



Full wwPDB EM Validation Report ⓘ

May 20, 2025 – 02:31 AM EDT

PDB ID : 9B29 / pdb_00009b29
EMDB ID : EMD-44101
Title : Cryo-EM structure of the mouse TRPM3 alpha 2 channel in complex with
cholesteryl hemisuccinate
Authors : Yin, Y.; Park, C.G.; Feng, S.; Zhang, F.; Guan, Z.; Sharma, K.; Borgnia, M.J.;
Im, W.; Lee, S.-Y.
Deposited on : 2024-03-14
Resolution : 3.13 Å(reported)

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

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

A user guide is available at

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

The types of validation reports are described at

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

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

EMDB validation analysis : 0.0.1.dev118
Mogul : 2022.3.0, CSD as543be (2022)
MolProbity : 4-5-2 with Phenix2.0rc1
buster-report : 1.1.7 (2018)
Percentile statistics : 20231227.v01 (using entries in the PDB archive December 27th 2023)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.43.1

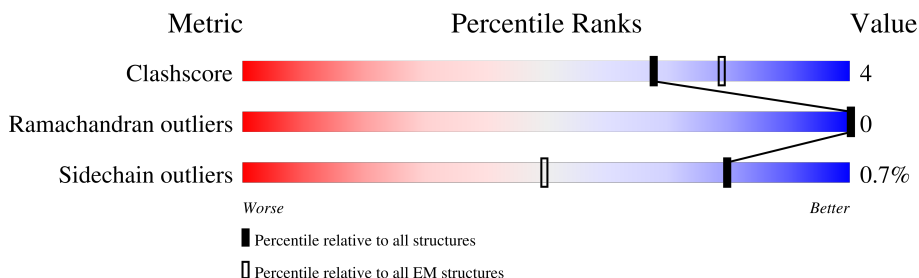
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 3.13 Å.

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



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

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

Mol	Chain	Length	Quality of chain
1	A	1739	
1	B	1739	
1	C	1739	
1	D	1739	

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 43604 atoms, of which 20568 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 Transient receptor potential cation channel, subfamily M, member 3.

Mol	Chain	Residues	Atoms						AltConf	Trace
1	A	798	Total	C	H	N	O	S	0	0
			10426	3626	4863	937	958	42		
1	B	798	Total	C	H	N	O	S	0	0
			10426	3626	4863	937	958	42		
1	C	798	Total	C	H	N	O	S	0	0
			10426	3626	4863	937	958	42		
1	D	798	Total	C	H	N	O	S	0	0
			10426	3626	4863	937	958	42		

There are 120 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	1710	SER	-	expression tag	UNP Q5F4S7
A	1711	ASN	-	expression tag	UNP Q5F4S7
A	1712	SER	-	expression tag	UNP Q5F4S7
A	1713	LEU	-	expression tag	UNP Q5F4S7
A	1714	GLU	-	expression tag	UNP Q5F4S7
A	1715	VAL	-	expression tag	UNP Q5F4S7
A	1716	LEU	-	expression tag	UNP Q5F4S7
A	1717	PHE	-	expression tag	UNP Q5F4S7
A	1718	GLN	-	expression tag	UNP Q5F4S7
A	1719	GLY	-	expression tag	UNP Q5F4S7
A	1720	PRO	-	expression tag	UNP Q5F4S7
A	1721	ASP	-	expression tag	UNP Q5F4S7
A	1722	TYR	-	expression tag	UNP Q5F4S7
A	1723	LYS	-	expression tag	UNP Q5F4S7
A	1724	ASP	-	expression tag	UNP Q5F4S7
A	1725	ASP	-	expression tag	UNP Q5F4S7
A	1726	ASP	-	expression tag	UNP Q5F4S7
A	1727	ASP	-	expression tag	UNP Q5F4S7
A	1728	LYS	-	expression tag	UNP Q5F4S7
A	1729	ALA	-	expression tag	UNP Q5F4S7
A	1730	HIS	-	expression tag	UNP Q5F4S7

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Chain	Residue	Modelled	Actual	Comment	Reference
A	1731	HIS	-	expression tag	UNP Q5F4S7
A	1732	HIS	-	expression tag	UNP Q5F4S7
A	1733	HIS	-	expression tag	UNP Q5F4S7
A	1734	HIS	-	expression tag	UNP Q5F4S7
A	1735	HIS	-	expression tag	UNP Q5F4S7
A	1736	HIS	-	expression tag	UNP Q5F4S7
A	1737	HIS	-	expression tag	UNP Q5F4S7
A	1738	HIS	-	expression tag	UNP Q5F4S7
A	1739	HIS	-	expression tag	UNP Q5F4S7
B	1710	SER	-	expression tag	UNP Q5F4S7
B	1711	ASN	-	expression tag	UNP Q5F4S7
B	1712	SER	-	expression tag	UNP Q5F4S7
B	1713	LEU	-	expression tag	UNP Q5F4S7
B	1714	GLU	-	expression tag	UNP Q5F4S7
B	1715	VAL	-	expression tag	UNP Q5F4S7
B	1716	LEU	-	expression tag	UNP Q5F4S7
B	1717	PHE	-	expression tag	UNP Q5F4S7
B	1718	GLN	-	expression tag	UNP Q5F4S7
B	1719	GLY	-	expression tag	UNP Q5F4S7
B	1720	PRO	-	expression tag	UNP Q5F4S7
B	1721	ASP	-	expression tag	UNP Q5F4S7
B	1722	TYR	-	expression tag	UNP Q5F4S7
B	1723	LYS	-	expression tag	UNP Q5F4S7
B	1724	ASP	-	expression tag	UNP Q5F4S7
B	1725	ASP	-	expression tag	UNP Q5F4S7
B	1726	ASP	-	expression tag	UNP Q5F4S7
B	1727	ASP	-	expression tag	UNP Q5F4S7
B	1728	LYS	-	expression tag	UNP Q5F4S7
B	1729	ALA	-	expression tag	UNP Q5F4S7
B	1730	HIS	-	expression tag	UNP Q5F4S7
B	1731	HIS	-	expression tag	UNP Q5F4S7
B	1732	HIS	-	expression tag	UNP Q5F4S7
B	1733	HIS	-	expression tag	UNP Q5F4S7
B	1734	HIS	-	expression tag	UNP Q5F4S7
B	1735	HIS	-	expression tag	UNP Q5F4S7
B	1736	HIS	-	expression tag	UNP Q5F4S7
B	1737	HIS	-	expression tag	UNP Q5F4S7
B	1738	HIS	-	expression tag	UNP Q5F4S7
B	1739	HIS	-	expression tag	UNP Q5F4S7
C	1710	SER	-	expression tag	UNP Q5F4S7
C	1711	ASN	-	expression tag	UNP Q5F4S7
C	1712	SER	-	expression tag	UNP Q5F4S7

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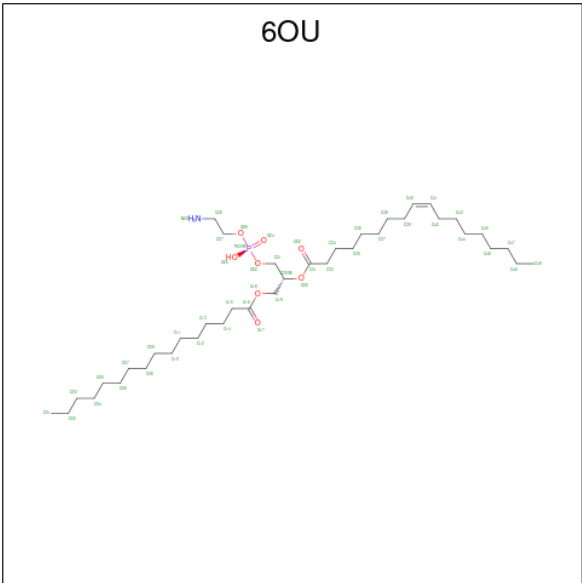
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C	1713	LEU	-	expression tag	UNP Q5F4S7
C	1714	GLU	-	expression tag	UNP Q5F4S7
C	1715	VAL	-	expression tag	UNP Q5F4S7
C	1716	LEU	-	expression tag	UNP Q5F4S7
C	1717	PHE	-	expression tag	UNP Q5F4S7
C	1718	GLN	-	expression tag	UNP Q5F4S7
C	1719	GLY	-	expression tag	UNP Q5F4S7
C	1720	PRO	-	expression tag	UNP Q5F4S7
C	1721	ASP	-	expression tag	UNP Q5F4S7
C	1722	TYR	-	expression tag	UNP Q5F4S7
C	1723	LYS	-	expression tag	UNP Q5F4S7
C	1724	ASP	-	expression tag	UNP Q5F4S7
C	1725	ASP	-	expression tag	UNP Q5F4S7
C	1726	ASP	-	expression tag	UNP Q5F4S7
C	1727	ASP	-	expression tag	UNP Q5F4S7
C	1728	LYS	-	expression tag	UNP Q5F4S7
C	1729	ALA	-	expression tag	UNP Q5F4S7
C	1730	HIS	-	expression tag	UNP Q5F4S7
C	1731	HIS	-	expression tag	UNP Q5F4S7
C	1732	HIS	-	expression tag	UNP Q5F4S7
C	1733	HIS	-	expression tag	UNP Q5F4S7
C	1734	HIS	-	expression tag	UNP Q5F4S7
C	1735	HIS	-	expression tag	UNP Q5F4S7
C	1736	HIS	-	expression tag	UNP Q5F4S7
C	1737	HIS	-	expression tag	UNP Q5F4S7
C	1738	HIS	-	expression tag	UNP Q5F4S7
C	1739	HIS	-	expression tag	UNP Q5F4S7
D	1710	SER	-	expression tag	UNP Q5F4S7
D	1711	ASN	-	expression tag	UNP Q5F4S7
D	1712	SER	-	expression tag	UNP Q5F4S7
D	1713	LEU	-	expression tag	UNP Q5F4S7
D	1714	GLU	-	expression tag	UNP Q5F4S7
D	1715	VAL	-	expression tag	UNP Q5F4S7
D	1716	LEU	-	expression tag	UNP Q5F4S7
D	1717	PHE	-	expression tag	UNP Q5F4S7
D	1718	GLN	-	expression tag	UNP Q5F4S7
D	1719	GLY	-	expression tag	UNP Q5F4S7
D	1720	PRO	-	expression tag	UNP Q5F4S7
D	1721	ASP	-	expression tag	UNP Q5F4S7
D	1722	TYR	-	expression tag	UNP Q5F4S7
D	1723	LYS	-	expression tag	UNP Q5F4S7
D	1724	ASP	-	expression tag	UNP Q5F4S7

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Chain	Residue	Modelled	Actual	Comment	Reference
D	1725	ASP	-	expression tag	UNP Q5F4S7
D	1726	ASP	-	expression tag	UNP Q5F4S7
D	1727	ASP	-	expression tag	UNP Q5F4S7
D	1728	LYS	-	expression tag	UNP Q5F4S7
D	1729	ALA	-	expression tag	UNP Q5F4S7
D	1730	HIS	-	expression tag	UNP Q5F4S7
D	1731	HIS	-	expression tag	UNP Q5F4S7
D	1732	HIS	-	expression tag	UNP Q5F4S7
D	1733	HIS	-	expression tag	UNP Q5F4S7
D	1734	HIS	-	expression tag	UNP Q5F4S7
D	1735	HIS	-	expression tag	UNP Q5F4S7
D	1736	HIS	-	expression tag	UNP Q5F4S7
D	1737	HIS	-	expression tag	UNP Q5F4S7
D	1738	HIS	-	expression tag	UNP Q5F4S7
D	1739	HIS	-	expression tag	UNP Q5F4S7

- Molecule 2 is [(2 {R})-1-[2-azanylethoxy(oxidanyl)phosphoryl]oxy-3-hexadecanoyloxy-prop an-2-yl] ({Z})-octadec-9-enoate (CCD ID: 6OU) (formula: C₃₉H₇₆NO₈P).



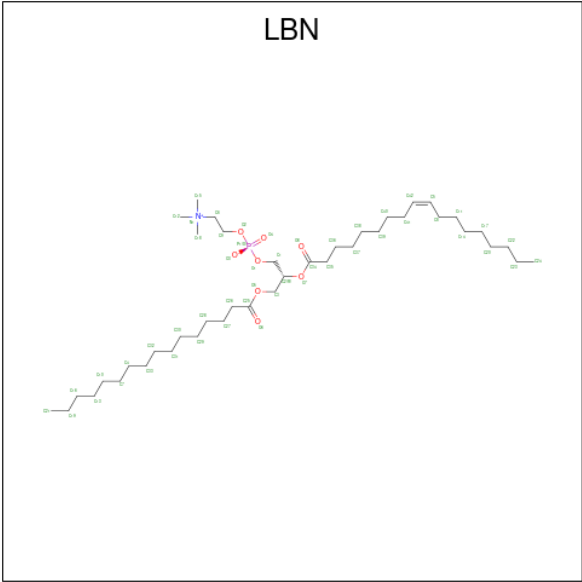
Mol	Chain	Residues	Atoms						AltConf
2	A	1	Total	C	H	N	O	P	0
			124	39	75	1	8	1	
2	B	1	Total	C	H	N	O	P	0
			124	39	75	1	8	1	
2	C	1	Total	C	H	N	O	P	0
			124	39	75	1	8	1	

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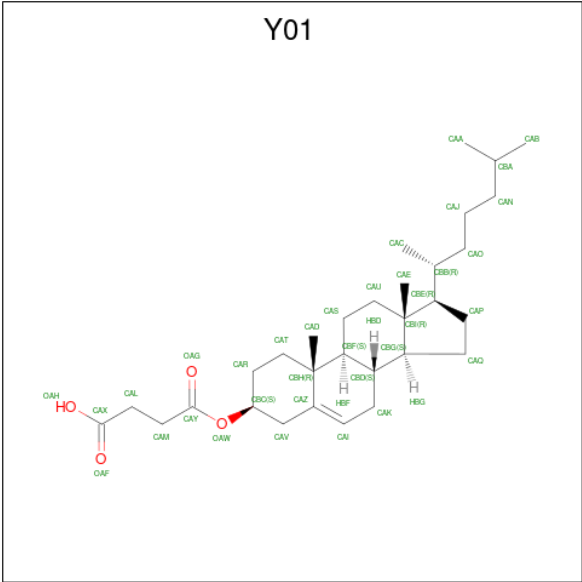
Mol	Chain	Residues	Atoms						AltConf
2	D	1	Total	C	H	N	O	P	0
			124	39	75	1	8	1	

- Molecule 3 is 1-palmitoyl-2-oleoyl-sn-glycero-3-phosphocholine (CCD ID: LBN) (formula: C₄₂H₈₂NO₈P).



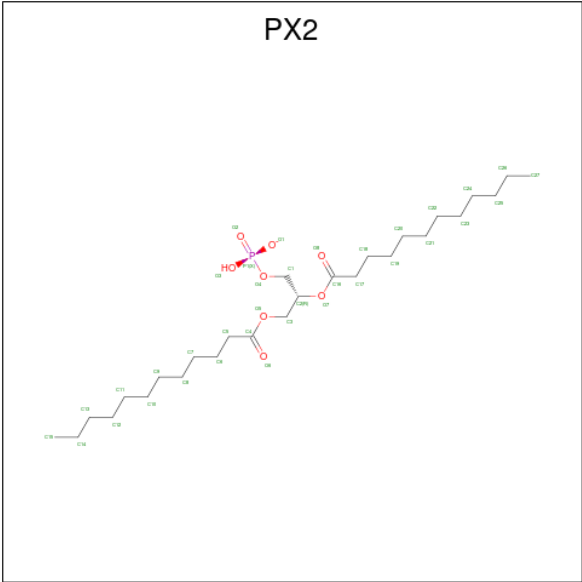
Mol	Chain	Residues	Atoms						AltConf
3	A	1	Total	C	H	N	O	P	0
			101	32	59	1	8	1	
3	B	1	Total	C	H	N	O	P	0
			101	32	59	1	8	1	
3	C	1	Total	C	H	N	O	P	0
			101	32	59	1	8	1	
3	D	1	Total	C	H	N	O	P	0
			101	32	59	1	8	1	

- Molecule 4 is CHOLESTEROL HEMISUCCINATE (CCD ID: Y01) (formula: C₃₁H₅₀O₄).

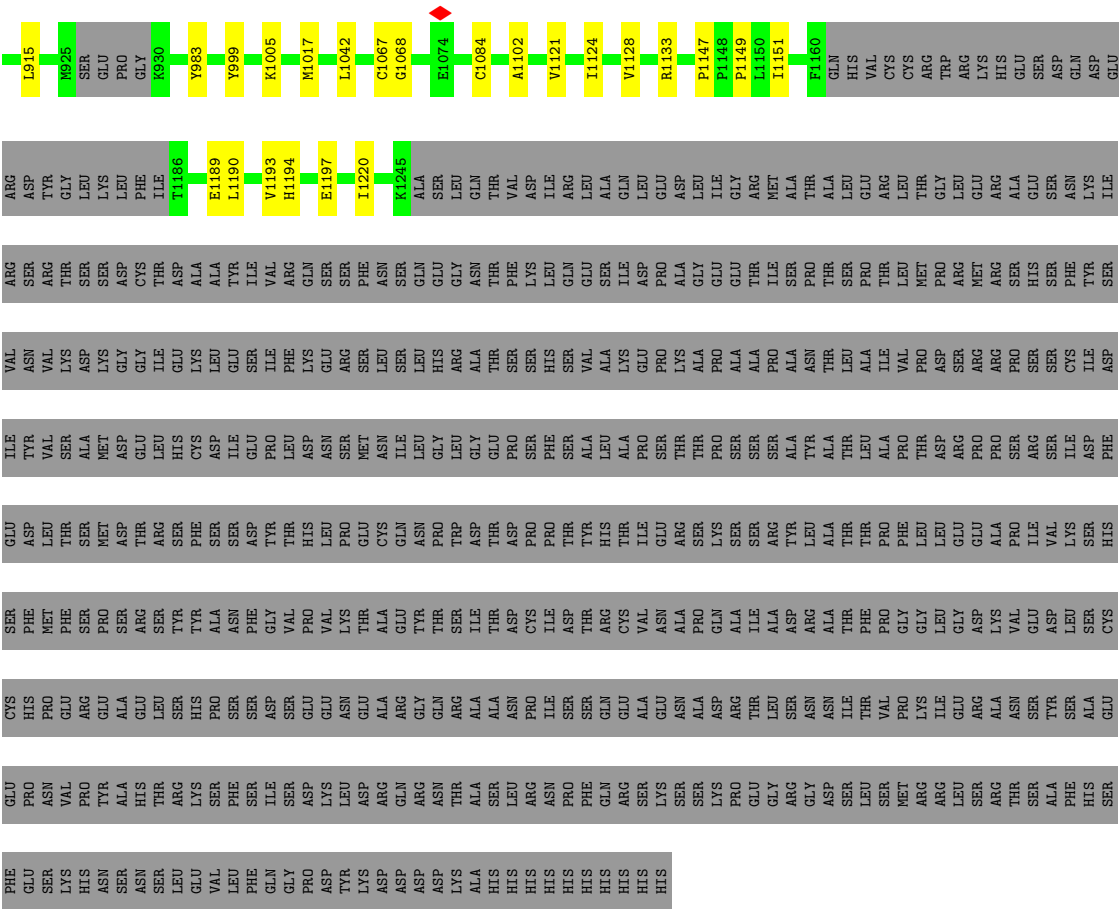


Mol	Chain	Residues	Atoms				AltConf
4	A	1	Total	C	H	O	0
			84	31	49	4	
4	A	1	Total	C	H	O	0
			84	31	49	4	
4	B	1	Total	C	H	O	0
			84	31	49	4	
4	B	1	Total	C	H	O	0
			84	31	49	4	
4	C	1	Total	C	H	O	0
			84	31	49	4	
4	C	1	Total	C	H	O	0
			84	31	49	4	
4	D	1	Total	C	H	O	0
			84	31	49	4	
4	D	1	Total	C	H	O	0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

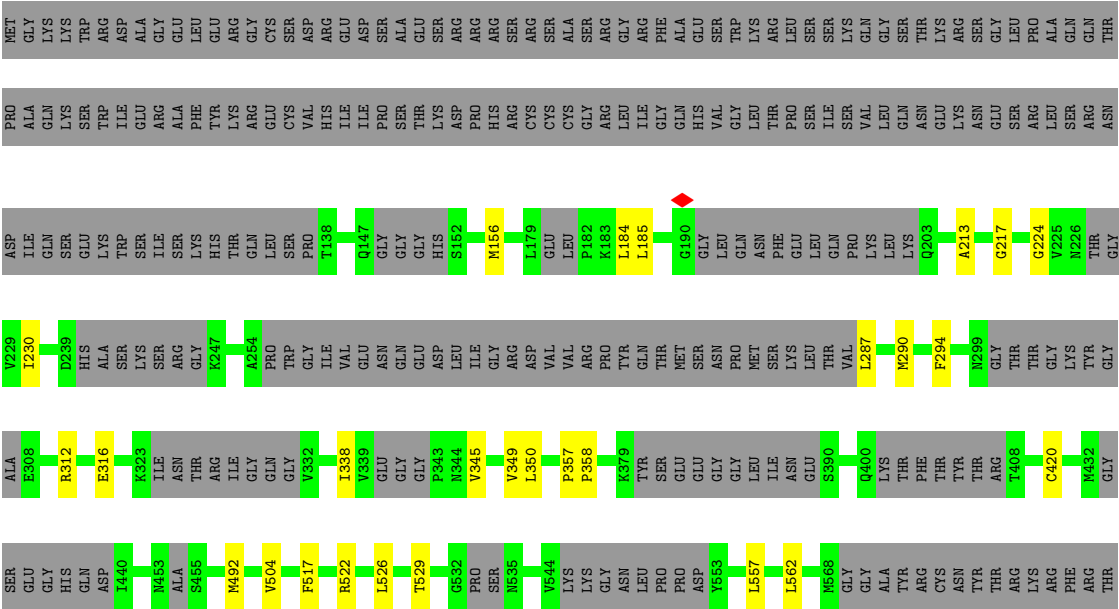
- Molecule 5 is 1,2-DILAUROYL-SN-GLYCERO-3-PHOSPHATE (CCD ID: PX2) (formula: C₂₇H₅₂O₈P).



Mol	Chain	Residues	Atoms					AltConf
5	A	1	Total	C	H	O	P	0
			82	26	47	8	1	
5	B	1	Total	C	H	O	P	0
			82	26	47	8	1	
5	C	1	Total	C	H	O	P	0
			82	26	47	8	1	
5	D	1	Total	C	H	O	P	0
			82	26	47	8	1	



● Molecule 1: Transient receptor potential cation channel, subfamily M, member 3





4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C4	Depositor
Number of particles used	69009	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)	800	Depositor
Maximum defocus (nm)	2000	Depositor
Magnification	81000	Depositor
Image detector	GATAN K3 BIOQUANTUM (6k x 4k)	Depositor
Maximum map value	1.568	Depositor
Minimum map value	-0.844	Depositor
Average map value	0.001	Depositor
Map value standard deviation	0.034	Depositor
Recommended contour level	0.1	Depositor
Map size (Å)	358.4, 358.4, 358.4	wwPDB
Map dimensions	320, 320, 320	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.12, 1.12, 1.12	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: Y01, PX2, 6OU, LBN

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	0.09	0/5668	0.23	0/7737
1	B	0.09	0/5668	0.23	0/7737
1	C	0.09	0/5668	0.23	0/7737
1	D	0.09	0/5668	0.23	0/7737
All	All	0.09	0/22672	0.23	0/30948

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	5563	4863	4882	38	0
1	B	5563	4863	4882	39	0
1	C	5563	4863	4882	39	0
1	D	5563	4863	4882	40	0
2	A	49	75	0	0	0
2	B	49	75	0	0	0
2	C	49	75	0	0	0
2	D	49	75	0	0	0
3	A	42	59	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	B	42	59	0	0	0
3	C	42	59	0	0	0
3	D	42	59	0	0	0
4	A	70	98	98	1	0
4	B	70	98	98	3	0
4	C	70	98	98	2	0
4	D	70	98	98	1	0
5	A	35	47	47	0	0
5	B	35	47	47	0	0
5	C	35	47	47	0	0
5	D	35	47	47	0	0
All	All	23036	20568	20108	157	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 4.

All (157) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1068:GLY:N	1:B:1084:CYS:SG	2.60	0.74
1:A:1068:GLY:N	1:A:1084:CYS:SG	2.60	0.74
1:C:1068:GLY:N	1:C:1084:CYS:SG	2.60	0.73
1:D:1068:GLY:N	1:D:1084:CYS:SG	2.60	0.73
1:C:767:LEU:HD12	1:C:767:LEU:O	1.93	0.69
1:A:767:LEU:HD12	1:A:767:LEU:O	1.93	0.69
1:C:184:LEU:HD23	1:C:185:LEU:N	2.08	0.69
1:D:184:LEU:HD23	1:D:185:LEU:N	2.08	0.68
1:B:184:LEU:HD23	1:B:185:LEU:N	2.08	0.68
1:A:184:LEU:HD23	1:A:185:LEU:N	2.08	0.68
1:B:767:LEU:HD12	1:B:767:LEU:O	1.93	0.68
1:D:767:LEU:O	1:D:767:LEU:HD12	1.93	0.67
1:D:1147:PRO:O	1:D:1151:ILE:HG23	1.95	0.67
1:C:1147:PRO:O	1:C:1151:ILE:HG23	1.95	0.67
1:B:1147:PRO:O	1:B:1151:ILE:HG23	1.95	0.66
1:A:1147:PRO:O	1:A:1151:ILE:HG23	1.95	0.66
1:A:1067:CYS:SG	1:A:1068:GLY:N	2.70	0.65
1:B:1067:CYS:SG	1:B:1068:GLY:N	2.70	0.65
1:D:1067:CYS:SG	1:D:1068:GLY:N	2.69	0.65
1:B:750:ILE:O	1:B:755:SER:OG	2.13	0.62
1:C:1067:CYS:SG	1:C:1068:GLY:N	2.70	0.62
1:C:750:ILE:O	1:C:755:SER:OG	2.13	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:664:ALA:N	1:D:1197:GLU:OE2	2.33	0.62
1:A:750:ILE:O	1:A:755:SER:OG	2.13	0.62
1:B:664:ALA:N	1:B:1197:GLU:OE2	2.33	0.61
4:A:2101:Y01:HAC1	4:A:2101:Y01:HAU2	1.83	0.61
1:A:664:ALA:N	1:A:1197:GLU:OE2	2.33	0.61
1:C:664:ALA:N	1:C:1197:GLU:OE2	2.33	0.61
4:B:2101:Y01:HAC1	4:B:2101:Y01:HAU2	1.83	0.61
1:B:345:VAL:O	1:B:349:VAL:HG23	2.02	0.60
1:D:345:VAL:O	1:D:349:VAL:HG23	2.02	0.60
4:C:2101:Y01:HAU2	4:C:2101:Y01:HAC1	1.83	0.60
1:C:345:VAL:O	1:C:349:VAL:HG23	2.02	0.60
4:D:2101:Y01:HAC1	4:D:2101:Y01:HAU2	1.83	0.58
1:A:345:VAL:O	1:A:349:VAL:HG23	2.02	0.58
1:D:1189:GLU:O	1:D:1193:VAL:HG23	2.05	0.57
1:A:1189:GLU:O	1:A:1193:VAL:HG23	2.05	0.57
1:C:1189:GLU:O	1:C:1193:VAL:HG23	2.05	0.56
1:D:750:ILE:O	1:D:755:SER:OG	2.13	0.56
1:B:1189:GLU:O	1:B:1193:VAL:HG23	2.05	0.56
1:B:517:PHE:O	1:B:522:ARG:NH2	2.39	0.56
1:B:1190:LEU:O	1:B:1194:HIS:ND1	2.39	0.56
1:A:290:MET:HA	1:A:290:MET:HE2	1.87	0.56
1:B:290:MET:HA	1:B:290:MET:HE2	1.87	0.56
1:D:1190:LEU:O	1:D:1194:HIS:ND1	2.39	0.56
1:C:517:PHE:O	1:C:522:ARG:NH2	2.39	0.55
1:D:517:PHE:O	1:D:522:ARG:NH2	2.39	0.55
1:A:517:PHE:O	1:A:522:ARG:NH2	2.39	0.55
1:C:290:MET:HE2	1:C:290:MET:HA	1.87	0.55
1:B:156:MET:O	1:B:294:PHE:N	2.40	0.54
1:D:290:MET:HA	1:D:290:MET:HE2	1.87	0.54
1:A:526:LEU:O	1:A:529:THR:HG22	2.08	0.54
1:C:1190:LEU:O	1:C:1194:HIS:ND1	2.39	0.54
1:C:526:LEU:O	1:C:529:THR:HG22	2.08	0.54
1:D:526:LEU:O	1:D:529:THR:HG22	2.08	0.53
1:A:1190:LEU:O	1:A:1194:HIS:ND1	2.39	0.53
1:A:156:MET:O	1:A:294:PHE:N	2.40	0.53
1:B:184:LEU:HD23	1:B:185:LEU:H	1.73	0.53
1:D:184:LEU:HD23	1:D:185:LEU:H	1.73	0.53
1:B:526:LEU:O	1:B:529:THR:HG22	2.08	0.53
1:A:184:LEU:HD23	1:A:185:LEU:H	1.73	0.52
1:C:156:MET:O	1:C:294:PHE:N	2.40	0.52
1:D:156:MET:O	1:D:294:PHE:N	2.40	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:338:ILE:CD1	1:D:349:VAL:HG22	2.41	0.51
1:A:338:ILE:CD1	1:A:349:VAL:HG22	2.41	0.51
1:C:184:LEU:HD23	1:C:185:LEU:H	1.73	0.51
1:A:312:ARG:NH1	1:A:316:GLU:OE2	2.44	0.51
1:C:312:ARG:NH1	1:C:316:GLU:OE2	2.44	0.51
1:C:338:ILE:CD1	1:C:349:VAL:HG22	2.41	0.51
1:B:338:ILE:CD1	1:B:349:VAL:HG22	2.41	0.50
1:D:312:ARG:NH1	1:D:316:GLU:OE2	2.44	0.50
1:B:312:ARG:NH1	1:B:316:GLU:OE2	2.44	0.50
1:A:1124:ILE:O	1:A:1128:VAL:HG23	2.12	0.50
1:B:1124:ILE:O	1:B:1128:VAL:HG23	2.12	0.50
1:C:1124:ILE:O	1:C:1128:VAL:HG23	2.12	0.49
1:B:224:GLY:O	1:B:287:LEU:N	2.46	0.49
1:D:562:LEU:C	1:D:562:LEU:HD23	2.37	0.49
1:A:562:LEU:C	1:A:562:LEU:HD23	2.37	0.49
1:D:1124:ILE:O	1:D:1128:VAL:HG23	2.12	0.49
1:B:562:LEU:C	1:B:562:LEU:HD23	2.37	0.49
1:C:562:LEU:C	1:C:562:LEU:HD23	2.37	0.48
1:A:492:MET:HE1	1:A:504:VAL:HG22	1.95	0.48
1:C:224:GLY:O	1:C:287:LEU:N	2.46	0.48
1:D:224:GLY:O	1:D:287:LEU:N	2.46	0.48
1:A:224:GLY:O	1:A:287:LEU:N	2.46	0.48
1:C:492:MET:HE1	1:C:504:VAL:HG22	1.95	0.48
1:D:492:MET:HE1	1:D:504:VAL:HG22	1.95	0.47
1:B:492:MET:HE1	1:B:504:VAL:HG22	1.95	0.47
1:B:1151:ILE:HD12	1:B:1151:ILE:C	2.40	0.47
1:C:1151:ILE:C	1:C:1151:ILE:HD12	2.40	0.47
1:A:1151:ILE:C	1:A:1151:ILE:HD12	2.40	0.47
1:C:1017:MET:HE1	1:C:1102:ALA:HB2	1.97	0.46
1:D:1151:ILE:C	1:D:1151:ILE:HD12	2.40	0.46
1:D:1017:MET:HE1	1:D:1102:ALA:HB2	1.97	0.46
1:B:1017:MET:HE1	1:B:1102:ALA:HB2	1.97	0.46
1:B:350:LEU:HD21	1:B:420:CYS:SG	2.56	0.46
1:C:710:LEU:HD13	1:C:749:PHE:CE1	2.52	0.45
1:A:1017:MET:HE1	1:A:1102:ALA:HB2	1.97	0.45
1:D:350:LEU:HD21	1:D:420:CYS:SG	2.56	0.45
1:D:710:LEU:HD13	1:D:749:PHE:CE1	2.51	0.45
1:B:710:LEU:HD13	1:B:749:PHE:CE1	2.51	0.45
1:C:350:LEU:HD21	1:C:420:CYS:SG	2.56	0.45
1:A:350:LEU:HD21	1:A:420:CYS:SG	2.56	0.45
1:A:710:LEU:HD13	1:A:749:PHE:CE1	2.51	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1042:LEU:HD23	1:D:894:LEU:HB3	1.99	0.45
1:C:894:LEU:HB3	1:D:1042:LEU:HD23	1.99	0.45
1:A:894:LEU:HB3	1:B:1042:LEU:HD23	1.98	0.44
1:B:492:MET:HA	1:B:492:MET:HE3	1.99	0.44
1:D:492:MET:HE3	1:D:492:MET:HA	2.00	0.44
1:A:557:LEU:C	1:A:557:LEU:HD13	2.43	0.44
1:A:492:MET:HE3	1:A:492:MET:HA	2.00	0.44
1:C:557:LEU:C	1:C:557:LEU:HD13	2.43	0.44
1:B:557:LEU:C	1:B:557:LEU:HD13	2.43	0.43
1:B:894:LEU:HB3	1:C:1042:LEU:HD23	1.99	0.43
1:D:557:LEU:C	1:D:557:LEU:HD13	2.43	0.43
1:B:526:LEU:HD21	1:B:644:TRP:CZ2	2.54	0.43
1:C:526:LEU:HD21	1:C:644:TRP:CZ2	2.54	0.43
1:C:655:LEU:HD23	1:C:655:LEU:O	2.19	0.43
1:D:526:LEU:HD21	1:D:644:TRP:CZ2	2.54	0.43
1:D:655:LEU:O	1:D:655:LEU:HD23	2.19	0.43
1:A:526:LEU:HD21	1:A:644:TRP:CZ2	2.54	0.43
4:B:2102:Y01:HAE2	4:B:2102:Y01:HBB	1.95	0.43
1:B:655:LEU:HD23	1:B:655:LEU:O	2.19	0.43
1:A:906:TRP:O	1:A:909:ILE:HG13	2.19	0.43
1:C:492:MET:HA	1:C:492:MET:HE3	2.00	0.43
1:D:230:ILE:HD12	1:D:230:ILE:N	2.34	0.43
1:A:230:ILE:N	1:A:230:ILE:HD12	2.34	0.42
1:C:906:TRP:O	1:C:909:ILE:HG13	2.19	0.42
1:B:906:TRP:O	1:B:909:ILE:HG13	2.19	0.42
1:C:230:ILE:HD12	1:C:230:ILE:N	2.34	0.42
1:B:230:ILE:HD12	1:B:230:ILE:N	2.34	0.42
4:B:2102:Y01:HAD2	4:B:2102:Y01:HAS2	1.92	0.42
1:D:906:TRP:O	1:D:909:ILE:HG13	2.19	0.42
1:A:655:LEU:O	1:A:655:LEU:HD23	2.19	0.42
1:B:915:LEU:HD13	1:B:915:LEU:O	2.20	0.41
4:C:2102:Y01:HAD2	4:C:2102:Y01:HAS2	1.92	0.41
1:D:729:LEU:O	1:D:734:ASN:N	2.45	0.41
1:C:915:LEU:HD13	1:C:915:LEU:O	2.20	0.41
1:D:1005:LYS:CD	1:D:1121:VAL:HG13	2.51	0.41
1:B:892:ILE:HD11	1:B:904:GLN:C	2.46	0.41
1:A:915:LEU:O	1:A:915:LEU:HD13	2.20	0.41
1:A:1005:LYS:CD	1:A:1121:VAL:HG13	2.51	0.41
1:C:1005:LYS:CD	1:C:1121:VAL:HG13	2.51	0.41
1:A:1220:ILE:HD11	1:B:1220:ILE:HD12	2.03	0.41
1:D:915:LEU:HD13	1:D:915:LEU:O	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:892:ILE:HD11	1:A:904:GLN:C	2.46	0.40
1:B:710:LEU:CD1	1:B:725:LEU:HD21	2.51	0.40
1:C:904:GLN:OE1	1:C:904:GLN:N	2.45	0.40
1:C:1148:PRO:N	1:C:1149:PRO:CD	2.85	0.40
1:D:892:ILE:HD11	1:D:904:GLN:C	2.46	0.40
1:B:1147:PRO:HB2	1:B:1149:PRO:HD2	2.03	0.40
1:D:1117:THR:O	1:D:1117:THR:HG22	2.22	0.40
1:A:1220:ILE:HD12	1:D:1220:ILE:HD11	2.03	0.40
1:B:1005:LYS:CD	1:B:1121:VAL:HG13	2.51	0.40
1:C:213:ALA:O	1:C:217:GLY:N	2.52	0.40
1:D:1088:ALA:O	1:D:1092:PRO:HD2	2.22	0.40
1:C:357:PRO:N	1:C:358:PRO:CD	2.84	0.40

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	756/1739 (44%)	736 (97%)	20 (3%)	0	100	100
1	B	756/1739 (44%)	736 (97%)	20 (3%)	0	100	100
1	C	756/1739 (44%)	736 (97%)	20 (3%)	0	100	100
1	D	756/1739 (44%)	736 (97%)	20 (3%)	0	100	100
All	All	3024/6956 (44%)	2944 (97%)	80 (3%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains ⓘ

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

entries.

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	457/1545 (30%)	454 (99%)	3 (1%)	81	89
1	B	457/1545 (30%)	454 (99%)	3 (1%)	81	89
1	C	457/1545 (30%)	454 (99%)	3 (1%)	81	89
1	D	457/1545 (30%)	454 (99%)	3 (1%)	81	89
All	All	1828/6180 (30%)	1816 (99%)	12 (1%)	80	89

All (12) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	983	TYR
1	A	999	TYR
1	A	1133	ARG
1	B	983	TYR
1	B	999	TYR
1	B	1133	ARG
1	C	983	TYR
1	C	999	TYR
1	C	1133	ARG
1	D	983	TYR
1	D	999	TYR
1	D	1133	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (24) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	639	HIS
1	A	697	HIS
1	A	890	ASN
1	A	1062	GLN
1	A	1115	ASN
1	A	1135	GLN
1	B	639	HIS
1	B	697	HIS
1	B	890	ASN
1	B	1062	GLN
1	B	1115	ASN

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Mol	Chain	Res	Type
1	B	1135	GLN
1	C	639	HIS
1	C	697	HIS
1	C	890	ASN
1	C	1062	GLN
1	C	1115	ASN
1	C	1135	GLN
1	D	639	HIS
1	D	697	HIS
1	D	890	ASN
1	D	1062	GLN
1	D	1115	ASN
1	D	1135	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 oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

20 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	$\# Z > 2$
5	PX2	C	2201	-	34,34,35	1.00	4 (11%)	37,39,40	1.04	2 (5%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
3	LBN	A	2004	-	41,41,51	1.12	3 (7%)	47,49,59	0.87	2 (4%)
5	PX2	D	2201	-	34,34,35	1.00	4 (11%)	37,39,40	1.05	2 (5%)
4	Y01	C	2102	-	38,38,38	1.15	3 (7%)	57,57,57	2.49	16 (28%)
2	6OU	C	2001	-	48,48,48	0.90	4 (8%)	51,53,53	0.86	2 (3%)
4	Y01	D	2102	-	38,38,38	1.14	3 (7%)	57,57,57	2.49	17 (29%)
4	Y01	A	2102	-	38,38,38	1.15	3 (7%)	57,57,57	2.49	17 (29%)
4	Y01	B	2102	-	38,38,38	1.15	3 (7%)	57,57,57	2.49	16 (28%)
5	PX2	A	2201	-	34,34,35	0.99	4 (11%)	37,39,40	1.05	2 (5%)
5	PX2	B	2201	-	34,34,35	1.00	4 (11%)	37,39,40	1.04	2 (5%)
3	LBN	C	2004	-	41,41,51	1.12	3 (7%)	47,49,59	0.87	2 (4%)
3	LBN	D	2004	-	41,41,51	1.12	3 (7%)	47,49,59	0.87	2 (4%)
3	LBN	B	2004	-	41,41,51	1.12	3 (7%)	47,49,59	0.87	2 (4%)
4	Y01	C	2101	-	38,38,38	1.09	3 (7%)	57,57,57	2.32	15 (26%)
4	Y01	D	2101	-	38,38,38	1.10	3 (7%)	57,57,57	2.32	15 (26%)
2	6OU	B	2001	-	48,48,48	0.90	4 (8%)	51,53,53	0.86	2 (3%)
4	Y01	A	2101	-	38,38,38	1.09	3 (7%)	57,57,57	2.31	15 (26%)
4	Y01	B	2101	-	38,38,38	1.09	3 (7%)	57,57,57	2.32	15 (26%)
2	6OU	D	2001	-	48,48,48	0.91	4 (8%)	51,53,53	0.85	2 (3%)
2	6OU	A	2001	-	48,48,48	0.91	4 (8%)	51,53,53	0.86	2 (3%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	PX2	C	2201	-	-	17/36/36/37	-
3	LBN	A	2004	-	-	22/45/45/55	-
5	PX2	D	2201	-	-	17/36/36/37	-
4	Y01	C	2102	-	-	15/19/77/77	0/4/4/4
2	6OU	C	2001	-	-	30/52/52/52	-
4	Y01	D	2102	-	-	15/19/77/77	0/4/4/4
4	Y01	A	2102	-	-	15/19/77/77	0/4/4/4
4	Y01	B	2102	-	-	15/19/77/77	0/4/4/4
5	PX2	A	2201	-	-	17/36/36/37	-
5	PX2	B	2201	-	-	17/36/36/37	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	LBN	C	2004	-	-	22/45/45/55	-
3	LBN	D	2004	-	-	22/45/45/55	-
3	LBN	B	2004	-	-	22/45/45/55	-
4	Y01	C	2101	-	-	5/19/77/77	0/4/4/4
4	Y01	D	2101	-	-	5/19/77/77	0/4/4/4
2	6OU	B	2001	-	-	29/52/52/52	-
4	Y01	A	2101	-	-	5/19/77/77	0/4/4/4
4	Y01	B	2101	-	-	5/19/77/77	0/4/4/4
2	6OU	D	2001	-	-	30/52/52/52	-
2	6OU	A	2001	-	-	30/52/52/52	-

All (68) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	B	2102	Y01	OAW-CAY	3.31	1.43	1.34
4	C	2102	Y01	OAW-CAY	3.31	1.43	1.34
4	D	2102	Y01	OAW-CAY	3.31	1.43	1.34
4	A	2102	Y01	OAW-CAY	3.29	1.43	1.34
4	C	2101	Y01	OAW-CAY	3.28	1.43	1.34
4	D	2101	Y01	OAW-CAY	3.26	1.43	1.34
4	A	2101	Y01	OAW-CAY	3.25	1.43	1.34
4	B	2101	Y01	OAW-CAY	3.25	1.43	1.34
4	A	2101	Y01	OAH-CAX	-2.86	1.21	1.30
4	D	2101	Y01	OAH-CAX	-2.86	1.21	1.30
4	B	2101	Y01	OAH-CAX	-2.85	1.21	1.30
4	A	2102	Y01	OAH-CAX	-2.83	1.21	1.30
4	D	2102	Y01	OAH-CAX	-2.83	1.21	1.30
4	B	2102	Y01	OAH-CAX	-2.82	1.21	1.30
4	C	2101	Y01	OAH-CAX	-2.82	1.21	1.30
4	C	2102	Y01	OAH-CAX	-2.82	1.21	1.30
3	A	2004	LBN	O5-C25	2.80	1.41	1.33
3	D	2004	LBN	O5-C25	2.80	1.41	1.33
3	B	2004	LBN	O5-C25	2.78	1.41	1.33
3	C	2004	LBN	O5-C25	2.78	1.41	1.33
2	A	2001	6OU	O30-C20	-2.69	1.40	1.46
2	D	2001	6OU	O30-C20	-2.69	1.40	1.46
2	C	2001	6OU	O30-C20	-2.67	1.40	1.46
2	B	2001	6OU	O30-C20	-2.65	1.40	1.46
3	C	2004	LBN	O7-C34	2.56	1.41	1.34
3	A	2004	LBN	O7-C34	2.52	1.41	1.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	2004	LBN	O7-C34	2.52	1.41	1.34
3	D	2004	LBN	O7-C34	2.52	1.41	1.34
2	B	2001	6OU	O18-C16	2.45	1.40	1.33
2	D	2001	6OU	O18-C16	2.45	1.40	1.33
2	A	2001	6OU	O18-C16	2.42	1.40	1.33
2	C	2001	6OU	O18-C16	2.42	1.40	1.33
5	D	2201	PX2	O5-C4	2.41	1.40	1.33
5	B	2201	PX2	O5-C4	2.41	1.40	1.33
5	C	2201	PX2	O5-C4	2.41	1.40	1.33
5	B	2201	PX2	O7-C2	-2.39	1.41	1.46
5	C	2201	PX2	O7-C2	-2.39	1.41	1.46
5	A	2201	PX2	O5-C4	2.39	1.40	1.33
5	A	2201	PX2	O7-C2	-2.38	1.41	1.46
5	D	2201	PX2	O7-C2	-2.38	1.41	1.46
4	A	2102	Y01	CAS-CBF	2.32	1.57	1.53
4	C	2102	Y01	CAS-CBF	2.32	1.57	1.53
4	B	2102	Y01	CAS-CBF	2.27	1.57	1.53
3	C	2004	LBN	O7-C2	-2.26	1.41	1.46
3	A	2004	LBN	O7-C2	-2.25	1.41	1.46
3	B	2004	LBN	O7-C2	-2.25	1.41	1.46
4	D	2102	Y01	CAS-CBF	2.24	1.57	1.53
3	D	2004	LBN	O7-C2	-2.21	1.41	1.46
5	A	2201	PX2	O7-C16	2.19	1.40	1.34
5	D	2201	PX2	O7-C16	2.19	1.40	1.34
2	C	2001	6OU	O18-C19	-2.18	1.40	1.45
5	B	2201	PX2	O7-C16	2.18	1.40	1.34
5	C	2201	PX2	O7-C16	2.18	1.40	1.34
5	B	2201	PX2	O5-C3	-2.18	1.40	1.45
5	C	2201	PX2	O5-C3	-2.18	1.40	1.45
2	A	2001	6OU	O18-C19	-2.17	1.40	1.45
2	D	2001	6OU	O18-C19	-2.17	1.40	1.45
5	A	2201	PX2	O5-C3	-2.16	1.40	1.45
5	D	2201	PX2	O5-C3	-2.16	1.40	1.45
2	B	2001	6OU	O18-C19	-2.13	1.40	1.45
2	D	2001	6OU	O30-C31	2.10	1.40	1.34
2	A	2001	6OU	O30-C31	2.08	1.40	1.34
2	B	2001	6OU	O30-C31	2.08	1.40	1.34
2	C	2001	6OU	O30-C31	2.05	1.40	1.34
4	A	2101	Y01	CAK-CAI	2.04	1.54	1.50
4	B	2101	Y01	CAK-CAI	2.04	1.54	1.50
4	C	2101	Y01	CAK-CAI	2.04	1.54	1.50
4	D	2101	Y01	CAK-CAI	2.04	1.54	1.50

All (150) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	B	2101	Y01	CAT-CBH-CBF	-9.42	96.27	108.74
4	C	2101	Y01	CAT-CBH-CBF	-9.42	96.28	108.74
4	D	2101	Y01	CAT-CBH-CBF	-9.41	96.28	108.74
4	A	2101	Y01	CAT-CBH-CBF	-9.40	96.30	108.74
4	B	2102	Y01	CAT-CBH-CBF	-8.45	97.55	108.74
4	D	2102	Y01	CAT-CBH-CBF	-8.45	97.55	108.74
4	A	2102	Y01	CAT-CBH-CBF	-8.45	97.56	108.74
4	C	2102	Y01	CAT-CBH-CBF	-8.42	97.59	108.74
4	B	2102	Y01	CAV-CAZ-CAI	7.72	131.04	120.57
4	C	2102	Y01	CAV-CAZ-CAI	7.72	131.04	120.57
4	D	2102	Y01	CAV-CAZ-CAI	7.71	131.02	120.57
4	A	2102	Y01	CAV-CAZ-CAI	7.70	131.01	120.57
4	C	2101	Y01	CAV-CAZ-CAI	6.66	129.60	120.57
4	A	2101	Y01	CAV-CAZ-CAI	6.62	129.54	120.57
4	D	2101	Y01	CAV-CAZ-CAI	6.61	129.53	120.57
4	B	2101	Y01	CAV-CAZ-CAI	6.61	129.53	120.57
4	B	2102	Y01	CBH-CBF-CBD	-5.65	104.45	112.71
4	D	2102	Y01	CBH-CBF-CBD	-5.65	104.46	112.71
4	C	2102	Y01	CBH-CBF-CBD	-5.62	104.50	112.71
4	A	2102	Y01	CBH-CBF-CBD	-5.61	104.51	112.71
4	B	2101	Y01	CBH-CBF-CBD	-5.31	104.95	112.71
4	C	2101	Y01	CBH-CBF-CBD	-5.31	104.96	112.71
4	D	2101	Y01	CBH-CBF-CBD	-5.30	104.97	112.71
4	A	2101	Y01	CBH-CBF-CBD	-5.30	104.97	112.71
4	B	2102	Y01	CAV-CAZ-CBH	-4.74	110.35	116.42
4	C	2102	Y01	CAV-CAZ-CBH	-4.74	110.35	116.42
4	D	2102	Y01	CAV-CAZ-CBH	-4.73	110.37	116.42
4	A	2102	Y01	CAV-CAZ-CBH	-4.69	110.42	116.42
4	D	2101	Y01	CAD-CBH-CBF	4.19	116.37	111.66
4	A	2101	Y01	CAD-CBH-CBF	4.14	116.31	111.66
4	B	2101	Y01	CAD-CBH-CBF	4.14	116.31	111.66
4	C	2101	Y01	CAD-CBH-CBF	4.14	116.31	111.66
4	A	2102	Y01	CAU-CBI-CBE	-4.12	110.54	116.60
4	C	2102	Y01	CAU-CBI-CBE	-4.12	110.54	116.60
4	C	2101	Y01	CBH-CAZ-CAI	-4.09	116.96	122.93
5	A	2201	PX2	O7-C16-C17	4.09	120.32	111.48
5	D	2201	PX2	O7-C16-C17	4.09	120.32	111.48
4	D	2101	Y01	CBH-CAZ-CAI	-4.08	116.97	122.93
4	A	2101	Y01	CBH-CAZ-CAI	-4.07	116.99	122.93
4	D	2102	Y01	CAU-CBI-CBE	-4.07	110.61	116.60
5	B	2201	PX2	O7-C16-C17	4.06	120.27	111.48
5	C	2201	PX2	O7-C16-C17	4.06	120.27	111.48

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	B	2102	Y01	CAU-CBI-CBE	-4.05	110.63	116.60
4	B	2101	Y01	CBH-CAZ-CAI	-4.05	117.01	122.93
4	B	2102	Y01	OAW-CAY-CAM	4.05	120.23	111.48
4	D	2102	Y01	OAW-CAY-CAM	4.05	120.23	111.48
4	C	2102	Y01	OAW-CAY-CAM	4.03	120.20	111.48
4	A	2102	Y01	OAW-CAY-CAM	4.02	120.19	111.48
3	D	2004	LBN	O7-C34-C35	3.87	119.86	111.48
3	A	2004	LBN	O7-C34-C35	3.87	119.85	111.48
3	B	2004	LBN	O7-C34-C35	3.87	119.85	111.48
3	C	2004	LBN	O7-C34-C35	3.85	119.80	111.48
4	C	2101	Y01	OAW-CAY-CAM	3.74	119.57	111.48
4	B	2101	Y01	OAW-CAY-CAM	3.73	119.55	111.48
4	A	2101	Y01	OAW-CAY-CAM	3.72	119.53	111.48
4	D	2101	Y01	OAW-CAY-CAM	3.70	119.49	111.48
2	B	2001	6OU	O30-C31-C33	3.69	119.47	111.48
2	A	2001	6OU	O30-C31-C33	3.69	119.45	111.48
2	C	2001	6OU	O30-C31-C33	3.68	119.44	111.48
2	D	2001	6OU	O30-C31-C33	3.66	119.39	111.48
4	D	2102	Y01	CBI-CBE-CBB	-3.48	114.12	119.50
4	A	2102	Y01	CBI-CBE-CBB	-3.47	114.14	119.50
4	C	2102	Y01	CBI-CBE-CBB	-3.47	114.14	119.50
4	B	2102	Y01	CBI-CBE-CBB	-3.46	114.15	119.50
4	D	2101	Y01	CAU-CBI-CBE	-3.43	111.54	116.60
4	C	2101	Y01	CAU-CBI-CBE	-3.41	111.57	116.60
4	A	2101	Y01	CAU-CBI-CBE	-3.41	111.58	116.60
4	B	2101	Y01	CAU-CBI-CBE	-3.41	111.58	116.60
4	A	2102	Y01	CAU-CAS-CBF	3.36	118.85	113.14
4	B	2102	Y01	CAU-CAS-CBF	3.34	118.82	113.14
4	C	2102	Y01	CAU-CAS-CBF	3.34	118.81	113.14
4	D	2102	Y01	CAU-CAS-CBF	3.34	118.81	113.14
4	A	2102	Y01	CAT-CAR-CBC	3.20	115.55	110.33
4	C	2102	Y01	CAT-CAR-CBC	3.18	115.51	110.33
4	B	2102	Y01	CAT-CAR-CBC	3.17	115.50	110.33
4	D	2102	Y01	CAT-CAR-CBC	3.16	115.48	110.33
4	A	2102	Y01	CAC-CBB-CBE	-3.14	108.17	112.88
4	C	2102	Y01	CAC-CBB-CBE	-3.14	108.17	112.88
4	B	2102	Y01	CAC-CBB-CBE	-3.13	108.19	112.88
4	D	2102	Y01	CAC-CBB-CBE	-3.12	108.20	112.88
4	B	2101	Y01	CAK-CBD-CBF	-3.08	106.17	109.72
4	B	2101	Y01	CAD-CBH-CAZ	3.07	113.08	108.38
4	A	2101	Y01	CAK-CBD-CBF	-3.06	106.18	109.72
4	D	2101	Y01	CAK-CBD-CBF	-3.06	106.18	109.72

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	C	2101	Y01	CAD-CBH-CAZ	3.06	113.06	108.38
4	D	2101	Y01	CAD-CBH-CAZ	3.04	113.03	108.38
4	A	2101	Y01	CAD-CBH-CAZ	3.04	113.03	108.38
4	C	2101	Y01	CAK-CBD-CBF	-3.02	106.23	109.72
4	A	2102	Y01	CBH-CAZ-CAI	-2.98	118.58	122.93
4	B	2102	Y01	CBH-CAZ-CAI	-2.96	118.61	122.93
4	C	2102	Y01	CBH-CAZ-CAI	-2.96	118.61	122.93
4	D	2102	Y01	CBH-CAZ-CAI	-2.96	118.61	122.93
4	C	2102	Y01	CAD-CBH-CAT	2.89	113.82	109.43
4	A	2102	Y01	CAD-CBH-CAT	2.88	113.81	109.43
4	B	2102	Y01	CAD-CBH-CAT	2.87	113.79	109.43
4	D	2102	Y01	CAD-CBH-CAT	2.86	113.78	109.43
4	A	2102	Y01	CBD-CAK-CAI	-2.78	108.90	112.76
4	C	2102	Y01	CBD-CAK-CAI	-2.77	108.92	112.76
4	B	2102	Y01	CBD-CAK-CAI	-2.76	108.94	112.76
4	D	2102	Y01	CBD-CAK-CAI	-2.76	108.94	112.76
4	C	2101	Y01	CBI-CBE-CBB	-2.76	115.24	119.50
4	D	2101	Y01	CBI-CBE-CBB	-2.74	115.26	119.50
4	A	2101	Y01	CBI-CBE-CBB	-2.72	115.30	119.50
4	A	2102	Y01	CAK-CBD-CBF	-2.71	106.58	109.72
4	C	2102	Y01	CAK-CBD-CBF	-2.71	106.59	109.72
4	B	2102	Y01	CAK-CBD-CBF	-2.71	106.59	109.72
4	B	2101	Y01	CBI-CBE-CBB	-2.70	115.32	119.50
4	D	2102	Y01	CAK-CBD-CBF	-2.66	106.64	109.72
5	D	2201	PX2	O5-C4-C5	2.66	119.95	111.83
5	A	2201	PX2	O5-C4-C5	2.65	119.92	111.83
2	B	2001	6OU	O18-C16-C15	2.65	119.92	111.83
2	C	2001	6OU	O18-C16-C15	2.65	119.91	111.83
2	A	2001	6OU	O18-C16-C15	2.65	119.90	111.83
4	B	2101	Y01	CAU-CAS-CBF	2.65	117.63	113.14
5	B	2201	PX2	O5-C4-C5	2.64	119.89	111.83
2	D	2001	6OU	O18-C16-C15	2.64	119.89	111.83
5	C	2201	PX2	O5-C4-C5	2.64	119.88	111.83
4	A	2101	Y01	CAU-CAS-CBF	2.63	117.61	113.14
4	D	2101	Y01	CAU-CAS-CBF	2.63	117.61	113.14
4	C	2101	Y01	CAU-CAS-CBF	2.63	117.60	113.14
4	A	2102	Y01	CAD-CBH-CBF	2.57	114.55	111.66
4	C	2102	Y01	CAD-CBH-CBF	2.57	114.54	111.66
4	D	2102	Y01	CAD-CBH-CBF	2.56	114.53	111.66
4	B	2102	Y01	CAD-CBH-CBF	2.55	114.52	111.66
3	B	2004	LBN	O5-C25-C26	2.54	119.58	111.83
3	C	2004	LBN	O5-C25-C26	2.54	119.58	111.83

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	2004	LBN	O5-C25-C26	2.53	119.56	111.83
3	D	2004	LBN	O5-C25-C26	2.53	119.56	111.83
4	C	2101	Y01	CAV-CAZ-CBH	-2.36	113.40	116.42
4	B	2101	Y01	CAV-CAZ-CBH	-2.34	113.42	116.42
4	A	2101	Y01	CAV-CAZ-CBH	-2.33	113.44	116.42
4	B	2102	Y01	CAD-CBH-CAZ	2.32	111.93	108.38
4	D	2102	Y01	CAD-CBH-CAZ	2.32	111.92	108.38
4	D	2101	Y01	CAV-CAZ-CBH	-2.31	113.47	116.42
4	B	2101	Y01	CAC-CBB-CBE	-2.30	109.43	112.88
4	A	2101	Y01	CAC-CBB-CBE	-2.30	109.43	112.88
4	D	2101	Y01	CAC-CBB-CBE	-2.30	109.43	112.88
4	C	2101	Y01	CAC-CBB-CBE	-2.30	109.44	112.88
4	C	2102	Y01	CAD-CBH-CAZ	2.30	111.89	108.38
4	A	2102	Y01	CAD-CBH-CAZ	2.29	111.88	108.38
4	C	2101	Y01	CBC-CAV-CAZ	2.17	114.65	111.45
4	A	2101	Y01	CBC-CAV-CAZ	2.16	114.65	111.45
4	B	2101	Y01	CBC-CAV-CAZ	2.16	114.65	111.45
4	D	2101	Y01	CBC-CAV-CAZ	2.14	114.62	111.45
4	C	2101	Y01	CAS-CBF-CBD	2.09	114.69	111.78
4	A	2101	Y01	CAS-CBF-CBD	2.04	114.63	111.78
4	D	2101	Y01	CAS-CBF-CBD	2.04	114.63	111.78
4	B	2101	Y01	CAS-CBF-CBD	2.04	114.63	111.78
4	D	2102	Y01	CAS-CBF-CBD	2.02	114.60	111.78
4	A	2102	Y01	CAP-CBE-CBI	-2.02	101.46	103.84

There are no chirality outliers.

All (355) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	2001	6OU	C21-O22-P23-O24
2	A	2001	6OU	C21-O22-P23-O25
2	A	2001	6OU	C21-O22-P23-O26
2	A	2001	6OU	C27-O26-P23-O22
2	A	2001	6OU	C27-O26-P23-O25
2	A	2001	6OU	O26-C27-C28-N29
2	A	2001	6OU	C33-C31-O30-C20
2	B	2001	6OU	C21-O22-P23-O24
2	B	2001	6OU	C21-O22-P23-O25
2	B	2001	6OU	C21-O22-P23-O26
2	B	2001	6OU	C27-O26-P23-O22
2	B	2001	6OU	C27-O26-P23-O25
2	B	2001	6OU	O26-C27-C28-N29

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Mol	Chain	Res	Type	Atoms
2	B	2001	6OU	C33-C31-O30-C20
2	C	2001	6OU	C21-O22-P23-O24
2	C	2001	6OU	C21-O22-P23-O25
2	C	2001	6OU	C21-O22-P23-O26
2	C	2001	6OU	C27-O26-P23-O22
2	C	2001	6OU	C27-O26-P23-O25
2	C	2001	6OU	O26-C27-C28-N29
2	C	2001	6OU	C33-C31-O30-C20
2	D	2001	6OU	C21-O22-P23-O24
2	D	2001	6OU	C21-O22-P23-O25
2	D	2001	6OU	C21-O22-P23-O26
2	D	2001	6OU	C27-O26-P23-O22
2	D	2001	6OU	C27-O26-P23-O25
2	D	2001	6OU	O26-C27-C28-N29
2	D	2001	6OU	C33-C31-O30-C20
3	A	2004	LBN	C1-O1-P1-O2
3	A	2004	LBN	C1-O1-P1-O3
3	A	2004	LBN	N1-C6-C9-O2
3	B	2004	LBN	C1-O1-P1-O2
3	B	2004	LBN	C1-O1-P1-O3
3	B	2004	LBN	N1-C6-C9-O2
3	C	2004	LBN	C1-O1-P1-O2
3	C	2004	LBN	C1-O1-P1-O3
3	C	2004	LBN	N1-C6-C9-O2
3	D	2004	LBN	C1-O1-P1-O2
3	D	2004	LBN	C1-O1-P1-O3
3	D	2004	LBN	N1-C6-C9-O2
5	A	2201	PX2	C17-C16-O7-C2
5	B	2201	PX2	C17-C16-O7-C2
5	C	2201	PX2	C17-C16-O7-C2
5	D	2201	PX2	C17-C16-O7-C2
5	A	2201	PX2	O6-C4-O5-C3
5	B	2201	PX2	O6-C4-O5-C3
5	C	2201	PX2	O6-C4-O5-C3
5	D	2201	PX2	O6-C4-O5-C3
2	A	2001	6OU	O32-C31-O30-C20
2	B	2001	6OU	O32-C31-O30-C20
2	C	2001	6OU	O32-C31-O30-C20
2	D	2001	6OU	O32-C31-O30-C20
2	A	2001	6OU	C15-C16-O18-C19
2	B	2001	6OU	C15-C16-O18-C19
2	C	2001	6OU	C15-C16-O18-C19

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Mol	Chain	Res	Type	Atoms
2	D	2001	6OU	C15-C16-O18-C19
4	A	2102	Y01	CAC-CBB-CBE-CBI
4	B	2102	Y01	CAC-CBB-CBE-CBI
4	C	2102	Y01	CAC-CBB-CBE-CBI
4	D	2102	Y01	CAC-CBB-CBE-CBI
4	A	2102	Y01	CAO-CBB-CBE-CBI
4	B	2102	Y01	CAO-CBB-CBE-CBI
4	C	2102	Y01	CAO-CBB-CBE-CBI
4	D	2102	Y01	CAO-CBB-CBE-CBI
5	A	2201	PX2	C5-C4-O5-C3
5	B	2201	PX2	C5-C4-O5-C3
5	C	2201	PX2	C5-C4-O5-C3
5	D	2201	PX2	C5-C4-O5-C3
2	A	2001	6OU	O17-C16-O18-C19
2	B	2001	6OU	O17-C16-O18-C19
2	C	2001	6OU	O17-C16-O18-C19
2	D	2001	6OU	O17-C16-O18-C19
5	A	2201	PX2	O8-C16-O7-C2
5	B	2201	PX2	O8-C16-O7-C2
5	C	2201	PX2	O8-C16-O7-C2
5	D	2201	PX2	O8-C16-O7-C2
3	A	2004	LBN	C34-C35-C36-C37
3	B	2004	LBN	C34-C35-C36-C37
3	C	2004	LBN	C34-C35-C36-C37
3	D	2004	LBN	C34-C35-C36-C37
2	A	2001	6OU	C13-C14-C15-C16
2	B	2001	6OU	C13-C14-C15-C16
2	C	2001	6OU	C13-C14-C15-C16
2	D	2001	6OU	C13-C14-C15-C16
4	A	2102	Y01	CAN-CAJ-CAO-CBB
4	B	2102	Y01	CAN-CAJ-CAO-CBB
4	C	2102	Y01	CAN-CAJ-CAO-CBB
4	D	2102	Y01	CAN-CAJ-CAO-CBB
4	A	2102	Y01	CAC-CBB-CBE-CAP
4	B	2102	Y01	CAC-CBB-CBE-CAP
4	C	2102	Y01	CAC-CBB-CBE-CAP
4	D	2102	Y01	CAC-CBB-CBE-CAP
5	A	2201	PX2	C3-C2-O7-C16
5	B	2201	PX2	C3-C2-O7-C16
5	C	2201	PX2	C3-C2-O7-C16
5	D	2201	PX2	C3-C2-O7-C16
4	A	2101	Y01	CAN-CAJ-CAO-CBB

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Mol	Chain	Res	Type	Atoms
4	B	2101	Y01	CAN-CAJ-CAO-CBB
4	C	2101	Y01	CAN-CAJ-CAO-CBB
4	D	2101	Y01	CAN-CAJ-CAO-CBB
2	C	2001	6OU	C42-C43-C44-C45
2	A	2001	6OU	C42-C43-C44-C45
2	B	2001	6OU	C42-C43-C44-C45
2	D	2001	6OU	C42-C43-C44-C45
3	A	2004	LBN	C25-C26-C27-C28
3	B	2004	LBN	C25-C26-C27-C28
3	C	2004	LBN	C25-C26-C27-C28
3	D	2004	LBN	C25-C26-C27-C28
3	B	2004	LBN	C30-C31-C32-C33
3	C	2004	LBN	C30-C31-C32-C33
2	A	2001	6OU	C35-C36-C37-C38
2	B	2001	6OU	C35-C36-C37-C38
2	C	2001	6OU	C35-C36-C37-C38
2	D	2001	6OU	C35-C36-C37-C38
3	A	2004	LBN	C30-C31-C32-C33
3	D	2004	LBN	C30-C31-C32-C33
3	A	2004	LBN	C29-C30-C31-C32
3	B	2004	LBN	C29-C30-C31-C32
3	C	2004	LBN	C29-C30-C31-C32
3	D	2004	LBN	C29-C30-C31-C32
3	A	2004	LBN	C31-C32-C33-C4
3	B	2004	LBN	C31-C32-C33-C4
3	C	2004	LBN	C31-C32-C33-C4
3	D	2004	LBN	C31-C32-C33-C4
3	A	2004	LBN	C35-C34-O7-C2
3	B	2004	LBN	C35-C34-O7-C2
3	C	2004	LBN	C35-C34-O7-C2
4	A	2102	Y01	CAM-CAY-OAW-CBC
4	B	2102	Y01	CAM-CAY-OAW-CBC
4	C	2102	Y01	CAM-CAY-OAW-CBC
4	D	2102	Y01	CAM-CAY-OAW-CBC
2	A	2001	6OU	C41-C42-C43-C44
2	B	2001	6OU	C41-C42-C43-C44
2	C	2001	6OU	C41-C42-C43-C44
2	D	2001	6OU	C41-C42-C43-C44
4	A	2101	Y01	CAJ-CAN-CBA-CAA
4	B	2101	Y01	CAJ-CAN-CBA-CAA
4	C	2101	Y01	CAJ-CAN-CBA-CAA
4	D	2101	Y01	CAJ-CAN-CBA-CAA

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Mol	Chain	Res	Type	Atoms
2	A	2001	6OU	C07-C08-C09-C10
2	B	2001	6OU	C07-C08-C09-C10
2	C	2001	6OU	C07-C08-C09-C10
2	D	2001	6OU	C07-C08-C09-C10
3	D	2004	LBN	C35-C34-O7-C2
3	A	2004	LBN	O1-C1-C2-C3
3	B	2004	LBN	O1-C1-C2-C3
3	C	2004	LBN	O1-C1-C2-C3
3	D	2004	LBN	O1-C1-C2-C3
4	A	2102	Y01	OAG-CAY-OAW-CBC
4	B	2102	Y01	OAG-CAY-OAW-CBC
4	C	2102	Y01	OAG-CAY-OAW-CBC
4	D	2102	Y01	OAG-CAY-OAW-CBC
5	B	2201	PX2	C11-C10-C9-C8
5	D	2201	PX2	C11-C10-C9-C8
5	A	2201	PX2	C11-C10-C9-C8
5	C	2201	PX2	C11-C10-C9-C8
2	A	2001	6OU	C08-C09-C10-C11
2	B	2001	6OU	C08-C09-C10-C11
2	C	2001	6OU	C08-C09-C10-C11
2	D	2001	6OU	C08-C09-C10-C11
2	B	2001	6OU	C45-C46-C47-C48
2	D	2001	6OU	C45-C46-C47-C48
2	A	2001	6OU	C45-C46-C47-C48
2	C	2001	6OU	C45-C46-C47-C48
2	A	2001	6OU	C04-C05-C06-C07
2	B	2001	6OU	C04-C05-C06-C07
2	C	2001	6OU	C04-C05-C06-C07
2	D	2001	6OU	C04-C05-C06-C07
3	A	2004	LBN	O8-C34-O7-C2
3	B	2004	LBN	O8-C34-O7-C2
3	C	2004	LBN	O8-C34-O7-C2
3	D	2004	LBN	O8-C34-O7-C2
2	A	2001	6OU	C05-C06-C07-C08
2	B	2001	6OU	C05-C06-C07-C08
2	D	2001	6OU	C05-C06-C07-C08
2	C	2001	6OU	C05-C06-C07-C08
5	A	2201	PX2	C5-C6-C7-C8
5	B	2201	PX2	C5-C6-C7-C8
5	C	2201	PX2	C5-C6-C7-C8
5	D	2201	PX2	C5-C6-C7-C8
3	B	2004	LBN	C27-C28-C29-C30

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Mol	Chain	Res	Type	Atoms
3	C	2004	LBN	C27-C28-C29-C30
3	A	2004	LBN	C27-C28-C29-C30
3	D	2004	LBN	C27-C28-C29-C30
4	A	2102	Y01	CAO-CBB-CBE-CAP
4	B	2102	Y01	CAO-CBB-CBE-CAP
4	C	2102	Y01	CAO-CBB-CBE-CAP
4	D	2102	Y01	CAO-CBB-CBE-CAP
5	A	2201	PX2	C10-C11-C12-C13
5	B	2201	PX2	C10-C11-C12-C13
5	D	2201	PX2	C10-C11-C12-C13
5	C	2201	PX2	C10-C11-C12-C13
3	A	2004	LBN	C2-C1-O1-P1
3	B	2004	LBN	C2-C1-O1-P1
3	C	2004	LBN	C2-C1-O1-P1
3	D	2004	LBN	C2-C1-O1-P1
5	A	2201	PX2	C17-C18-C19-C20
5	B	2201	PX2	C17-C18-C19-C20
5	C	2201	PX2	C17-C18-C19-C20
5	D	2201	PX2	C17-C18-C19-C20
3	C	2004	LBN	C26-C25-O5-C3
3	A	2004	LBN	C36-C37-C38-C39
3	B	2004	LBN	C36-C37-C38-C39
3	C	2004	LBN	C36-C37-C38-C39
3	D	2004	LBN	C36-C37-C38-C39
3	A	2004	LBN	C26-C25-O5-C3
3	B	2004	LBN	C26-C25-O5-C3
3	D	2004	LBN	C26-C25-O5-C3
4	B	2101	Y01	CAJ-CAN-CBA-CAB
3	A	2004	LBN	O6-C25-O5-C3
3	B	2004	LBN	O6-C25-O5-C3
3	C	2004	LBN	O6-C25-O5-C3
3	D	2004	LBN	O6-C25-O5-C3
4	A	2101	Y01	CAJ-CAN-CBA-CAB
4	C	2101	Y01	CAJ-CAN-CBA-CAB
4	D	2101	Y01	CAJ-CAN-CBA-CAB
2	A	2001	6OU	O30-C20-C21-O22
2	B	2001	6OU	O30-C20-C21-O22
2	C	2001	6OU	O30-C20-C21-O22
2	D	2001	6OU	O30-C20-C21-O22
5	A	2201	PX2	C20-C21-C22-C23
5	B	2201	PX2	C20-C21-C22-C23
2	A	2001	6OU	C11-C12-C13-C14

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Mol	Chain	Res	Type	Atoms
2	B	2001	6OU	C11-C12-C13-C14
2	C	2001	6OU	C11-C12-C13-C14
2	D	2001	6OU	C11-C12-C13-C14
5	D	2201	PX2	C20-C21-C22-C23
5	C	2201	PX2	C20-C21-C22-C23
2	A	2001	6OU	C19-C20-C21-O22
2	B	2001	6OU	C19-C20-C21-O22
2	C	2001	6OU	C19-C20-C21-O22
2	D	2001	6OU	C19-C20-C21-O22
2	A	2001	6OU	C43-C44-C45-C46
2	D	2001	6OU	C43-C44-C45-C46
2	B	2001	6OU	C43-C44-C45-C46
2	C	2001	6OU	C43-C44-C45-C46
5	A	2201	PX2	C19-C20-C21-C22
3	A	2004	LBN	O1-C1-C2-O7
3	B	2004	LBN	O1-C1-C2-O7
3	C	2004	LBN	O1-C1-C2-O7
3	D	2004	LBN	O1-C1-C2-O7
5	C	2201	PX2	C19-C20-C21-C22
5	D	2201	PX2	C19-C20-C21-C22
5	B	2201	PX2	C19-C20-C21-C22
5	C	2201	PX2	C21-C22-C23-C24
5	B	2201	PX2	C21-C22-C23-C24
3	A	2004	LBN	C42-C5-C8-C11
3	B	2004	LBN	C42-C5-C8-C11
3	C	2004	LBN	C42-C5-C8-C11
3	D	2004	LBN	C42-C5-C8-C11
5	A	2201	PX2	C21-C22-C23-C24
5	D	2201	PX2	C21-C22-C23-C24
2	A	2001	6OU	C27-O26-P23-O24
2	B	2001	6OU	C27-O26-P23-O24
2	C	2001	6OU	C27-O26-P23-O24
2	D	2001	6OU	C27-O26-P23-O24
3	A	2004	LBN	C1-O1-P1-O4
3	B	2004	LBN	C1-O1-P1-O4
3	C	2004	LBN	C1-O1-P1-O4
3	D	2004	LBN	C1-O1-P1-O4
5	A	2201	PX2	C6-C7-C8-C9
5	B	2201	PX2	C6-C7-C8-C9
5	C	2201	PX2	C6-C7-C8-C9
5	D	2201	PX2	C6-C7-C8-C9
4	A	2102	Y01	CAO-CAJ-CAN-CBA

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Mol	Chain	Res	Type	Atoms
4	B	2102	Y01	CAO-CAJ-CAN-CBA
4	C	2102	Y01	CAO-CAJ-CAN-CBA
4	D	2102	Y01	CAO-CAJ-CAN-CBA
5	A	2201	PX2	C23-C24-C25-C26
5	B	2201	PX2	C23-C24-C25-C26
5	C	2201	PX2	C23-C24-C25-C26
5	D	2201	PX2	C23-C24-C25-C26
5	A	2201	PX2	C11-C12-C13-C14
5	D	2201	PX2	C11-C12-C13-C14
5	B	2201	PX2	C11-C12-C13-C14
5	C	2201	PX2	C11-C12-C13-C14
4	A	2102	Y01	CAX-CAL-CAM-CAY
4	B	2102	Y01	CAX-CAL-CAM-CAY
4	C	2102	Y01	CAX-CAL-CAM-CAY
4	D	2102	Y01	CAX-CAL-CAM-CAY
4	A	2101	Y01	CAM-CAL-CAX-OAF
4	B	2101	Y01	CAM-CAL-CAX-OAF
4	C	2101	Y01	CAM-CAL-CAX-OAF
4	D	2101	Y01	CAM-CAL-CAX-OAF
3	D	2004	LBN	C28-C29-C30-C31
3	A	2004	LBN	C28-C29-C30-C31
3	B	2004	LBN	C28-C29-C30-C31
3	C	2004	LBN	C28-C29-C30-C31
5	C	2201	PX2	C22-C23-C24-C25
5	D	2201	PX2	C22-C23-C24-C25
5	A	2201	PX2	C22-C23-C24-C25
5	B	2201	PX2	C22-C23-C24-C25
4	A	2101	Y01	CAM-CAL-CAX-OAH
4	B	2101	Y01	CAM-CAL-CAX-OAH
4	C	2101	Y01	CAM-CAL-CAX-OAH
4	D	2101	Y01	CAM-CAL-CAX-OAH
5	A	2201	PX2	C18-C19-C20-C21
5	C	2201	PX2	C18-C19-C20-C21
5	D	2201	PX2	C18-C19-C20-C21
5	B	2201	PX2	C18-C19-C20-C21
3	A	2004	LBN	C39-C40-C41-C42
3	B	2004	LBN	C39-C40-C41-C42
3	C	2004	LBN	C39-C40-C41-C42
3	D	2004	LBN	C39-C40-C41-C42
4	B	2102	Y01	CAJ-CAN-CBA-CAA
4	C	2102	Y01	CAJ-CAN-CBA-CAA
4	A	2102	Y01	CAJ-CAN-CBA-CAA

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Mol	Chain	Res	Type	Atoms
2	A	2001	6OU	C38-C39-C40-C41
2	B	2001	6OU	C38-C39-C40-C41
2	C	2001	6OU	C38-C39-C40-C41
2	D	2001	6OU	C38-C39-C40-C41
2	C	2001	6OU	C14-C15-C16-O18
2	A	2001	6OU	C14-C15-C16-O18
2	B	2001	6OU	C14-C15-C16-O18
2	D	2001	6OU	C14-C15-C16-O18
4	D	2102	Y01	CAJ-CAN-CBA-CAA
2	A	2001	6OU	C20-C21-O22-P23
2	B	2001	6OU	C20-C21-O22-P23
2	C	2001	6OU	C20-C21-O22-P23
2	D	2001	6OU	C20-C21-O22-P23
4	C	2102	Y01	CAL-CAM-CAY-OAW
4	A	2102	Y01	CAM-CAL-CAX-OAF
4	D	2102	Y01	CAM-CAL-CAX-OAF
4	A	2102	Y01	CAL-CAM-CAY-OAW
4	B	2102	Y01	CAL-CAM-CAY-OAW
4	D	2102	Y01	CAL-CAM-CAY-OAW
4	B	2102	Y01	CAM-CAL-CAX-OAF
4	C	2102	Y01	CAM-CAL-CAX-OAF
4	B	2102	Y01	CAM-CAL-CAX-OAH
4	D	2102	Y01	CAM-CAL-CAX-OAH
4	A	2102	Y01	CAM-CAL-CAX-OAH
4	C	2102	Y01	CAM-CAL-CAX-OAH
2	C	2001	6OU	C14-C15-C16-O17
2	A	2001	6OU	C14-C15-C16-O17
2	B	2001	6OU	C14-C15-C16-O17
2	D	2001	6OU	C14-C15-C16-O17
4	B	2102	Y01	CAJ-CAN-CBA-CAB
4	A	2102	Y01	CAJ-CAN-CBA-CAB
4	C	2102	Y01	CAJ-CAN-CBA-CAB
4	D	2102	Y01	CAJ-CAN-CBA-CAB
3	D	2004	LBN	O5-C25-C26-C27
2	D	2001	6OU	C02-C03-C04-C05
2	B	2001	6OU	C02-C03-C04-C05
2	D	2001	6OU	C03-C04-C05-C06
3	A	2004	LBN	O5-C25-C26-C27
3	B	2004	LBN	O5-C25-C26-C27
3	C	2004	LBN	O5-C25-C26-C27
4	C	2102	Y01	CAL-CAM-CAY-OAG
2	A	2001	6OU	C03-C04-C05-C06

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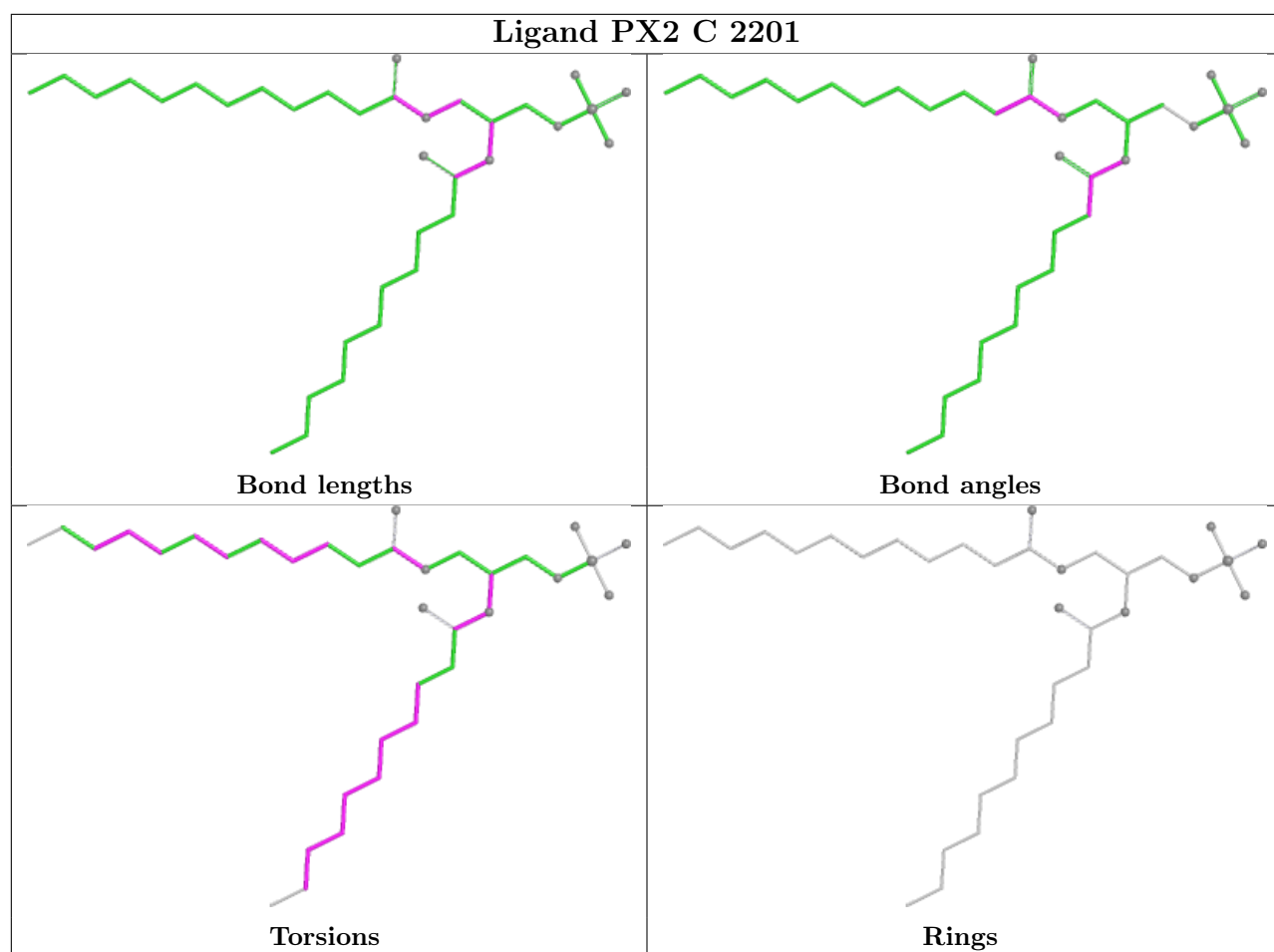
Mol	Chain	Res	Type	Atoms
2	A	2001	6OU	C02-C03-C04-C05
2	C	2001	6OU	C03-C04-C05-C06
4	A	2102	Y01	CAL-CAM-CAY-OAG
4	B	2102	Y01	CAL-CAM-CAY-OAG
4	D	2102	Y01	CAL-CAM-CAY-OAG
2	C	2001	6OU	C02-C03-C04-C05

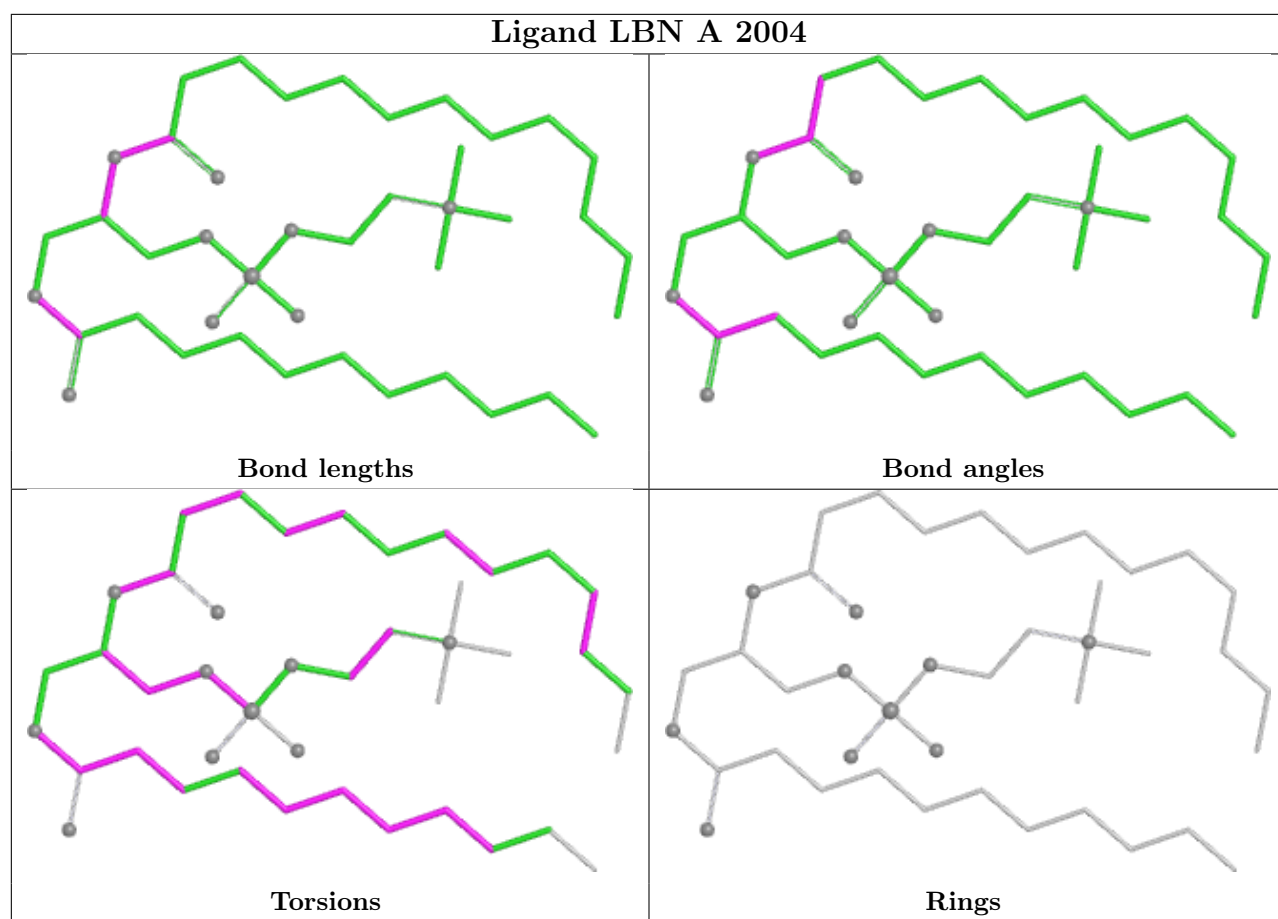
There are no ring outliers.

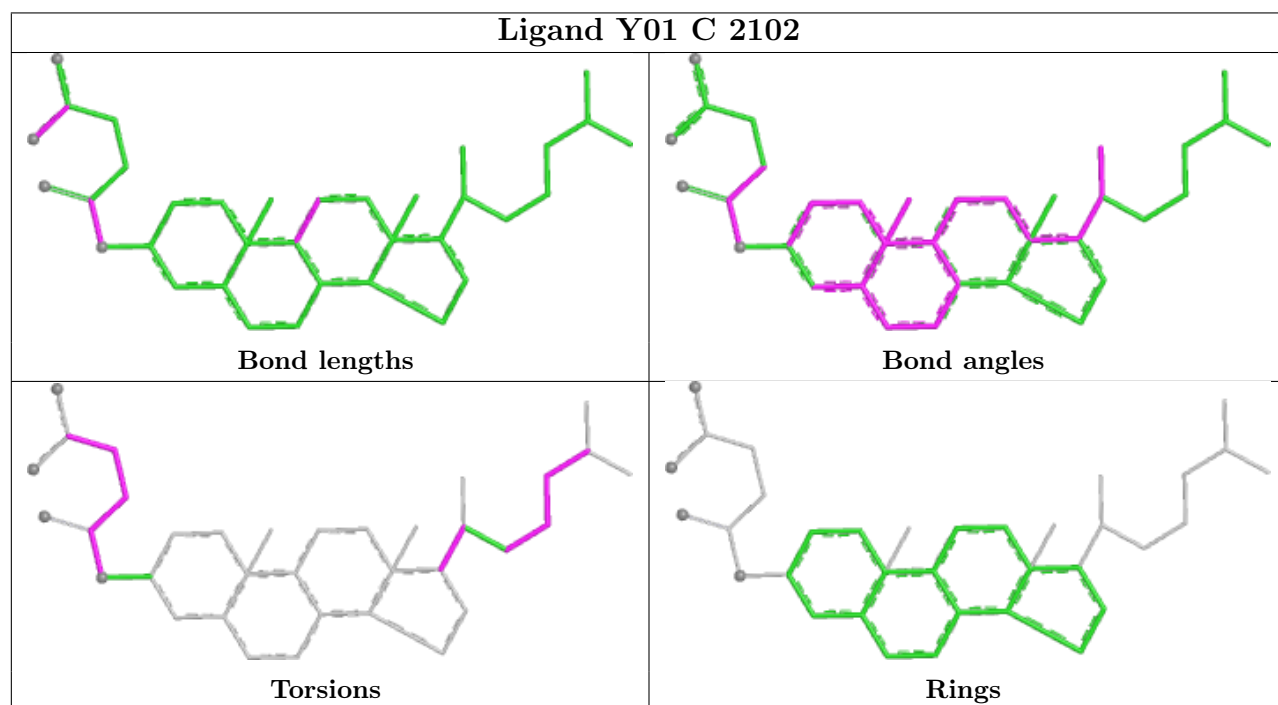
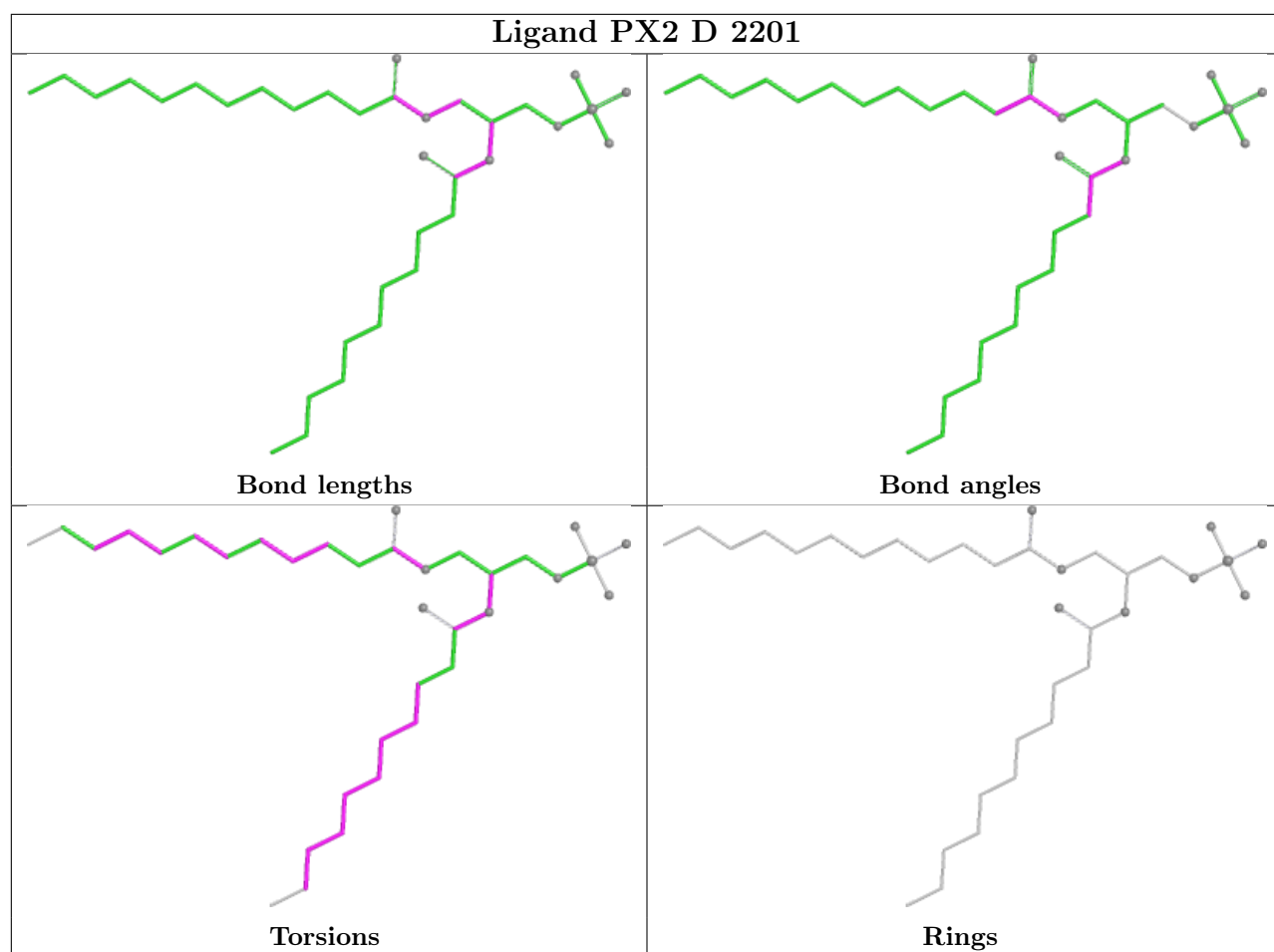
6 monomers are involved in 7 short contacts:

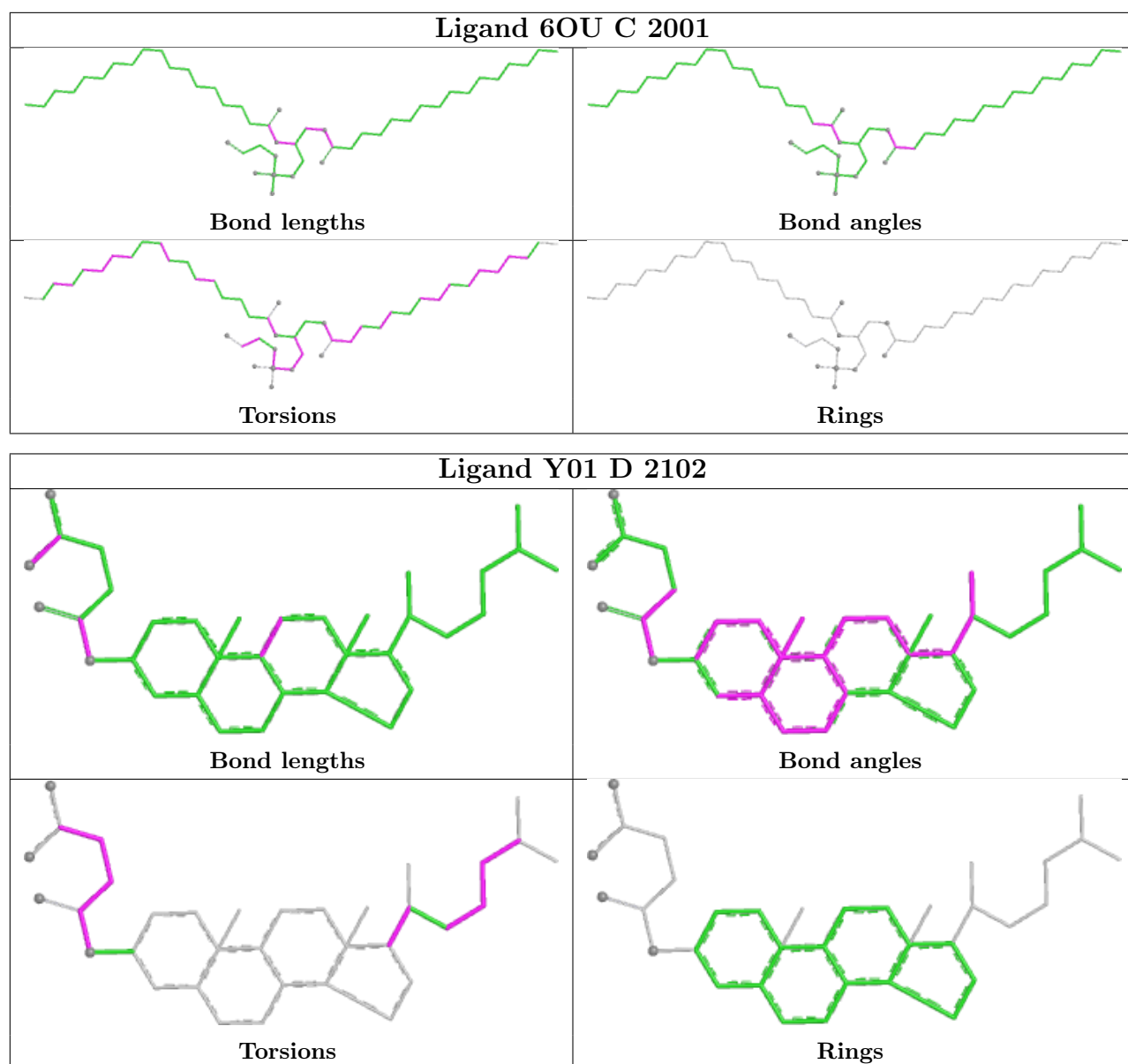
Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	C	2102	Y01	1	0
4	B	2102	Y01	2	0
4	C	2101	Y01	1	0
4	D	2101	Y01	1	0
4	A	2101	Y01	1	0
4	B	2101	Y01	1	0

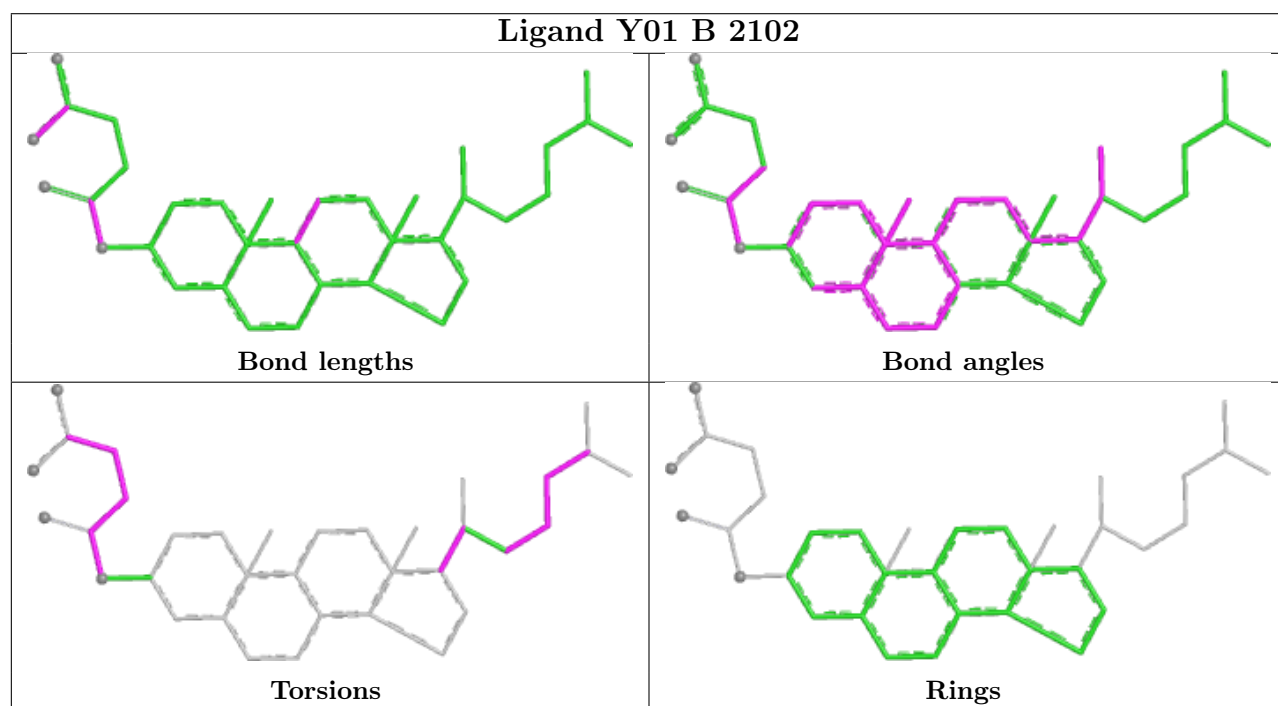
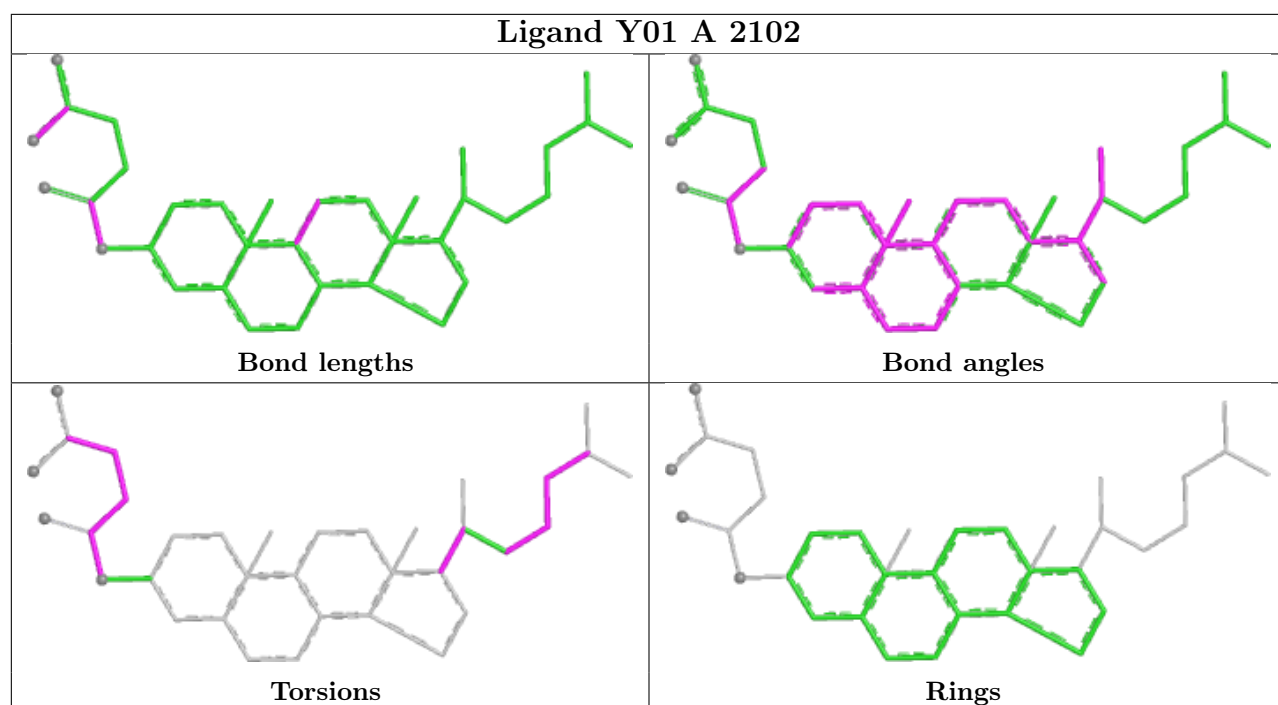
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

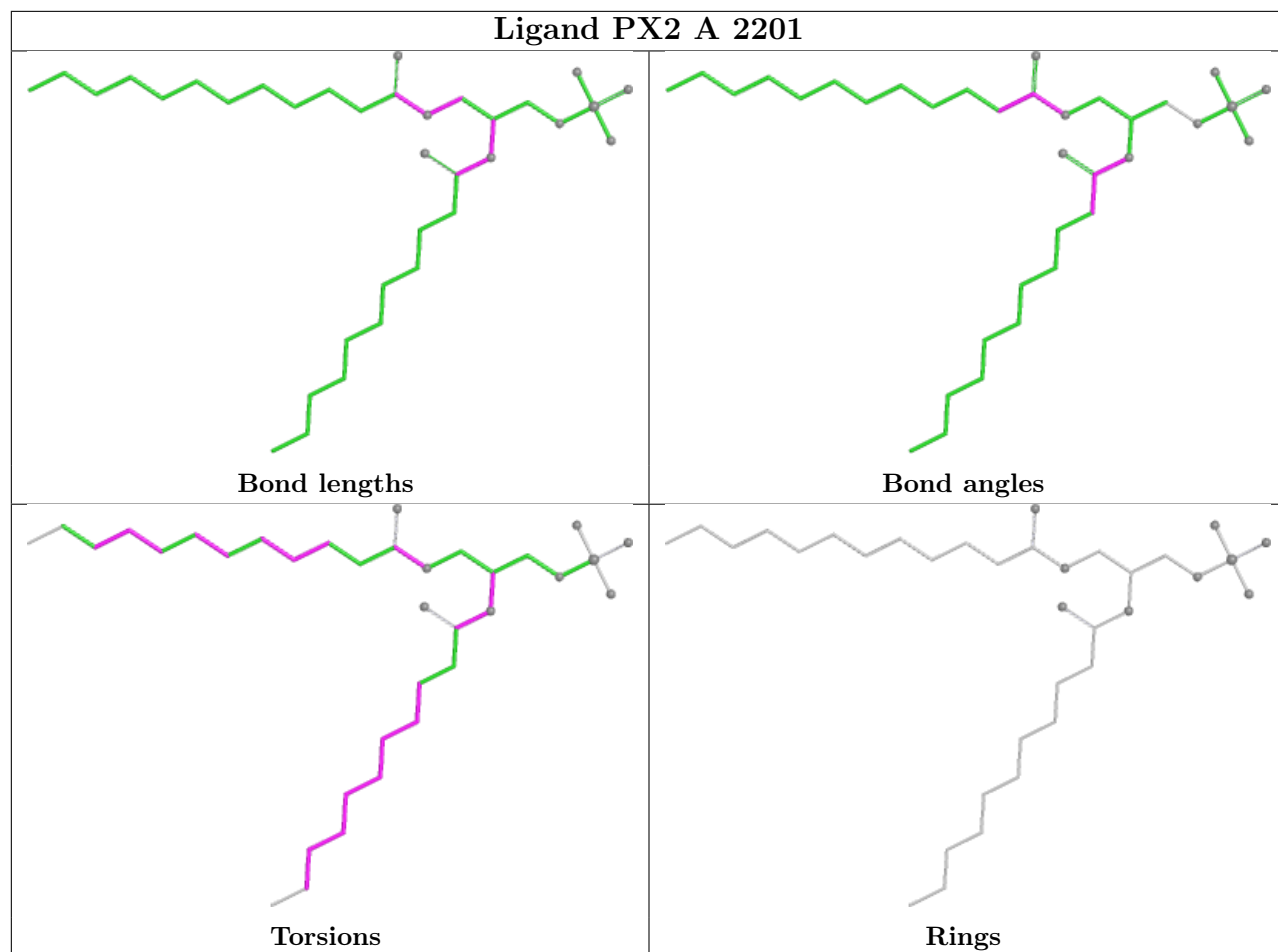


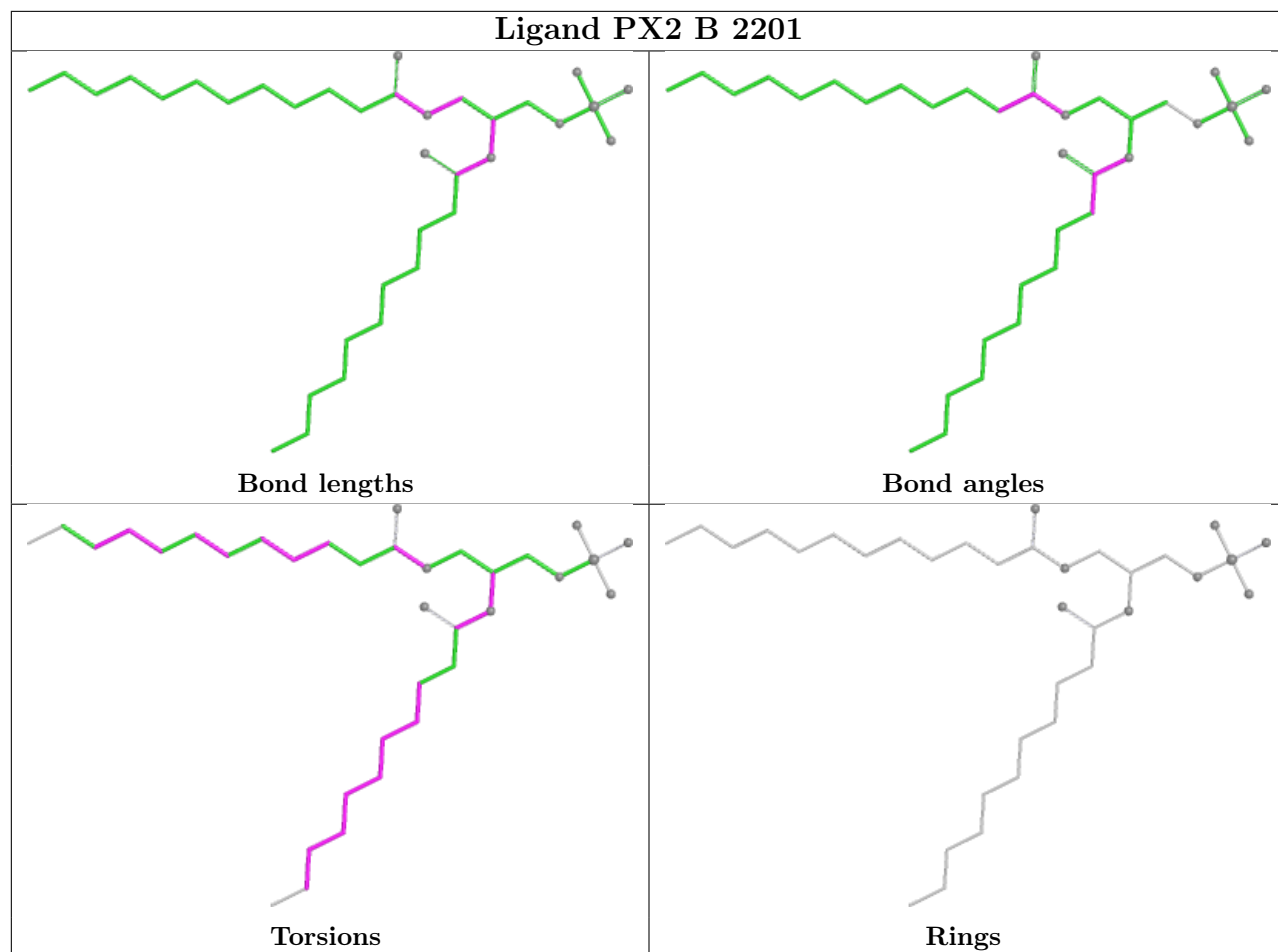


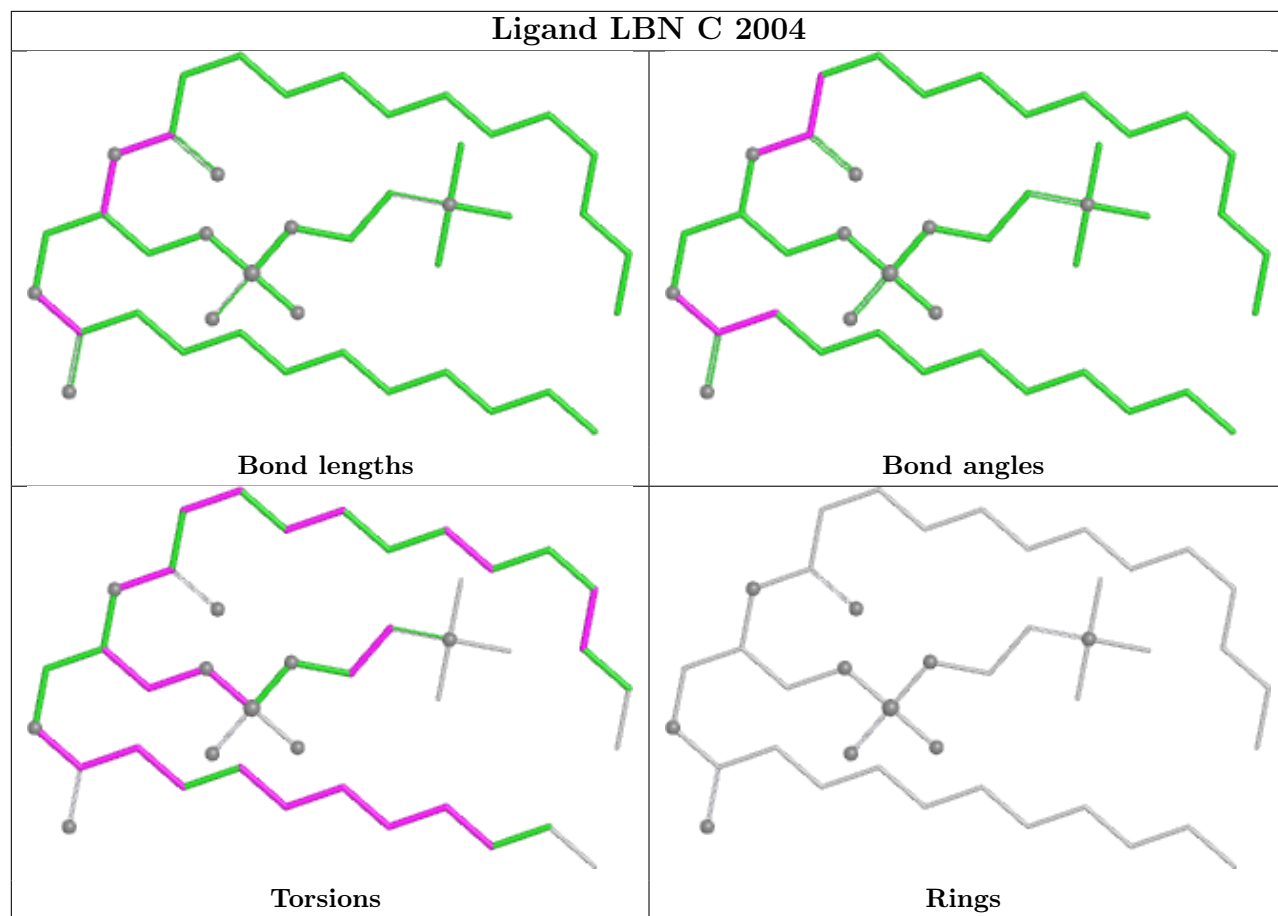


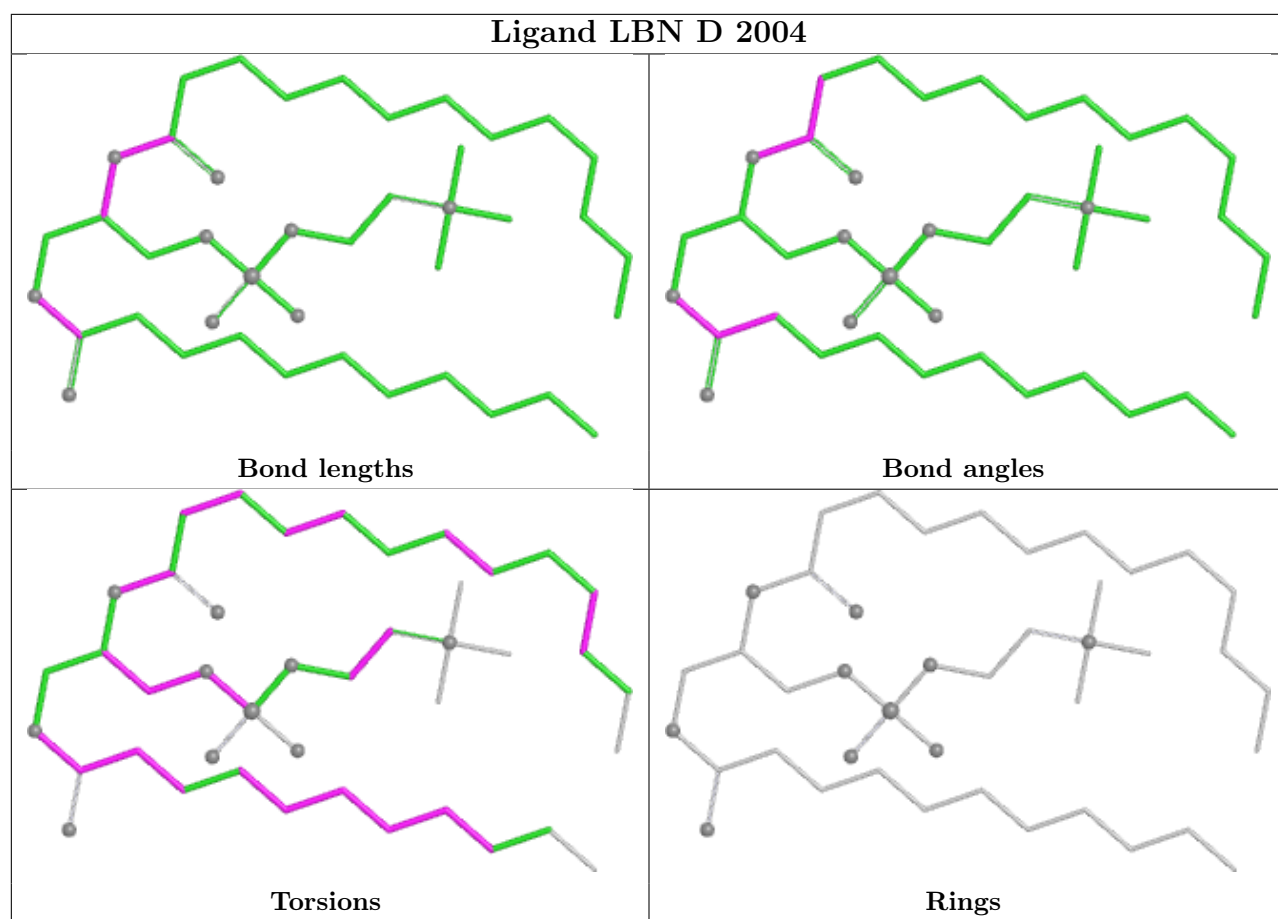


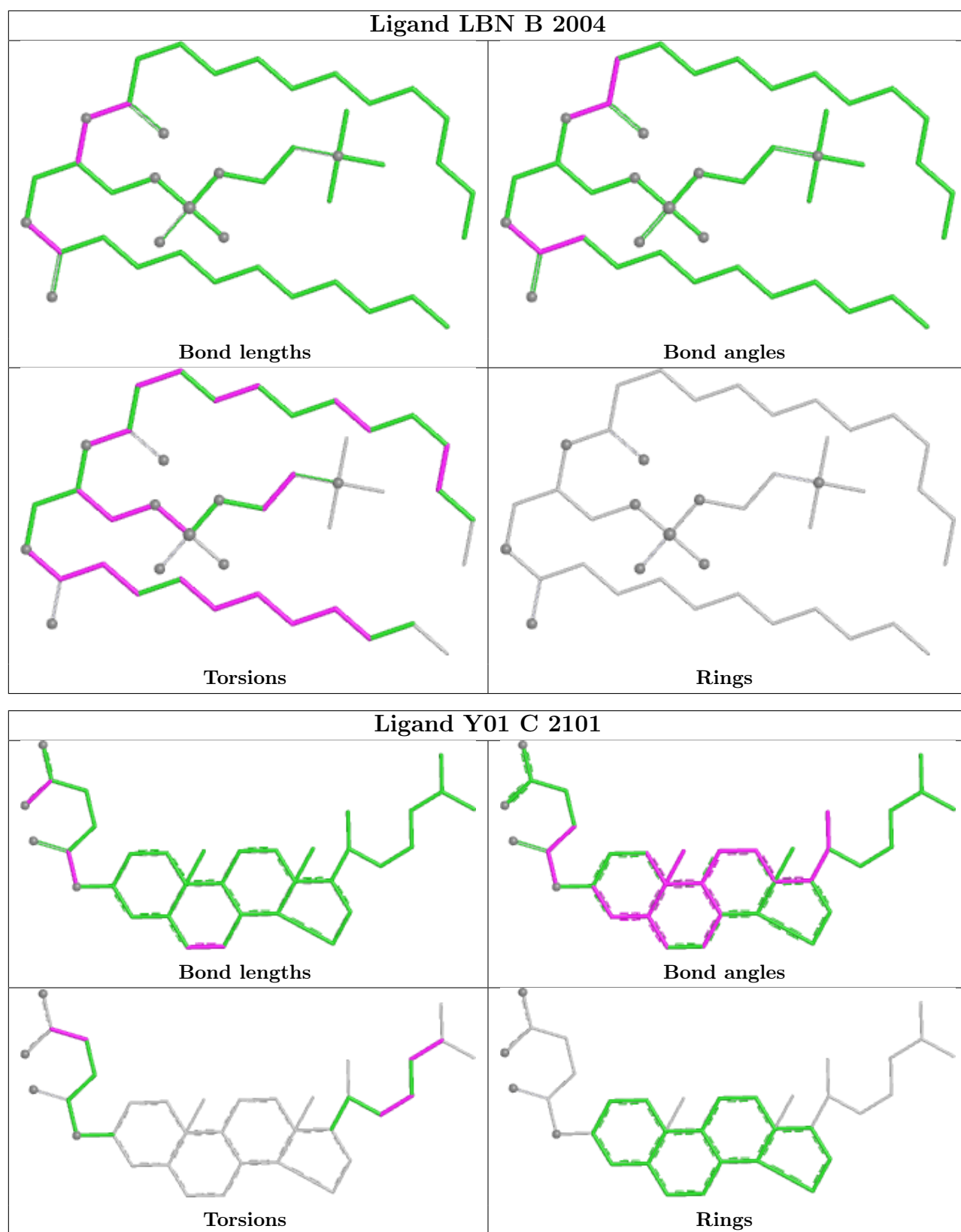


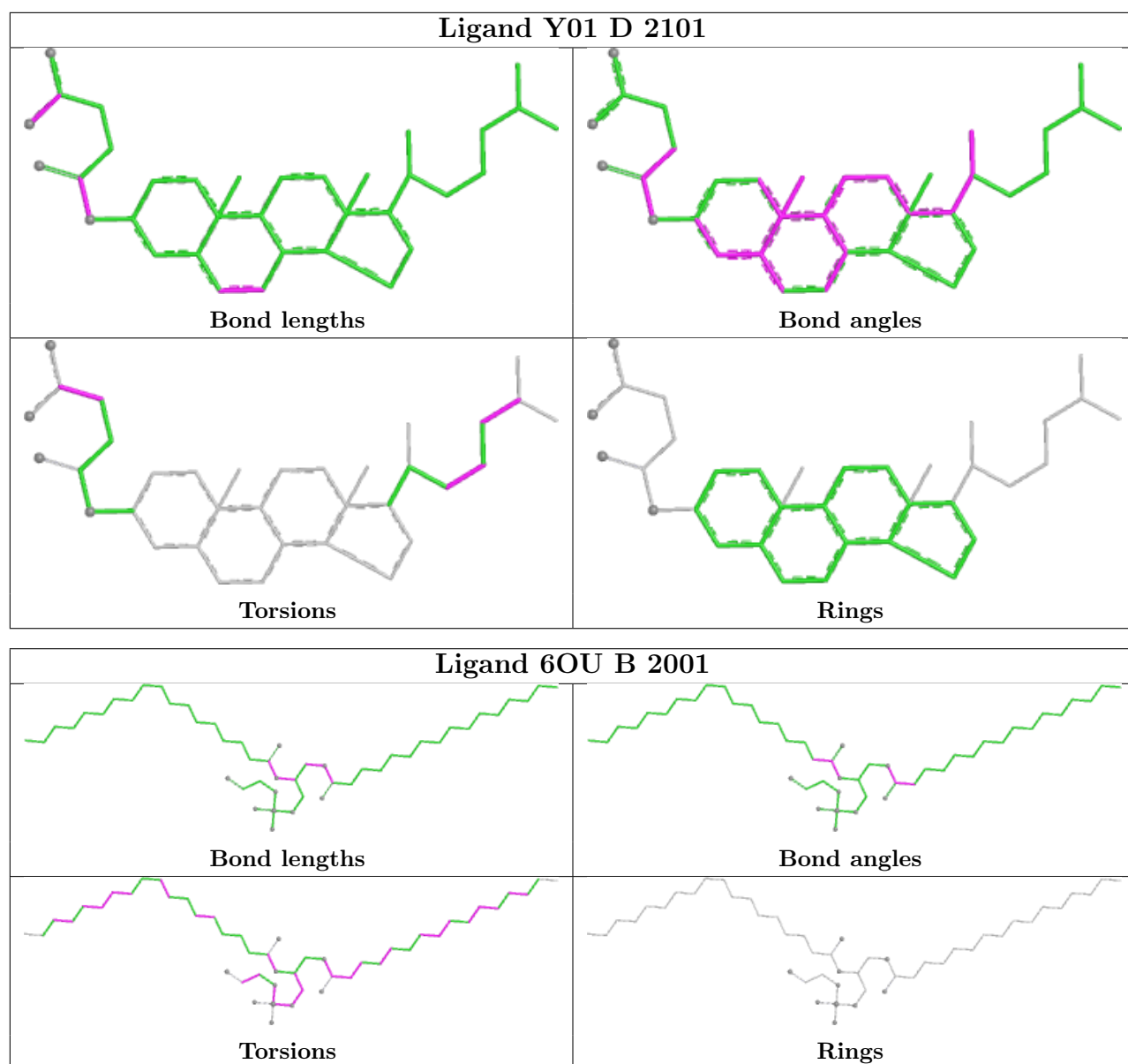


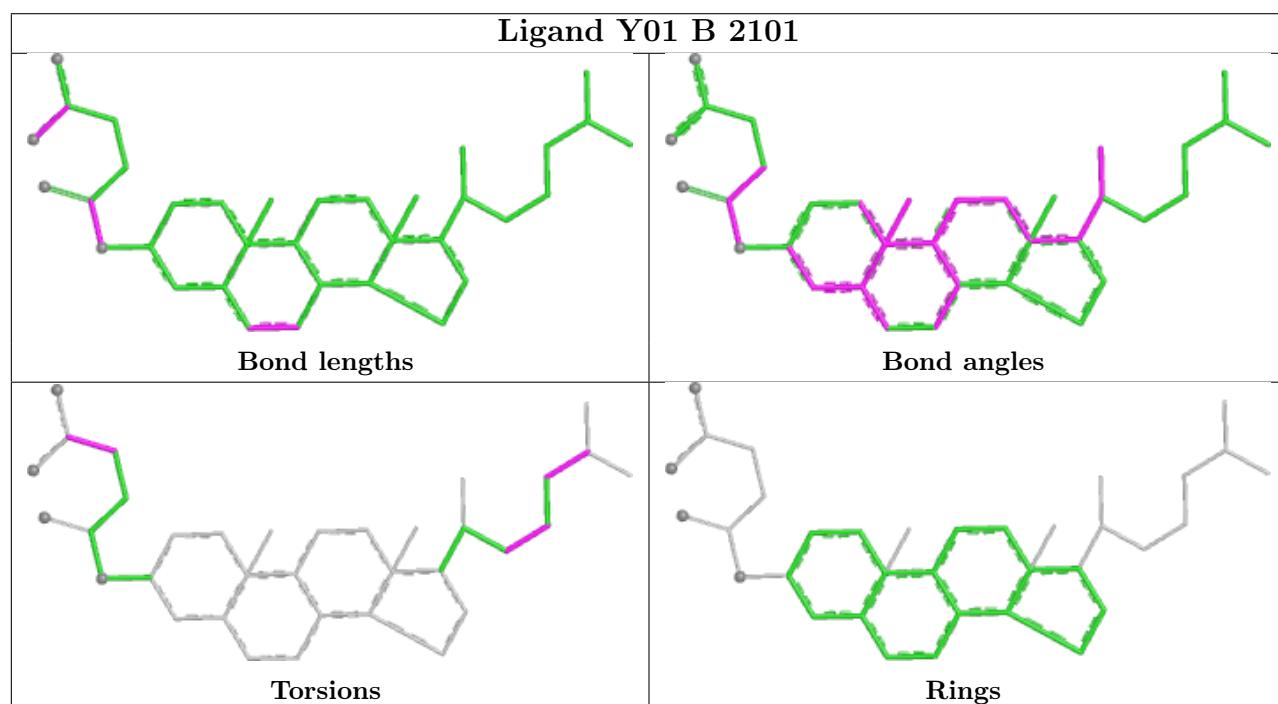
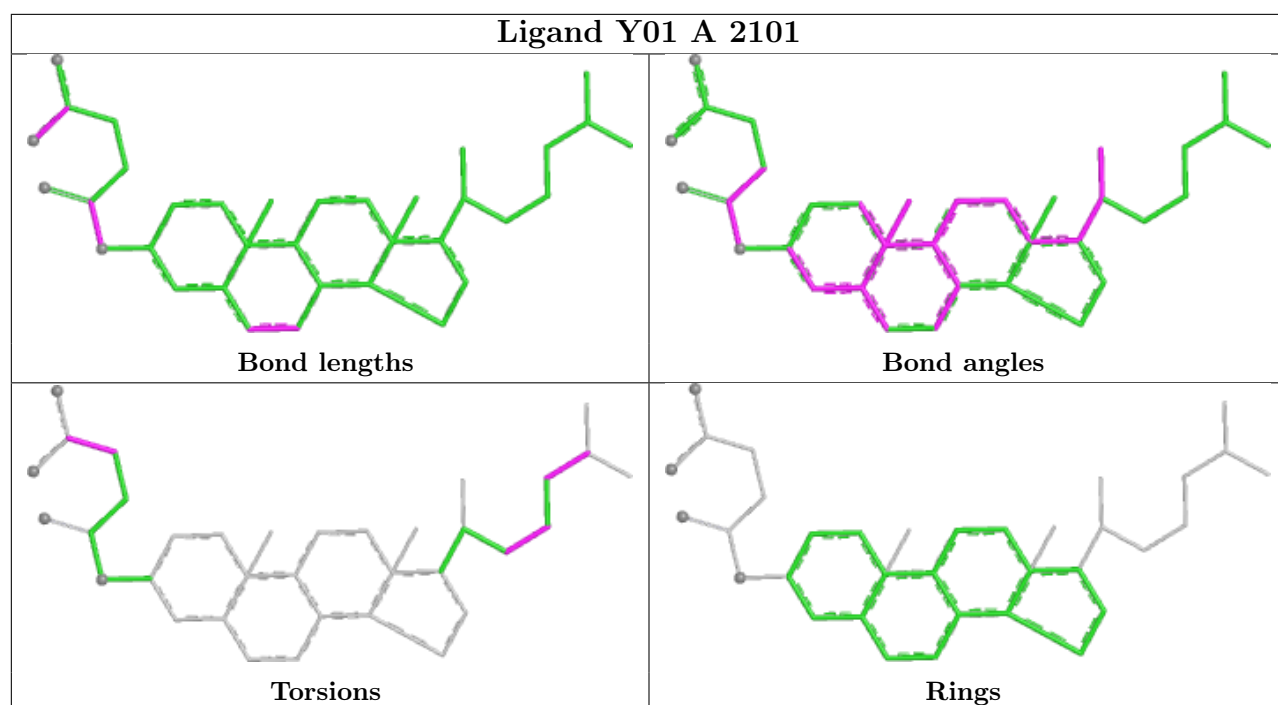


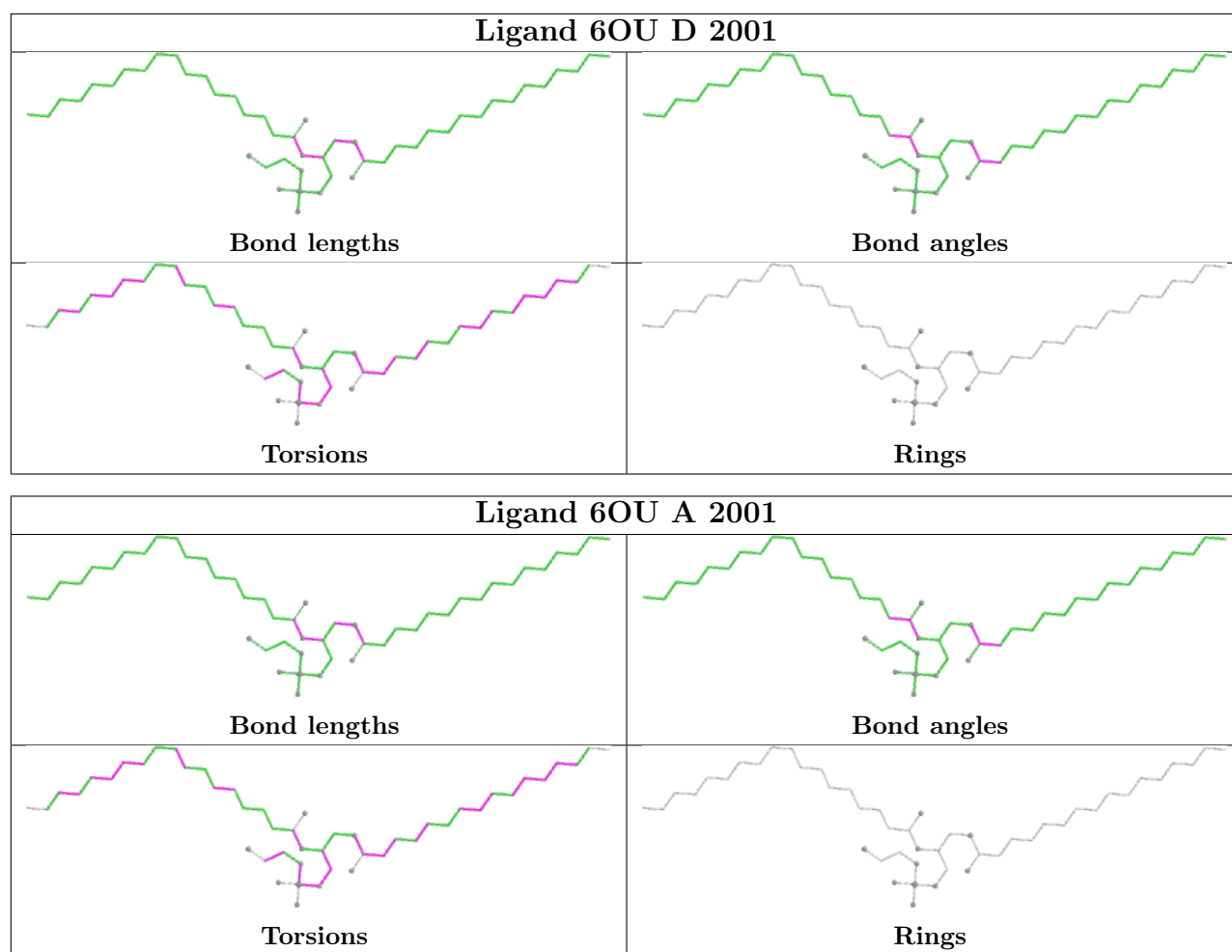












5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

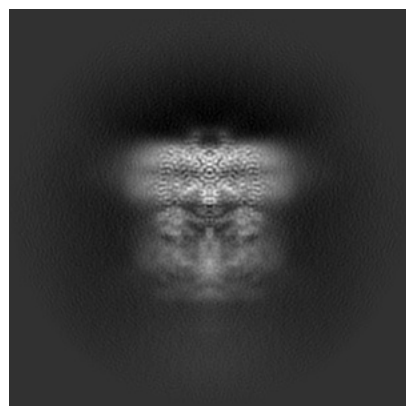
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-44101. These allow visual inspection of the internal detail of the map and identification of artifacts.

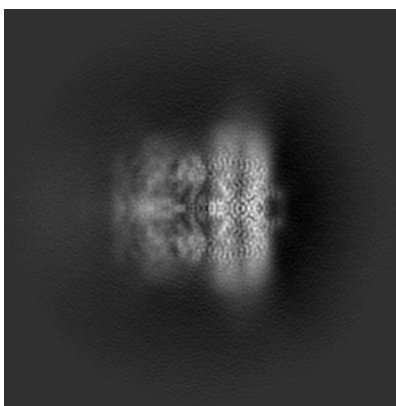
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

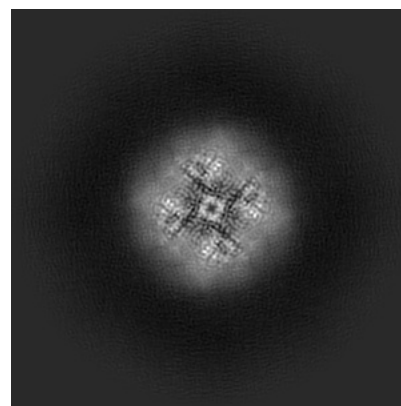
6.1.1 Primary map



X

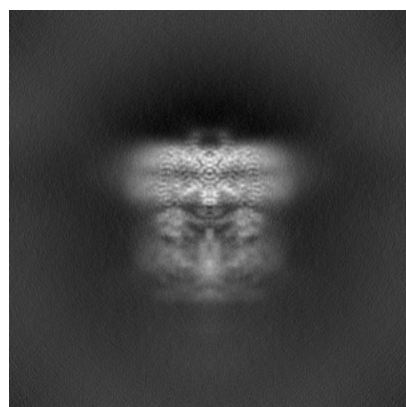


Y

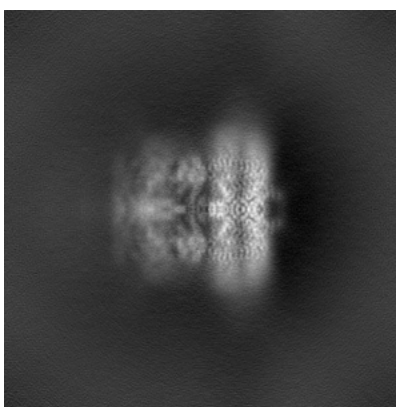


Z

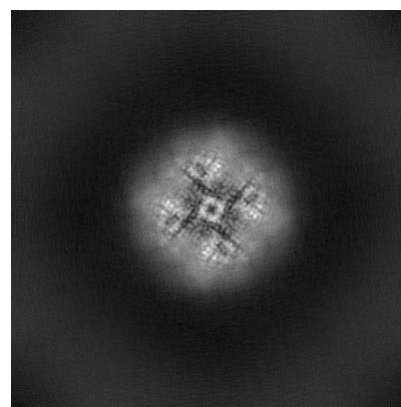
6.1.2 Raw map



X



Y

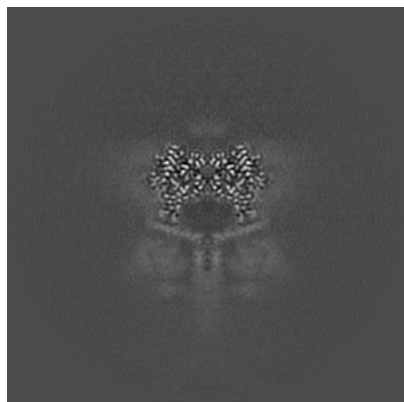


Z

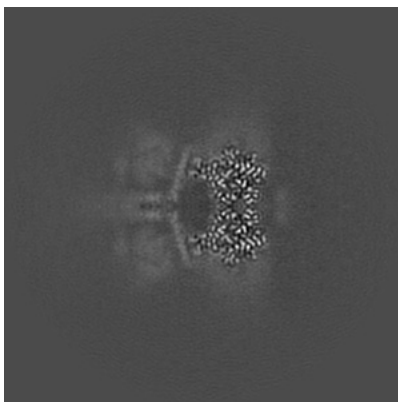
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

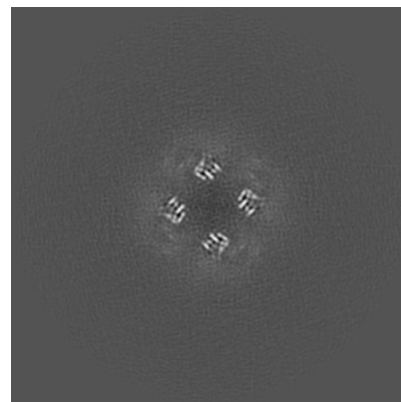
6.2.1 Primary map



X Index: 160

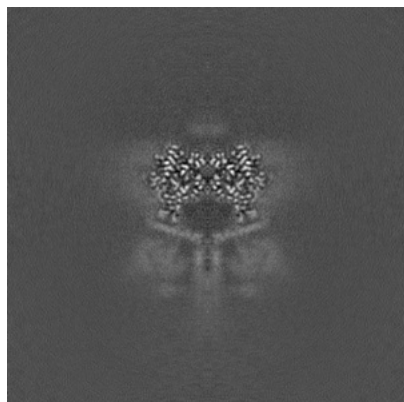


Y Index: 160

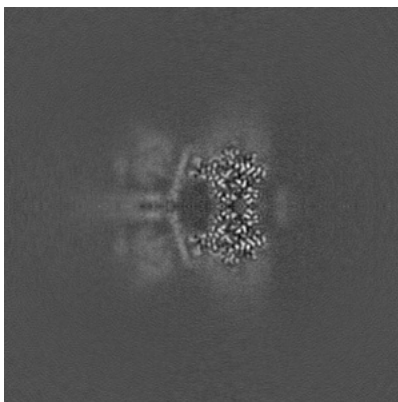


Z Index: 160

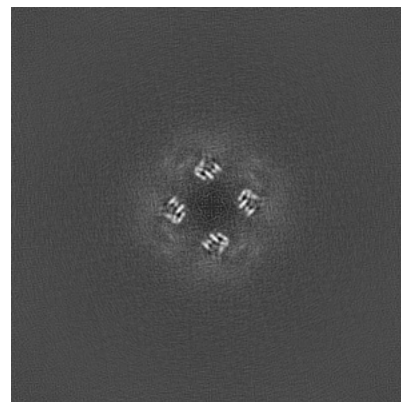
6.2.2 Raw map



X Index: 160



Y Index: 160

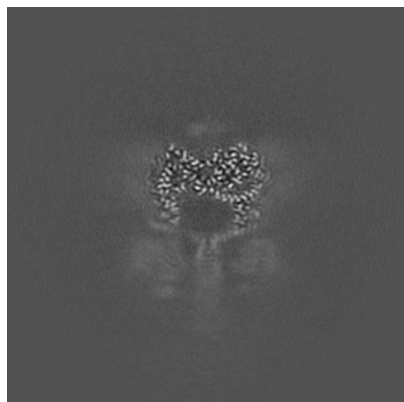


Z Index: 160

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

6.3 Largest variance slices [i](#)

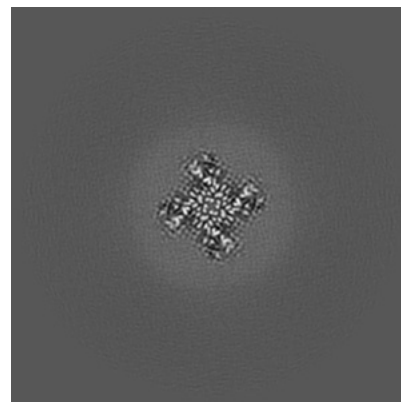
6.3.1 Primary map



X Index: 157

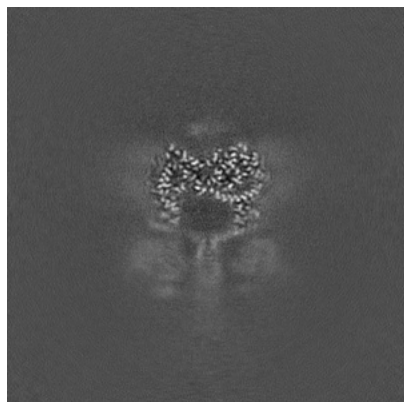


Y Index: 163

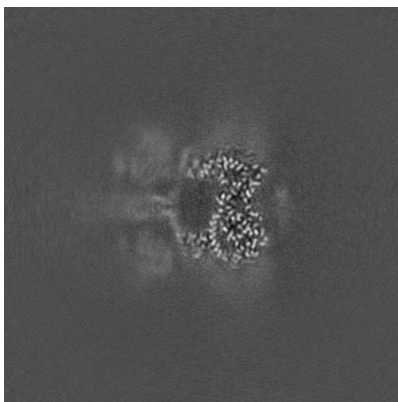


Z Index: 197

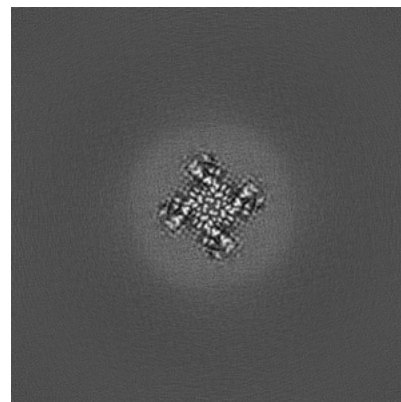
6.3.2 Raw map



X Index: 157



Y Index: 157

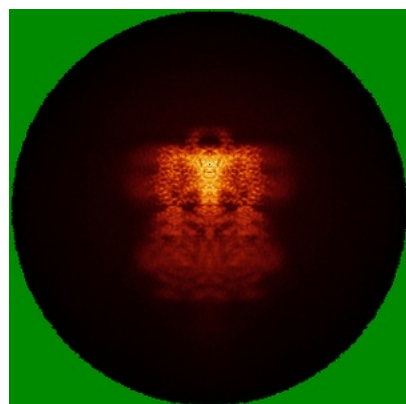


Z Index: 197

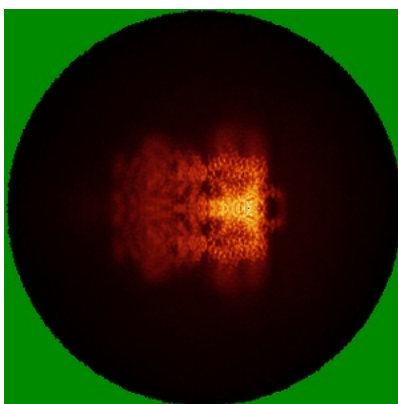
The images above show the largest variance slices of the map in three orthogonal directions.

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

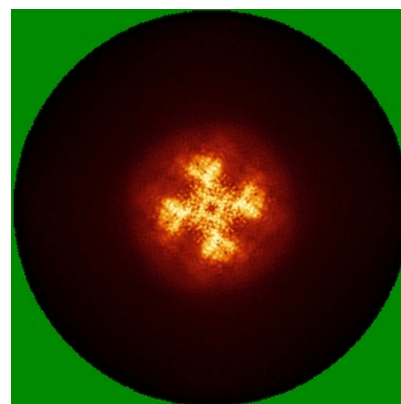
6.4.1 Primary map



X

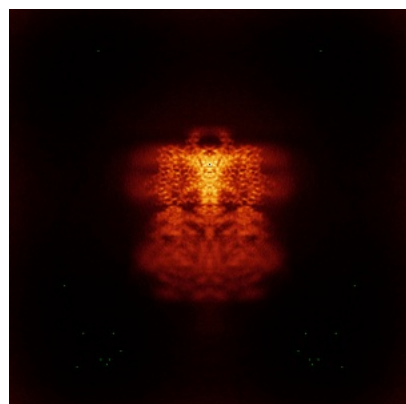


Y

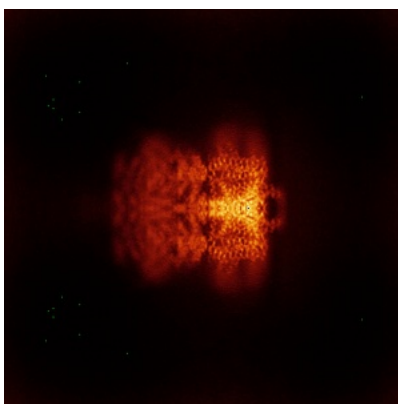


Z

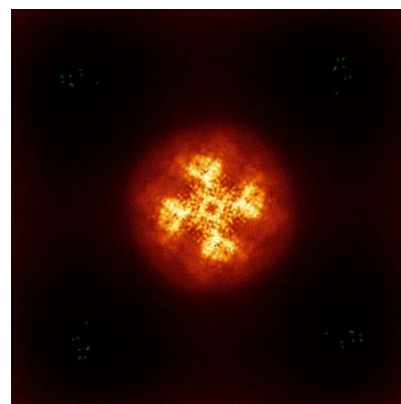
6.4.2 Raw map



X



Y

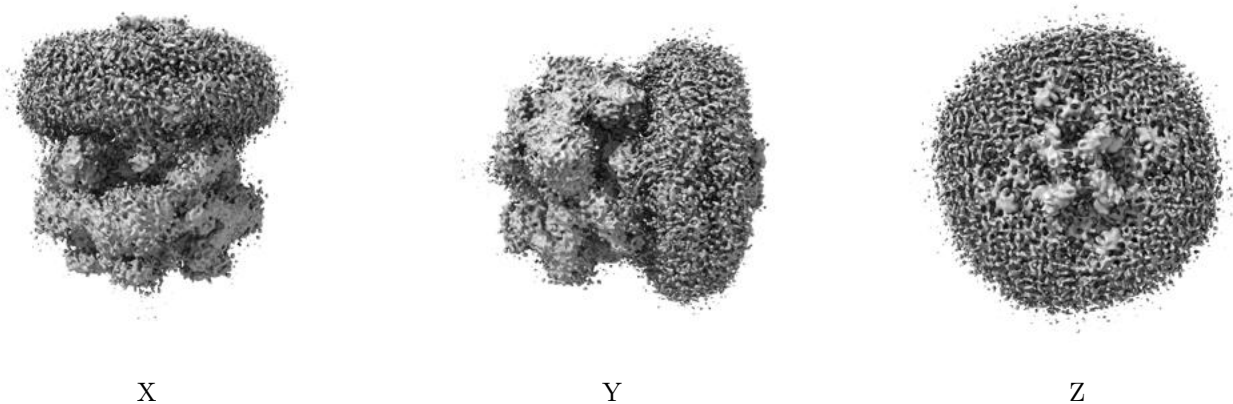


Z

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.

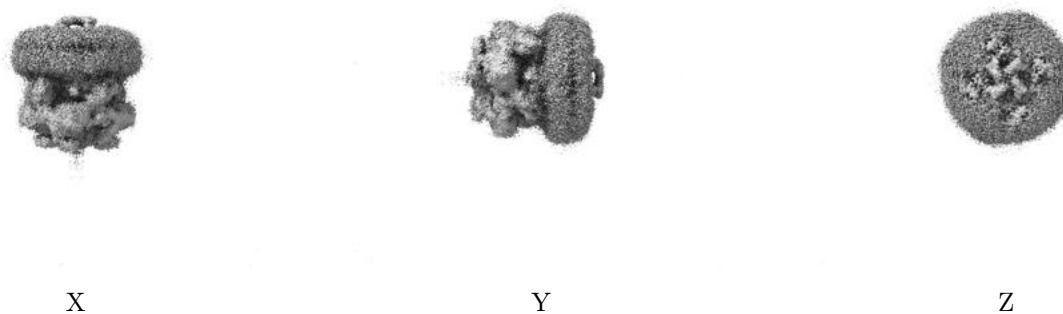
6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.1. 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.

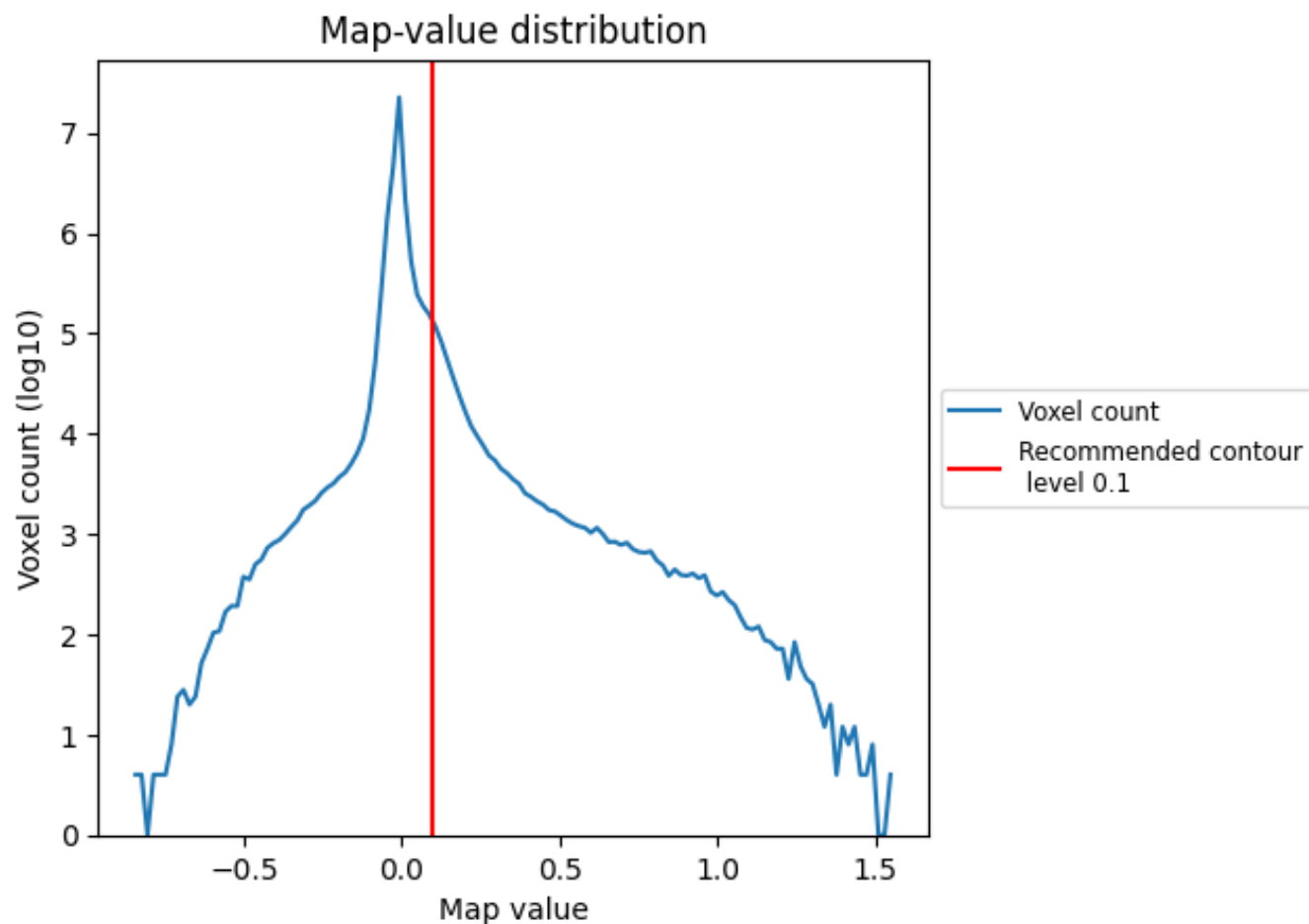
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

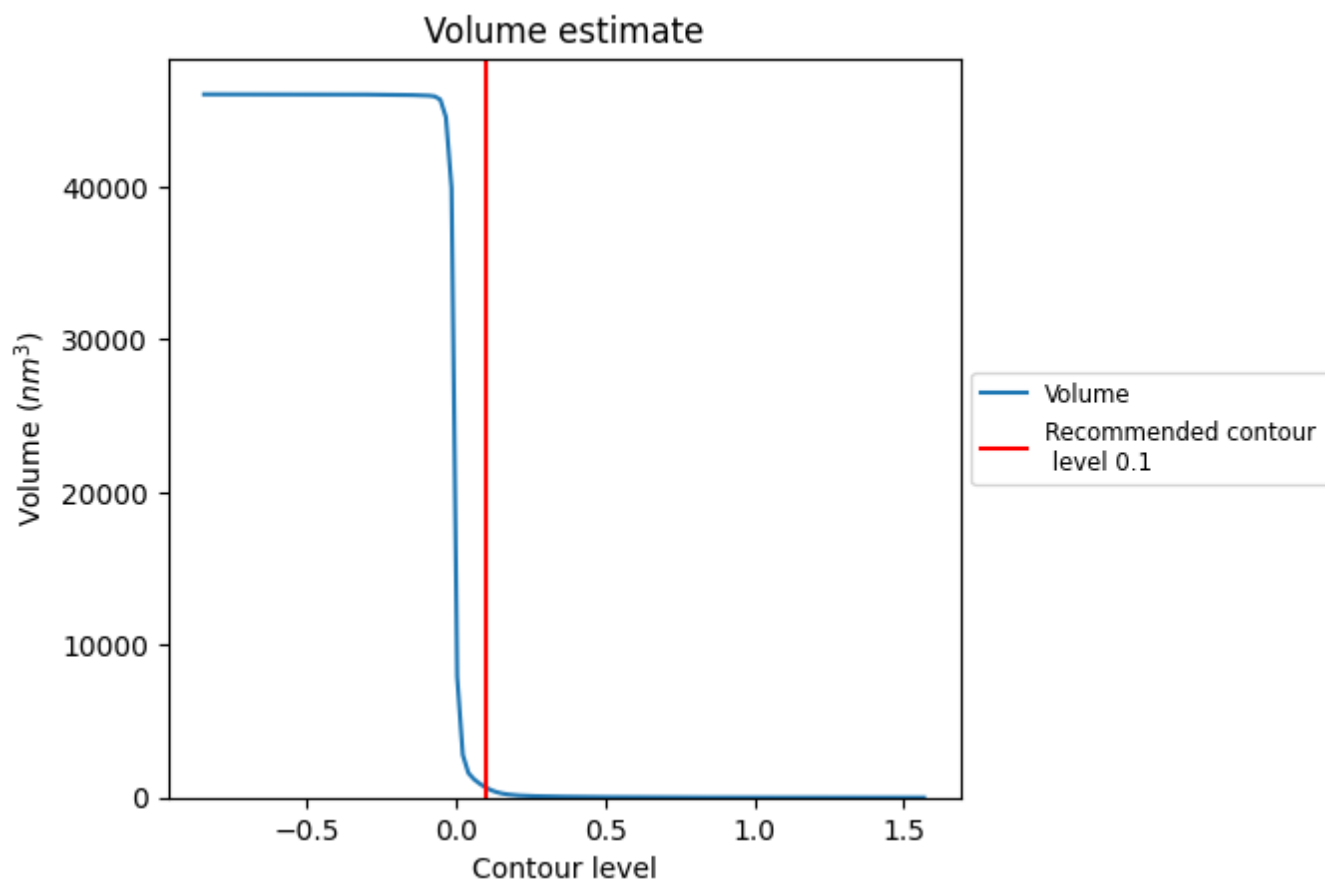
This section contains the results of statistical analysis of the map.

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.

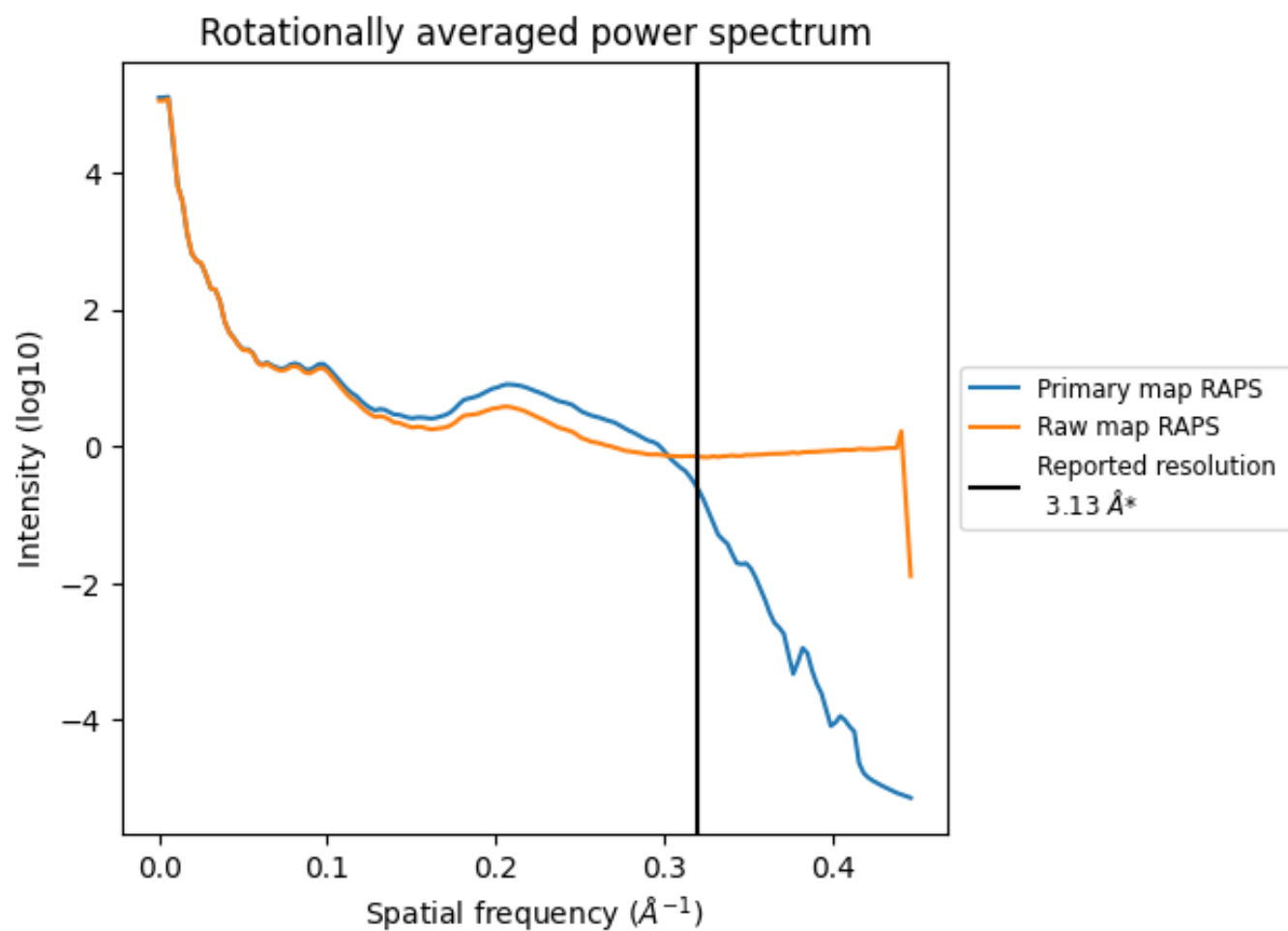
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 660 nm^3 ; this corresponds to an approximate mass of 597 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 ⓘ

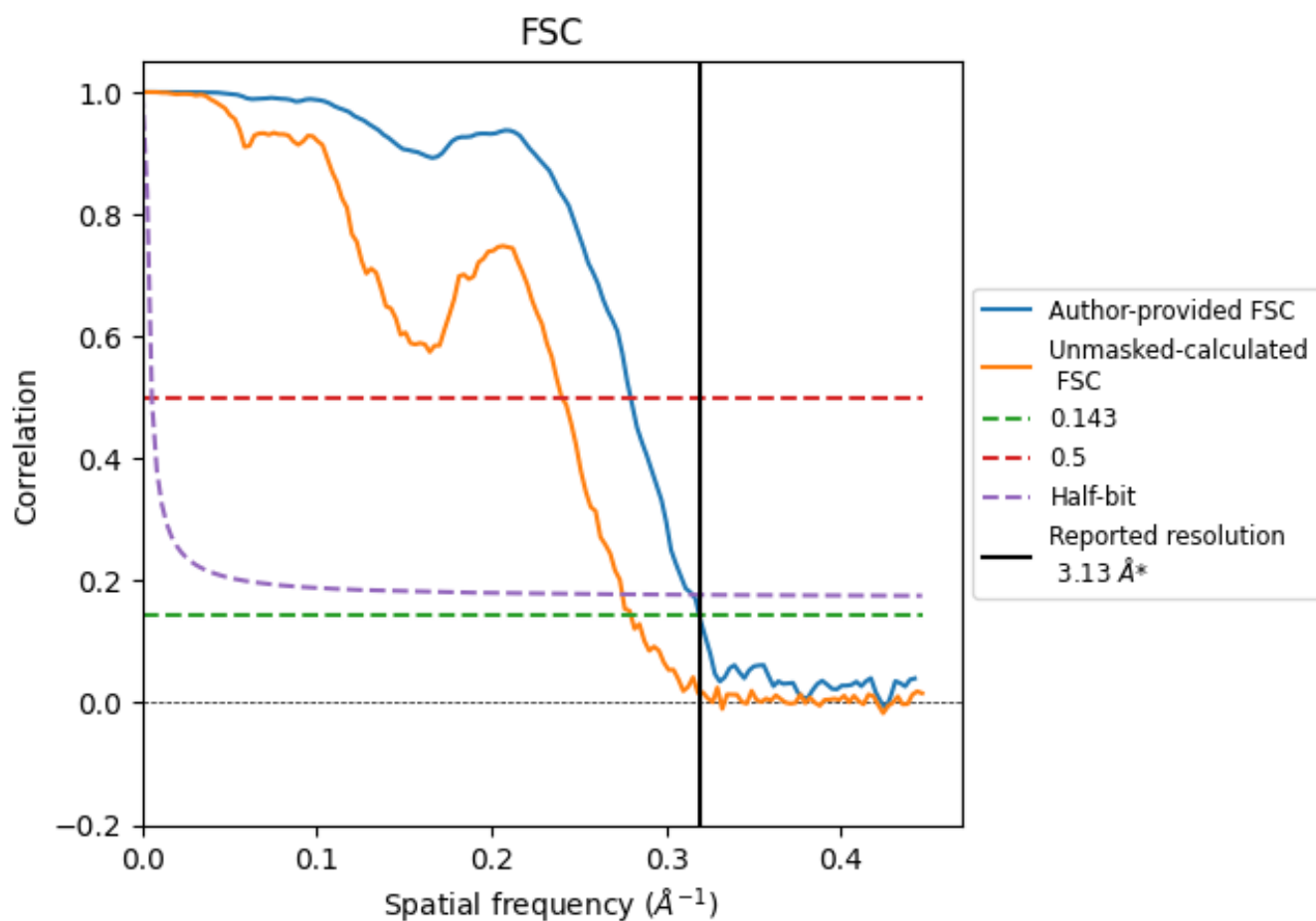


*Reported resolution corresponds to spatial frequency of 0.319 Å⁻¹

8 Fourier-Shell correlation [i](#)

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

8.1 FSC [i](#)



*Reported resolution corresponds to spatial frequency of 0.319 \AA^{-1}

8.2 Resolution estimates [i](#)

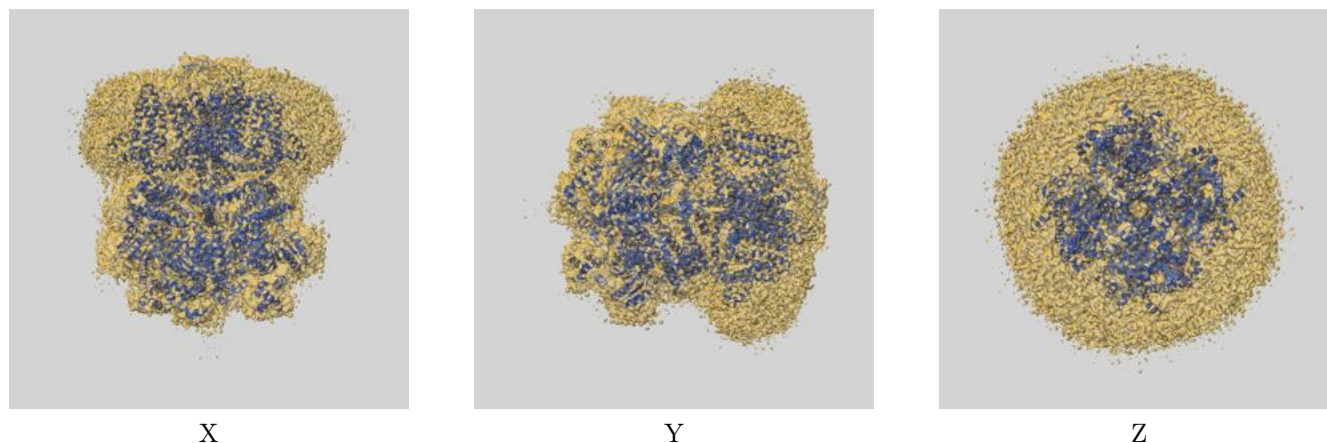
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.13	-	-
Author-provided FSC curve	3.14	3.58	3.18
Unmasked-calculated*	3.58	4.16	3.64

*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 3.58 differs from the reported value 3.13 by more than 10 %

9 Map-model fit [i](#)

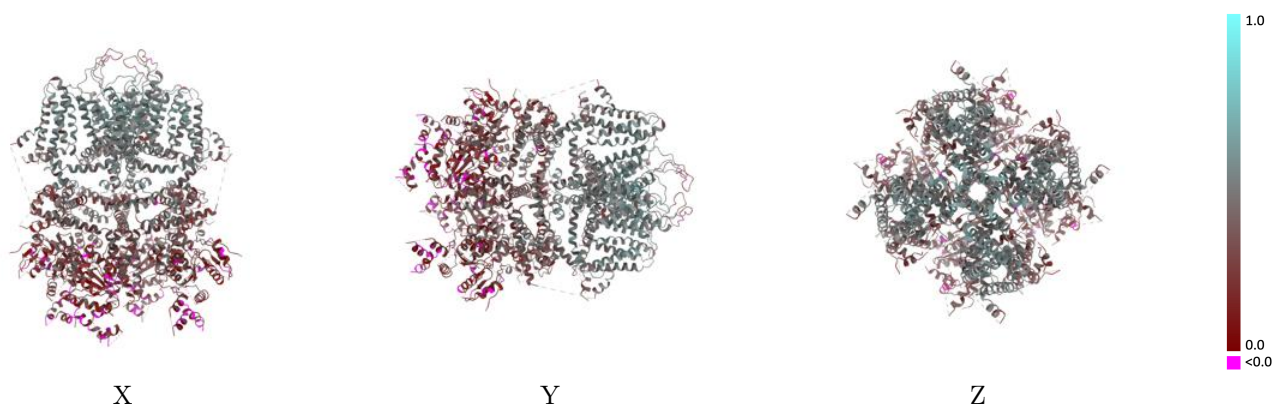
This section contains information regarding the fit between EMDB map EMD-44101 and PDB model 9B29. Per-residue inclusion information can be found in [section 3](#) on [page 10](#).

9.1 Map-model overlay [i](#)



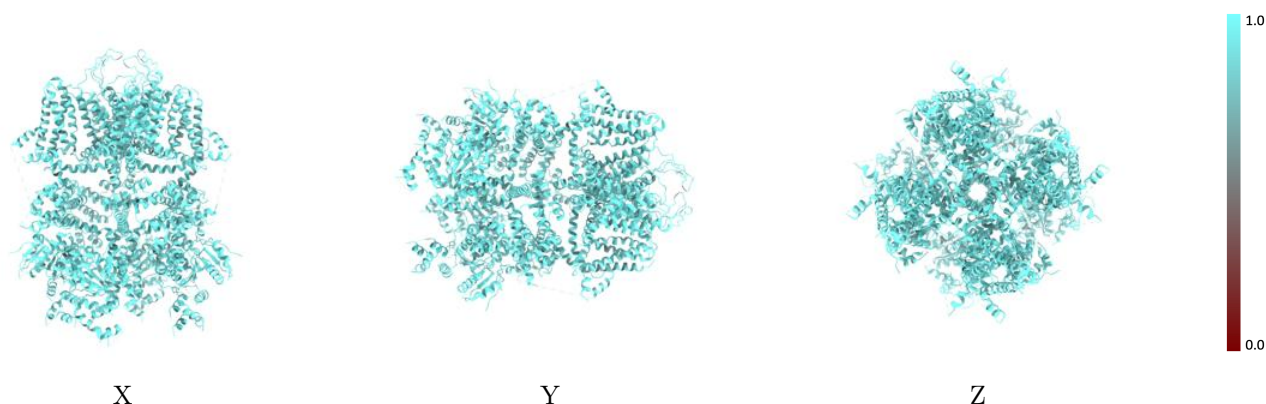
The images above show the 3D surface view of the map at the recommended contour level 0.1 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



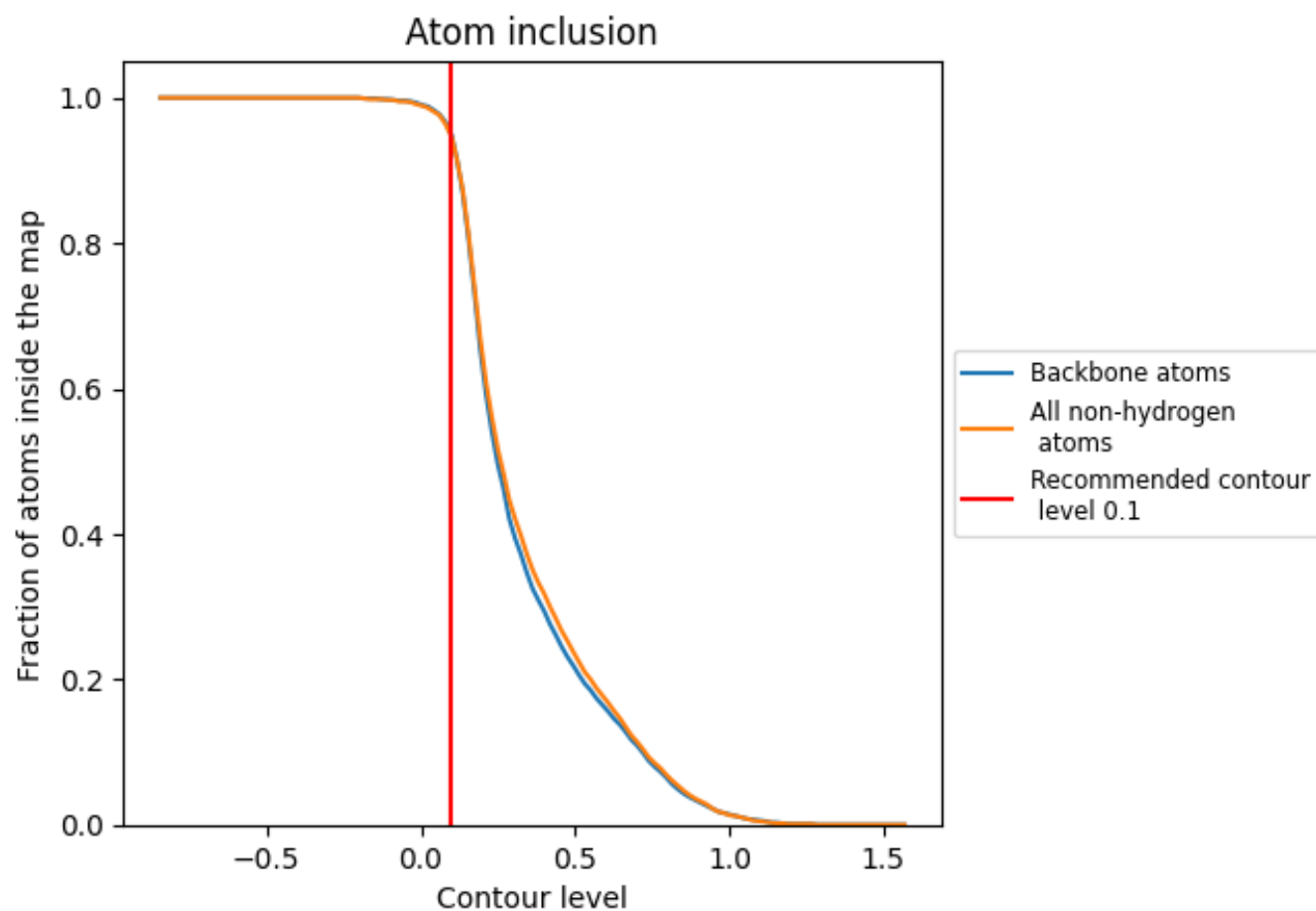
The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.1).

9.4 Atom inclusion [i](#)



At the recommended contour level, 95% of all backbone atoms, 95% 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 (0.1) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	<div></div> 0.9460	<div></div> 0.3940
A	<div></div> 0.9450	<div></div> 0.3930
B	<div></div> 0.9450	<div></div> 0.3940
C	<div></div> 0.9450	<div></div> 0.3940
D	<div></div> 0.9450	<div></div> 0.3930

