5 (10%)
2	PLX	D	5104	-	39,39,51	1.91	4 (10%)	43,47,59	1.58	5 (11%)
2	PLX	D	5105	-	36,36,51	1.99	4 (11%)	40,44,59	1.65	5 (12%)
2	PLX	A	2806	-	38,38,51	1.95	4 (10%)	42,46,59	1.63	5 (11%)
2	PLX	B	2802	-	35,35,51	2.02	4 (11%)	39,43,59	1.66	5 (12%)
2	PLX	D	5103	-	45,45,51	1.81	5 (11%)	49,53,59	1.52	5 (10%)
2	PLX	C	5102	-	36,36,51	1.99	4 (11%)	40,44,59	1.64	5 (12%)
2	PLX	C	5107	-	45,45,51	1.80	5 (11%)	49,53,59	1.52	5 (10%)
2	PLX	A	2803	-	39,39,51	1.92	4 (10%)	43,47,59	1.56	5 (11%)
2	PLX	B	2801	-	36,36,51	2.00	4 (11%)	40,44,59	1.61	6 (15%)
2	PLX	D	5106	-	35,35,51	2.02	4 (11%)	39,43,59	1.66	5 (12%)
2	PLX	C	5108	-	39,39,51	1.92	4 (10%)	43,47,59	1.58	5 (11%)
2	PLX	B	2807	-	39,39,51	1.92	5 (12%)	43,47,59	1.55	5 (11%)
2	PLX	B	2804	-	43,43,51	1.86	5 (11%)	47,51,59	1.50	5 (10%)
2	PLX	A	2805	-	35,35,51	2.02	5 (14%)	39,43,59	1.67	5 (12%)
2	PLX	B	2806	-	45,45,51	1.81	5 (11%)	49,53,59	1.52	5 (10%)
2	PLX	D	5102	-	45,45,51	1.80	4 (8%)	49,53,59	1.49	5 (10%)
2	PLX	C	5106	-	45,45,51	1.80	4 (8%)	49,53,59	1.48	5 (10%)
2	PLX	B	2803	-	38,38,51	1.96	4 (10%)	42,46,59	1.63	5 (11%)
2	PLX	A	2807	-	43,43,51	1.84	6 (13%)	47,51,59	1.81	7 (14%)
2	PLX	C	5103	-	35,35,51	2.02	4 (11%)	39,43,59	1.66	5 (12%)
2	PLX	C	5104	-	38,38,51	1.95	4 (10%)	42,46,59	1.63	5 (11%)
2	PLX	D	5108	-	43,43,51	1.87	5 (11%)	47,51,59	1.50	5 (10%)
2	PLX	A	2804	-	36,36,51	1.99	4 (11%)	40,44,59	1.64	5 (12%)
2	PLX	B	2805	-	45,45,51	1.80	4 (8%)	49,53,59	1.49	5 (10%)
2	PLX	C	5105	-	43,43,51	1.87	5 (11%)	47,51,59	1.50	5 (10%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	PLX	D	5107	-	3/3/5/5	27/42/42/55	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	PLX	A	2802	-	3/3/5/5	27/49/49/55	-
2	PLX	A	2801	-	3/3/5/5	25/49/49/55	-
2	PLX	D	5104	-	3/3/5/5	24/43/43/55	-
2	PLX	D	5105	-	3/3/5/5	25/40/40/55	-
2	PLX	A	2806	-	3/3/5/5	27/42/42/55	-
2	PLX	B	2802	-	3/3/5/5	24/39/39/55	-
2	PLX	D	5103	-	3/3/5/5	27/49/49/55	-
2	PLX	C	5102	-	3/3/5/5	25/40/40/55	-
2	PLX	C	5107	-	3/3/5/5	27/49/49/55	-
2	PLX	A	2803	-	3/3/5/5	21/43/43/55	-
2	PLX	B	2801	-	3/3/5/5	21/40/40/55	-
2	PLX	D	5106	-	3/3/5/5	24/39/39/55	-
2	PLX	C	5108	-	3/3/5/5	24/43/43/55	-
2	PLX	B	2807	-	3/3/5/5	26/43/43/55	-
2	PLX	B	2804	-	3/3/5/5	23/47/47/55	-
2	PLX	A	2805	-	3/3/5/5	26/39/39/55	-
2	PLX	B	2806	-	3/3/5/5	28/49/49/55	-
2	PLX	D	5102	-	3/3/5/5	25/49/49/55	-
2	PLX	C	5106	-	3/3/5/5	26/49/49/55	-
2	PLX	B	2803	-	3/3/5/5	25/42/42/55	-
2	PLX	A	2807	-	3/3/5/5	24/47/47/55	-
2	PLX	C	5103	-	3/3/5/5	25/39/39/55	-
2	PLX	C	5104	-	3/3/5/5	27/42/42/55	-
2	PLX	D	5108	-	3/3/5/5	22/47/47/55	-
2	PLX	A	2804	-	3/3/5/5	25/40/40/55	-
2	PLX	B	2805	-	3/3/5/5	25/49/49/55	-
2	PLX	C	5105	-	3/3/5/5	23/47/47/55	-

The worst 5 of 123 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	2801	PLX	O7-C6	-7.23	1.18	1.39
2	A	2805	PLX	O7-C6	-7.22	1.18	1.39
2	B	2802	PLX	O7-C6	-7.22	1.18	1.39
2	B	2803	PLX	O7-C6	-7.22	1.18	1.39
2	B	2806	PLX	O7-C6	-7.21	1.19	1.39

The worst 5 of 143 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed($^{\circ}$)	Ideal($^{\circ}$)
2	A	2807	PLX	O7-C6-C7	6.18	120.58	109.12
2	B	2803	PLX	O9-C24-C25	6.07	120.37	109.12
2	D	5107	PLX	O9-C24-C25	6.06	120.35	109.12
2	C	5104	PLX	O9-C24-C25	6.06	120.34	109.12
2	B	2806	PLX	O9-C24-C25	6.02	120.28	109.12

5 of 84 chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
2	A	2801	PLX	C24
2	A	2801	PLX	C4
2	A	2801	PLX	C6
2	A	2802	PLX	C24
2	A	2802	PLX	C4

5 of 698 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	2801	PLX	O7-C6-O6-C4
2	A	2801	PLX	O6-C4-C5-O8
2	A	2801	PLX	C3-O4-P1-O2
2	A	2801	PLX	C3-O4-P1-O3
2	A	2801	PLX	O9-C24-O8-C5

There are no ring outliers.

25 monomers are involved in 39 short contacts:

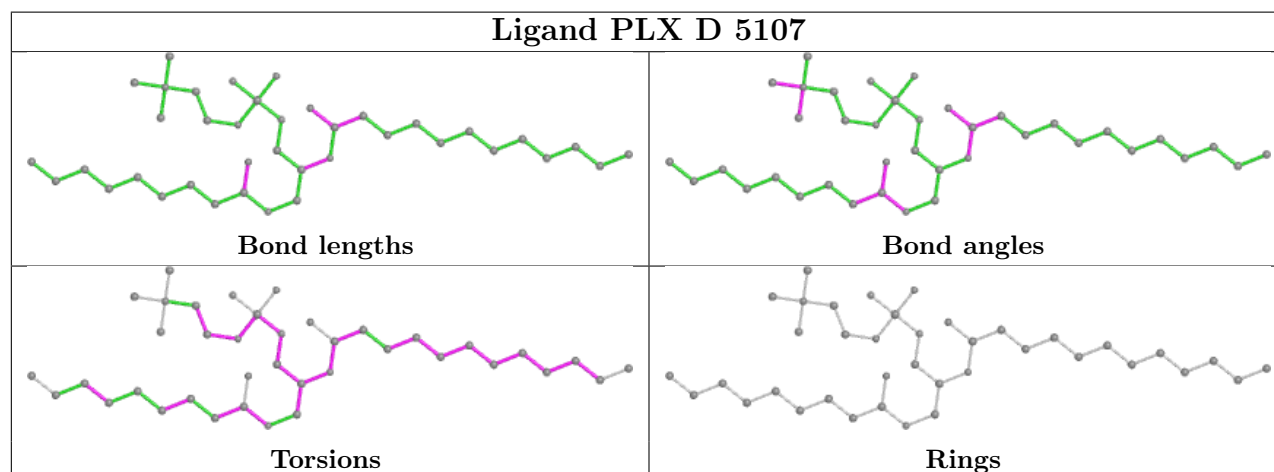
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	D	5107	PLX	2	0
2	A	2802	PLX	3	0
2	A	2801	PLX	1	0
2	D	5104	PLX	1	0
2	D	5105	PLX	1	0
2	A	2806	PLX	1	0
2	B	2802	PLX	1	0
2	D	5103	PLX	3	0
2	C	5102	PLX	1	0
2	C	5107	PLX	3	0
2	A	2803	PLX	1	0
2	B	2801	PLX	2	0
2	B	2807	PLX	1	0

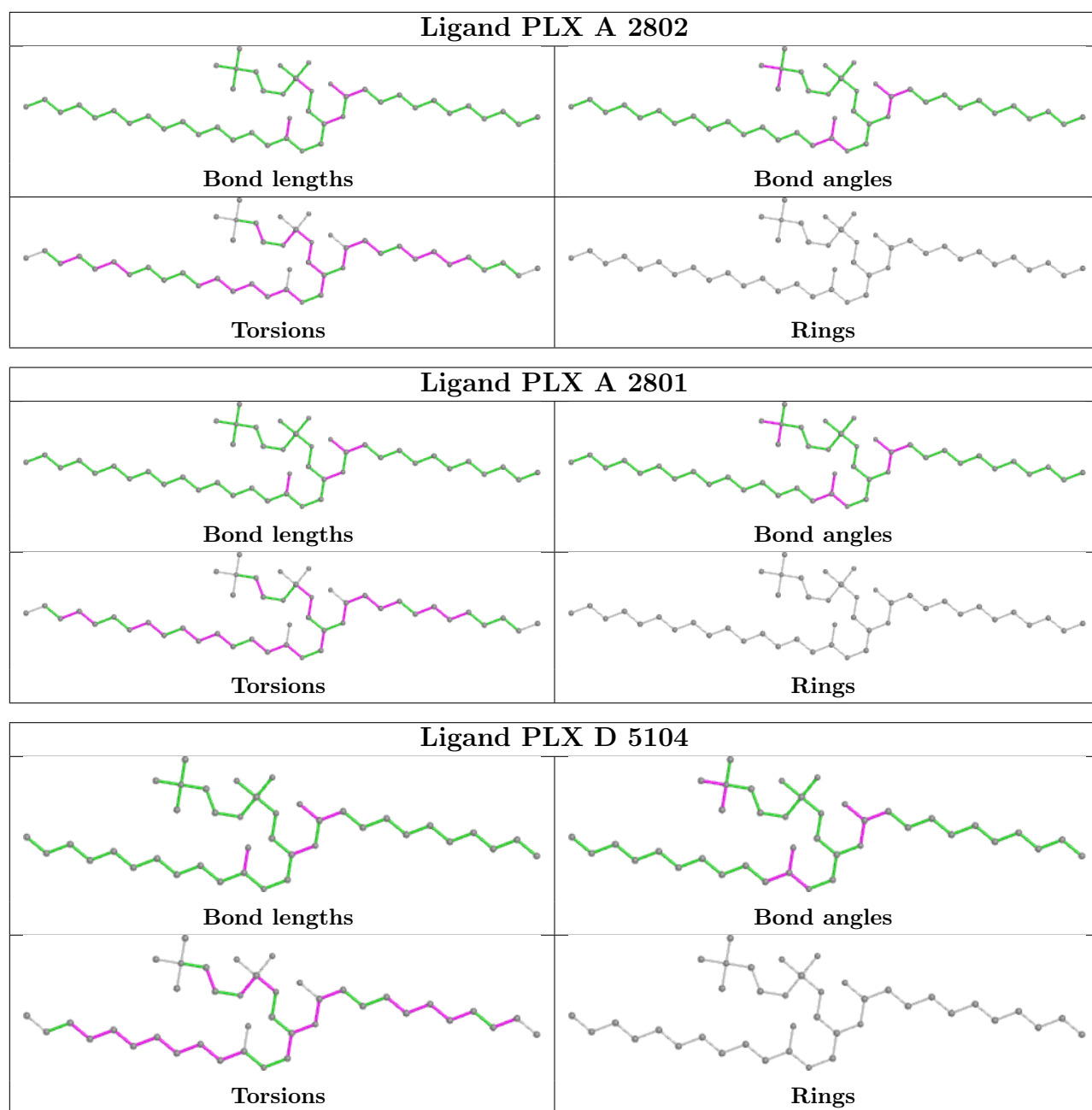
Continued on next page...

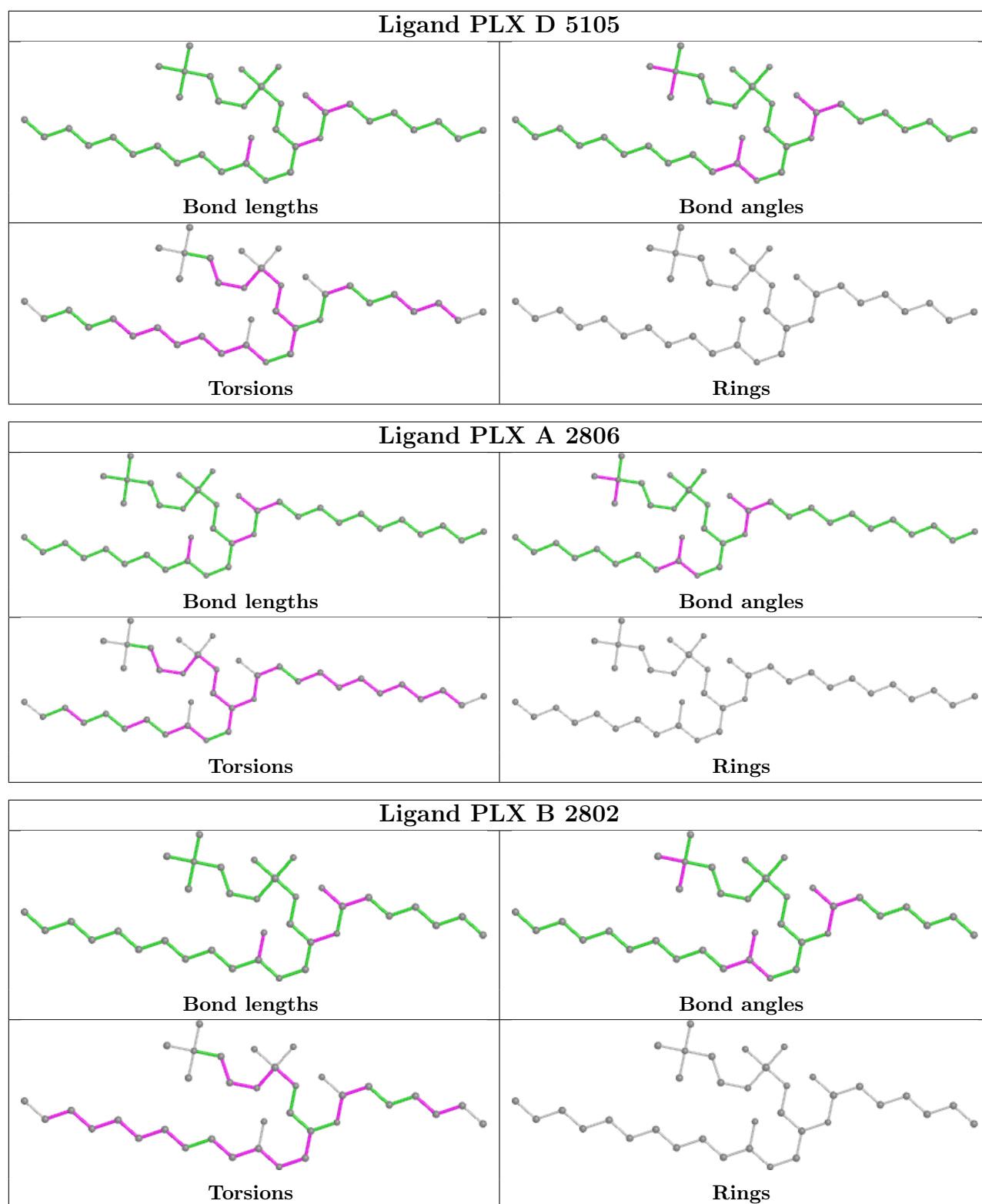
Continued from previous page...

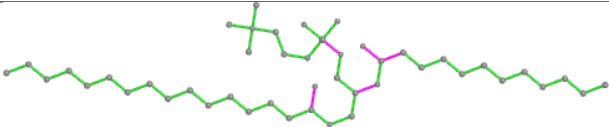
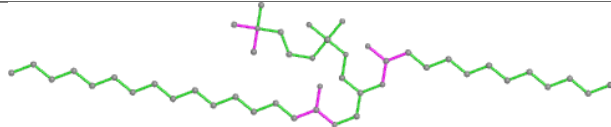
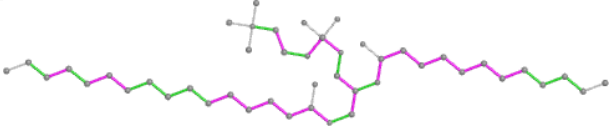
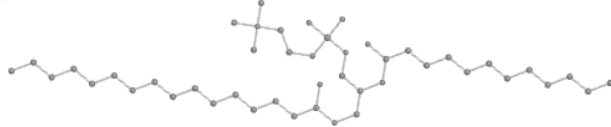
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	2805	PLX	2	0
2	B	2806	PLX	3	0
2	D	5102	PLX	1	0
2	C	5106	PLX	1	0
2	B	2803	PLX	1	0
2	A	2807	PLX	3	0
2	C	5103	PLX	1	0
2	C	5104	PLX	1	0
2	D	5108	PLX	1	0
2	A	2804	PLX	1	0
2	B	2805	PLX	3	0
2	C	5105	PLX	1	0

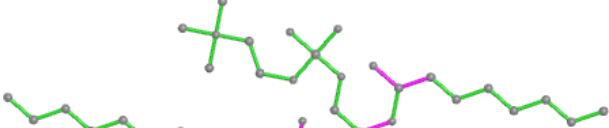
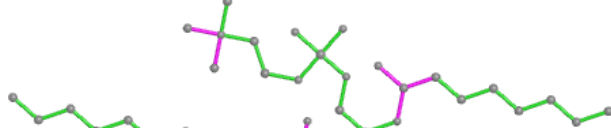
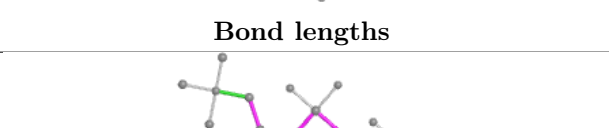
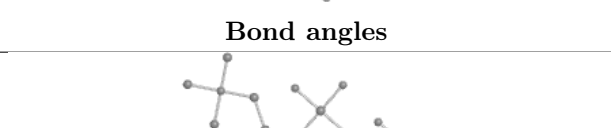
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

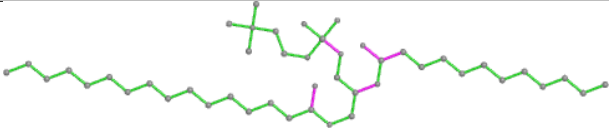
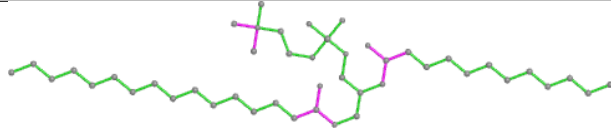
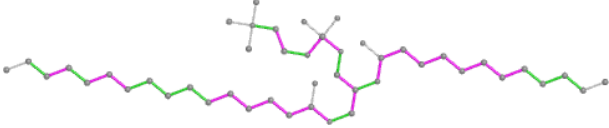
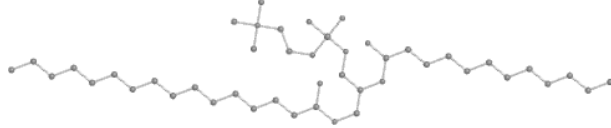


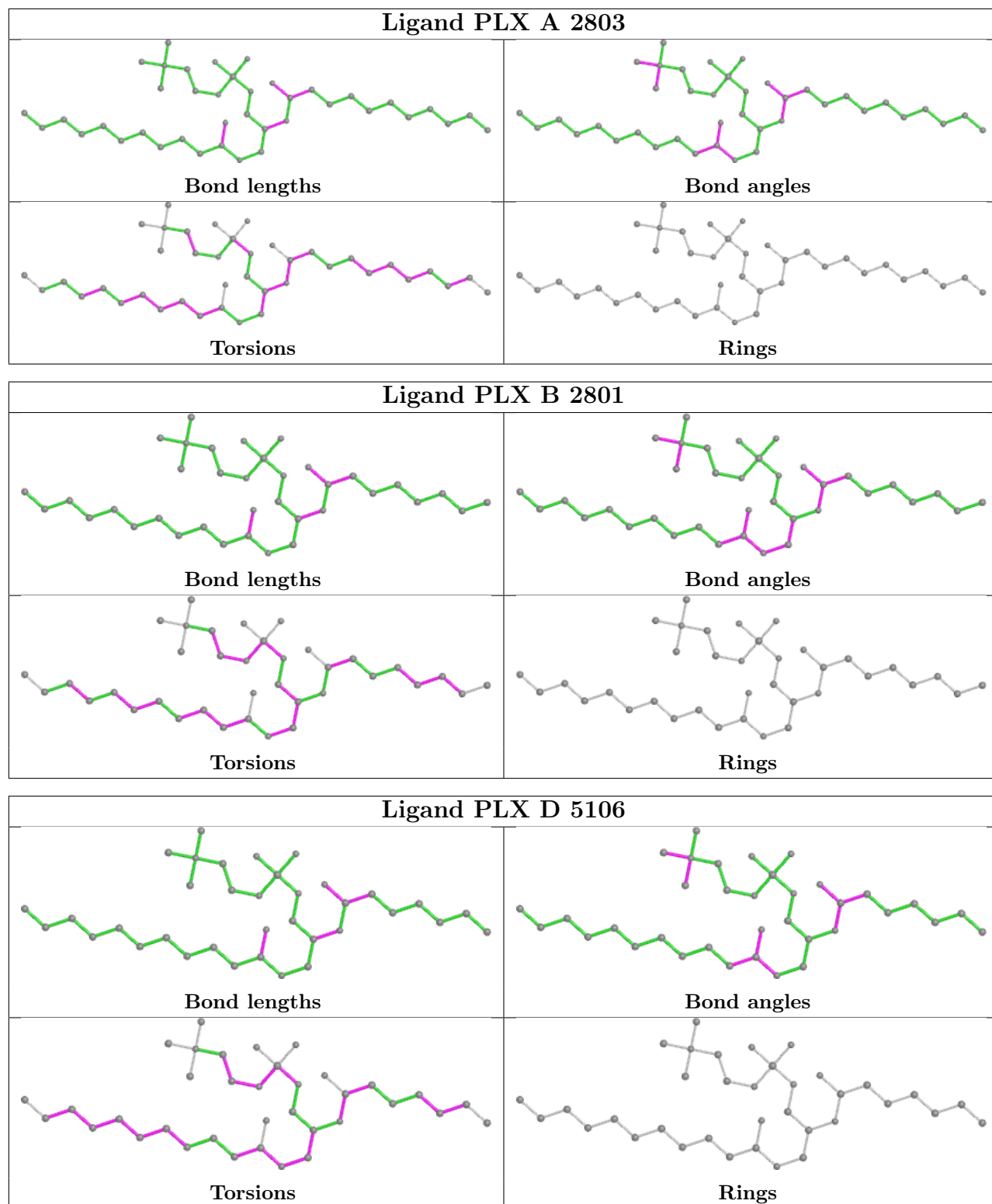


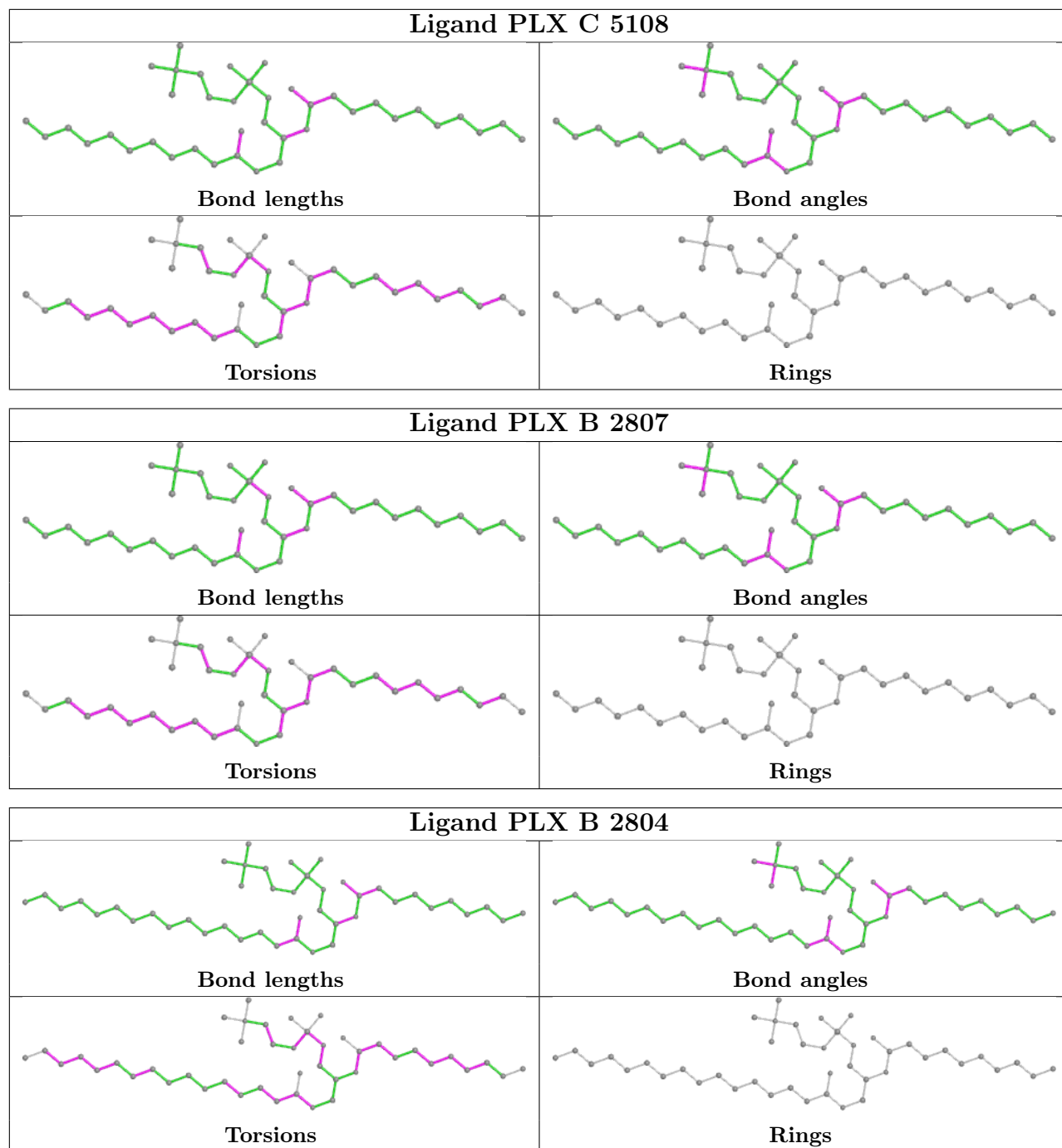


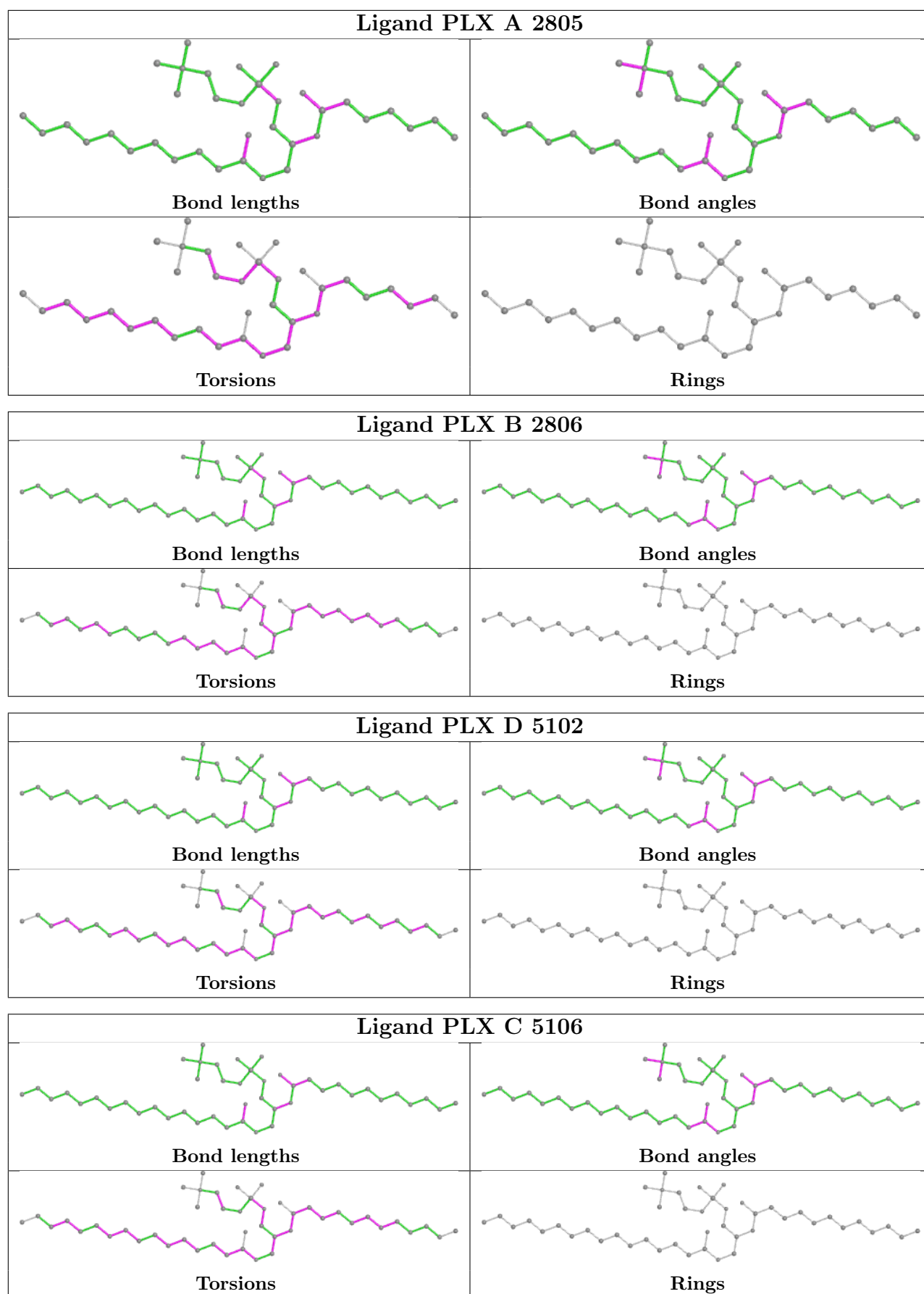
Ligand PLX D 5103	
	
Bond lengths	Bond angles
	
Torsions	Rings

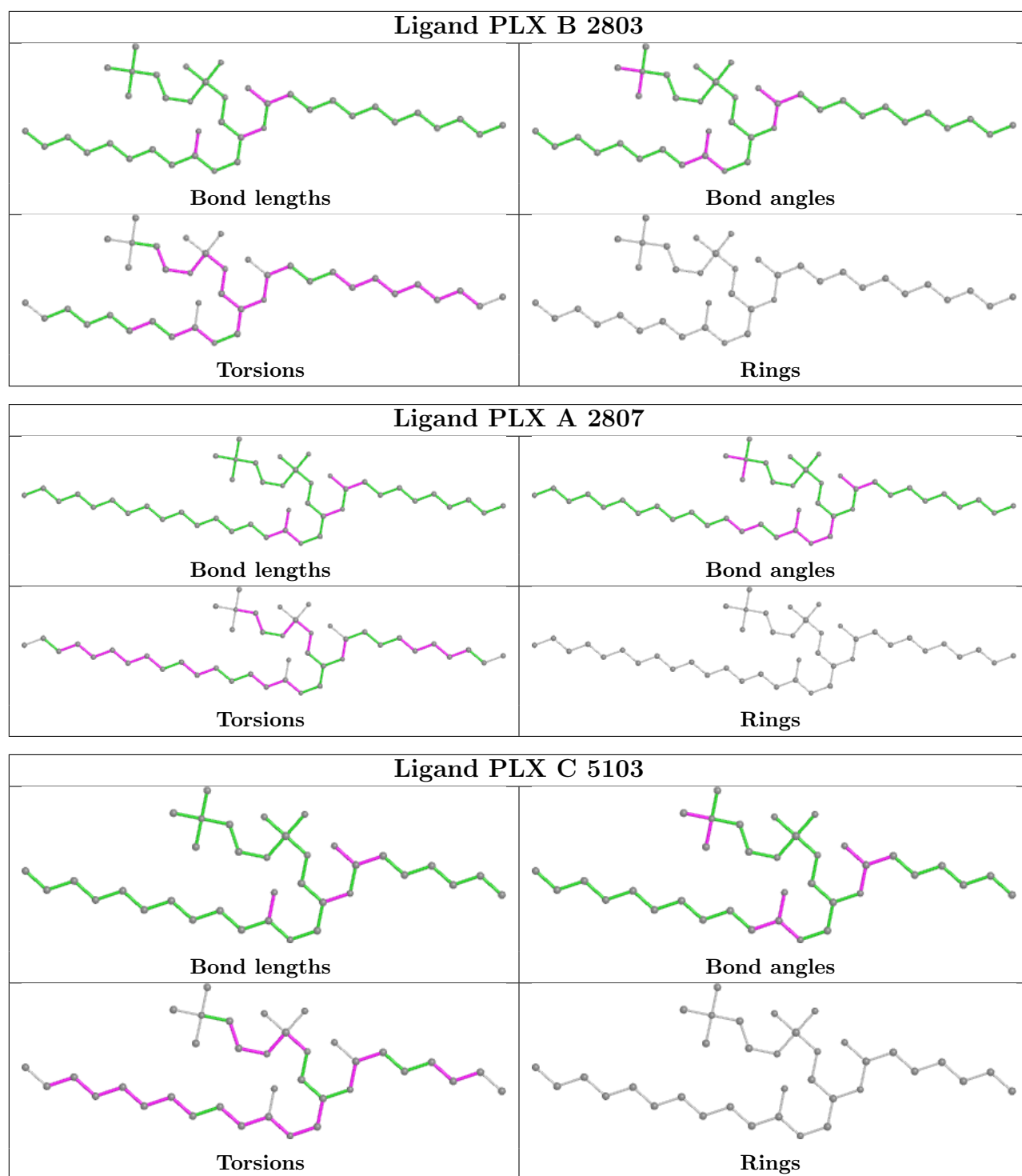
Ligand PLX C 5102	
	
Bond lengths	Bond angles
	
Torsions	Rings

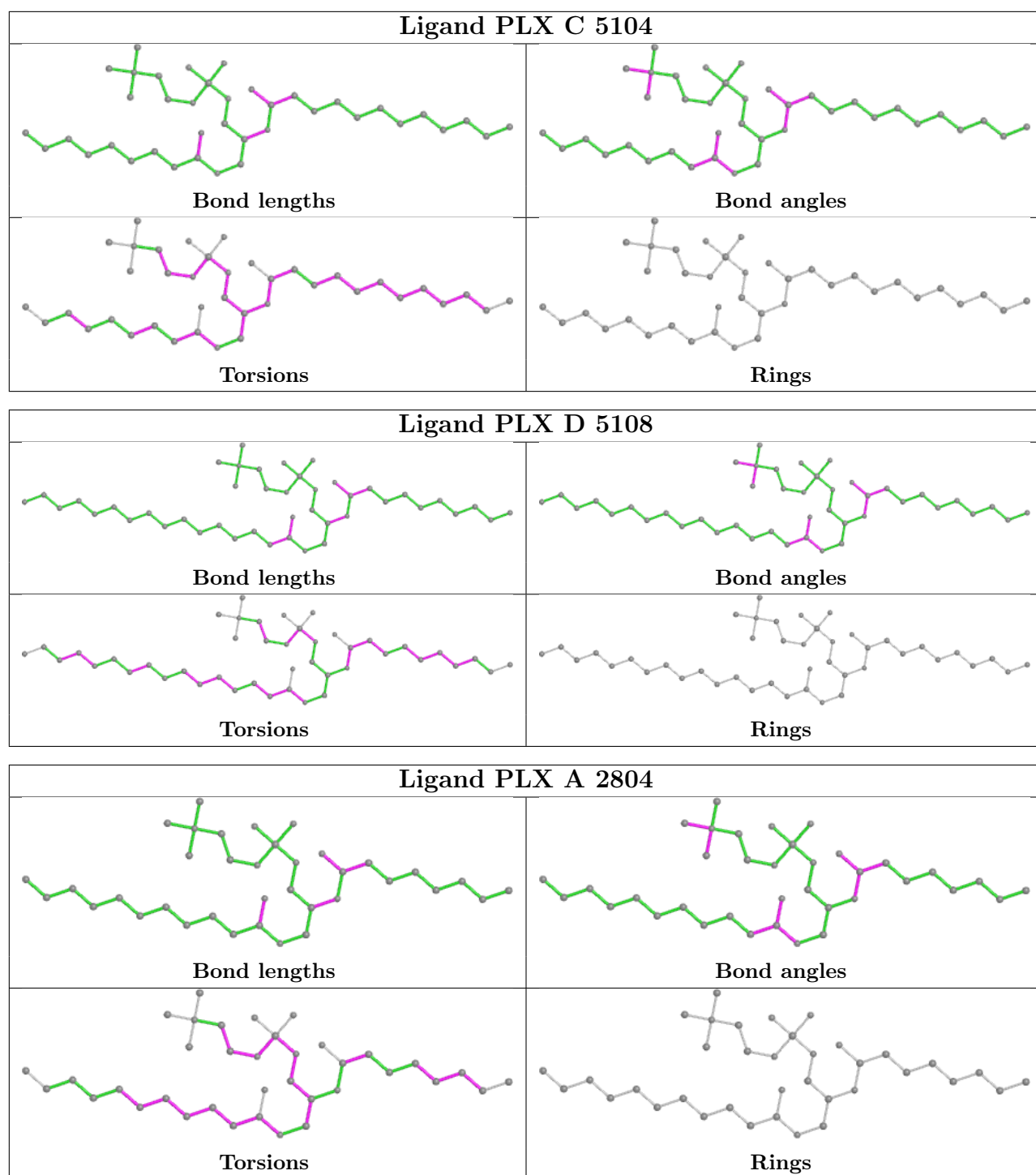
Ligand PLX C 5107	
	
Bond lengths	Bond angles
	
Torsions	Rings

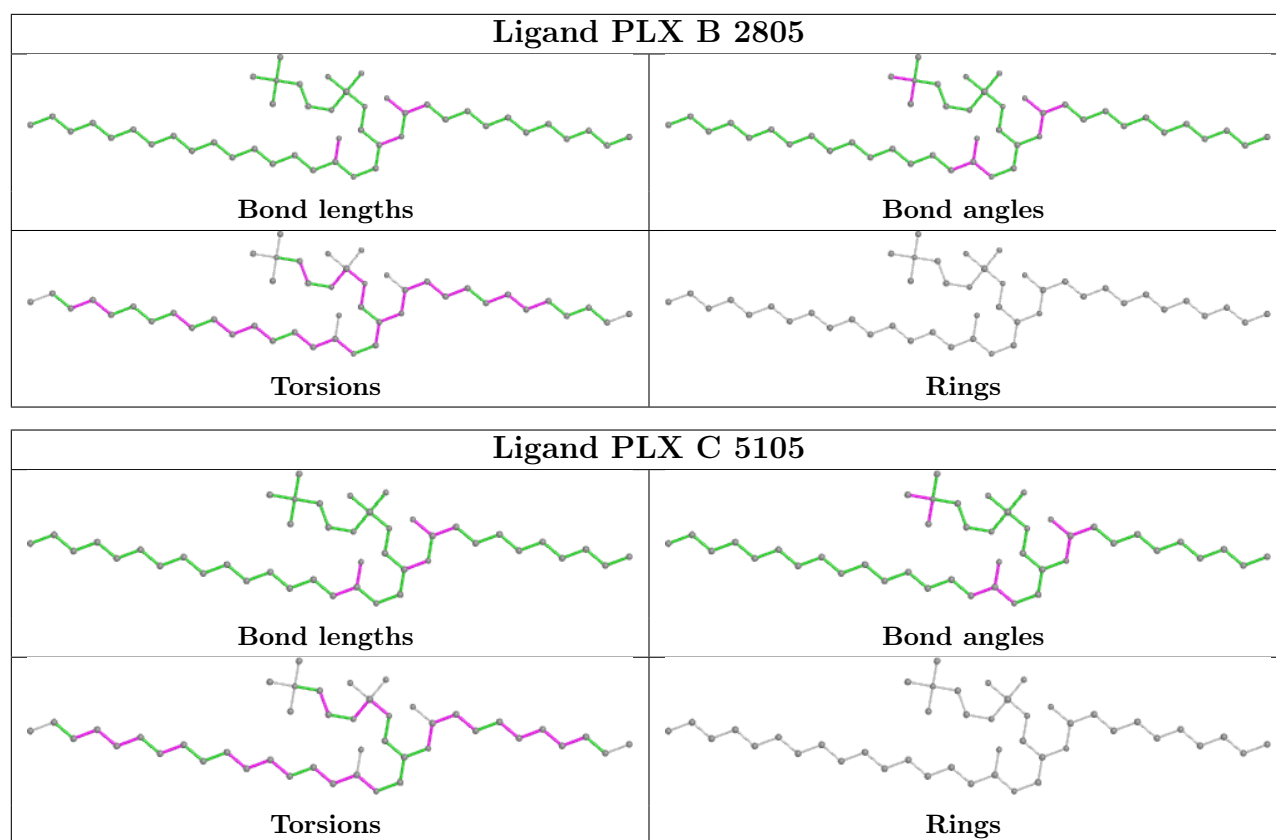












5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

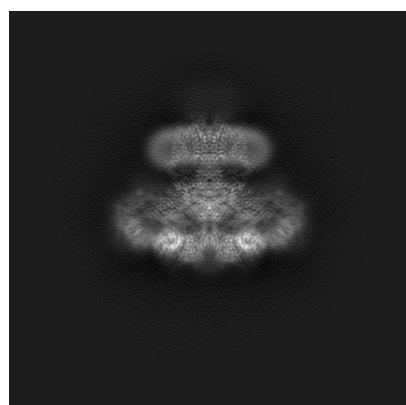
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-23338. These allow visual inspection of the internal detail of the map and identification of artifacts.

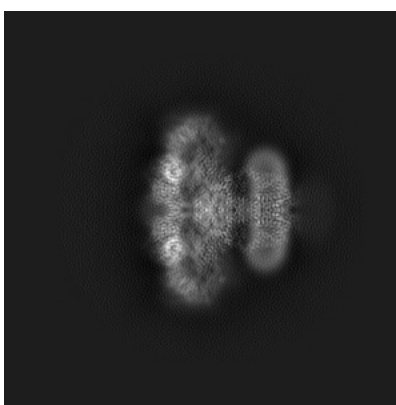
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

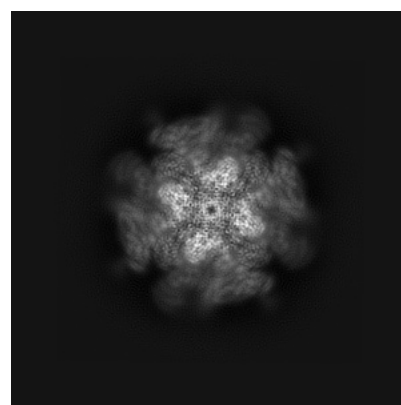
6.1.1 Primary map



X



Y

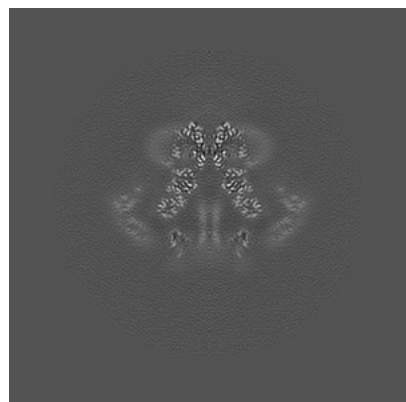


Z

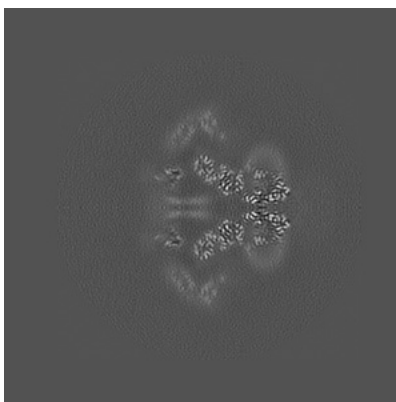
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

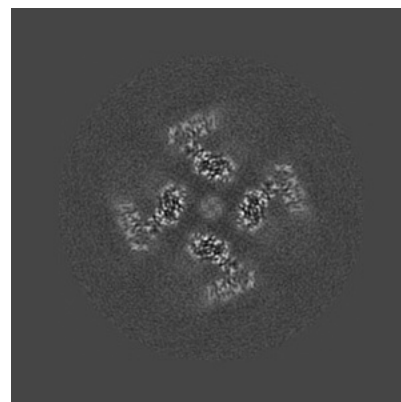
6.2.1 Primary map



X Index: 220



Y Index: 220

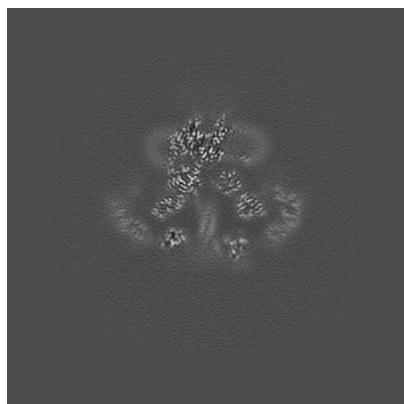


Z Index: 220

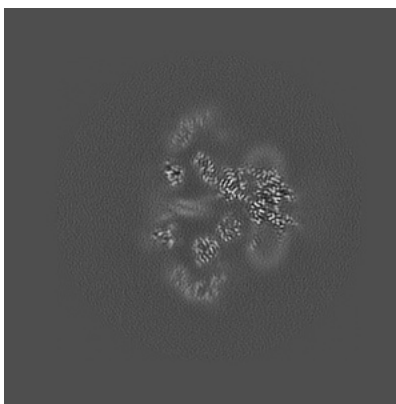
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

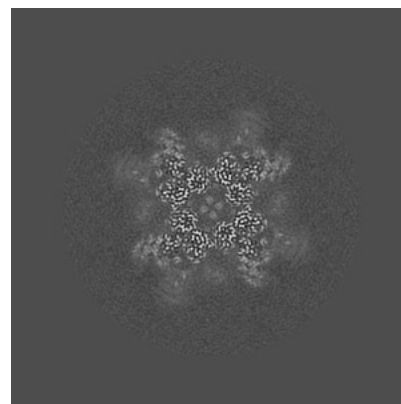
6.3.1 Primary map



X Index: 215



Y Index: 215

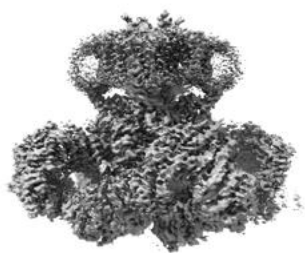


Z Index: 182

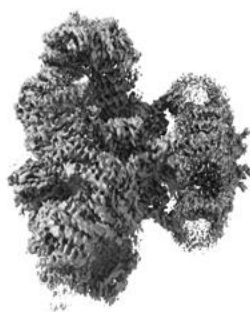
The images above show the largest variance slices of the map in three orthogonal directions.

6.4 Orthogonal surface views [i](#)

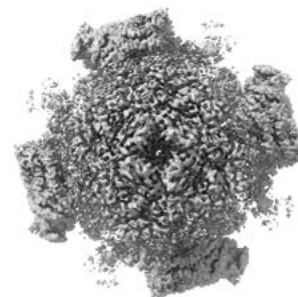
6.4.1 Primary map



X



Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.0112. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

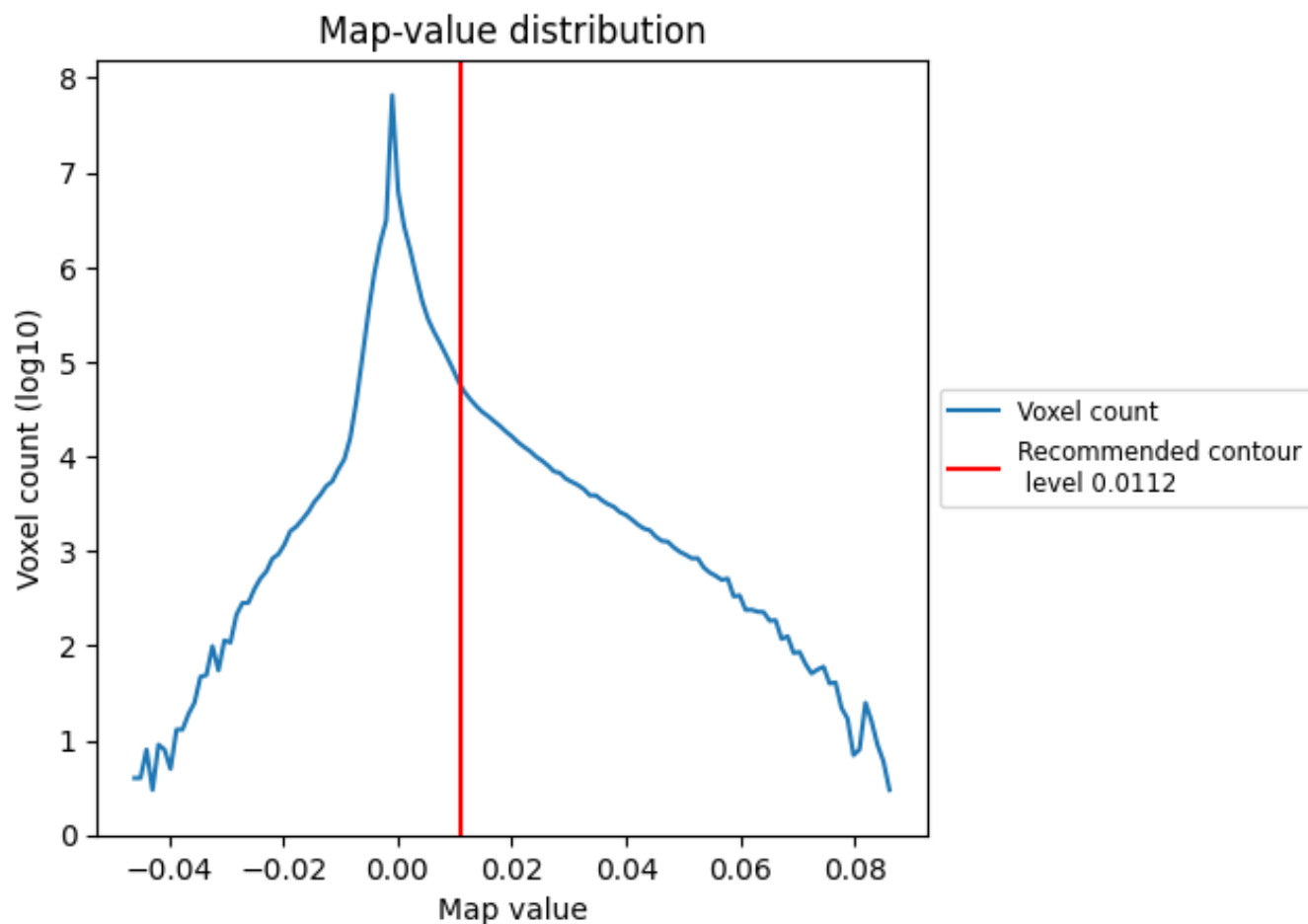
6.5 Mask visualisation

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

7 Map analysis [i](#)

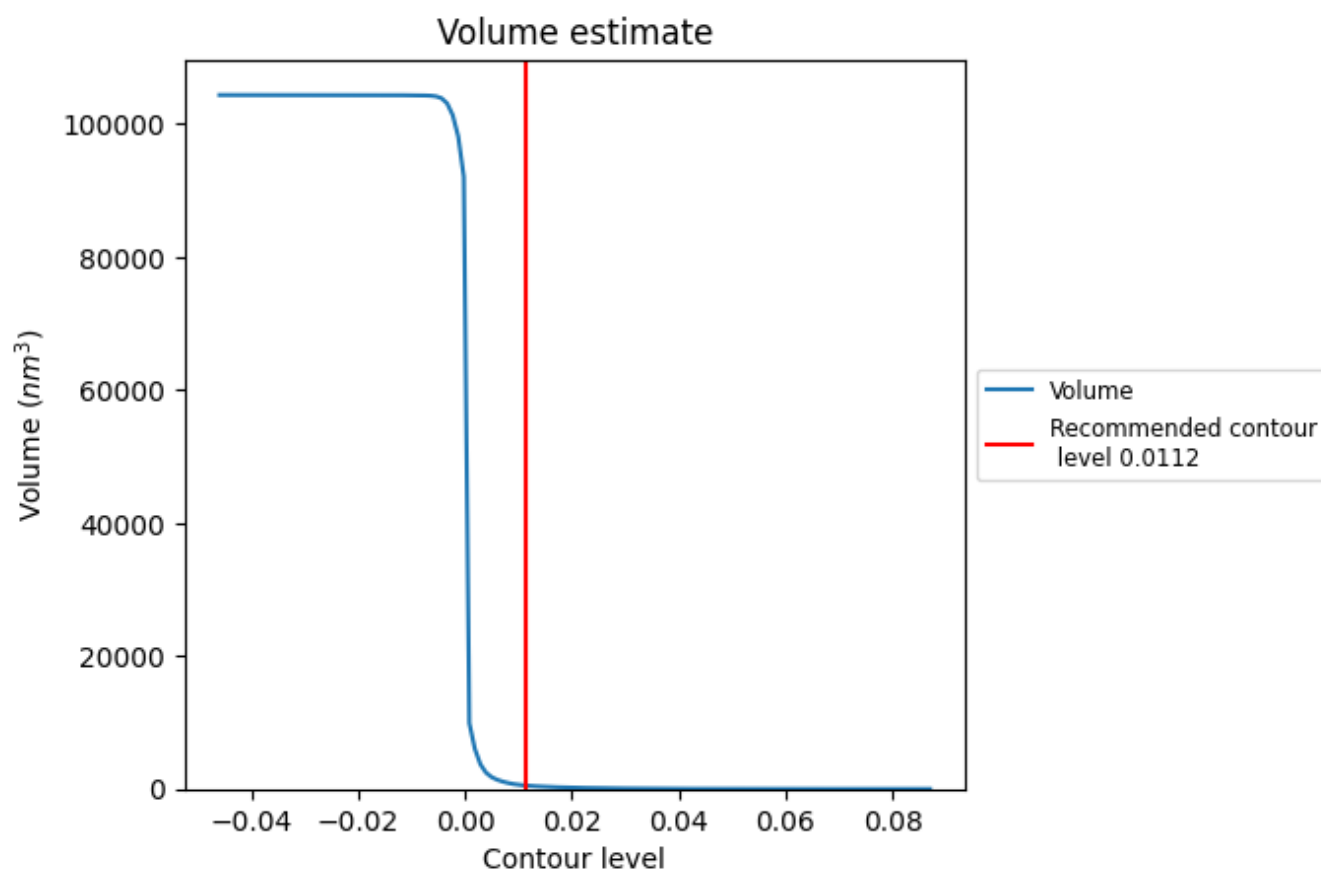
This section contains the results of statistical analysis of the map.

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.

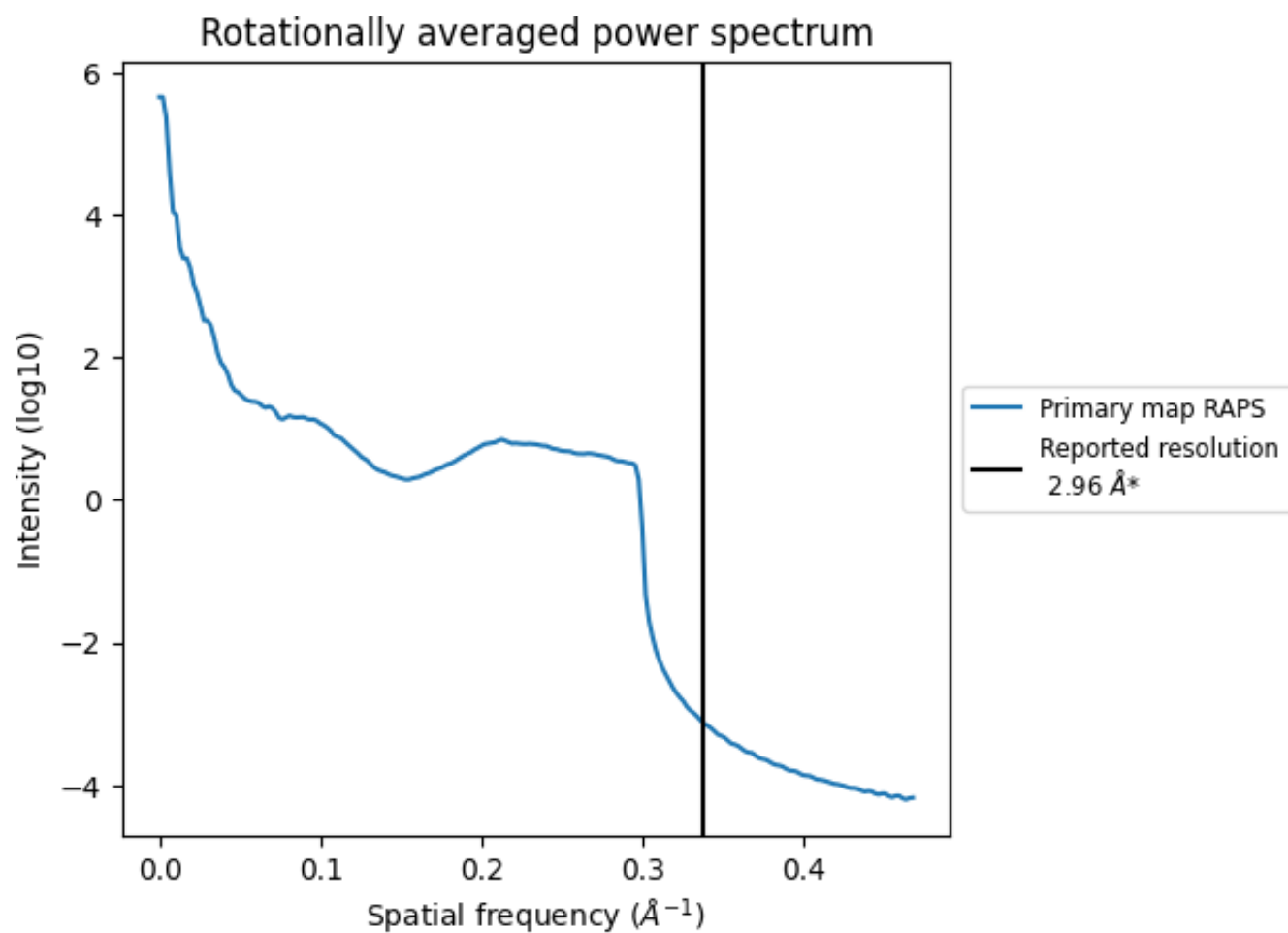
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 524 nm^3 ; this corresponds to an approximate mass of 474 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 0.338 Å⁻¹

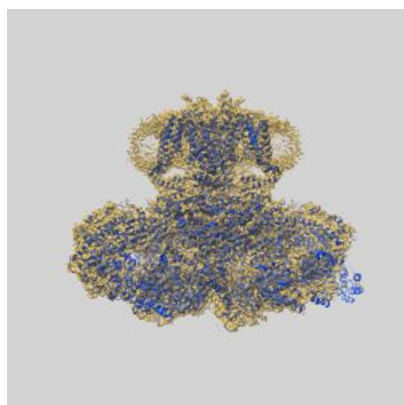
8 Fourier-Shell correlation

This section was not generated. No FSC curve or half-maps provided.

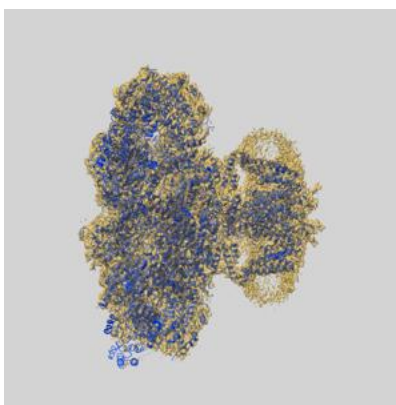
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-23338 and PDB model 7LHF. Per-residue inclusion information can be found in [section 3](#) on [page 7](#).

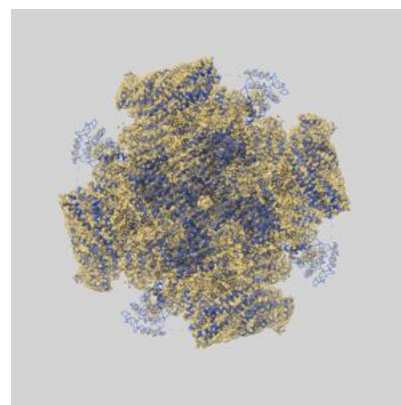
9.1 Map-model overlay [i](#)



X



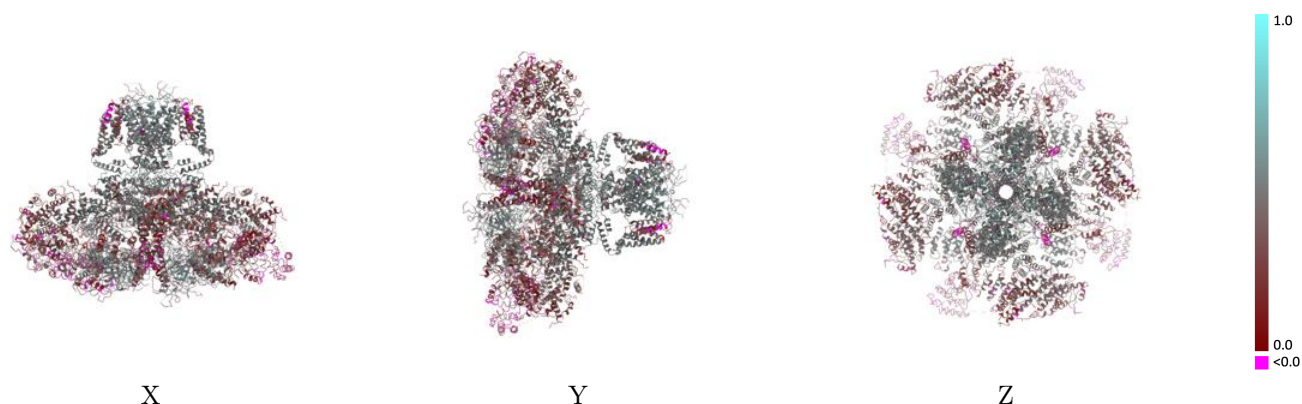
Y



Z

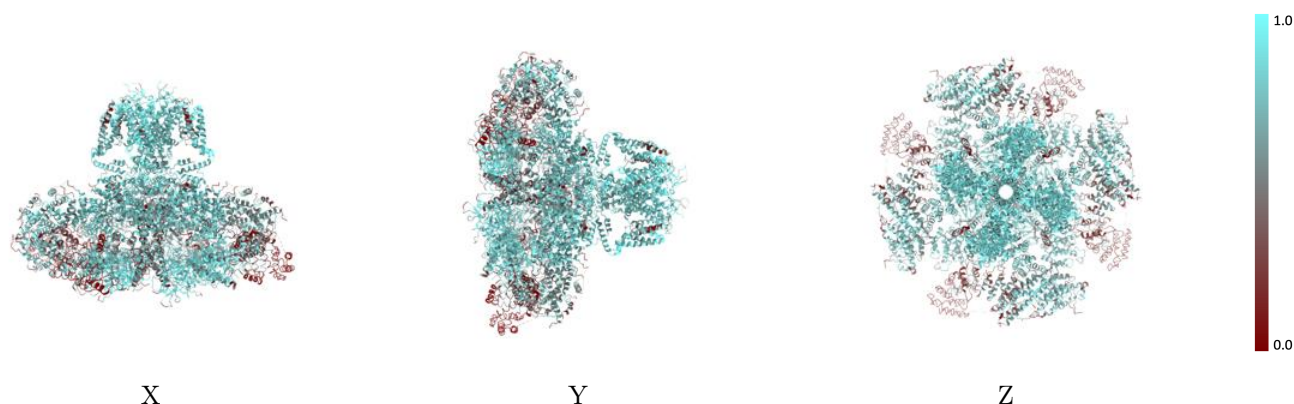
The images above show the 3D surface view of the map at the recommended contour level 0.0112 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



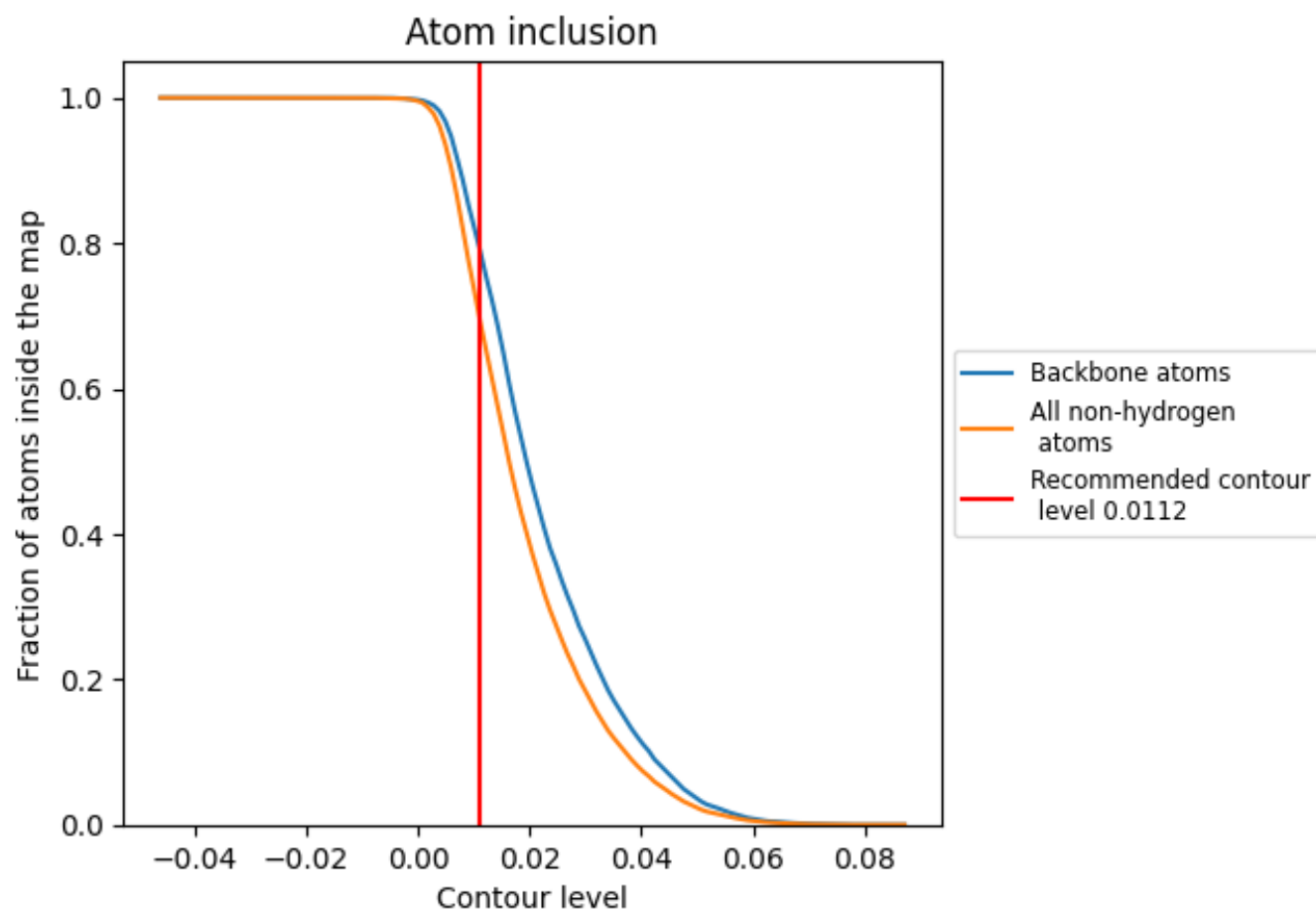
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.0112).

9.4 Atom inclusion [i](#)



At the recommended contour level, 79% of all backbone atoms, 69% 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 (0.0112) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	<div></div> 0.6921	<div></div> 0.3760
A	<div></div> 0.6926	<div></div> 0.3760
B	<div></div> 0.6912	<div></div> 0.3750
C	<div></div> 0.6924	<div></div> 0.3760
D	<div></div> 0.6923	<div></div> 0.3760

