



Full wwPDB EM Validation Report ⓘ

Nov 10, 2024 – 01:40 AM EST

PDB ID : 7LPA
EMDB ID : EMD-23474
Title : Cryo-EM structure of full-length TRPV1 with capsaicin at 4 degrees Celsius
Authors : Kwon, D.H.; Zhang, F.; Suo, Y.; Lee, S.-Y.
Deposited on : 2021-02-11
Resolution : 3.37 Å (reported)
Based on initial model : 5IRZ

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.dev113
Mogul : 2022.3.0, CSD as543be (2022)
MolProbity : 4.02b-467
buster-report : 1.1.7 (2018)
Percentile statistics : 20231227.v01 (using entries in the PDB archive December 27th 2023)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.39

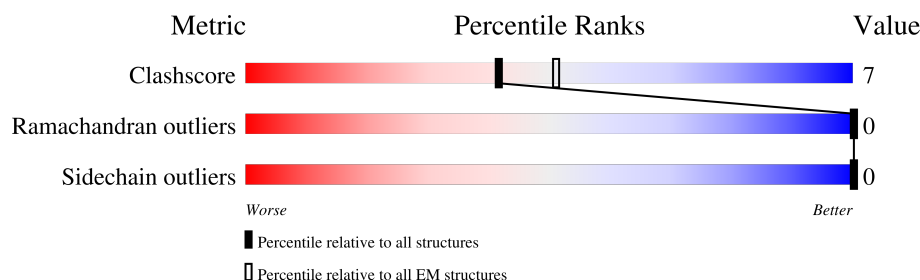
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 3.37 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	868	<div> <div>19%</div> <div>59%</div> <div>10%</div> <div>31%</div> </div>
1	B	868	<div> <div>19%</div> <div>59%</div> <div>10%</div> <div>31%</div> </div>
1	C	868	<div> <div>19%</div> <div>58%</div> <div>10%</div> <div>31%</div> </div>
1	D	868	<div> <div>19%</div> <div>59%</div> <div>10%</div> <div>31%</div> </div>

2 Entry composition [i](#)

There are 6 unique types of molecules in this entry. The entry contains 18634 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 Transient receptor potential cation channel subfamily V member 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	598	Total	C	N	O	S	0	0
			4467	2924	733	785	25		
1	B	598	Total	C	N	O	S	0	0
			4467	2924	733	785	25		
1	C	598	Total	C	N	O	S	0	0
			4467	2924	733	785	25		
1	D	598	Total	C	N	O	S	0	0
			4467	2924	733	785	25		

There are 120 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	839	GLU	-	expression tag	UNP O35433
A	840	ASN	-	expression tag	UNP O35433
A	841	SER	-	expression tag	UNP O35433
A	842	LEU	-	expression tag	UNP O35433
A	843	GLU	-	expression tag	UNP O35433
A	844	VAL	-	expression tag	UNP O35433
A	845	LEU	-	expression tag	UNP O35433
A	846	PHE	-	expression tag	UNP O35433
A	847	GLN	-	expression tag	UNP O35433
A	848	GLY	-	expression tag	UNP O35433
A	849	PRO	-	expression tag	UNP O35433
A	850	ASP	-	expression tag	UNP O35433
A	851	TYR	-	expression tag	UNP O35433
A	852	LYS	-	expression tag	UNP O35433
A	853	ASP	-	expression tag	UNP O35433
A	854	ASP	-	expression tag	UNP O35433
A	855	ASP	-	expression tag	UNP O35433
A	856	ASP	-	expression tag	UNP O35433
A	857	LYS	-	expression tag	UNP O35433
A	858	ALA	-	expression tag	UNP O35433
A	859	HIS	-	expression tag	UNP O35433

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Chain	Residue	Modelled	Actual	Comment	Reference
A	860	HIS	-	expression tag	UNP O35433
A	861	HIS	-	expression tag	UNP O35433
A	862	HIS	-	expression tag	UNP O35433
A	863	HIS	-	expression tag	UNP O35433
A	864	HIS	-	expression tag	UNP O35433
A	865	HIS	-	expression tag	UNP O35433
A	866	HIS	-	expression tag	UNP O35433
A	867	HIS	-	expression tag	UNP O35433
A	868	HIS	-	expression tag	UNP O35433
B	839	GLU	-	expression tag	UNP O35433
B	840	ASN	-	expression tag	UNP O35433
B	841	SER	-	expression tag	UNP O35433
B	842	LEU	-	expression tag	UNP O35433
B	843	GLU	-	expression tag	UNP O35433
B	844	VAL	-	expression tag	UNP O35433
B	845	LEU	-	expression tag	UNP O35433
B	846	PHE	-	expression tag	UNP O35433
B	847	GLN	-	expression tag	UNP O35433
B	848	GLY	-	expression tag	UNP O35433
B	849	PRO	-	expression tag	UNP O35433
B	850	ASP	-	expression tag	UNP O35433
B	851	TYR	-	expression tag	UNP O35433
B	852	LYS	-	expression tag	UNP O35433
B	853	ASP	-	expression tag	UNP O35433
B	854	ASP	-	expression tag	UNP O35433
B	855	ASP	-	expression tag	UNP O35433
B	856	ASP	-	expression tag	UNP O35433
B	857	LYS	-	expression tag	UNP O35433
B	858	ALA	-	expression tag	UNP O35433
B	859	HIS	-	expression tag	UNP O35433
B	860	HIS	-	expression tag	UNP O35433
B	861	HIS	-	expression tag	UNP O35433
B	862	HIS	-	expression tag	UNP O35433
B	863	HIS	-	expression tag	UNP O35433
B	864	HIS	-	expression tag	UNP O35433
B	865	HIS	-	expression tag	UNP O35433
B	866	HIS	-	expression tag	UNP O35433
B	867	HIS	-	expression tag	UNP O35433
B	868	HIS	-	expression tag	UNP O35433
C	839	GLU	-	expression tag	UNP O35433
C	840	ASN	-	expression tag	UNP O35433
C	841	SER	-	expression tag	UNP O35433

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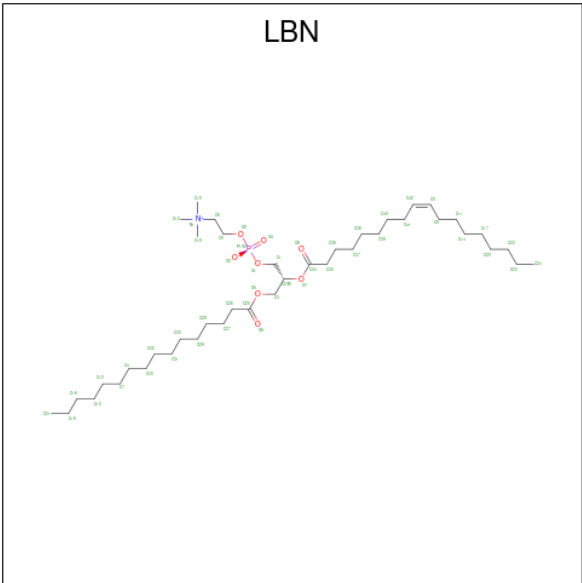
Chain	Residue	Modelled	Actual	Comment	Reference
C	842	LEU	-	expression tag	UNP O35433
C	843	GLU	-	expression tag	UNP O35433
C	844	VAL	-	expression tag	UNP O35433
C	845	LEU	-	expression tag	UNP O35433
C	846	PHE	-	expression tag	UNP O35433
C	847	GLN	-	expression tag	UNP O35433
C	848	GLY	-	expression tag	UNP O35433
C	849	PRO	-	expression tag	UNP O35433
C	850	ASP	-	expression tag	UNP O35433
C	851	TYR	-	expression tag	UNP O35433
C	852	LYS	-	expression tag	UNP O35433
C	853	ASP	-	expression tag	UNP O35433
C	854	ASP	-	expression tag	UNP O35433
C	855	ASP	-	expression tag	UNP O35433
C	856	ASP	-	expression tag	UNP O35433
C	857	LYS	-	expression tag	UNP O35433
C	858	ALA	-	expression tag	UNP O35433
C	859	HIS	-	expression tag	UNP O35433
C	860	HIS	-	expression tag	UNP O35433
C	861	HIS	-	expression tag	UNP O35433
C	862	HIS	-	expression tag	UNP O35433
C	863	HIS	-	expression tag	UNP O35433
C	864	HIS	-	expression tag	UNP O35433
C	865	HIS	-	expression tag	UNP O35433
C	866	HIS	-	expression tag	UNP O35433
C	867	HIS	-	expression tag	UNP O35433
C	868	HIS	-	expression tag	UNP O35433
D	839	GLU	-	expression tag	UNP O35433
D	840	ASN	-	expression tag	UNP O35433
D	841	SER	-	expression tag	UNP O35433
D	842	LEU	-	expression tag	UNP O35433
D	843	GLU	-	expression tag	UNP O35433
D	844	VAL	-	expression tag	UNP O35433
D	845	LEU	-	expression tag	UNP O35433
D	846	PHE	-	expression tag	UNP O35433
D	847	GLN	-	expression tag	UNP O35433
D	848	GLY	-	expression tag	UNP O35433
D	849	PRO	-	expression tag	UNP O35433
D	850	ASP	-	expression tag	UNP O35433
D	851	TYR	-	expression tag	UNP O35433
D	852	LYS	-	expression tag	UNP O35433
D	853	ASP	-	expression tag	UNP O35433

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Chain	Residue	Modelled	Actual	Comment	Reference
D	854	ASP	-	expression tag	UNP O35433
D	855	ASP	-	expression tag	UNP O35433
D	856	ASP	-	expression tag	UNP O35433
D	857	LYS	-	expression tag	UNP O35433
D	858	ALA	-	expression tag	UNP O35433
D	859	HIS	-	expression tag	UNP O35433
D	860	HIS	-	expression tag	UNP O35433
D	861	HIS	-	expression tag	UNP O35433
D	862	HIS	-	expression tag	UNP O35433
D	863	HIS	-	expression tag	UNP O35433
D	864	HIS	-	expression tag	UNP O35433
D	865	HIS	-	expression tag	UNP O35433
D	866	HIS	-	expression tag	UNP O35433
D	867	HIS	-	expression tag	UNP O35433
D	868	HIS	-	expression tag	UNP O35433

- Molecule 2 is 1-palmitoyl-2-oleoyl-sn-glycero-3-phosphocholine (three-letter code: LBN) (formula: C₄₂H₈₂NO₈P).



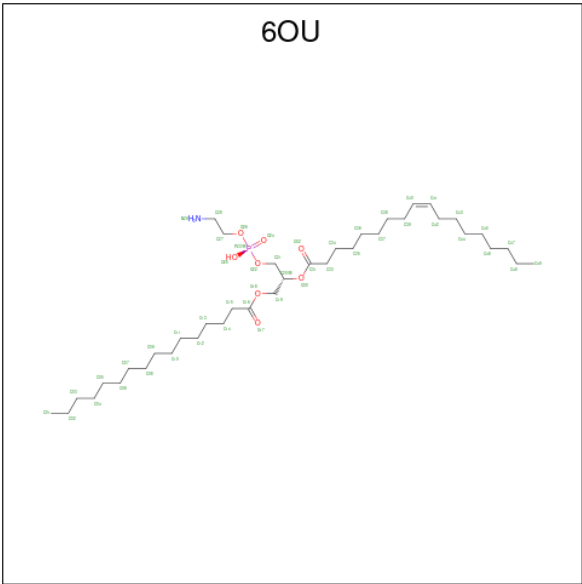
Mol	Chain	Residues	Atoms					AltConf
2	A	1	Total	C	N	O	P	0
			33	23	1	8	1	
2	A	1	Total	C	O			
			28	23	5			
2	B	1	Total	C	O			
			28	23	5			

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Mol	Chain	Residues	Atoms					AltConf
2	B	1	Total	C	N	O	P	0
			33	23	1	8	1	
2	C	1	Total	C	O			0
			28	23	5			
2	C	1	Total	C	N	O	P	0
			33	23	1	8	1	
2	D	1	Total	C	O			0
			28	23	5			
2	D	1	Total	C	N	O	P	0
			33	23	1	8	1	

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



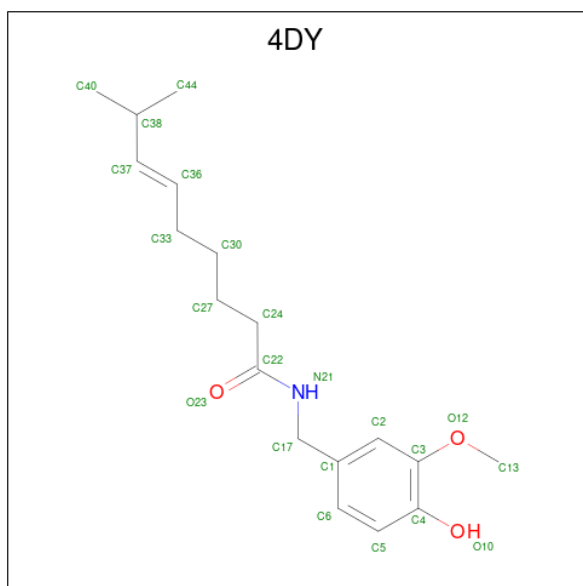
Mol	Chain	Residues	Atoms				AltConf
3	A	1	Total	C	O	P	0
			35	26	8	1	
3	A	1	Total	C	O	P	0
			31	22	8	1	
3	A	1	Total	C	O		0
			13	12	1		
3	A	1	Total	C	O	P	0
			31	22	8	1	
3	B	1	Total	C	O	P	0
			35	26	8	1	
3	B	1	Total	C	O	P	0
			31	22	8	1	

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Mol	Chain	Residues	Atoms			AltConf
3	B	1	Total	C	O	0
			13	12	1	
3	C	1	Total	C	O	P
			35	26	8	1
3	C	1	Total	C	O	P
			31	22	8	1
3	C	1	Total	C	O	
			13	12	1	0
3	D	1	Total	C	O	P
			35	26	8	1
3	D	1	Total	C	O	
			13	12	1	0

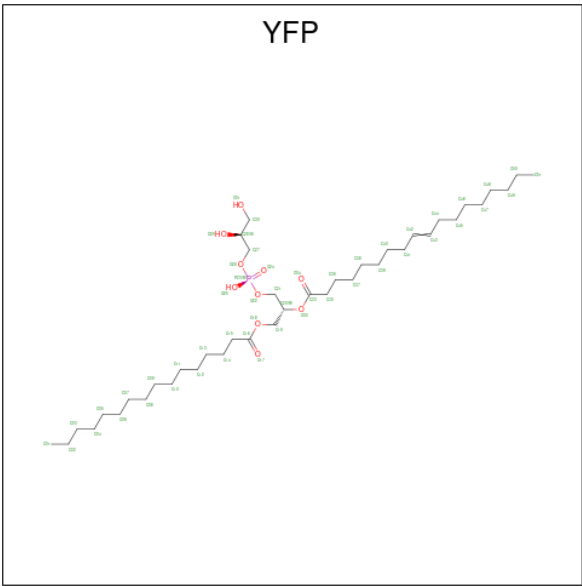
- Molecule 4 is (6E)-N-(4-hydroxy-3-methoxybenzyl)-8-methylnon-6-enamide (three-letter code: 4DY) (formula: C₁₈H₂₇NO₃).



Mol	Chain	Residues	Atoms			AltConf
4	A	1	Total	C	N	O
			22	18	1	3
4	B	1	Total	C	N	O
			22	18	1	3
4	C	1	Total	C	N	O
			22	18	1	3
4	D	1	Total	C	N	O
			22	18	1	3

- Molecule 5 is 1-palmitoyl-2-oleoyl-sn-glycero-3-phosphoglycerol (three-letter code: YFP)

(formula: C₄₀H₇₇O₁₀P).



Mol	Chain	Residues	Atoms				AltConf
5	A	1	Total	C	O	P	0
			29	20	8	1	
5	B	1	Total	C	O	P	0
			29	20	8	1	
5	C	1	Total	C	O	P	0
			29	20	8	1	
5	D	1	Total	C	O	P	0
			29	20	8	1	

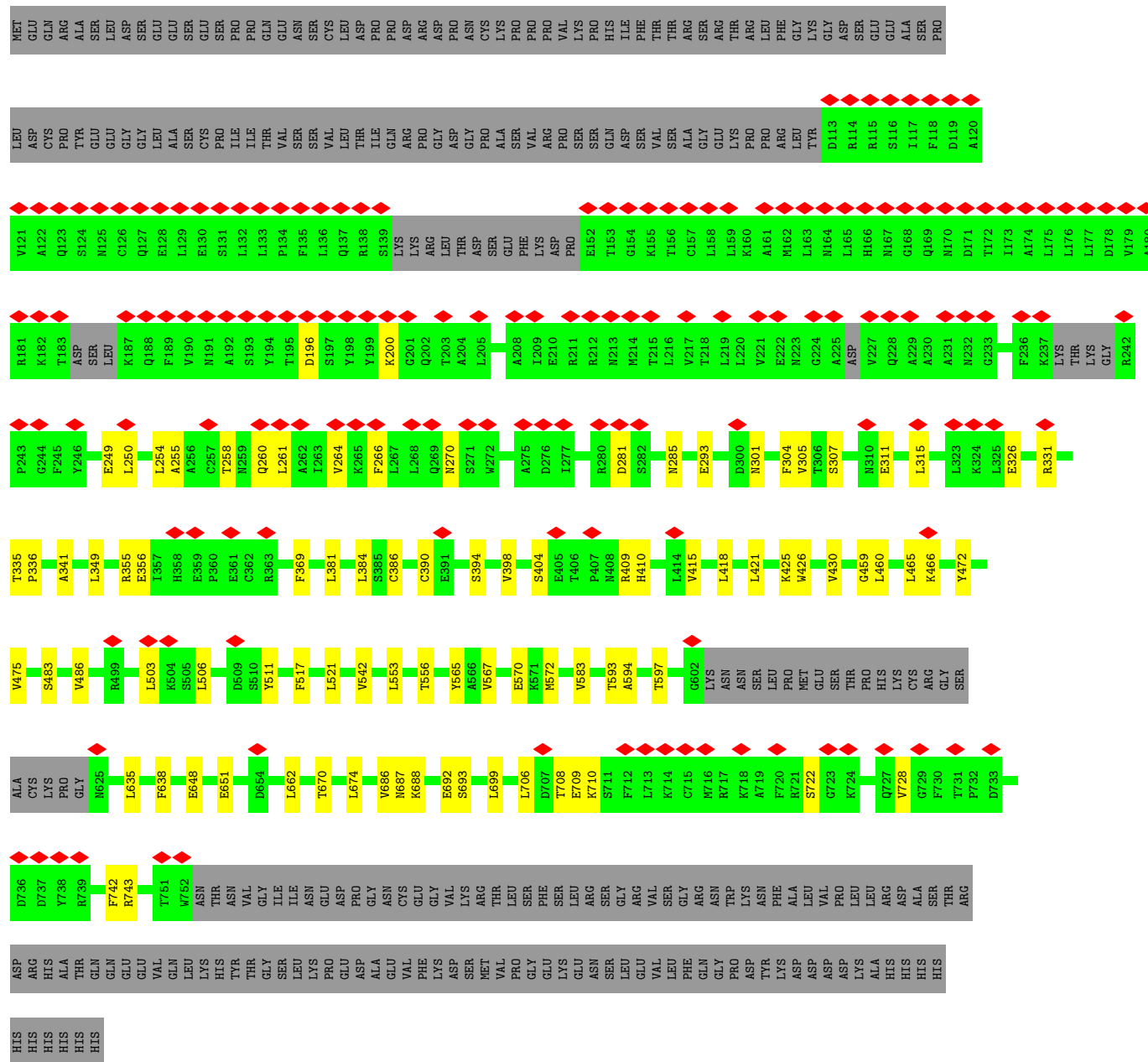
- Molecule 6 is SODIUM ION (three-letter code: NA) (formula: Na).

Mol	Chain	Residues	Atoms		AltConf
6	A	2	Total	Na	0
			2	2	

HIS
HIS
HIS

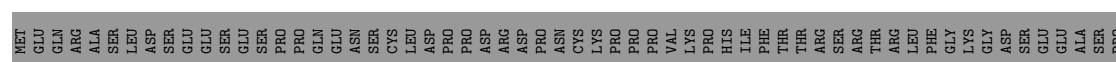
- Molecule 1: Transient receptor potential cation channel subfamily V member 1

Chain B: 



- Molecule 1: Transient receptor potential cation channel subfamily V member 1

Chain C: 







4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	114269	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)	750	Depositor
Maximum defocus (nm)	2500	Depositor
Magnification	81000	Depositor
Image detector	GATAN K3 BIOQUANTUM (6k x 4k)	Depositor
Maximum map value	0.169	Depositor
Minimum map value	-0.117	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.004	Depositor
Recommended contour level	0.014	Depositor
Map size (Å)	276.48, 276.48, 276.48	wwPDB
Map dimensions	256, 256, 256	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.08, 1.08, 1.08	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: YFP, 6OU, 4DY, NA, 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	0.28	0/4567	0.43	0/6213
1	B	0.29	0/4567	0.43	0/6213
1	C	0.29	0/4567	0.43	0/6213
1	D	0.29	0/4567	0.43	0/6213
All	All	0.29	0/18268	0.43	0/24852

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	4467	0	4164	63	0
1	B	4467	0	4164	62	0
1	C	4467	0	4164	62	0
1	D	4467	0	4164	61	0
2	A	61	0	0	1	0
2	B	61	0	0	0	0
2	C	61	0	0	0	0
2	D	61	0	0	0	0
3	A	110	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	B	79	0	0	0	0
3	C	79	0	0	0	0
3	D	48	0	0	0	0
4	A	22	0	0	0	0
4	B	22	0	0	0	0
4	C	22	0	0	0	0
4	D	22	0	0	0	0
5	A	29	0	0	0	0
5	B	29	0	0	0	0
5	C	29	0	0	0	0
5	D	29	0	0	0	0
6	A	2	0	0	0	0
All	All	18634	0	16656	232	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 7.

All (232) 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:430:VAL:HG23	1:A:708:THR:HG21	1.69	0.75
1:B:430:VAL:HG23	1:B:708:THR:HG21	1.69	0.75
1:C:430:VAL:HG23	1:C:708:THR:HG21	1.69	0.74
1:D:430:VAL:HG23	1:D:708:THR:HG21	1.69	0.74
1:B:356:GLU:N	1:B:356:GLU:OE1	2.24	0.71
1:A:356:GLU:N	1:A:356:GLU:OE1	2.24	0.71
1:C:356:GLU:N	1:C:356:GLU:OE1	2.24	0.70
1:D:356:GLU:N	1:D:356:GLU:OE1	2.24	0.69
1:B:260:GLN:O	1:B:264:VAL:HG13	2.00	0.62
1:A:260:GLN:O	1:A:264:VAL:HG13	2.00	0.61
1:C:260:GLN:O	1:C:264:VAL:HG13	2.00	0.61
1:D:260:GLN:O	1:D:264:VAL:HG13	2.00	0.61
1:B:687:ASN:OD1	1:B:688:LYS:NZ	2.37	0.58
1:D:687:ASN:OD1	1:D:688:LYS:NZ	2.37	0.58
1:C:687:ASN:OD1	1:C:688:LYS:NZ	2.37	0.58
1:A:687:ASN:OD1	1:A:688:LYS:NZ	2.37	0.57
1:C:583:VAL:HG21	1:D:565:TYR:CE2	2.40	0.56
1:B:583:VAL:HG21	1:C:565:TYR:CE2	2.41	0.56
1:A:583:VAL:HG21	1:B:565:TYR:CD2	2.41	0.56
1:A:593:THR:O	1:A:597:THR:HG23	2.06	0.56
1:B:593:THR:O	1:B:597:THR:HG23	2.06	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:593:THR:O	1:D:597:THR:HG23	2.06	0.56
1:A:583:VAL:HG21	1:B:565:TYR:CE2	2.42	0.55
1:B:583:VAL:HG21	1:C:565:TYR:CD2	2.42	0.55
1:C:583:VAL:HG21	1:D:565:TYR:CD2	2.41	0.55
1:C:593:THR:O	1:C:597:THR:HG23	2.06	0.54
1:A:565:TYR:CE2	1:D:583:VAL:HG21	2.42	0.54
1:A:565:TYR:CD2	1:D:583:VAL:HG21	2.43	0.54
1:C:511:TYR:HD1	1:C:570:GLU:HG3	1.73	0.54
1:A:511:TYR:HD1	1:A:570:GLU:HG3	1.73	0.53
1:B:511:TYR:HD1	1:B:570:GLU:HG3	1.73	0.53
1:B:255:ALA:CB	1:B:264:VAL:HG12	2.39	0.53
1:C:503:LEU:O	1:C:506:LEU:HD22	2.09	0.53
1:D:511:TYR:HD1	1:D:570:GLU:HG3	1.73	0.53
1:D:255:ALA:CB	1:D:264:VAL:HG12	2.39	0.52
1:D:503:LEU:O	1:D:506:LEU:HD22	2.09	0.52
1:C:255:ALA:CB	1:C:264:VAL:HG12	2.39	0.52
1:B:503:LEU:O	1:B:506:LEU:HD22	2.09	0.52
1:A:255:ALA:CB	1:A:264:VAL:HG12	2.39	0.52
1:A:572:MET:CE	1:A:686:VAL:HG23	2.40	0.51
1:B:572:MET:CE	1:B:686:VAL:HG23	2.40	0.51
1:D:261:LEU:O	1:D:264:VAL:HG22	2.11	0.51
1:A:261:LEU:O	1:A:264:VAL:HG22	2.11	0.51
1:A:503:LEU:O	1:A:506:LEU:HD22	2.09	0.51
1:C:261:LEU:O	1:C:264:VAL:HG22	2.11	0.51
1:B:261:LEU:O	1:B:264:VAL:HG22	2.11	0.51
1:D:301:ASN:HA	1:D:304:PHE:CE1	2.46	0.51
1:B:465:LEU:HD23	1:B:466:LYS:O	2.11	0.51
1:C:301:ASN:HA	1:C:304:PHE:CE1	2.46	0.51
1:C:465:LEU:HD23	1:C:466:LYS:O	2.11	0.51
1:C:572:MET:CE	1:C:686:VAL:HG23	2.40	0.51
1:B:511:TYR:CD1	1:B:570:GLU:HG3	2.46	0.50
1:C:511:TYR:CD1	1:C:570:GLU:HG3	2.46	0.50
1:D:706:LEU:O	1:D:710:LYS:HD3	2.11	0.50
1:A:465:LEU:HD23	1:A:466:LYS:O	2.11	0.50
1:A:706:LEU:O	1:A:710:LYS:HD3	2.11	0.50
1:D:572:MET:CE	1:D:686:VAL:HG23	2.40	0.50
1:C:706:LEU:O	1:C:710:LYS:HD3	2.11	0.50
1:D:511:TYR:CD1	1:D:570:GLU:HG3	2.46	0.50
1:D:465:LEU:HD23	1:D:466:LYS:O	2.11	0.50
1:A:255:ALA:HB3	1:A:264:VAL:HG12	1.94	0.49
1:A:301:ASN:HA	1:A:304:PHE:CE1	2.46	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:511:TYR:CD1	1:A:570:GLU:HG3	2.46	0.49
1:B:301:ASN:HA	1:B:304:PHE:CE1	2.46	0.49
1:B:384:LEU:HD11	1:B:742:PHE:HB2	1.95	0.49
1:D:651:GLU:HG3	1:D:651:GLU:O	2.12	0.49
1:B:706:LEU:O	1:B:710:LYS:HD3	2.11	0.49
1:C:651:GLU:O	1:C:651:GLU:HG3	2.13	0.49
1:D:281:ASP:OD1	1:D:285:ASN:N	2.45	0.49
1:D:384:LEU:HD11	1:D:742:PHE:HB2	1.95	0.49
1:D:506:LEU:H	1:D:506:LEU:HD23	1.77	0.49
1:B:506:LEU:HD23	1:B:506:LEU:H	1.77	0.49
1:A:281:ASP:OD1	1:A:285:ASN:N	2.45	0.49
1:A:542:VAL:HG13	1:D:594:ALA:O	2.12	0.49
1:B:255:ALA:HB3	1:B:264:VAL:HG12	1.94	0.49
1:B:651:GLU:HG3	1:B:651:GLU:O	2.13	0.49
1:C:384:LEU:HD11	1:C:742:PHE:HB2	1.95	0.49
1:C:255:ALA:HB3	1:C:264:VAL:HG12	1.94	0.49
1:C:281:ASP:OD1	1:C:285:ASN:N	2.45	0.49
1:B:281:ASP:OD1	1:B:285:ASN:N	2.46	0.49
1:D:459:GLY:O	1:D:460:LEU:HD12	2.13	0.49
1:A:651:GLU:O	1:A:651:GLU:HG3	2.13	0.48
1:C:594:ALA:O	1:D:542:VAL:HG13	2.13	0.48
1:A:384:LEU:HD11	1:A:742:PHE:HB2	1.95	0.48
1:B:459:GLY:O	1:B:460:LEU:HD12	2.13	0.48
1:A:459:GLY:O	1:A:460:LEU:HD12	2.13	0.48
1:D:255:ALA:HB3	1:D:264:VAL:HG12	1.94	0.48
1:A:415:VAL:CG2	1:A:418:LEU:HD13	2.43	0.48
1:A:506:LEU:H	1:A:506:LEU:HD23	1.77	0.48
1:A:369:PHE:CZ	1:A:728:VAL:HG21	2.49	0.48
1:A:555:TYR:OH	2:A:901:LBN:O4	2.20	0.48
1:B:415:VAL:CG2	1:B:418:LEU:HD13	2.43	0.48
1:A:254:LEU:O	1:A:258:THR:HG23	2.14	0.48
1:B:369:PHE:CZ	1:B:728:VAL:HG21	2.49	0.48
1:C:415:VAL:CG2	1:C:418:LEU:HD13	2.43	0.48
1:D:415:VAL:CG2	1:D:418:LEU:HD13	2.43	0.48
1:C:254:LEU:O	1:C:258:THR:HG23	2.14	0.48
1:B:594:ALA:O	1:C:542:VAL:HG13	2.14	0.47
1:C:506:LEU:HD23	1:C:506:LEU:H	1.77	0.47
1:D:254:LEU:O	1:D:258:THR:HG23	2.14	0.47
1:C:369:PHE:CZ	1:C:728:VAL:HG21	2.49	0.47
1:C:459:GLY:O	1:C:460:LEU:HD12	2.13	0.47
1:B:648:GLU:O	1:B:648:GLU:HG3	2.15	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:369:PHE:CZ	1:D:728:VAL:HG21	2.49	0.47
1:A:648:GLU:HG3	1:A:648:GLU:O	2.15	0.47
1:B:254:LEU:O	1:B:258:THR:HG23	2.14	0.47
1:D:326:GLU:OE1	1:D:355:ARG:NH1	2.48	0.47
1:A:326:GLU:OE1	1:A:355:ARG:NH1	2.48	0.47
1:C:648:GLU:HG3	1:C:648:GLU:O	2.15	0.47
1:B:415:VAL:HG21	1:B:418:LEU:HD13	1.98	0.46
1:C:415:VAL:HG21	1:C:418:LEU:HD13	1.98	0.46
1:A:381:LEU:HD21	1:A:743:ARG:NH1	2.31	0.46
1:B:381:LEU:HD21	1:B:743:ARG:NH1	2.31	0.46
1:A:594:ALA:O	1:B:542:VAL:HG13	2.14	0.46
1:D:381:LEU:HD21	1:D:743:ARG:NH1	2.31	0.46
1:A:415:VAL:HG21	1:A:418:LEU:HD13	1.98	0.46
1:C:381:LEU:HD21	1:C:743:ARG:NH1	2.30	0.46
1:B:425:LYS:O	1:B:430:VAL:HG12	2.16	0.46
1:D:415:VAL:HG21	1:D:418:LEU:HD13	1.98	0.46
1:B:553:LEU:O	1:B:556:THR:OG1	2.33	0.45
1:C:425:LYS:O	1:C:430:VAL:HG12	2.16	0.45
1:A:542:VAL:CG1	1:D:662:LEU:HD11	2.47	0.45
1:D:648:GLU:O	1:D:648:GLU:HG3	2.15	0.45
1:A:425:LYS:O	1:A:430:VAL:HG12	2.16	0.45
1:D:425:LYS:O	1:D:430:VAL:HG12	2.16	0.45
1:B:662:LEU:HD11	1:C:542:VAL:CG1	2.47	0.45
1:A:341:ALA:HB2	1:A:349:LEU:HD12	1.99	0.45
1:A:662:LEU:HD11	1:B:542:VAL:CG1	2.47	0.45
1:B:341:ALA:HB2	1:B:349:LEU:HD12	1.99	0.44
1:A:692:GLU:OE1	1:A:692:GLU:N	2.49	0.44
1:D:335:THR:HG23	1:D:336:PRO:HD2	2.00	0.44
1:A:335:THR:HG23	1:A:336:PRO:HD2	2.00	0.44
1:B:410:HIS:ND1	1:B:699:LEU:HD13	2.33	0.44
1:B:567:VAL:HG11	1:B:693:SER:HA	1.99	0.44
1:C:335:THR:HG23	1:C:336:PRO:HD2	2.00	0.44
1:B:335:THR:HG23	1:B:336:PRO:HD2	2.00	0.44
1:B:326:GLU:OE1	1:B:355:ARG:NH1	2.48	0.44
1:D:341:ALA:HB2	1:D:349:LEU:HD12	1.99	0.44
1:A:517:PHE:O	1:A:520:SER:OG	2.30	0.43
1:A:553:LEU:O	1:A:556:THR:OG1	2.33	0.43
1:C:662:LEU:HD11	1:D:542:VAL:CG1	2.48	0.43
1:D:386:CYS:O	1:D:390:CYS:HB2	2.18	0.43
1:A:426:TRP:HA	1:A:430:VAL:CG1	2.48	0.43
1:B:386:CYS:O	1:B:390:CYS:HB2	2.19	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:426:TRP:HA	1:B:430:VAL:CG1	2.48	0.43
1:C:410:HIS:ND1	1:C:699:LEU:HD13	2.33	0.43
1:A:410:HIS:ND1	1:A:699:LEU:HD13	2.33	0.43
1:C:341:ALA:HB2	1:C:349:LEU:HD12	1.99	0.43
1:C:635:LEU:O	1:C:638:PHE:N	2.52	0.43
1:D:567:VAL:HG11	1:D:693:SER:HA	1.99	0.43
1:A:567:VAL:HG11	1:A:693:SER:HA	1.99	0.43
1:C:311:GLU:O	1:C:315:LEU:HD13	2.19	0.43
1:C:426:TRP:HA	1:C:430:VAL:CG1	2.49	0.43
1:D:410:HIS:ND1	1:D:699:LEU:HD13	2.33	0.43
1:A:386:CYS:O	1:A:390:CYS:HB2	2.18	0.43
1:C:567:VAL:HG11	1:C:693:SER:HA	1.99	0.43
1:A:394:SER:O	1:A:398:VAL:HG23	2.19	0.43
1:B:635:LEU:O	1:B:638:PHE:N	2.52	0.43
1:D:553:LEU:O	1:D:556:THR:OG1	2.33	0.43
1:B:311:GLU:O	1:B:315:LEU:HD13	2.19	0.43
1:D:311:GLU:O	1:D:315:LEU:HD13	2.19	0.42
1:A:662:LEU:HD23	1:A:662:LEU:HA	1.80	0.42
1:B:394:SER:O	1:B:398:VAL:HG23	2.19	0.42
1:A:635:LEU:O	1:A:638:PHE:N	2.52	0.42
1:D:426:TRP:HA	1:D:430:VAL:CG1	2.48	0.42
1:A:404:SER:HA	1:A:409:ARG:HD3	2.01	0.42
1:C:394:SER:O	1:C:398:VAL:HG23	2.19	0.42
1:D:394:SER:O	1:D:398:VAL:HG23	2.19	0.42
1:C:386:CYS:O	1:C:390:CYS:HB2	2.18	0.42
1:C:692:GLU:OE1	1:C:692:GLU:N	2.49	0.42
1:D:635:LEU:O	1:D:638:PHE:N	2.52	0.42
1:A:196:ASP:O	1:A:200:LYS:N	2.53	0.42
1:A:311:GLU:O	1:A:315:LEU:HD13	2.19	0.42
1:B:196:ASP:O	1:B:200:LYS:N	2.53	0.42
1:B:692:GLU:OE1	1:B:692:GLU:N	2.49	0.42
1:C:301:ASN:O	1:C:305:VAL:HG23	2.20	0.42
1:D:196:ASP:O	1:D:200:LYS:N	2.53	0.42
1:D:692:GLU:OE1	1:D:692:GLU:N	2.49	0.42
1:C:326:GLU:OE1	1:C:355:ARG:NH1	2.48	0.42
1:D:249:GLU:O	1:D:250:LEU:HD23	2.20	0.42
1:D:293:GLU:HG3	1:D:293:GLU:O	2.20	0.42
1:D:301:ASN:O	1:D:305:VAL:HG23	2.20	0.42
1:C:196:ASP:O	1:C:200:LYS:N	2.53	0.42
1:C:293:GLU:O	1:C:293:GLU:HG3	2.20	0.42
1:C:404:SER:HA	1:C:409:ARG:HD3	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:301:ASN:O	1:B:305:VAL:HG23	2.20	0.41
1:C:249:GLU:O	1:C:250:LEU:HD23	2.20	0.41
1:C:553:LEU:O	1:C:556:THR:OG1	2.33	0.41
1:A:249:GLU:O	1:A:250:LEU:HD23	2.20	0.41
1:B:662:LEU:HD23	1:B:662:LEU:HA	1.80	0.41
1:C:662:LEU:HD23	1:C:662:LEU:HA	1.80	0.41
1:A:293:GLU:O	1:A:293:GLU:HG3	2.20	0.41
1:C:421:LEU:HD11	1:C:722:SER:OG	2.21	0.41
1:D:266:PHE:O	1:D:270:ASN:N	2.54	0.41
1:C:266:PHE:O	1:C:270:ASN:N	2.54	0.41
1:C:517:PHE:O	1:C:521:LEU:HG	2.21	0.41
1:C:670:THR:HA	1:C:674:LEU:HB2	2.02	0.41
1:D:331:ARG:HA	1:D:331:ARG:NE	2.36	0.41
1:D:421:LEU:HD11	1:D:722:SER:OG	2.21	0.41
1:A:307:SER:O	1:A:311:GLU:HG2	2.21	0.41
1:A:421:LEU:HD11	1:A:722:SER:OG	2.21	0.41
1:A:517:PHE:O	1:A:521:LEU:HG	2.21	0.41
1:B:293:GLU:O	1:B:293:GLU:HG3	2.20	0.41
1:C:307:SER:O	1:C:311:GLU:HG2	2.21	0.41
1:D:404:SER:HA	1:D:409:ARG:HD3	2.01	0.41
1:D:483:SER:O	1:D:486:VAL:HG12	2.20	0.41
1:A:266:PHE:O	1:A:270:ASN:N	2.54	0.41
1:A:483:SER:O	1:A:486:VAL:HG12	2.20	0.41
1:B:249:GLU:O	1:B:250:LEU:HD23	2.20	0.41
1:B:404:SER:HA	1:B:409:ARG:HD3	2.01	0.41
1:B:421:LEU:HD11	1:B:722:SER:OG	2.21	0.41
1:B:483:SER:O	1:B:486:VAL:HG12	2.20	0.41
1:C:331:ARG:NE	1:C:331:ARG:HA	2.36	0.41
1:C:483:SER:O	1:C:486:VAL:HG12	2.20	0.41
1:D:517:PHE:O	1:D:521:LEU:HG	2.21	0.41
1:B:472:TYR:O	1:B:475:VAL:HG12	2.21	0.41
1:C:472:TYR:O	1:C:475:VAL:HG12	2.21	0.41
1:B:266:PHE:O	1:B:270:ASN:N	2.54	0.40
1:B:517:PHE:O	1:B:521:LEU:HG	2.21	0.40
1:B:709:GLU:HG3	1:B:710:LYS:HD2	2.03	0.40
1:B:670:THR:HA	1:B:674:LEU:HB2	2.02	0.40
1:D:307:SER:O	1:D:311:GLU:HG2	2.21	0.40
1:D:472:TYR:O	1:D:475:VAL:HG12	2.21	0.40
1:A:301:ASN:O	1:A:305:VAL:HG23	2.20	0.40
1:A:331:ARG:HA	1:A:331:ARG:NE	2.36	0.40
1:A:709:GLU:HG3	1:A:710:LYS:HD2	2.03	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:670:THR:HA	1:D:674:LEU:HB2	2.02	0.40
1:A:670:THR:HA	1:A:674:LEU:HB2	2.02	0.40
1:B:307:SER:O	1:B:311:GLU:HG2	2.21	0.40
1:B:331:ARG:NE	1:B:331:ARG:HA	2.36	0.40
1:C:539:ALA:O	1:C:543:PHE:CD2	2.75	0.40
1:D:709:GLU:HG3	1:D:710:LYS:HD2	2.03	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	586/868 (68%)	562 (96%)	24 (4%)	0	100	100
1	B	586/868 (68%)	562 (96%)	24 (4%)	0	100	100
1	C	586/868 (68%)	562 (96%)	24 (4%)	0	100	100
1	D	586/868 (68%)	562 (96%)	24 (4%)	0	100	100
All	All	2344/3472 (68%)	2248 (96%)	96 (4%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains [i](#)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	418/770 (54%)	418 (100%)	0	100	100
1	B	418/770 (54%)	418 (100%)	0	100	100
1	C	418/770 (54%)	418 (100%)	0	100	100
1	D	418/770 (54%)	418 (100%)	0	100	100
All	All	1672/3080 (54%)	1672 (100%)	0	100	100

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

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

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry ⓘ

Of 30 ligands modelled in this entry, 2 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	$\# Z > 2$
3	6OU	C	906	-	11,12,48	0.84	0	10,11,53	0.60	0
3	6OU	D	904	-	34,34,48	1.70	4 (11%)	37,39,53	0.91	2 (5%)
2	LBN	D	903	-	32,32,51	1.45	4 (12%)	38,40,59	0.97	1 (2%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	LBN	B	901	-	27,27,51	0.99	1 (3%)	29,29,59	0.77	0
2	LBN	B	903	-	32,32,51	1.46	4 (12%)	38,40,59	0.97	1 (2%)
4	4DY	D	906	-	22,22,22	1.41	3 (13%)	27,27,27	1.32	3 (11%)
2	LBN	A	907	-	27,27,51	0.99	1 (3%)	29,29,59	0.77	0
2	LBN	D	901	-	27,27,51	0.99	1 (3%)	29,29,59	0.77	0
4	4DY	A	905	-	22,22,22	1.41	3 (13%)	27,27,27	1.32	3 (11%)
2	LBN	C	903	-	32,32,51	1.45	4 (12%)	38,40,59	0.97	1 (2%)
5	YFP	D	902	-	28,28,50	1.72	5 (17%)	31,33,56	1.48	4 (12%)
3	6OU	A	904	-	11,12,48	0.84	0	10,11,53	0.60	0
5	YFP	A	908	-	28,28,50	1.72	5 (17%)	31,33,56	1.48	4 (12%)
3	6OU	D	905	-	11,12,48	0.84	0	10,11,53	0.60	0
5	YFP	B	902	-	28,28,50	1.72	5 (17%)	31,33,56	1.48	4 (12%)
2	LBN	A	901	-	32,32,51	1.45	4 (12%)	38,40,59	0.97	1 (2%)
3	6OU	B	904	-	34,34,48	1.73	4 (11%)	37,39,53	0.93	2 (5%)
3	6OU	A	906	-	30,30,48	1.78	4 (13%)	33,35,53	0.95	2 (6%)
4	4DY	B	907	-	22,22,22	1.40	3 (13%)	27,27,27	1.32	3 (11%)
3	6OU	A	902	-	34,34,48	1.72	5 (14%)	37,39,53	0.91	2 (5%)
3	6OU	B	906	-	11,12,48	0.84	0	10,11,53	0.60	0
3	6OU	B	905	-	30,30,48	1.78	4 (13%)	33,35,53	0.95	2 (6%)
2	LBN	C	901	-	27,27,51	0.99	1 (3%)	29,29,59	0.76	0
3	6OU	A	903	-	30,30,48	1.77	4 (13%)	33,35,53	0.95	2 (6%)
3	6OU	C	905	-	30,30,48	1.77	4 (13%)	33,35,53	0.95	2 (6%)
4	4DY	C	907	-	22,22,22	1.40	3 (13%)	27,27,27	1.32	3 (11%)
5	YFP	C	902	-	28,28,50	1.72	5 (17%)	31,33,56	1.48	4 (12%)
3	6OU	C	904	-	34,34,48	1.71	5 (14%)	37,39,53	0.91	2 (5%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	6OU	C	906	-	-	7/10/10/52	-
3	6OU	D	904	-	-	20/36/36/52	-
2	LBN	D	903	-	-	22/36/36/55	-
2	LBN	B	901	-	-	17/29/29/55	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	LBN	B	903	-	-	22/36/36/55	-
4	4DY	D	906	-	-	1/16/16/16	0/1/1/1
2	LBN	A	907	-	-	17/29/29/55	-
2	LBN	D	901	-	-	17/29/29/55	-
4	4DY	A	905	-	-	1/16/16/16	0/1/1/1
2	LBN	C	903	-	-	22/36/36/55	-
5	YFP	D	902	-	-	14/30/30/55	-
3	6OU	A	904	-	-	7/10/10/52	-
5	YFP	A	908	-	-	14/30/30/55	-
3	6OU	D	905	-	-	7/10/10/52	-
5	YFP	B	902	-	-	14/30/30/55	-
2	LBN	A	901	-	-	22/36/36/55	-
3	6OU	B	904	-	-	15/36/36/52	-
3	6OU	A	906	-	-	8/32/32/52	-
4	4DY	B	907	-	-	1/16/16/16	0/1/1/1
3	6OU	A	902	-	-	23/36/36/52	-
3	6OU	B	906	-	-	7/10/10/52	-
3	6OU	B	905	-	-	8/32/32/52	-
2	LBN	C	901	-	-	17/29/29/55	-
3	6OU	A	903	-	-	8/32/32/52	-
3	6OU	C	905	-	-	8/32/32/52	-
4	4DY	C	907	-	-	1/16/16/16	0/1/1/1
5	YFP	C	902	-	-	14/30/30/55	-
3	6OU	C	904	-	-	19/36/36/52	-

All (86) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	904	6OU	P23-O22	5.53	1.77	1.60
3	A	902	6OU	P23-O22	5.48	1.77	1.60
3	C	904	6OU	P23-O22	5.44	1.77	1.60
3	D	904	6OU	P23-O22	5.32	1.77	1.60
3	B	905	6OU	P23-O22	5.31	1.77	1.60
3	A	903	6OU	P23-O22	5.29	1.77	1.60
3	A	906	6OU	P23-O22	5.28	1.77	1.60
3	C	905	6OU	P23-O22	5.26	1.76	1.60
4	D	906	4DY	C22-N21	5.09	1.45	1.33
4	A	905	4DY	C22-N21	5.07	1.45	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	903	LBN	P1-O2	5.06	1.79	1.59
4	B	907	4DY	C22-N21	5.06	1.45	1.33
4	C	907	4DY	C22-N21	5.06	1.45	1.33
2	A	901	LBN	P1-O2	5.04	1.79	1.59
2	D	903	LBN	P1-O2	5.04	1.79	1.59
2	C	903	LBN	P1-O2	5.04	1.79	1.59
3	A	906	6OU	P23-O26	4.99	1.73	1.54
3	A	903	6OU	P23-O26	4.98	1.73	1.54
3	C	905	6OU	P23-O26	4.97	1.73	1.54
3	B	905	6OU	P23-O26	4.96	1.73	1.54
3	A	902	6OU	P23-O26	4.94	1.73	1.54
3	D	904	6OU	P23-O26	4.94	1.73	1.54
3	B	904	6OU	P23-O26	4.93	1.73	1.54
3	C	904	6OU	P23-O26	4.86	1.72	1.54
5	A	908	YFP	P23-O26	4.40	1.71	1.54
5	B	902	YFP	P23-O26	4.38	1.71	1.54
5	C	902	YFP	P23-O26	4.38	1.71	1.54
5	D	902	YFP	P23-O26	4.36	1.71	1.54
5	A	908	YFP	C19-C20	3.47	1.61	1.50
5	B	902	YFP	C19-C20	3.46	1.61	1.50
5	D	902	YFP	C19-C20	3.45	1.61	1.50
5	C	902	YFP	C19-C20	3.44	1.61	1.50
5	A	908	YFP	P23-O22	3.06	1.70	1.60
5	B	902	YFP	P23-O22	3.05	1.69	1.60
5	D	902	YFP	P23-O22	3.05	1.69	1.60
5	C	902	YFP	P23-O22	3.04	1.69	1.60
2	A	907	LBN	C1-C2	2.67	1.57	1.51
2	D	901	LBN	C1-C2	2.67	1.57	1.51
2	C	901	LBN	C1-C2	2.66	1.57	1.51
3	B	904	6OU	C21-C20	2.66	1.59	1.50
2	B	901	LBN	C1-C2	2.65	1.57	1.51
3	A	902	6OU	C21-C20	2.53	1.58	1.50
3	C	904	6OU	C21-C20	2.49	1.58	1.50
4	D	906	4DY	O23-C22	-2.46	1.18	1.23
3	D	904	6OU	C21-C20	2.46	1.58	1.50
4	A	905	4DY	O23-C22	-2.44	1.18	1.23
3	B	905	6OU	C21-C20	2.43	1.58	1.50
4	B	907	4DY	O23-C22	-2.40	1.18	1.23
4	C	907	4DY	O23-C22	-2.40	1.18	1.23
3	A	906	6OU	C21-C20	2.40	1.58	1.50
3	A	903	6OU	C21-C20	2.39	1.58	1.50
3	C	905	6OU	C21-C20	2.39	1.58	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	902	6OU	C19-C20	2.29	1.58	1.50
5	D	902	YFP	C21-C20	2.28	1.58	1.50
5	B	902	YFP	C21-C20	2.28	1.57	1.50
5	C	902	YFP	C21-C20	2.28	1.57	1.50
5	A	908	YFP	C21-C20	2.25	1.57	1.50
2	B	903	LBN	P1-O1	2.23	1.68	1.59
2	C	903	LBN	P1-O1	2.22	1.68	1.59
2	A	901	LBN	P1-O1	2.22	1.68	1.59
2	D	903	LBN	P1-O1	2.22	1.68	1.59
3	B	904	6OU	C19-C20	2.22	1.57	1.50
5	C	902	YFP	O18-C16	2.20	1.39	1.33
5	D	902	YFP	O18-C16	2.20	1.39	1.33
5	A	908	YFP	O18-C16	2.18	1.39	1.33
5	B	902	YFP	O18-C16	2.18	1.39	1.33
2	B	903	LBN	O2-C9	-2.17	1.36	1.44
2	C	903	LBN	O2-C9	-2.17	1.36	1.44
2	A	901	LBN	O2-C9	-2.16	1.36	1.44
2	D	903	LBN	O2-C9	-2.15	1.36	1.44
3	A	903	6OU	C19-C20	2.10	1.57	1.50
3	C	905	6OU	C19-C20	2.10	1.57	1.50
3	A	906	6OU	C19-C20	2.10	1.57	1.50
3	D	904	6OU	O30-C31	2.09	1.40	1.34
3	B	905	6OU	C19-C20	2.08	1.57	1.50
2	C	903	LBN	C1-C2	2.08	1.57	1.50
2	D	903	LBN	C1-C2	2.08	1.57	1.50
2	A	901	LBN	C1-C2	2.07	1.57	1.50
2	B	903	LBN	C1-C2	2.06	1.57	1.50
4	C	907	4DY	O12-C3	2.05	1.40	1.37
4	B	907	4DY	O12-C3	2.05	1.40	1.37
4	D	906	4DY	O12-C3	2.05	1.40	1.37
4	A	905	4DY	O12-C3	2.04	1.40	1.37
3	C	904	6OU	C19-C20	2.01	1.57	1.50
3	A	902	6OU	O30-C31	2.01	1.40	1.34
3	C	904	6OU	O30-C31	2.00	1.39	1.34

All (48) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	C	902	YFP	O32-C33-C35	5.35	123.05	111.48
5	A	908	YFP	O32-C33-C35	5.34	123.04	111.48
5	B	902	YFP	O32-C33-C35	5.34	123.04	111.48
5	D	902	YFP	O32-C33-C35	5.33	123.02	111.48

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	903	LBN	O3-P1-O4	3.46	128.54	112.44
2	A	901	LBN	O3-P1-O4	3.45	128.49	112.44
2	D	903	LBN	O3-P1-O4	3.45	128.47	112.44
2	C	903	LBN	O3-P1-O4	3.44	128.46	112.44
3	D	904	6OU	O25-P23-O24	3.44	124.22	110.83
3	B	904	6OU	O25-P23-O24	3.43	124.20	110.83
3	A	906	6OU	O25-P23-O24	3.42	124.16	110.83
3	A	903	6OU	O25-P23-O24	3.41	124.12	110.83
3	B	905	6OU	O25-P23-O24	3.41	124.11	110.83
3	C	905	6OU	O25-P23-O24	3.40	124.07	110.83
3	C	904	6OU	O25-P23-O24	3.37	123.96	110.83
5	C	902	YFP	O18-C16-C15	3.36	122.07	111.83
5	D	902	YFP	O18-C16-C15	3.36	122.07	111.83
5	A	908	YFP	O18-C16-C15	3.35	122.04	111.83
5	B	902	YFP	O18-C16-C15	3.35	122.04	111.83
3	A	902	6OU	O25-P23-O24	3.34	123.85	110.83
4	B	907	4DY	C24-C22-N21	3.07	121.94	116.34
4	C	907	4DY	C24-C22-N21	3.06	121.93	116.34
4	A	905	4DY	C24-C22-N21	3.05	121.91	116.34
4	D	906	4DY	C24-C22-N21	3.04	121.89	116.34
4	D	906	4DY	O12-C3-C4	2.96	118.98	114.55
4	B	907	4DY	O12-C3-C4	2.96	118.98	114.55
4	A	905	4DY	O12-C3-C4	2.95	118.97	114.55
4	C	907	4DY	O12-C3-C4	2.95	118.97	114.55
5	D	902	YFP	O18-C16-O17	-2.81	116.59	123.63
5	C	902	YFP	O18-C16-O17	-2.80	116.61	123.63
5	A	908	YFP	O32-C33-O34	-2.79	117.17	123.70
5	B	902	YFP	O18-C16-O17	-2.79	116.64	123.63
5	A	908	YFP	O18-C16-O17	-2.79	116.66	123.63
5	B	902	YFP	O32-C33-O34	-2.78	117.19	123.70
5	D	902	YFP	O32-C33-O34	-2.78	117.19	123.70
5	C	902	YFP	O32-C33-O34	-2.77	117.22	123.70
3	B	904	6OU	O30-C31-C33	2.53	116.96	111.48
3	A	906	6OU	O30-C31-C33	2.48	116.85	111.48
3	A	903	6OU	O30-C31-C33	2.48	116.84	111.48
3	C	905	6OU	O30-C31-C33	2.48	116.84	111.48
3	B	905	6OU	O30-C31-C33	2.47	116.81	111.48
3	A	902	6OU	O30-C31-C33	2.45	116.77	111.48
3	D	904	6OU	O30-C31-C33	2.44	116.75	111.48
3	C	904	6OU	O30-C31-C33	2.39	116.65	111.48
4	D	906	4DY	O23-C22-C24	-2.08	118.25	122.02
4	A	905	4DY	O23-C22-C24	-2.08	118.26	122.02

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	B	907	4DY	O23-C22-C24	-2.07	118.28	122.02
4	C	907	4DY	O23-C22-C24	-2.06	118.28	122.02

There are no chirality outliers.

All (353) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	901	LBN	C1-O1-P1-O2
2	A	901	LBN	C9-O2-P1-O1
2	A	901	LBN	C9-O2-P1-O3
2	A	901	LBN	C3-C2-O7-C34
2	A	901	LBN	N1-C6-C9-O2
2	A	901	LBN	C26-C25-O5-C3
2	A	901	LBN	O6-C25-O5-C3
2	B	903	LBN	C1-O1-P1-O2
2	B	903	LBN	C9-O2-P1-O1
2	B	903	LBN	C9-O2-P1-O3
2	B	903	LBN	C3-C2-O7-C34
2	B	903	LBN	N1-C6-C9-O2
2	B	903	LBN	C26-C25-O5-C3
2	B	903	LBN	O6-C25-O5-C3
2	C	903	LBN	C1-O1-P1-O2
2	C	903	LBN	C9-O2-P1-O1
2	C	903	LBN	C9-O2-P1-O3
2	C	903	LBN	C3-C2-O7-C34
2	C	903	LBN	N1-C6-C9-O2
2	C	903	LBN	C26-C25-O5-C3
2	C	903	LBN	O6-C25-O5-C3
2	D	903	LBN	C1-O1-P1-O2
2	D	903	LBN	C9-O2-P1-O1
2	D	903	LBN	C9-O2-P1-O3
2	D	903	LBN	C3-C2-O7-C34
2	D	903	LBN	N1-C6-C9-O2
2	D	903	LBN	C26-C25-O5-C3
2	D	903	LBN	O6-C25-O5-C3
3	A	902	6OU	C21-O22-P23-O25
3	A	902	6OU	C21-O22-P23-O26
3	A	902	6OU	O32-C31-O30-C20
3	B	904	6OU	C33-C31-O30-C20
3	C	904	6OU	C15-C16-O18-C19
3	C	904	6OU	O17-C16-O18-C19
3	C	904	6OU	C21-O22-P23-O25

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Mol	Chain	Res	Type	Atoms
3	C	904	6OU	C21-O22-P23-O26
3	D	904	6OU	C21-O22-P23-O24
3	D	904	6OU	C21-O22-P23-O25
3	D	904	6OU	C21-O22-P23-O26
5	A	908	YFP	C21-O22-P23-O24
5	A	908	YFP	C21-O22-P23-O25
5	A	908	YFP	C21-O22-P23-O26
5	B	902	YFP	C21-O22-P23-O24
5	B	902	YFP	C21-O22-P23-O25
5	B	902	YFP	C21-O22-P23-O26
5	C	902	YFP	C21-O22-P23-O24
5	C	902	YFP	C21-O22-P23-O25
5	C	902	YFP	C21-O22-P23-O26
5	D	902	YFP	C21-O22-P23-O24
5	D	902	YFP	C21-O22-P23-O25
5	D	902	YFP	C21-O22-P23-O26
5	A	908	YFP	O17-C16-O18-C19
5	B	902	YFP	O17-C16-O18-C19
5	C	902	YFP	O17-C16-O18-C19
5	D	902	YFP	O17-C16-O18-C19
3	B	904	6OU	O32-C31-O30-C20
3	A	902	6OU	C33-C31-O30-C20
5	A	908	YFP	C15-C16-O18-C19
5	B	902	YFP	C15-C16-O18-C19
5	C	902	YFP	C15-C16-O18-C19
5	D	902	YFP	C15-C16-O18-C19
3	D	904	6OU	O17-C16-O18-C19
3	D	904	6OU	C15-C16-O18-C19
3	B	904	6OU	C09-C10-C11-C12
3	A	903	6OU	C15-C16-O18-C19
3	A	906	6OU	C15-C16-O18-C19
3	B	905	6OU	C15-C16-O18-C19
3	C	905	6OU	C15-C16-O18-C19
2	B	901	LBN	C38-C39-C40-C41
2	C	901	LBN	C38-C39-C40-C41
2	D	901	LBN	C38-C39-C40-C41
2	A	907	LBN	C38-C39-C40-C41
3	D	904	6OU	C36-C37-C38-C39
3	A	903	6OU	O17-C16-O18-C19
3	A	906	6OU	O17-C16-O18-C19
3	B	905	6OU	O17-C16-O18-C19
3	C	905	6OU	O17-C16-O18-C19

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Mol	Chain	Res	Type	Atoms
2	A	907	LBN	C34-C35-C36-C37
2	B	901	LBN	C34-C35-C36-C37
2	C	901	LBN	C34-C35-C36-C37
2	D	901	LBN	C34-C35-C36-C37
3	A	903	6OU	C31-C33-C34-C35
3	C	905	6OU	C31-C33-C34-C35
3	A	906	6OU	C31-C33-C34-C35
3	B	905	6OU	C31-C33-C34-C35
2	A	901	LBN	C34-C35-C36-C37
2	B	903	LBN	C34-C35-C36-C37
2	C	903	LBN	C34-C35-C36-C37
2	D	903	LBN	C34-C35-C36-C37
3	A	902	6OU	C13-C14-C15-C16
3	C	904	6OU	C31-C33-C34-C35
3	D	904	6OU	C13-C14-C15-C16
3	D	904	6OU	C31-C33-C34-C35
5	A	908	YFP	C13-C14-C15-C16
5	B	902	YFP	C13-C14-C15-C16
5	C	902	YFP	C13-C14-C15-C16
5	D	902	YFP	C13-C14-C15-C16
3	A	904	6OU	C37-C38-C39-C40
3	B	906	6OU	C37-C38-C39-C40
3	C	906	6OU	C37-C38-C39-C40
3	D	905	6OU	C37-C38-C39-C40
2	A	907	LBN	C26-C25-O5-C3
2	B	901	LBN	C26-C25-O5-C3
2	C	901	LBN	C26-C25-O5-C3
2	D	901	LBN	C26-C25-O5-C3
3	C	904	6OU	C19-C20-O30-C31
2	A	901	LBN	C29-C30-C31-C32
2	B	903	LBN	C29-C30-C31-C32
2	C	903	LBN	C26-C27-C28-C29
2	C	903	LBN	C29-C30-C31-C32
2	D	903	LBN	C29-C30-C31-C32
2	A	901	LBN	C26-C27-C28-C29
2	B	903	LBN	C26-C27-C28-C29
2	D	903	LBN	C26-C27-C28-C29
3	B	904	6OU	C11-C12-C13-C14
3	A	906	6OU	C36-C37-C38-C39
3	C	905	6OU	C36-C37-C38-C39
3	A	903	6OU	C36-C37-C38-C39
3	B	905	6OU	C36-C37-C38-C39

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Mol	Chain	Res	Type	Atoms
3	C	904	6OU	C34-C35-C36-C37
2	A	907	LBN	C26-C27-C28-C29
2	B	901	LBN	C26-C27-C28-C29
2	C	901	LBN	C26-C27-C28-C29
2	D	901	LBN	C26-C27-C28-C29
2	A	901	LBN	C35-C34-O7-C2
2	B	903	LBN	C35-C34-O7-C2
2	C	903	LBN	C35-C34-O7-C2
2	D	903	LBN	C35-C34-O7-C2
2	A	907	LBN	C29-C30-C31-C32
2	B	901	LBN	C29-C30-C31-C32
2	C	901	LBN	C29-C30-C31-C32
2	D	901	LBN	C29-C30-C31-C32
3	D	904	6OU	C34-C35-C36-C37
2	A	907	LBN	O6-C25-O5-C3
2	B	901	LBN	O6-C25-O5-C3
2	C	901	LBN	O6-C25-O5-C3
2	D	901	LBN	O6-C25-O5-C3
3	C	906	6OU	C34-C35-C36-C37
3	A	904	6OU	C34-C35-C36-C37
3	B	906	6OU	C34-C35-C36-C37
3	D	905	6OU	C34-C35-C36-C37
2	A	901	LBN	C36-C37-C38-C39
2	B	903	LBN	C36-C37-C38-C39
2	C	903	LBN	C36-C37-C38-C39
2	D	903	LBN	C36-C37-C38-C39
5	A	908	YFP	C09-C10-C11-C12
5	B	902	YFP	C09-C10-C11-C12
5	C	902	YFP	C09-C10-C11-C12
5	D	902	YFP	C09-C10-C11-C12
2	A	901	LBN	O8-C34-O7-C2
2	B	903	LBN	O8-C34-O7-C2
2	C	903	LBN	O8-C34-O7-C2
2	D	903	LBN	O8-C34-O7-C2
3	C	904	6OU	C40-C41-C42-C43
3	D	904	6OU	C40-C41-C42-C43
2	B	903	LBN	C35-C36-C37-C38
2	D	903	LBN	C35-C36-C37-C38
3	A	902	6OU	C34-C35-C36-C37
2	A	901	LBN	C35-C36-C37-C38
2	C	903	LBN	C35-C36-C37-C38
3	C	904	6OU	C33-C31-O30-C20

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Mol	Chain	Res	Type	Atoms
3	A	902	6OU	C11-C12-C13-C14
3	B	904	6OU	C13-C14-C15-C16
5	A	908	YFP	O18-C19-C20-O32
5	B	902	YFP	O18-C19-C20-O32
5	C	902	YFP	O18-C19-C20-O32
5	D	902	YFP	O18-C19-C20-O32
2	A	907	LBN	C30-C31-C32-C33
2	B	901	LBN	C30-C31-C32-C33
2	C	901	LBN	C30-C31-C32-C33
2	D	901	LBN	C30-C31-C32-C33
3	B	904	6OU	C07-C08-C09-C10
3	C	904	6OU	C33-C34-C35-C36
2	A	901	LBN	C27-C28-C29-C30
2	B	903	LBN	C27-C28-C29-C30
2	C	903	LBN	C27-C28-C29-C30
2	D	903	LBN	C27-C28-C29-C30
3	B	904	6OU	C33-C34-C35-C36
3	C	904	6OU	O32-C31-O30-C20
3	A	902	6OU	C35-C36-C37-C38
3	A	903	6OU	C12-C13-C14-C15
3	C	905	6OU	C12-C13-C14-C15
3	A	906	6OU	C12-C13-C14-C15
3	B	905	6OU	C12-C13-C14-C15
2	A	901	LBN	O1-C1-C2-C3
2	B	903	LBN	O1-C1-C2-C3
2	C	903	LBN	O1-C1-C2-C3
2	D	903	LBN	O1-C1-C2-C3
3	C	904	6OU	C12-C13-C14-C15
2	B	901	LBN	C27-C28-C29-C30
2	C	901	LBN	C27-C28-C29-C30
2	D	901	LBN	C27-C28-C29-C30
2	A	907	LBN	C27-C28-C29-C30
3	D	904	6OU	O18-C19-C20-C21
2	A	907	LBN	C39-C40-C41-C42
2	B	901	LBN	C39-C40-C41-C42
2	C	901	LBN	C39-C40-C41-C42
2	D	901	LBN	C39-C40-C41-C42
3	A	902	6OU	C21-O22-P23-O24
3	D	904	6OU	C11-C12-C13-C14
5	A	908	YFP	O32-C20-C21-O22
5	B	902	YFP	O32-C20-C21-O22
5	C	902	YFP	O32-C20-C21-O22

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Mol	Chain	Res	Type	Atoms
5	D	902	YFP	O32-C20-C21-O22
2	A	907	LBN	C31-C32-C33-C4
2	B	901	LBN	C31-C32-C33-C4
2	C	901	LBN	C31-C32-C33-C4
2	D	901	LBN	C31-C32-C33-C4
3	A	902	6OU	C09-C10-C11-C12
3	C	904	6OU	C07-C08-C09-C10
3	A	903	6OU	C10-C11-C12-C13
3	A	906	6OU	C10-C11-C12-C13
3	B	905	6OU	C10-C11-C12-C13
3	C	905	6OU	C10-C11-C12-C13
3	C	904	6OU	C06-C07-C08-C09
5	D	902	YFP	C36-C37-C38-C39
5	A	908	YFP	C36-C37-C38-C39
5	B	902	YFP	C36-C37-C38-C39
5	C	902	YFP	C36-C37-C38-C39
3	A	902	6OU	C12-C13-C14-C15
3	A	902	6OU	C10-C11-C12-C13
5	A	908	YFP	C19-C20-C21-O22
5	B	902	YFP	C19-C20-C21-O22
5	C	902	YFP	C19-C20-C21-O22
5	D	902	YFP	C19-C20-C21-O22
5	A	908	YFP	O18-C19-C20-C21
5	B	902	YFP	O18-C19-C20-C21
5	C	902	YFP	O18-C19-C20-C21
5	D	902	YFP	O18-C19-C20-C21
3	D	904	6OU	C12-C13-C14-C15
3	A	902	6OU	O30-C20-C21-O22
3	D	904	6OU	O18-C19-C20-O30
3	C	904	6OU	C36-C37-C38-C39
3	D	905	6OU	C35-C36-C37-C38
2	B	901	LBN	C28-C29-C30-C31
2	D	901	LBN	C28-C29-C30-C31
3	A	904	6OU	C35-C36-C37-C38
3	B	906	6OU	C35-C36-C37-C38
3	C	906	6OU	C35-C36-C37-C38
2	C	901	LBN	C28-C29-C30-C31
2	A	907	LBN	C28-C29-C30-C31
3	D	904	6OU	C08-C09-C10-C11
3	A	904	6OU	C40-C41-C42-C43
3	B	906	6OU	C40-C41-C42-C43
3	C	906	6OU	C40-C41-C42-C43

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Mol	Chain	Res	Type	Atoms
3	D	905	6OU	C40-C41-C42-C43
3	B	904	6OU	C36-C37-C38-C39
3	B	904	6OU	C21-O22-P23-O25
3	A	902	6OU	O18-C19-C20-C21
3	B	906	6OU	C33-C34-C35-C36
3	D	905	6OU	C33-C34-C35-C36
3	A	904	6OU	C33-C34-C35-C36
3	C	906	6OU	C33-C34-C35-C36
3	A	902	6OU	C06-C07-C08-C09
3	A	904	6OU	C31-C33-C34-C35
3	B	906	6OU	C31-C33-C34-C35
3	C	906	6OU	C31-C33-C34-C35
3	D	905	6OU	C31-C33-C34-C35
3	A	902	6OU	C19-C20-C21-O22
5	A	908	YFP	C35-C36-C37-C38
5	B	902	YFP	C35-C36-C37-C38
5	C	902	YFP	C35-C36-C37-C38
5	D	902	YFP	C35-C36-C37-C38
2	A	901	LBN	O1-C1-C2-O7
2	B	903	LBN	O1-C1-C2-O7
2	C	903	LBN	O1-C1-C2-O7
2	D	903	LBN	O1-C1-C2-O7
3	A	902	6OU	O18-C19-C20-O30
2	A	901	LBN	C1-O1-P1-O4
2	B	903	LBN	C1-O1-P1-O4
2	C	903	LBN	C1-O1-P1-O4
2	D	903	LBN	C1-O1-P1-O4
3	D	904	6OU	C09-C10-C11-C12
3	D	904	6OU	C19-C20-O30-C31
3	C	904	6OU	C09-C10-C11-C12
3	B	904	6OU	C35-C36-C37-C38
3	A	902	6OU	C31-C33-C34-C35
3	A	902	6OU	C14-C15-C16-O18
3	A	903	6OU	C40-C41-C42-C43
3	A	906	6OU	C40-C41-C42-C43
3	B	904	6OU	C40-C41-C42-C43
3	B	905	6OU	C40-C41-C42-C43
3	C	905	6OU	C40-C41-C42-C43
3	B	904	6OU	C14-C15-C16-O18
3	A	902	6OU	C37-C38-C39-C40
5	B	902	YFP	C07-C08-C09-C10
5	D	902	YFP	C07-C08-C09-C10

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Mol	Chain	Res	Type	Atoms
5	A	908	YFP	C07-C08-C09-C10
5	C	902	YFP	C07-C08-C09-C10
3	A	903	6OU	C20-C21-O22-P23
3	A	906	6OU	C20-C21-O22-P23
3	B	905	6OU	C20-C21-O22-P23
3	C	905	6OU	C20-C21-O22-P23
3	C	904	6OU	C10-C11-C12-C13
2	A	907	LBN	O1-C1-C2-C3
2	B	901	LBN	O1-C1-C2-C3
2	C	901	LBN	O1-C1-C2-C3
2	D	901	LBN	O1-C1-C2-C3
2	A	907	LBN	C40-C41-C42-C5
2	B	901	LBN	C40-C41-C42-C5
2	D	901	LBN	C40-C41-C42-C5
4	A	905	4DY	C22-C24-C27-C30
4	B	907	4DY	C22-C24-C27-C30
4	C	907	4DY	C22-C24-C27-C30
4	D	906	4DY	C22-C24-C27-C30
2	B	903	LBN	C30-C31-C32-C33
2	A	901	LBN	C30-C31-C32-C33
2	C	903	LBN	C30-C31-C32-C33
2	D	903	LBN	C30-C31-C32-C33
2	C	901	LBN	C40-C41-C42-C5
2	A	907	LBN	O1-C1-C2-O7
2	B	901	LBN	O1-C1-C2-O7
2	C	901	LBN	O1-C1-C2-O7
2	D	901	LBN	O1-C1-C2-O7
2	B	901	LBN	C35-C36-C37-C38
2	C	901	LBN	C35-C36-C37-C38
2	D	901	LBN	C35-C36-C37-C38
2	A	907	LBN	C35-C36-C37-C38
3	A	902	6OU	C38-C39-C40-C41
3	A	902	6OU	C07-C08-C09-C10
2	C	903	LBN	C28-C29-C30-C31
2	D	903	LBN	C28-C29-C30-C31
2	A	901	LBN	C28-C29-C30-C31
2	B	903	LBN	C28-C29-C30-C31
3	A	902	6OU	C33-C34-C35-C36
3	D	904	6OU	C33-C34-C35-C36
3	C	904	6OU	O30-C20-C21-O22
3	C	906	6OU	C38-C39-C40-C41
3	A	904	6OU	C38-C39-C40-C41

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Mol	Chain	Res	Type	Atoms
3	B	906	6OU	C38-C39-C40-C41
3	D	905	6OU	C38-C39-C40-C41
3	C	904	6OU	C19-C20-C21-O22
2	A	907	LBN	O5-C25-C26-C27
2	B	901	LBN	O5-C25-C26-C27
2	C	901	LBN	O5-C25-C26-C27
2	D	901	LBN	O5-C25-C26-C27
3	B	904	6OU	C38-C39-C40-C41
2	A	901	LBN	O5-C25-C26-C27
2	B	903	LBN	O5-C25-C26-C27
2	C	903	LBN	O5-C25-C26-C27
2	D	903	LBN	O5-C25-C26-C27
3	B	904	6OU	C12-C13-C14-C15
3	D	904	6OU	C14-C15-C16-O18
3	B	904	6OU	C31-C33-C34-C35
2	C	901	LBN	O6-C25-C26-C27
2	A	907	LBN	O6-C25-C26-C27
2	B	901	LBN	O6-C25-C26-C27
2	D	901	LBN	O6-C25-C26-C27
2	A	901	LBN	O6-C25-C26-C27
2	B	903	LBN	O6-C25-C26-C27
2	C	903	LBN	O6-C25-C26-C27
2	D	903	LBN	O6-C25-C26-C27
3	D	904	6OU	C14-C15-C16-O17

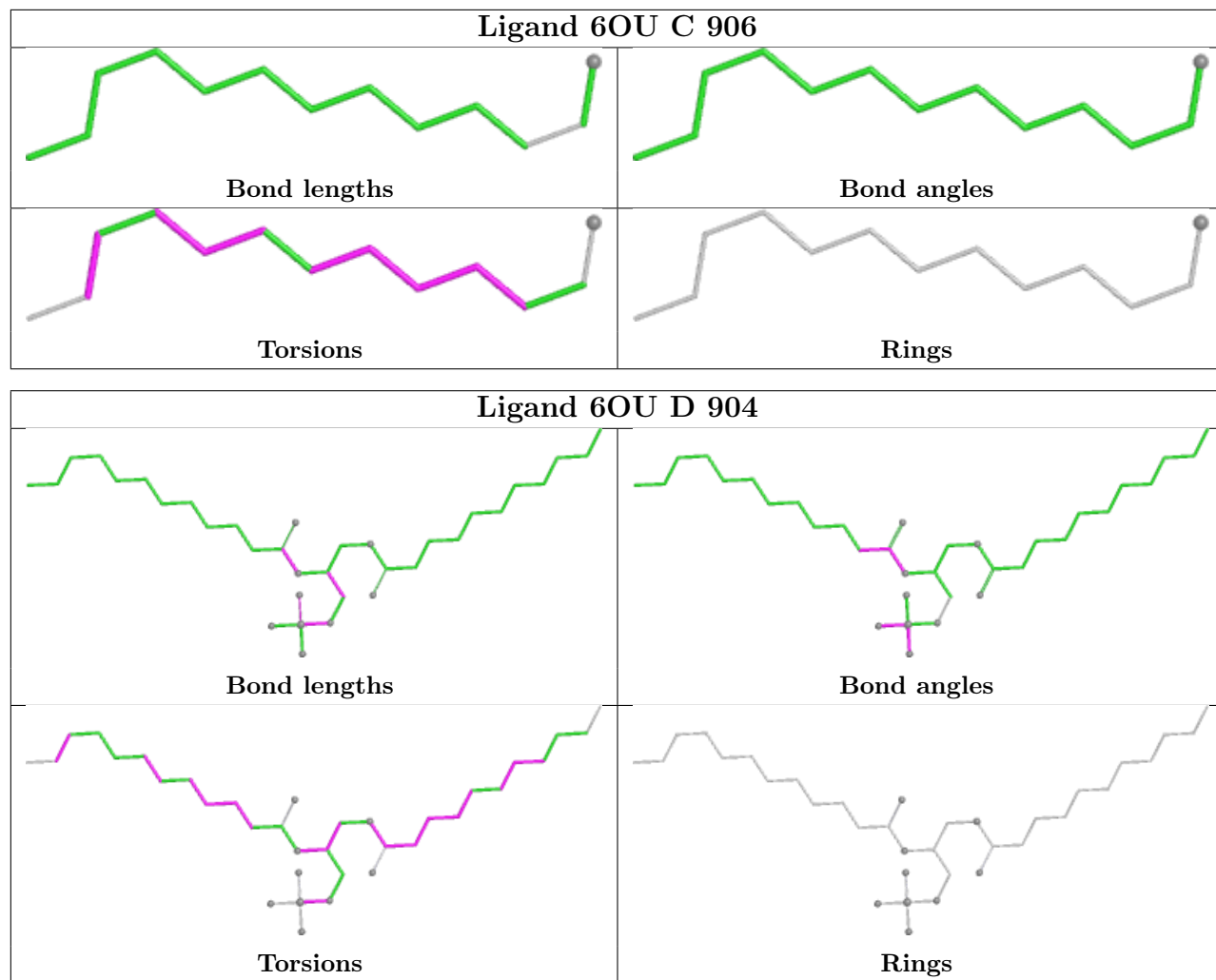
There are no ring outliers.

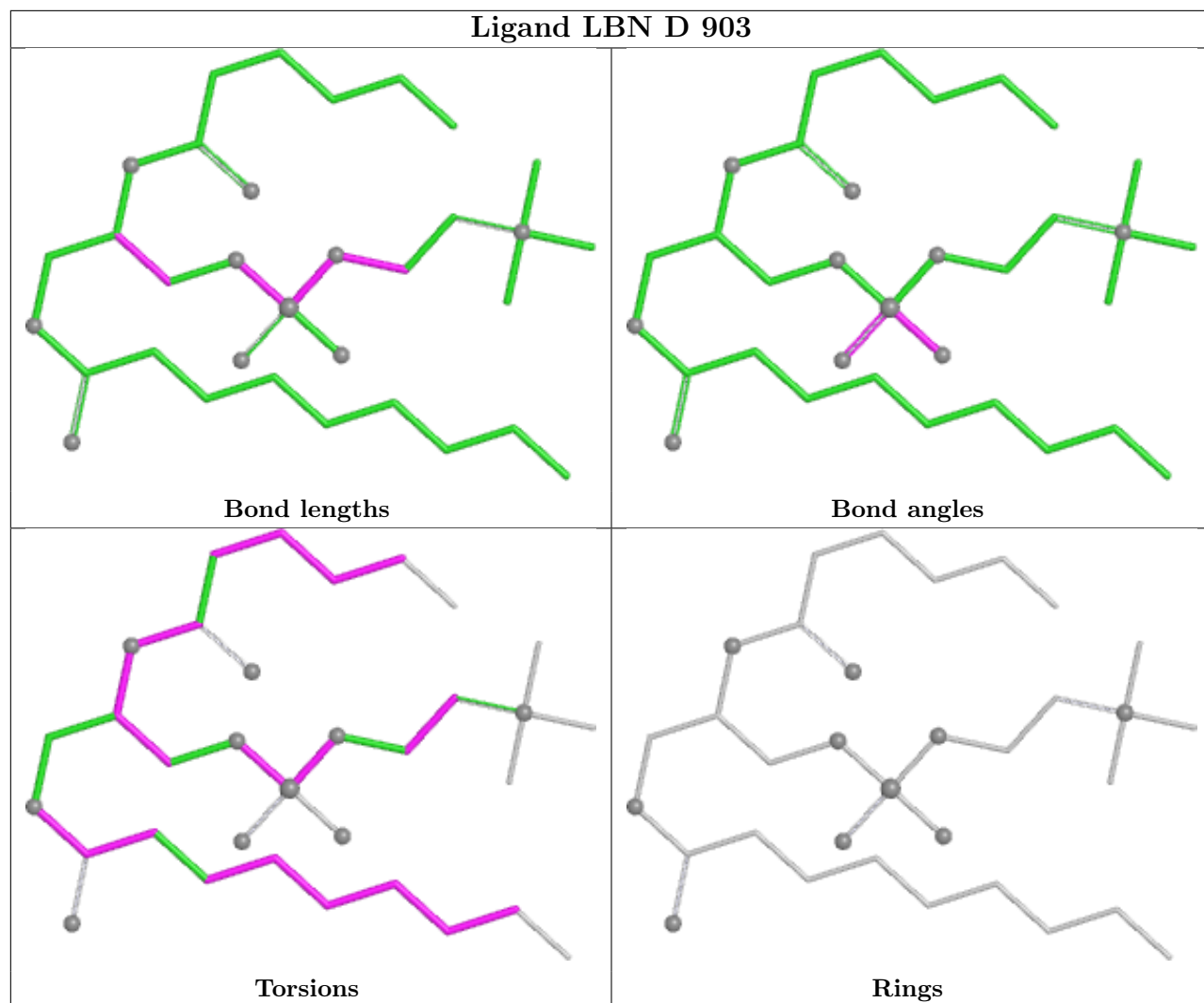
1 monomer is involved in 1 short contact:

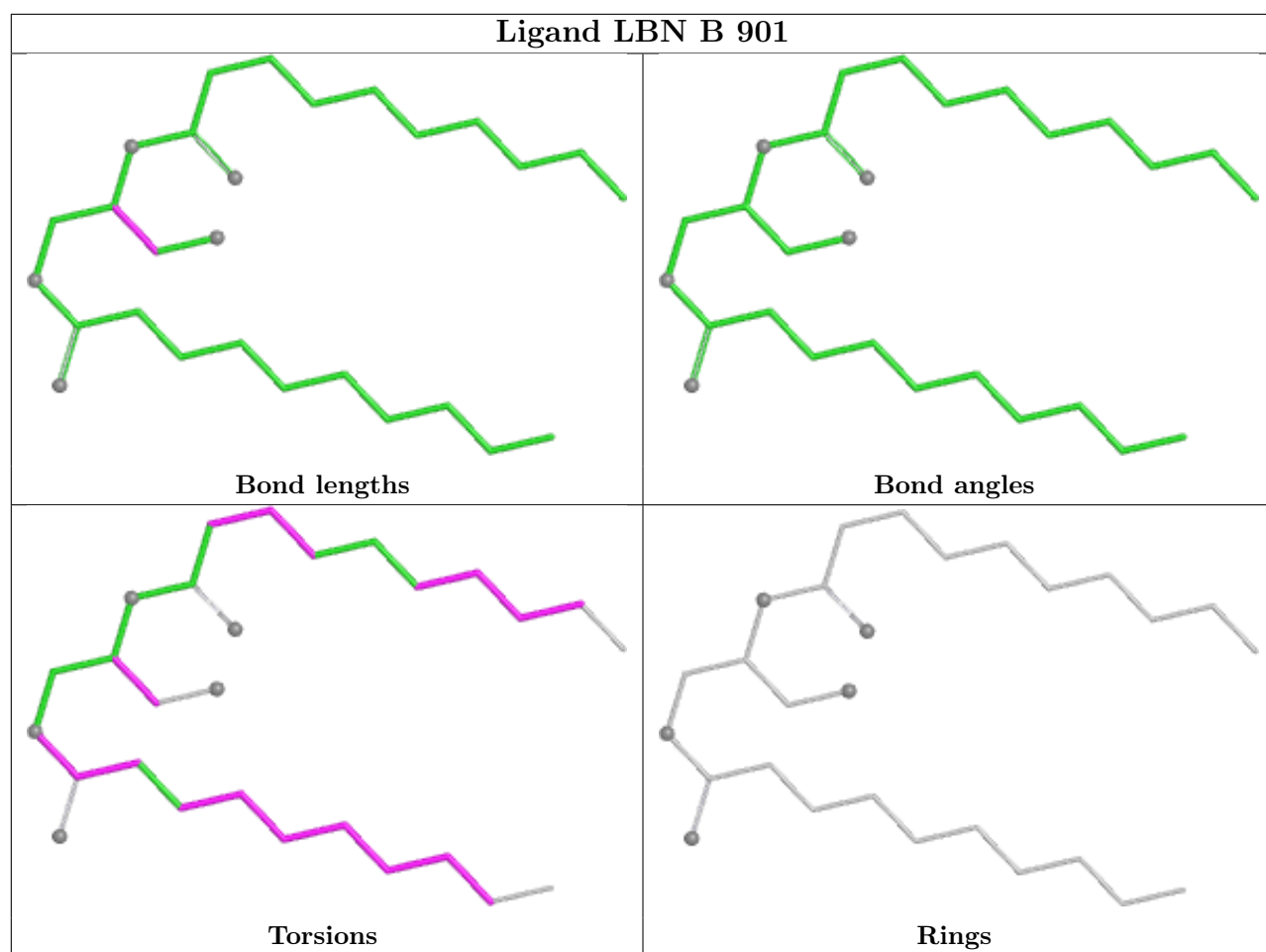
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	901	LBN	1	0

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

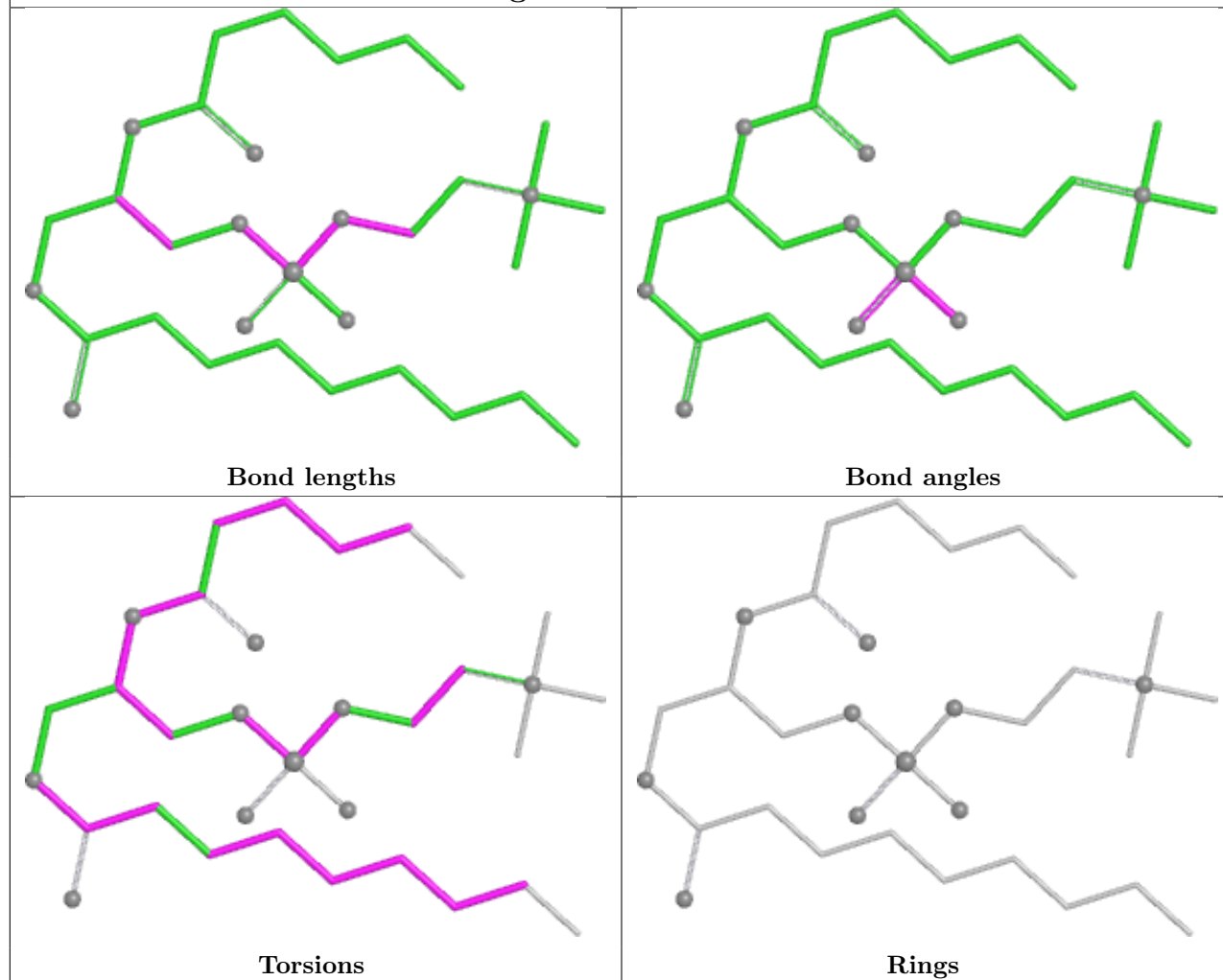
equivalents in the CSD to analyse the geometry.



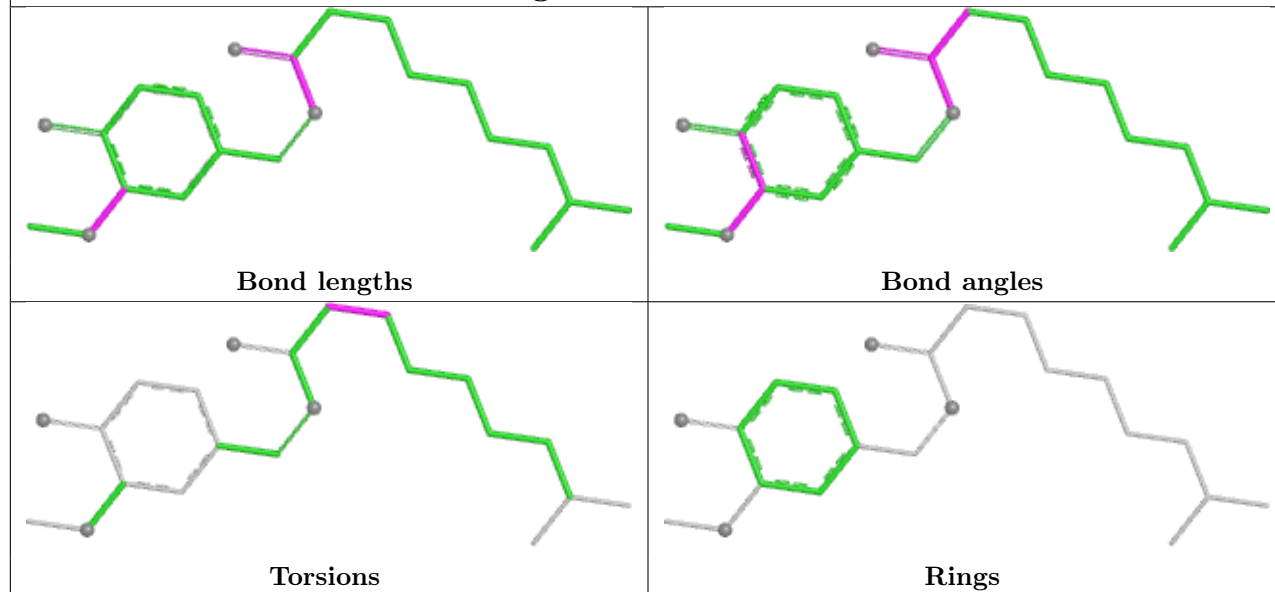


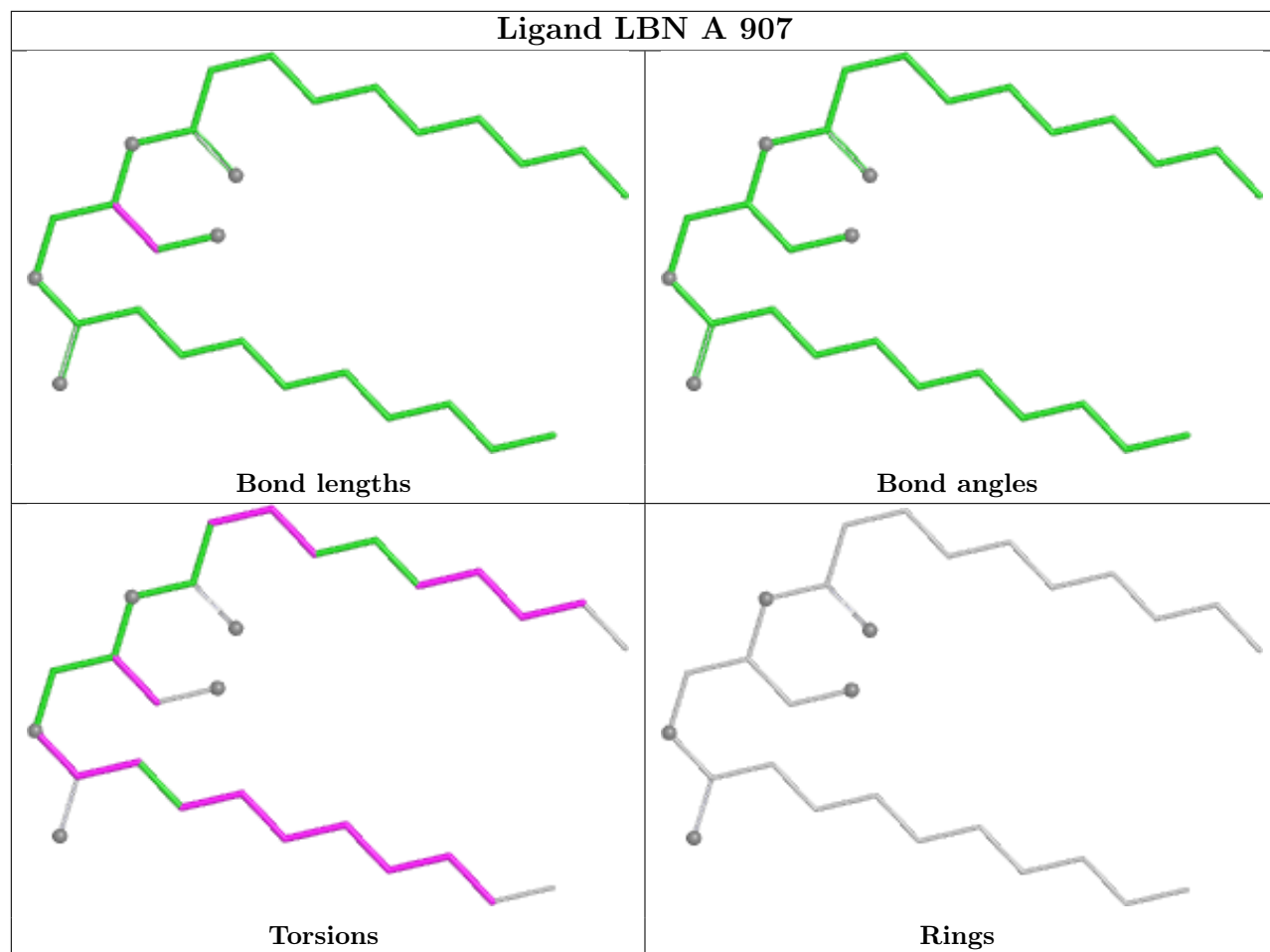


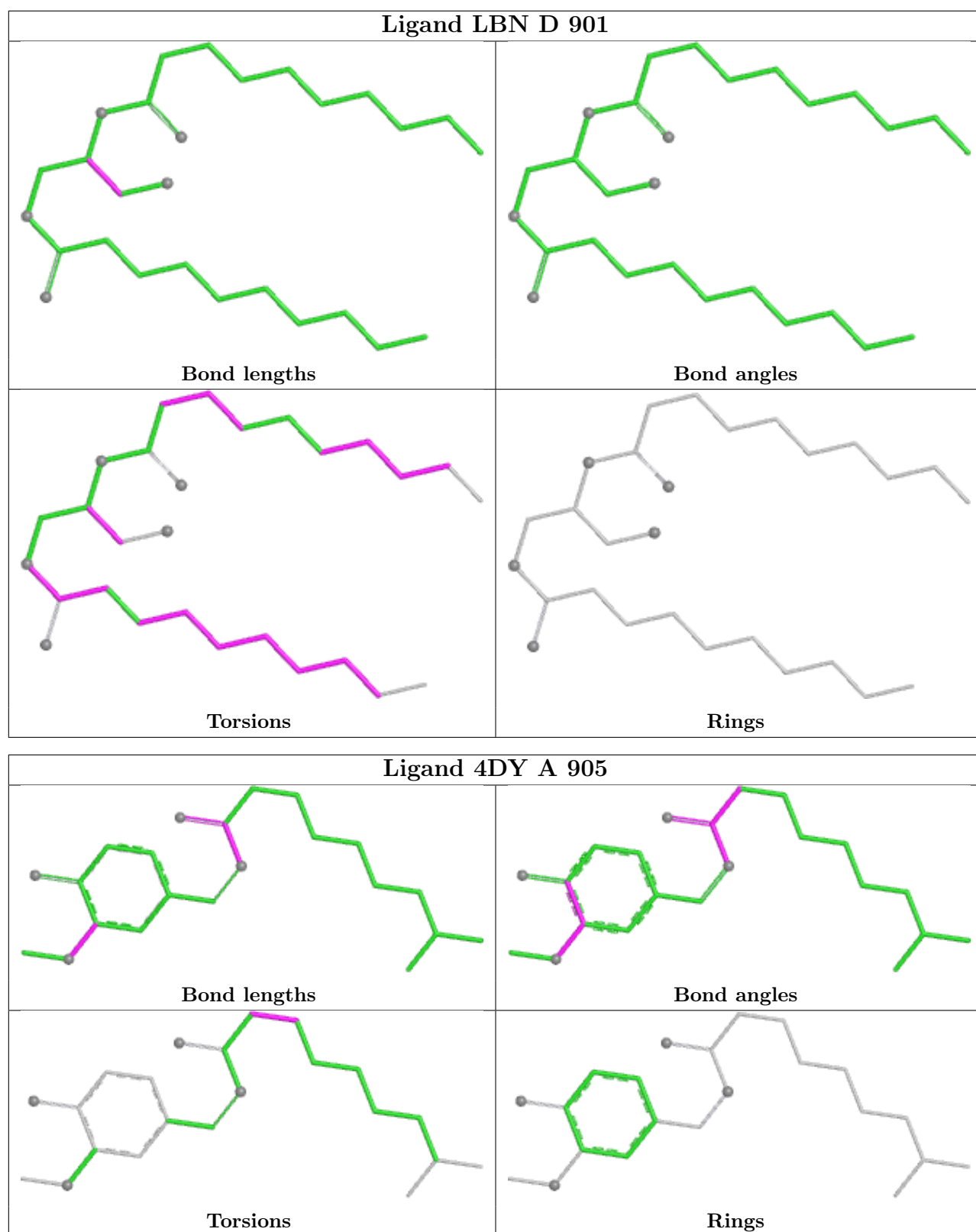
Ligand LBN B 903

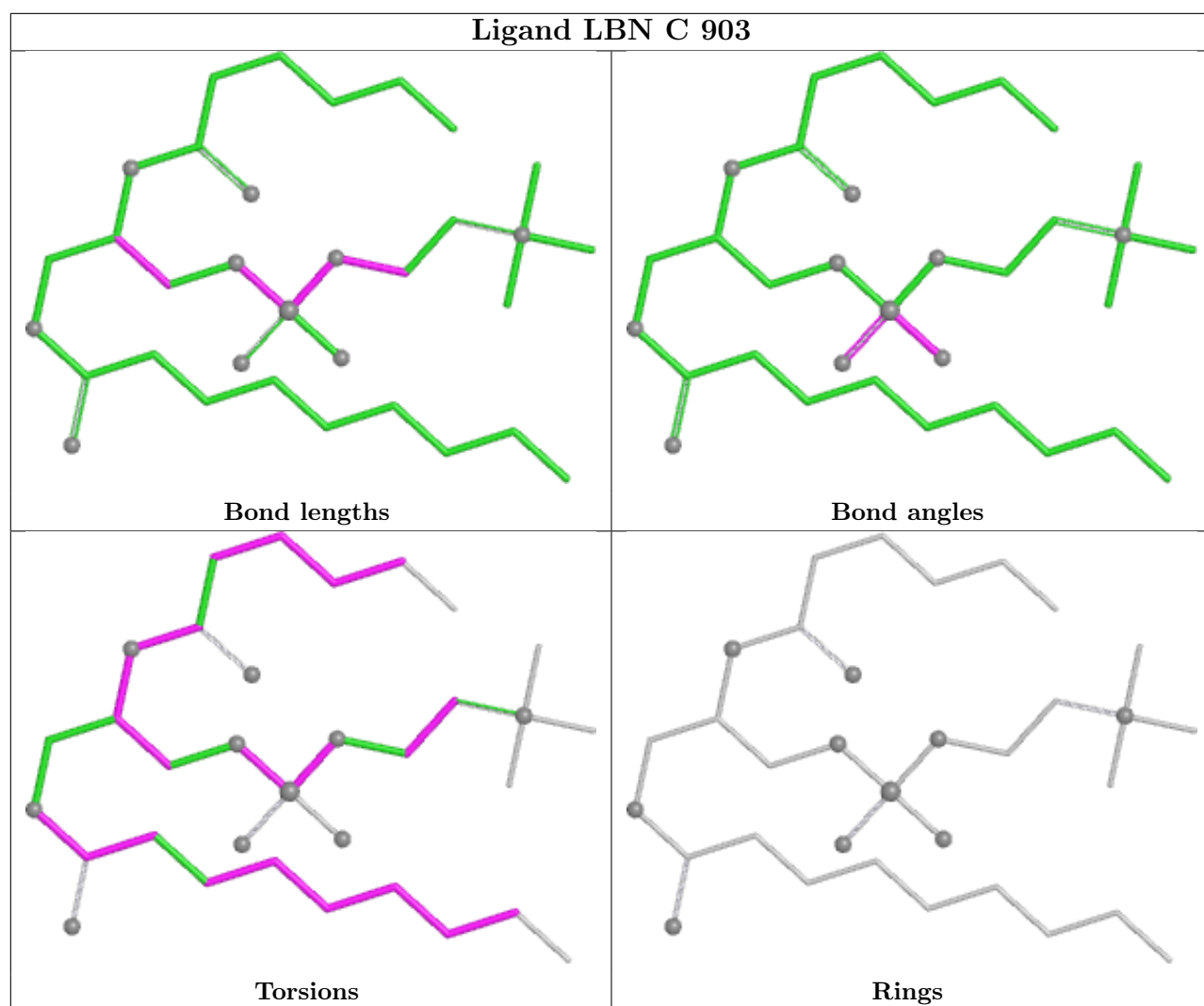


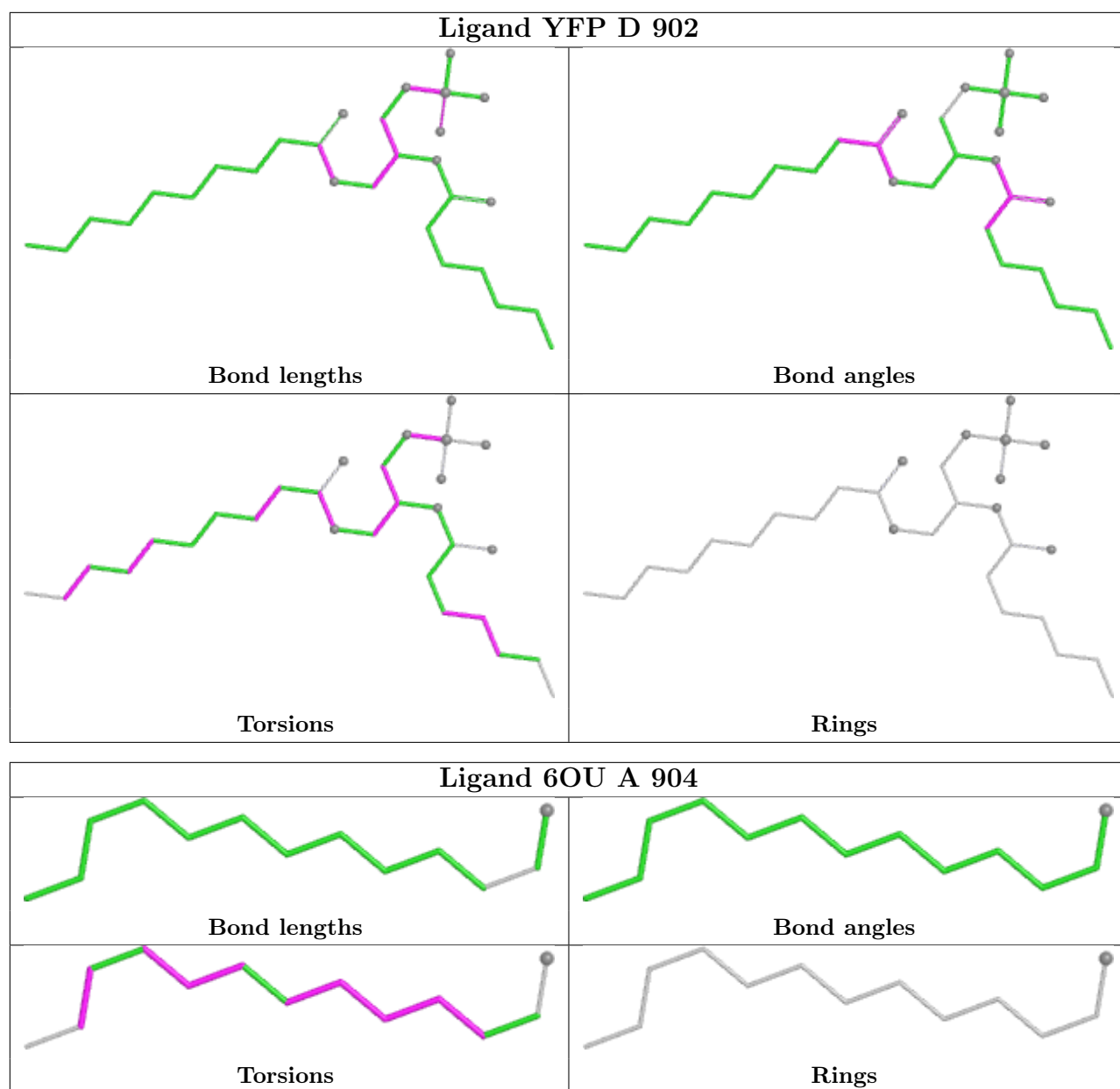
Ligand 4DY D 906

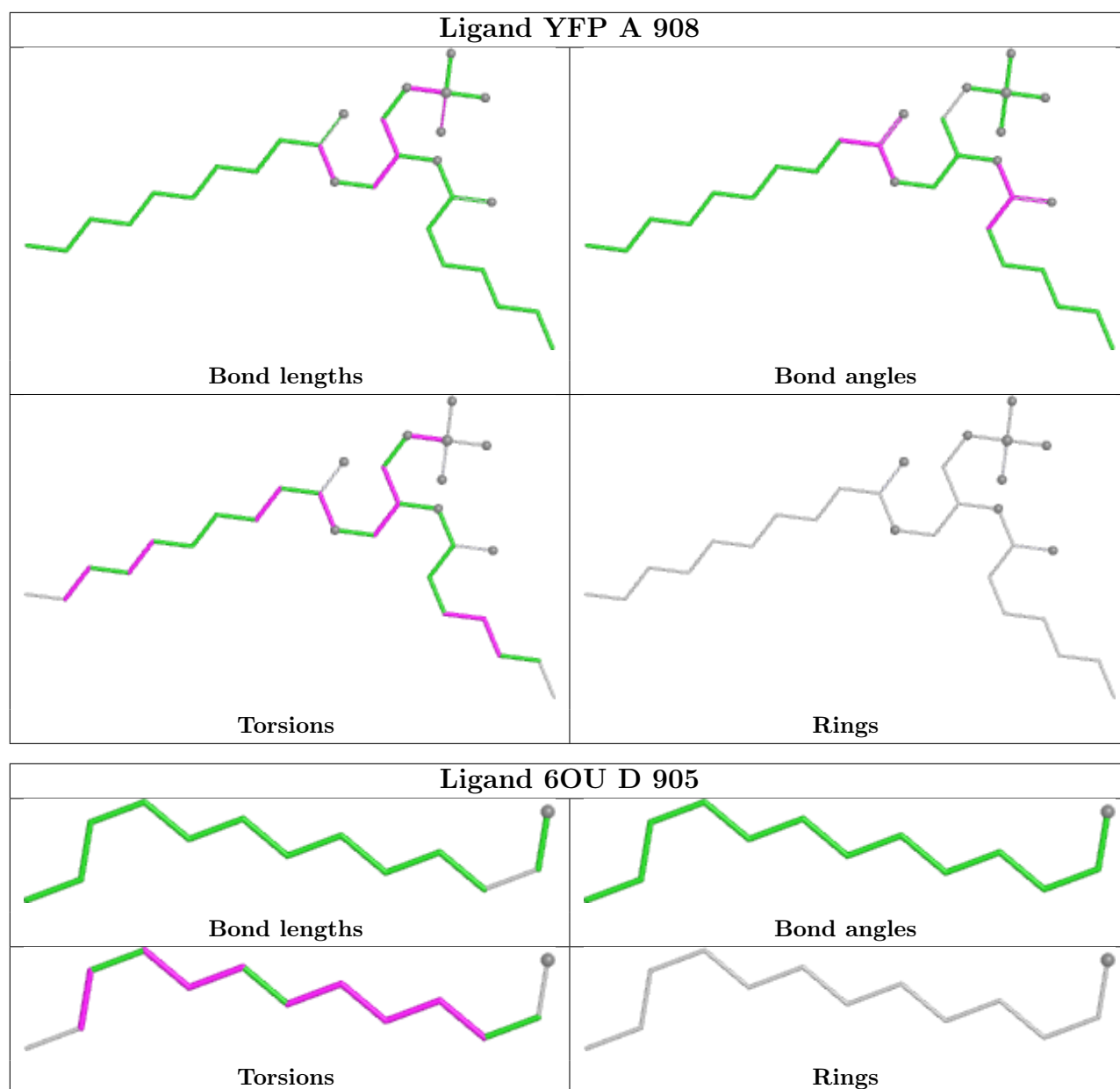


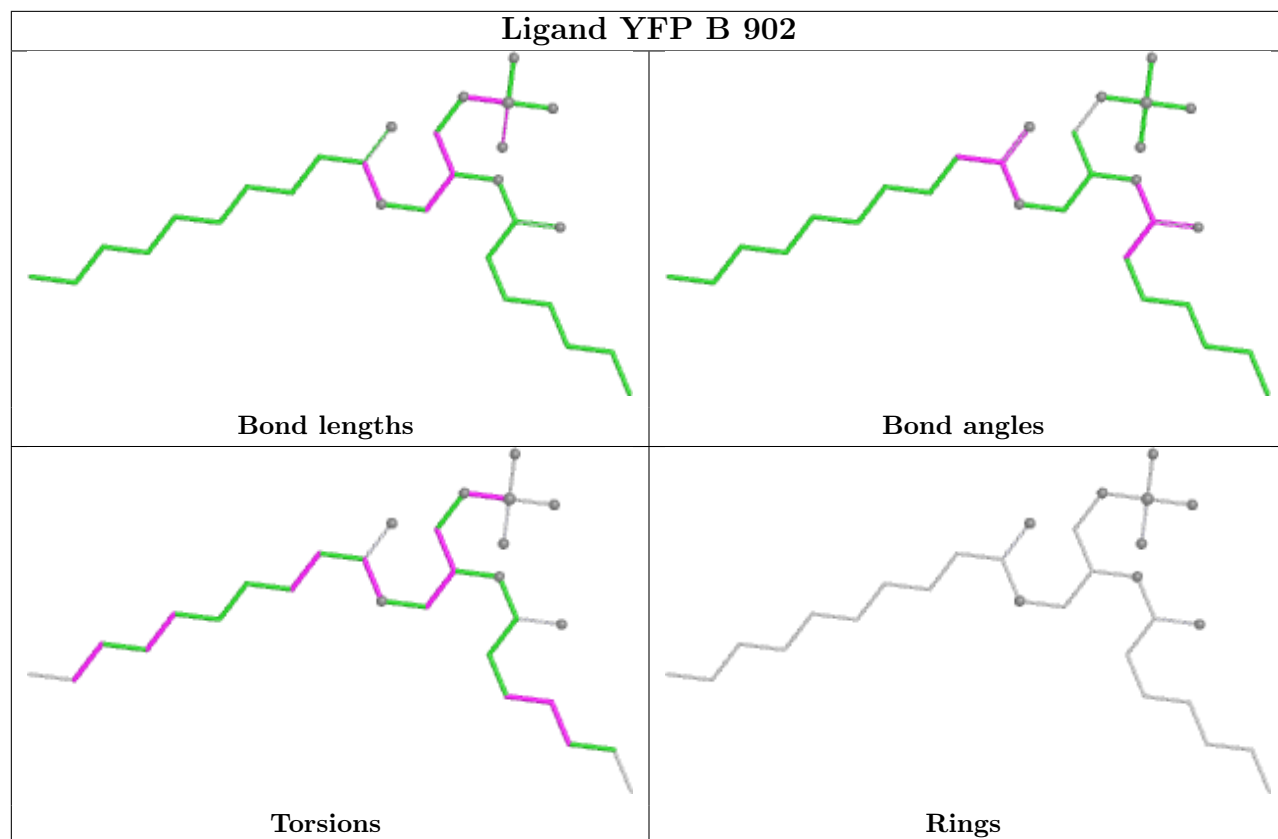


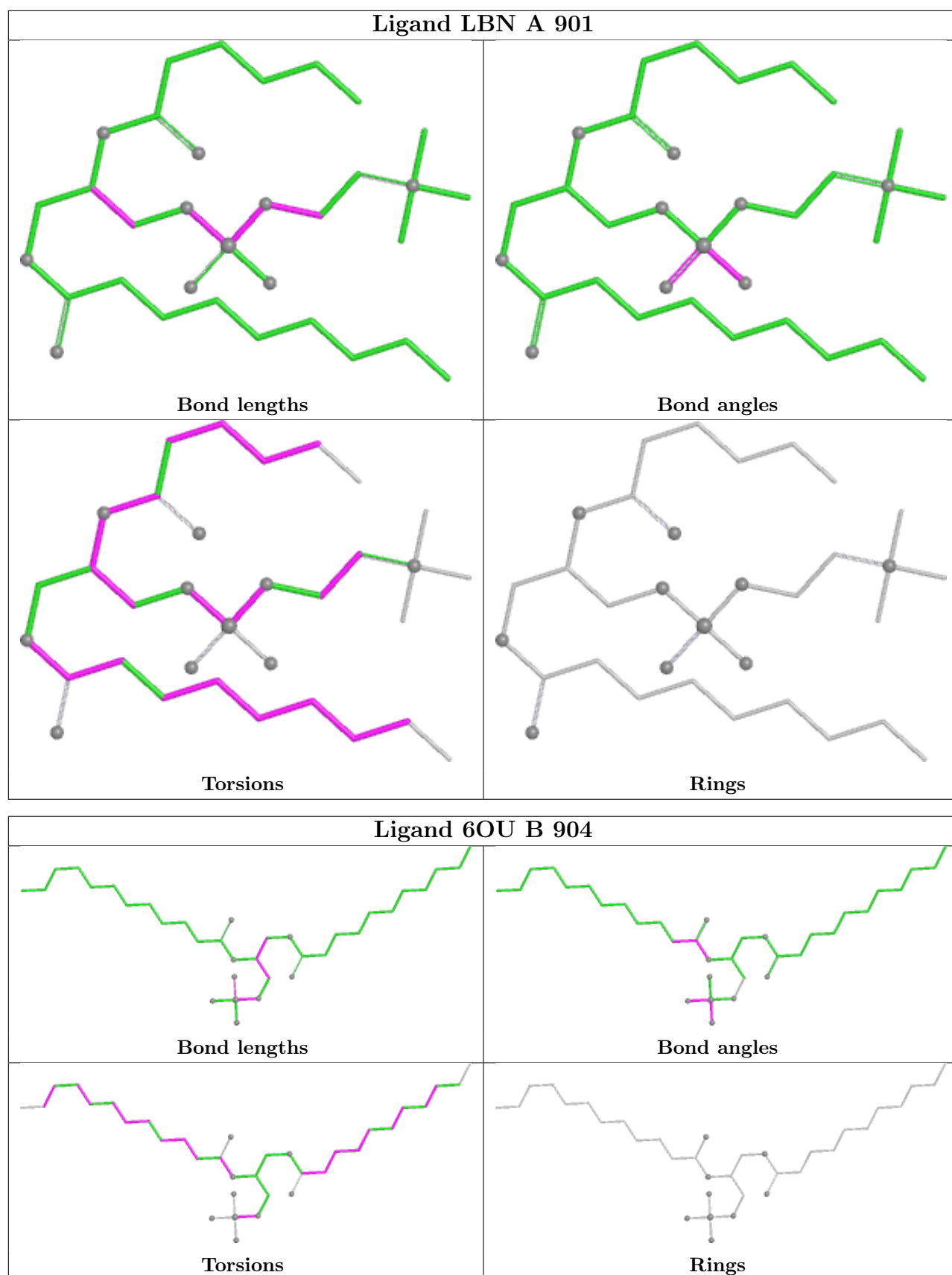


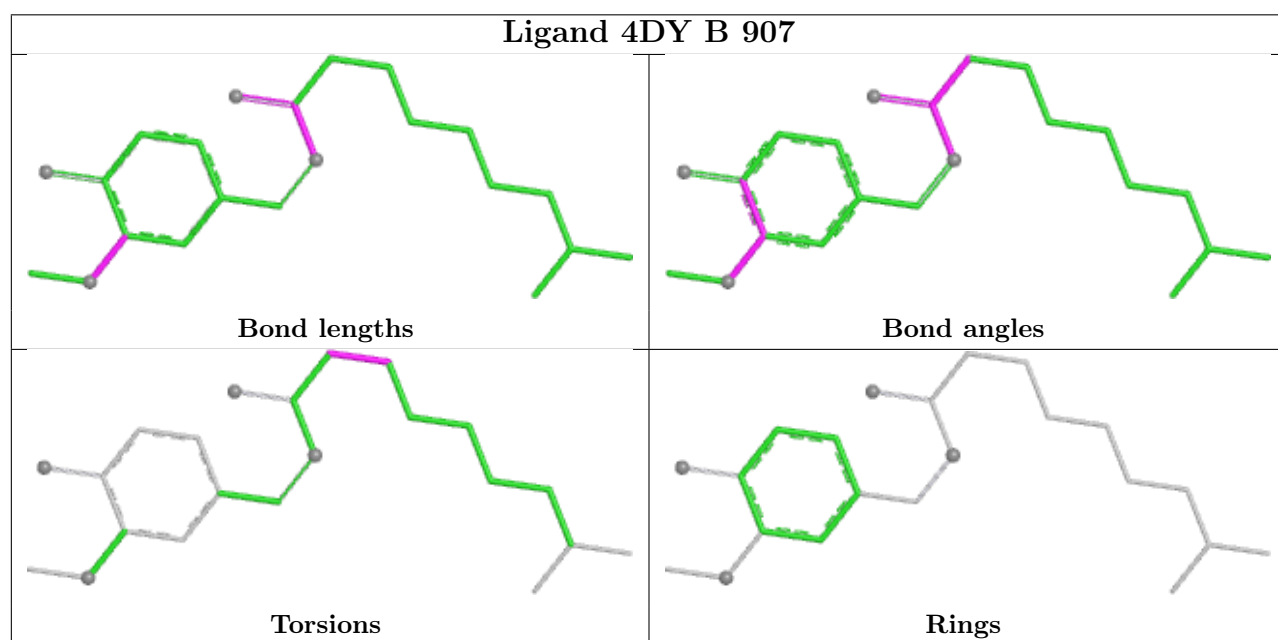
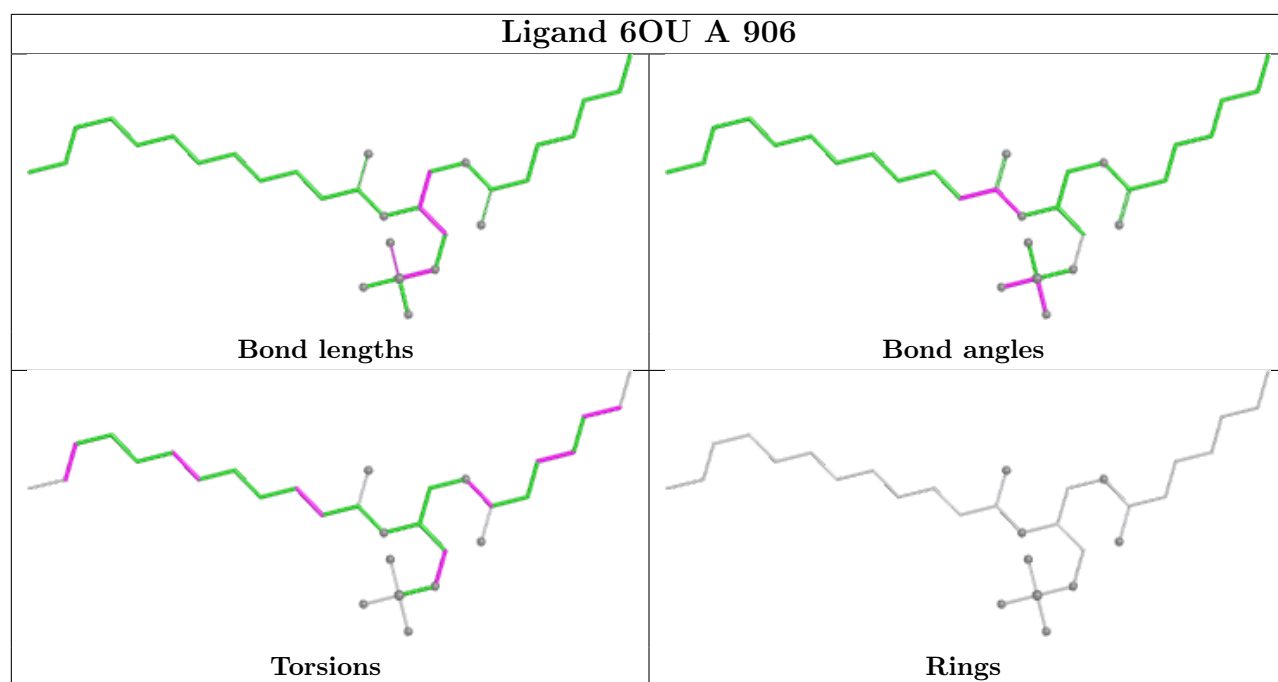


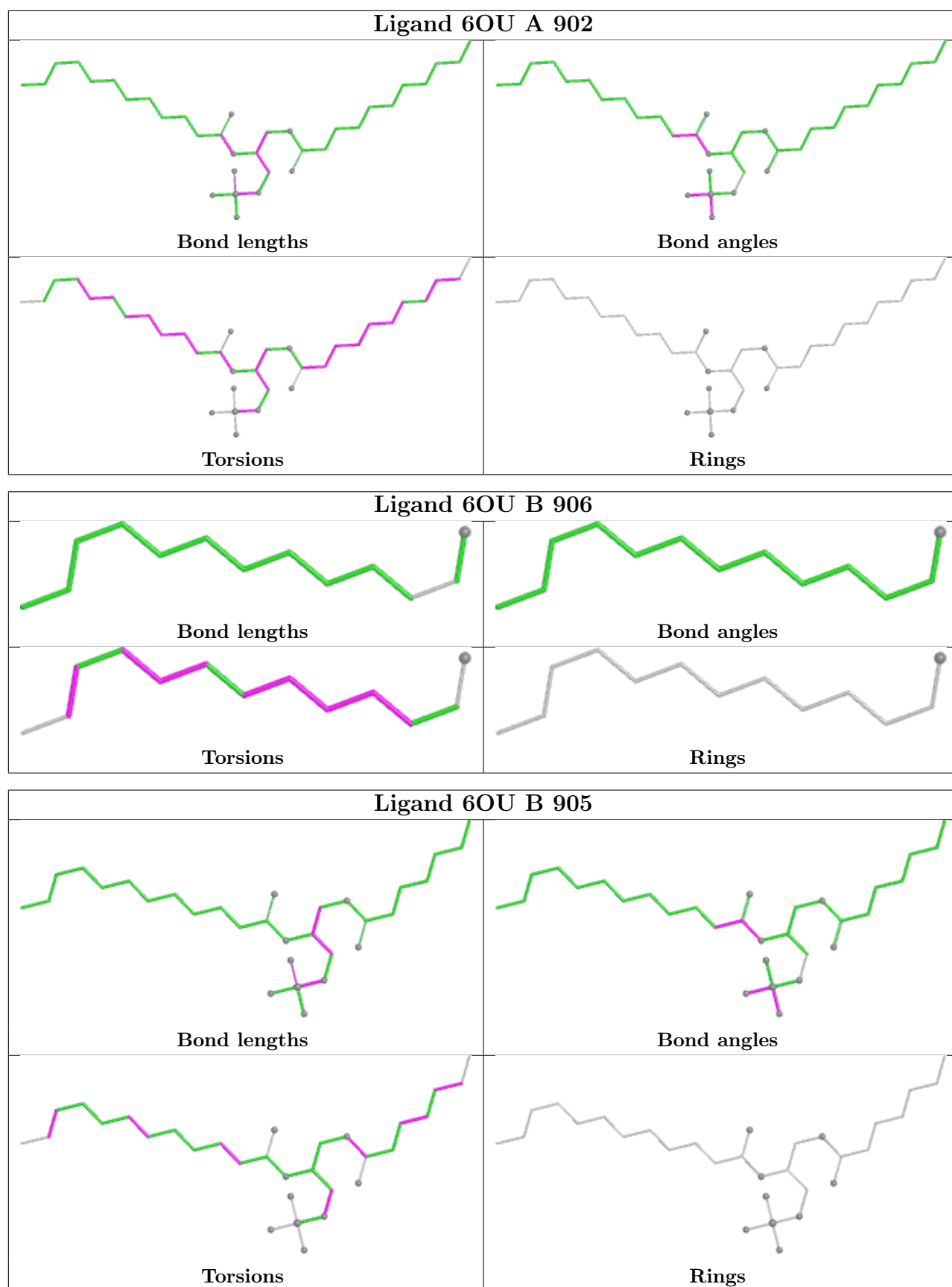


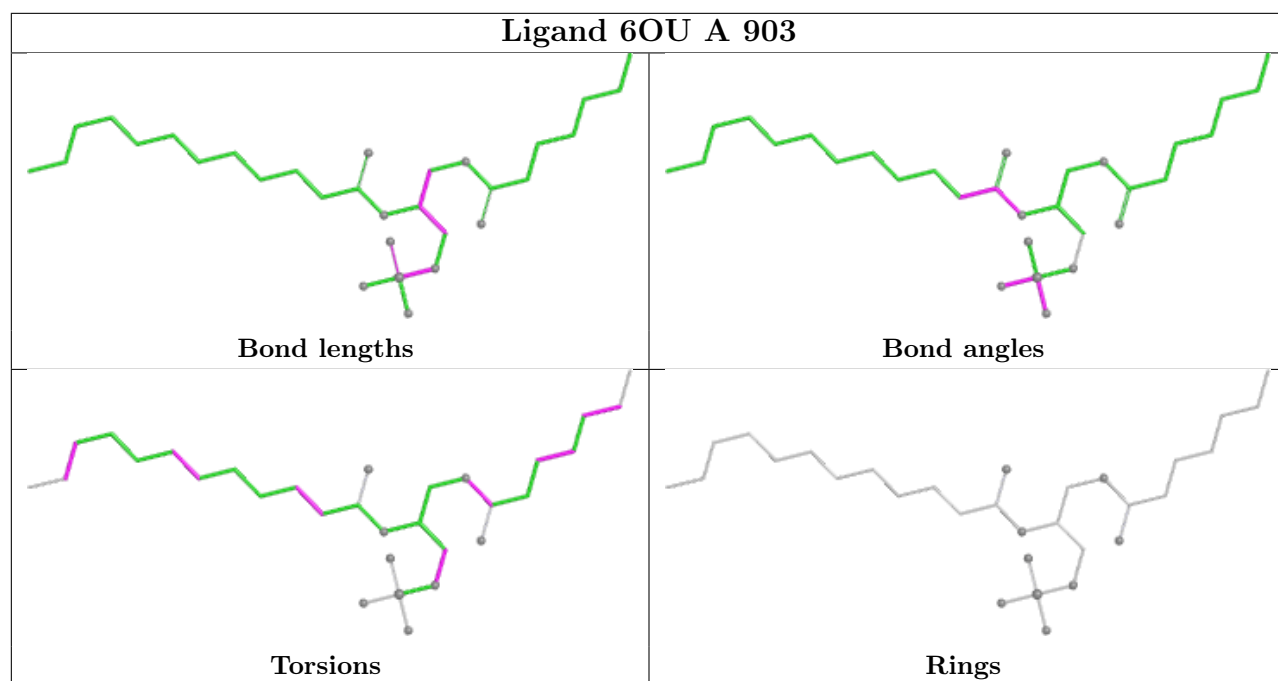
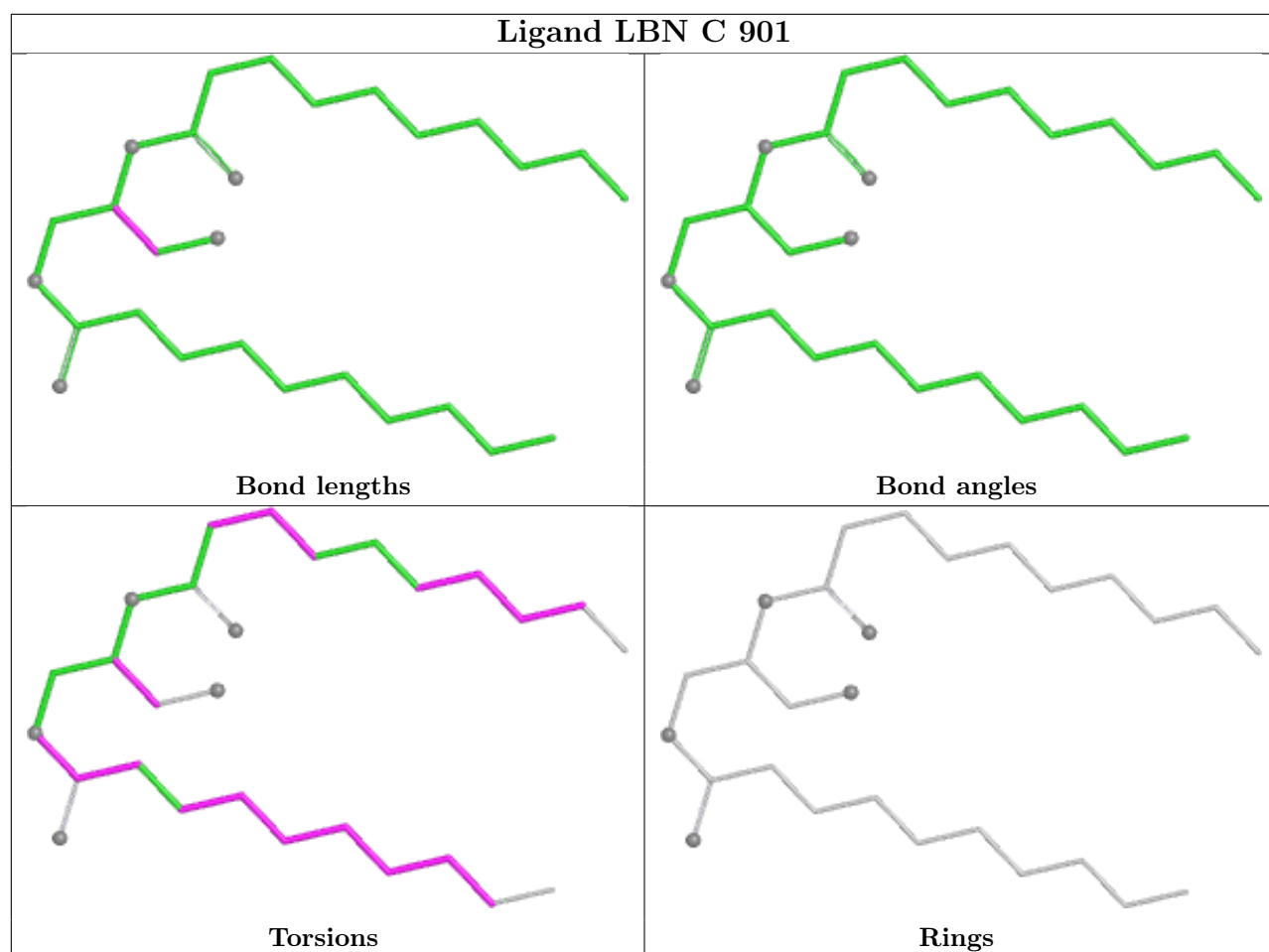


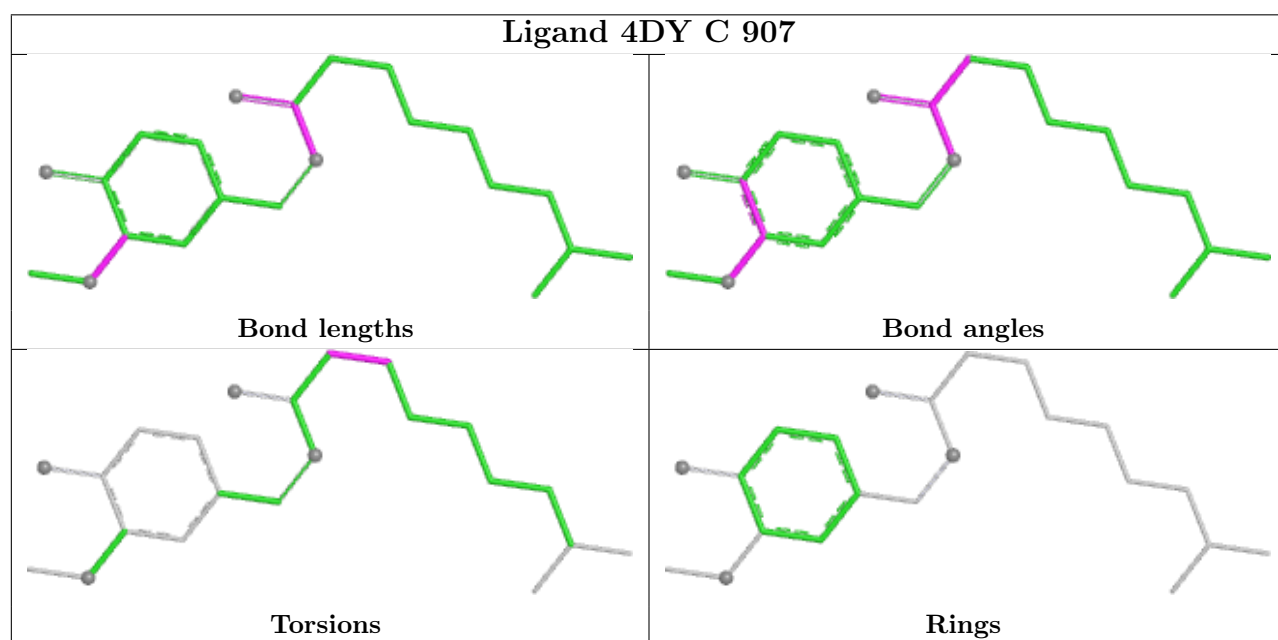
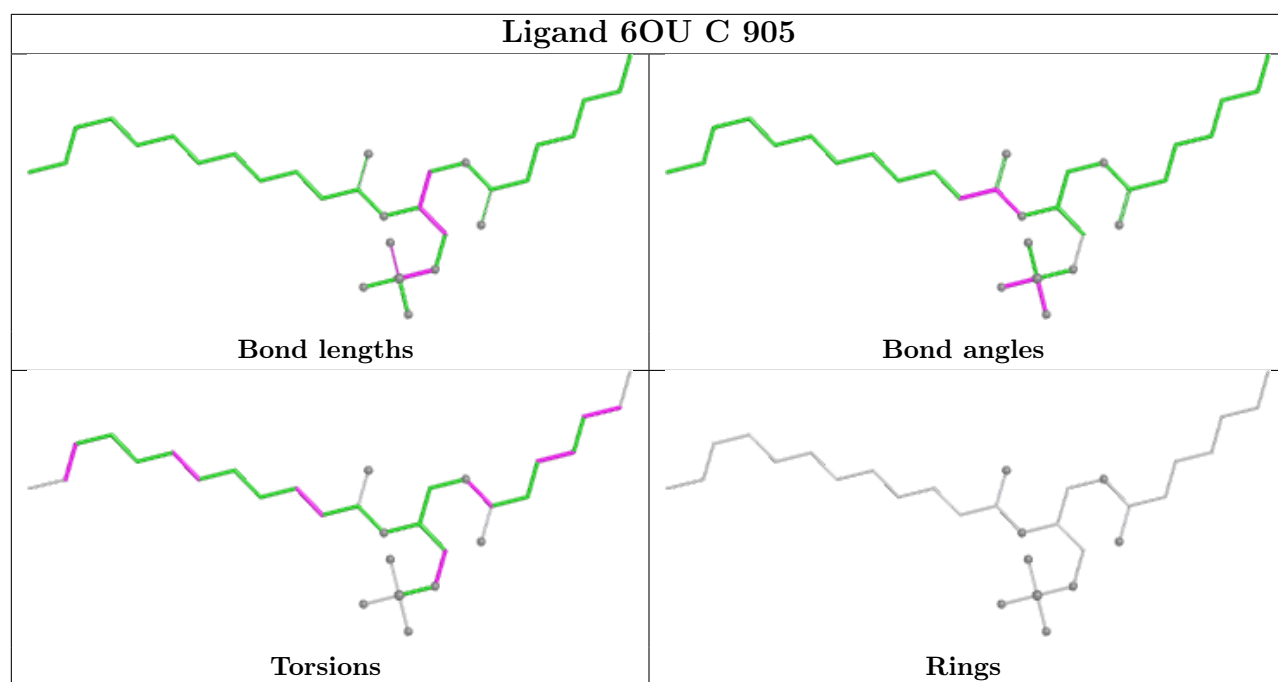


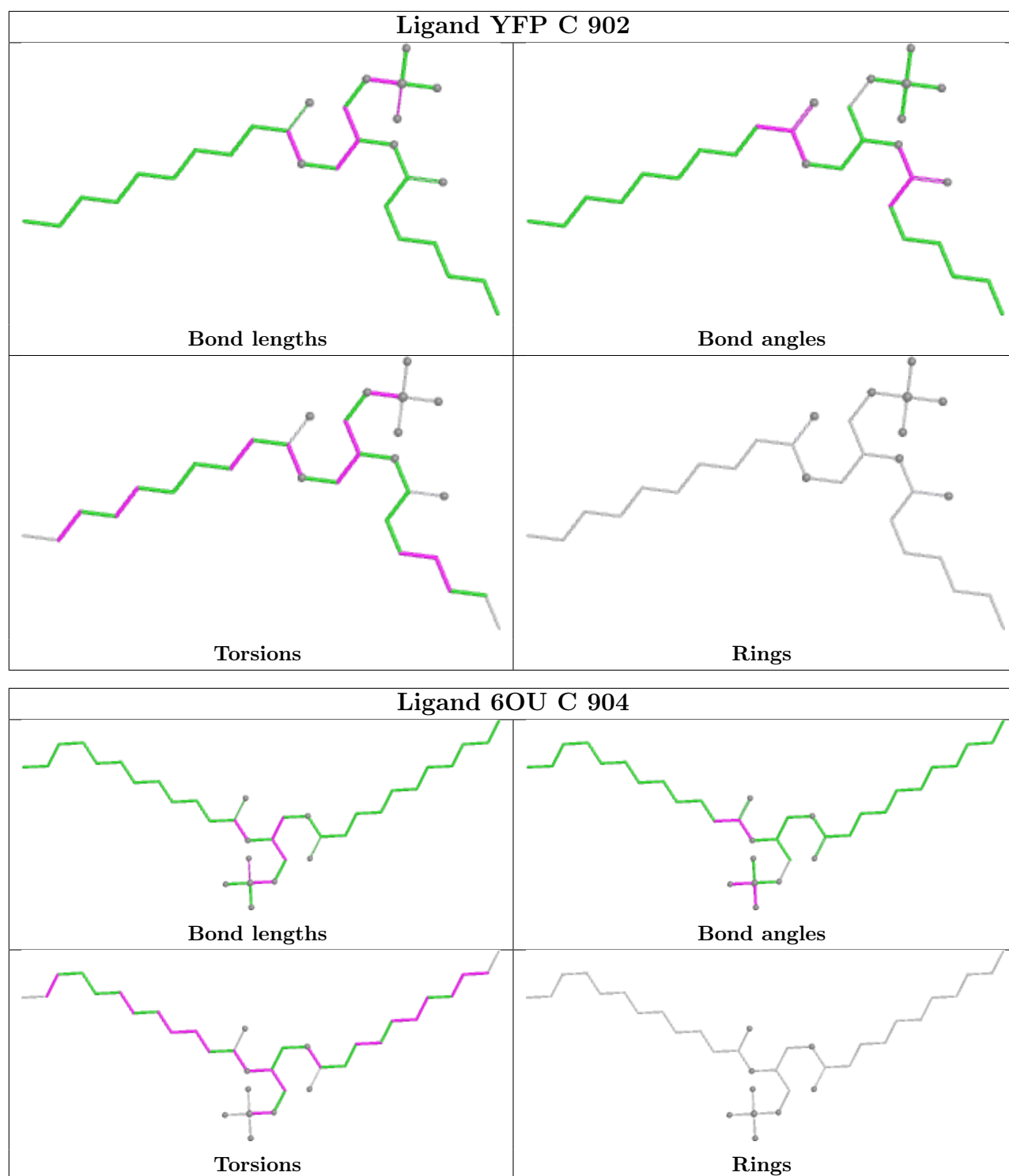












5.7 Other polymers ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

There are no chain breaks in this entry.

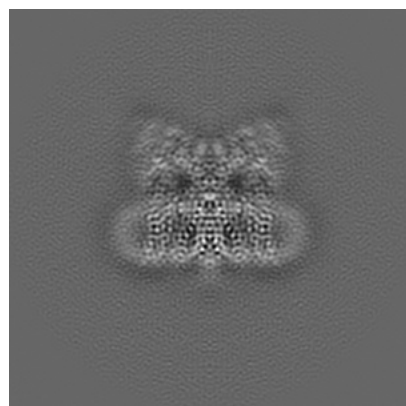
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-23474. These allow visual inspection of the internal detail of the map and identification of artifacts.

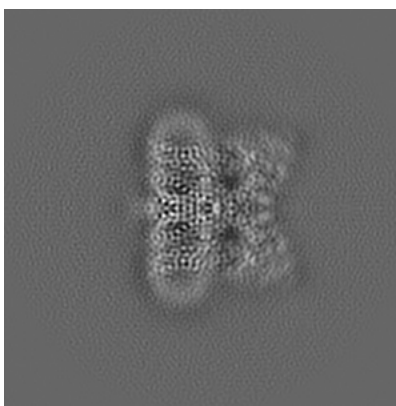
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

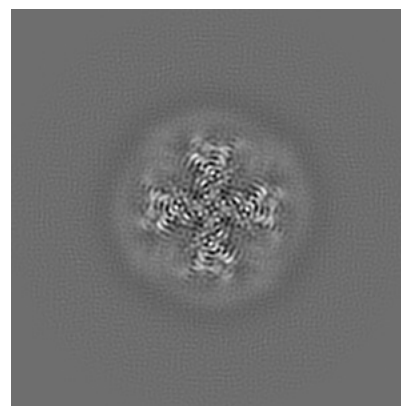
6.1.1 Primary map



X

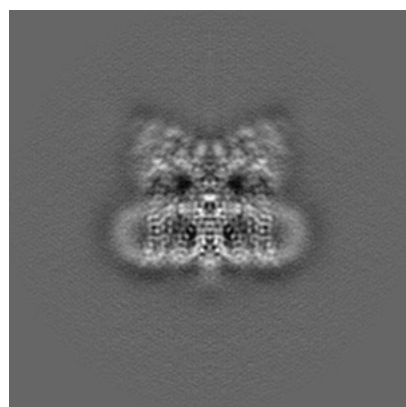


Y

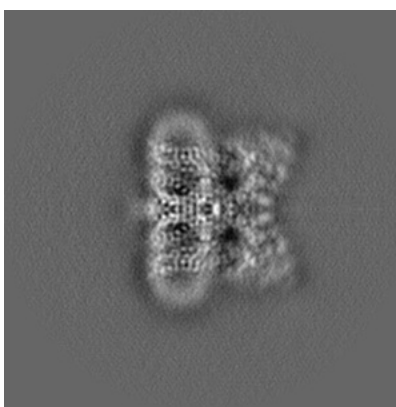


Z

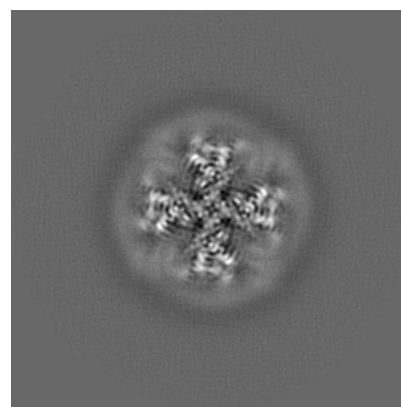
6.1.2 Raw map



X



Y

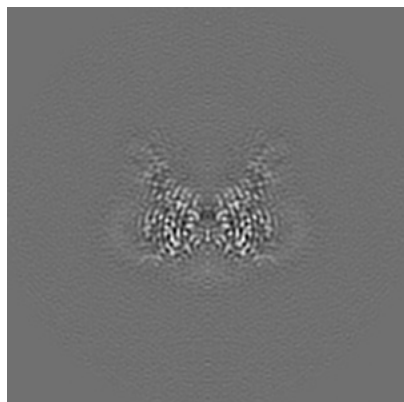


Z

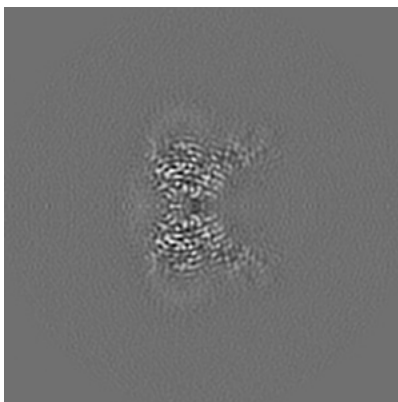
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

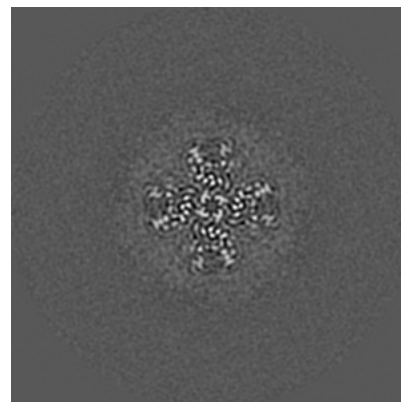
6.2.1 Primary map



X Index: 128

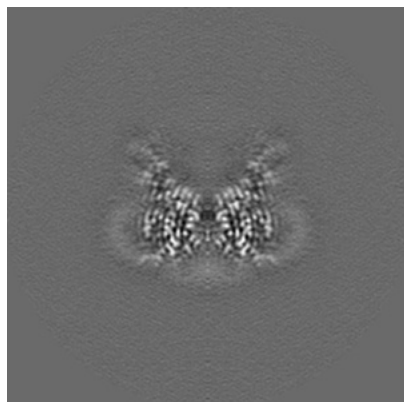


Y Index: 128

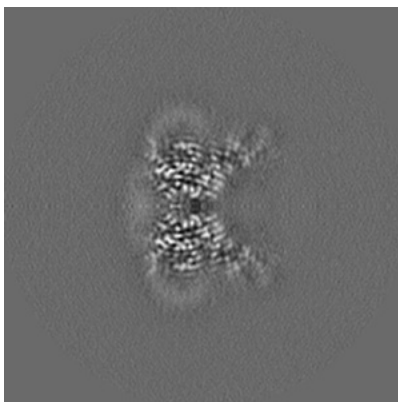


Z Index: 128

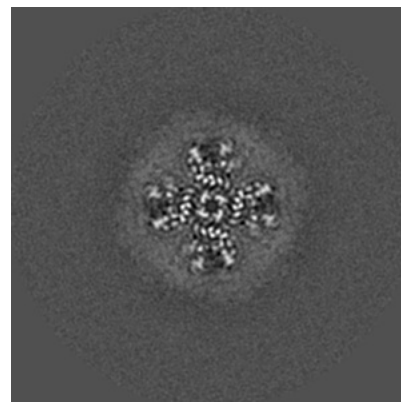
6.2.2 Raw map



X Index: 128



Y Index: 128

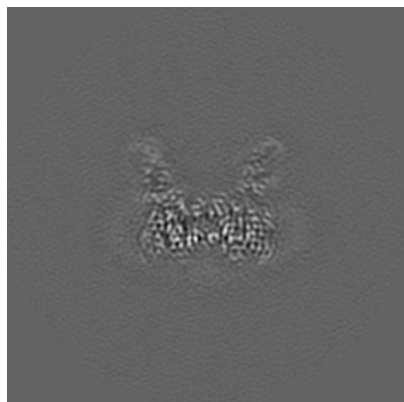


Z Index: 128

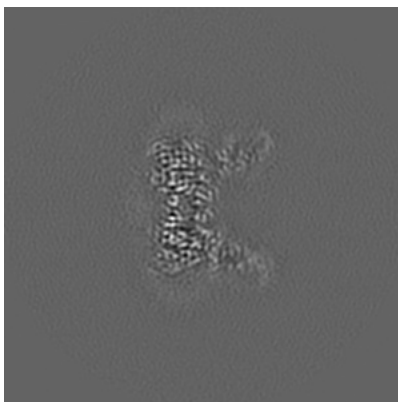
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

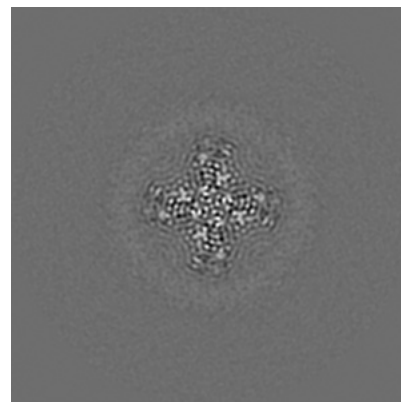
6.3.1 Primary map



X Index: 132

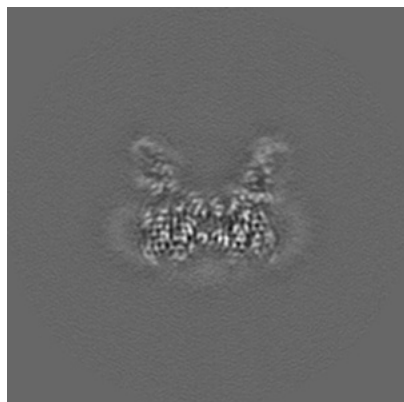


Y Index: 124

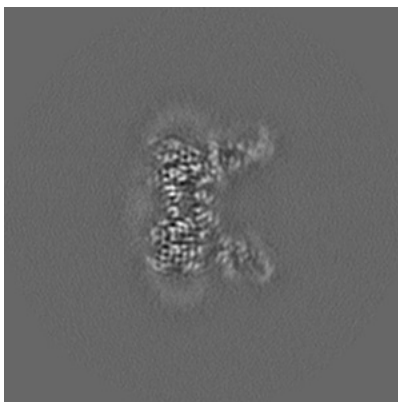


Z Index: 108

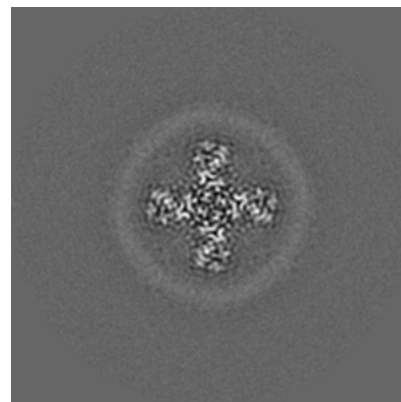
6.3.2 Raw map



X Index: 124



Y Index: 132

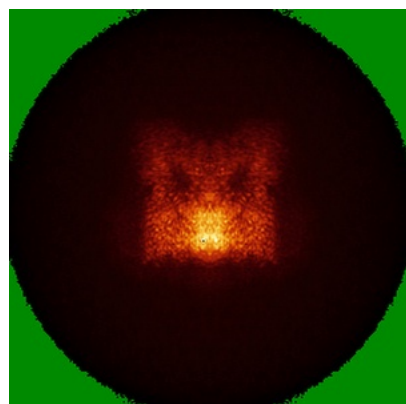


Z Index: 111

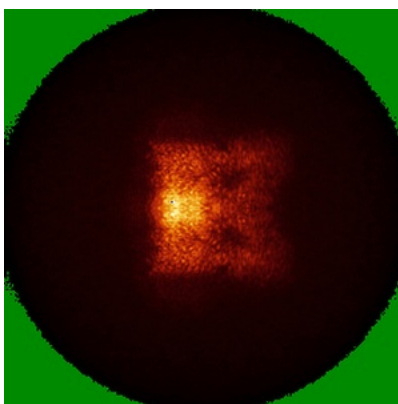
The images above show the largest variance slices of the map in three orthogonal directions.

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

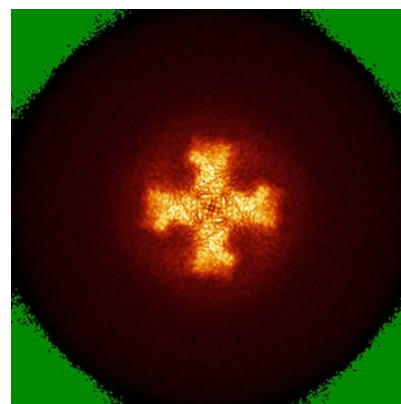
6.4.1 Primary map



X

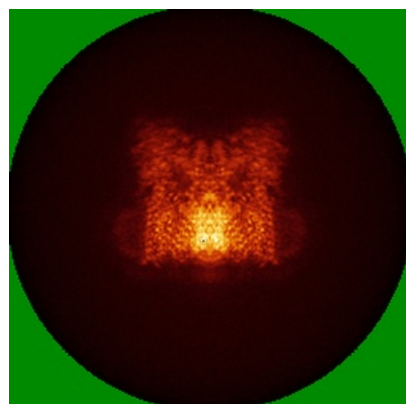


Y

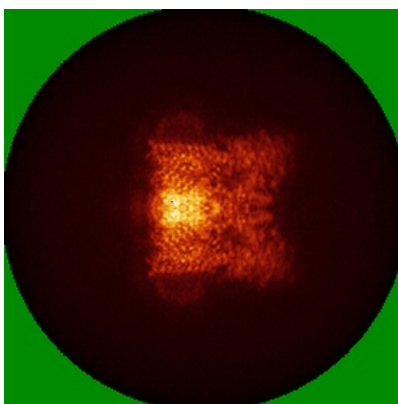


Z

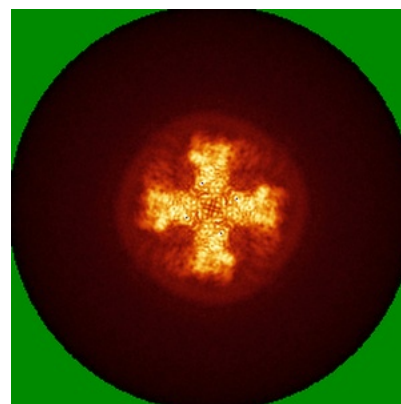
6.4.2 Raw map



X



Y

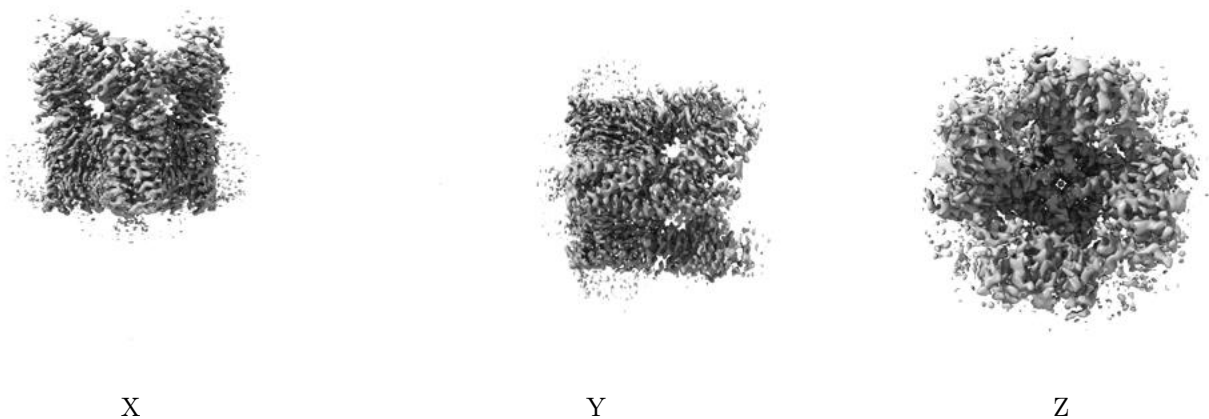


Z

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 0.014. 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.

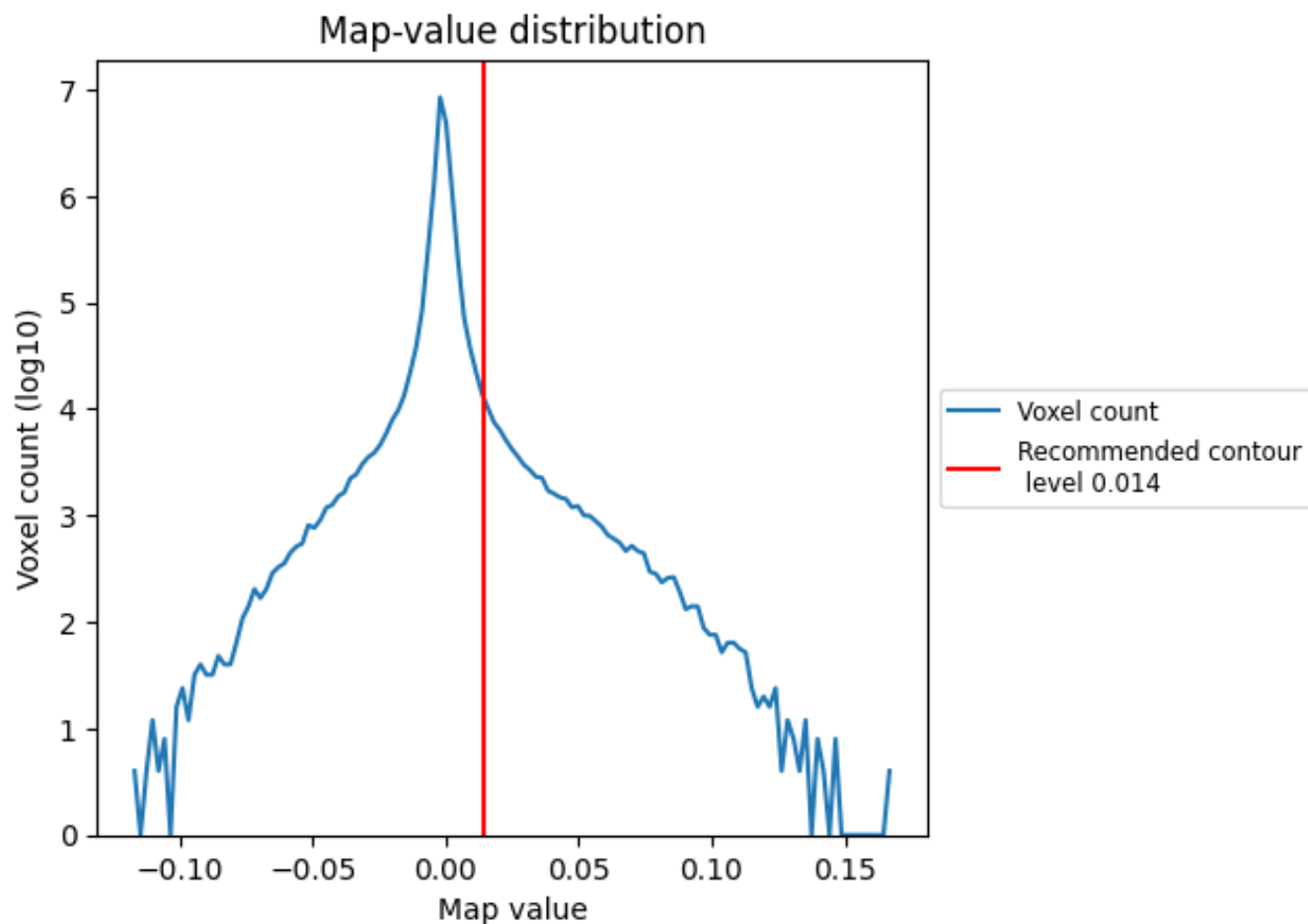
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

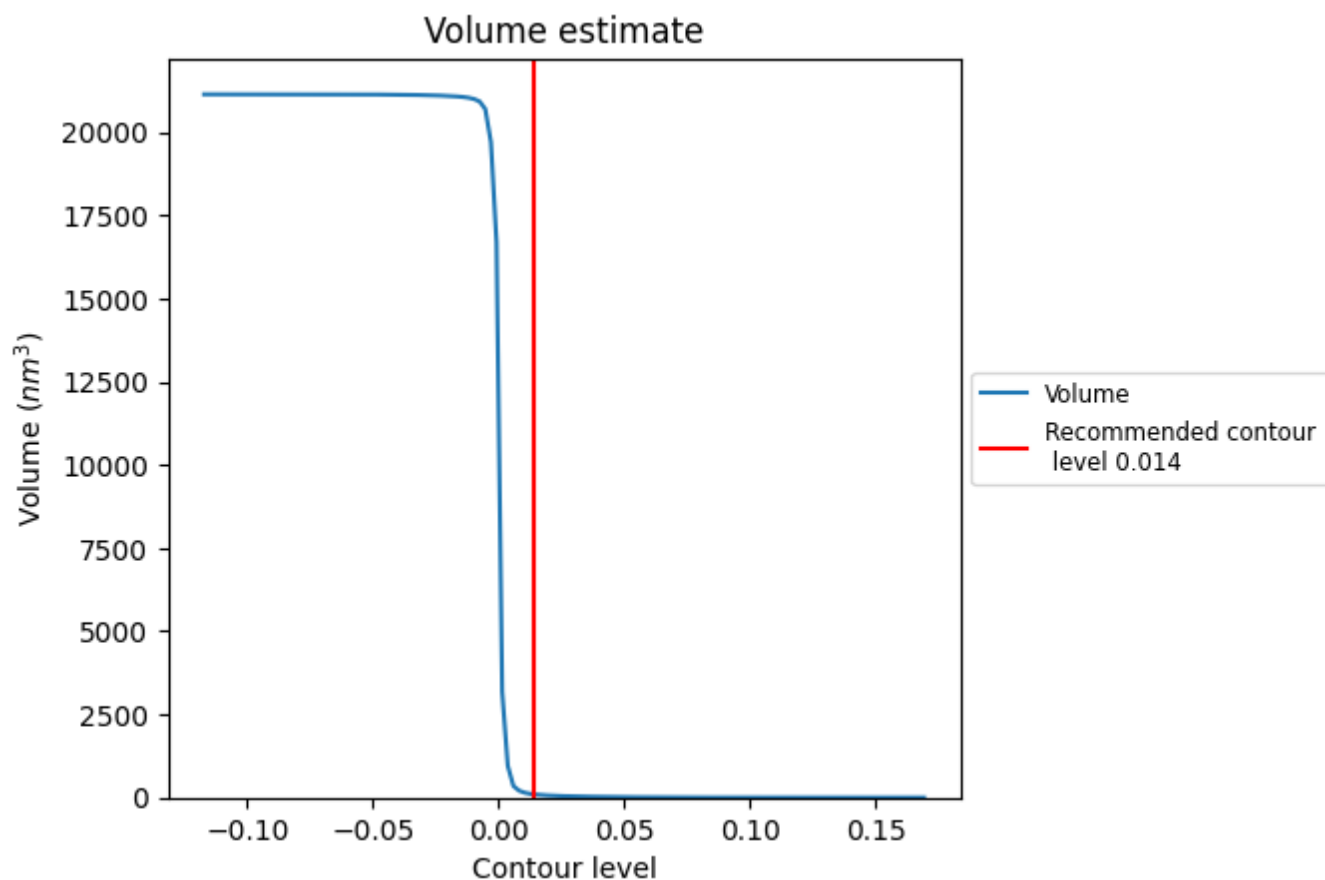
This section contains the results of statistical analysis of the map.

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.

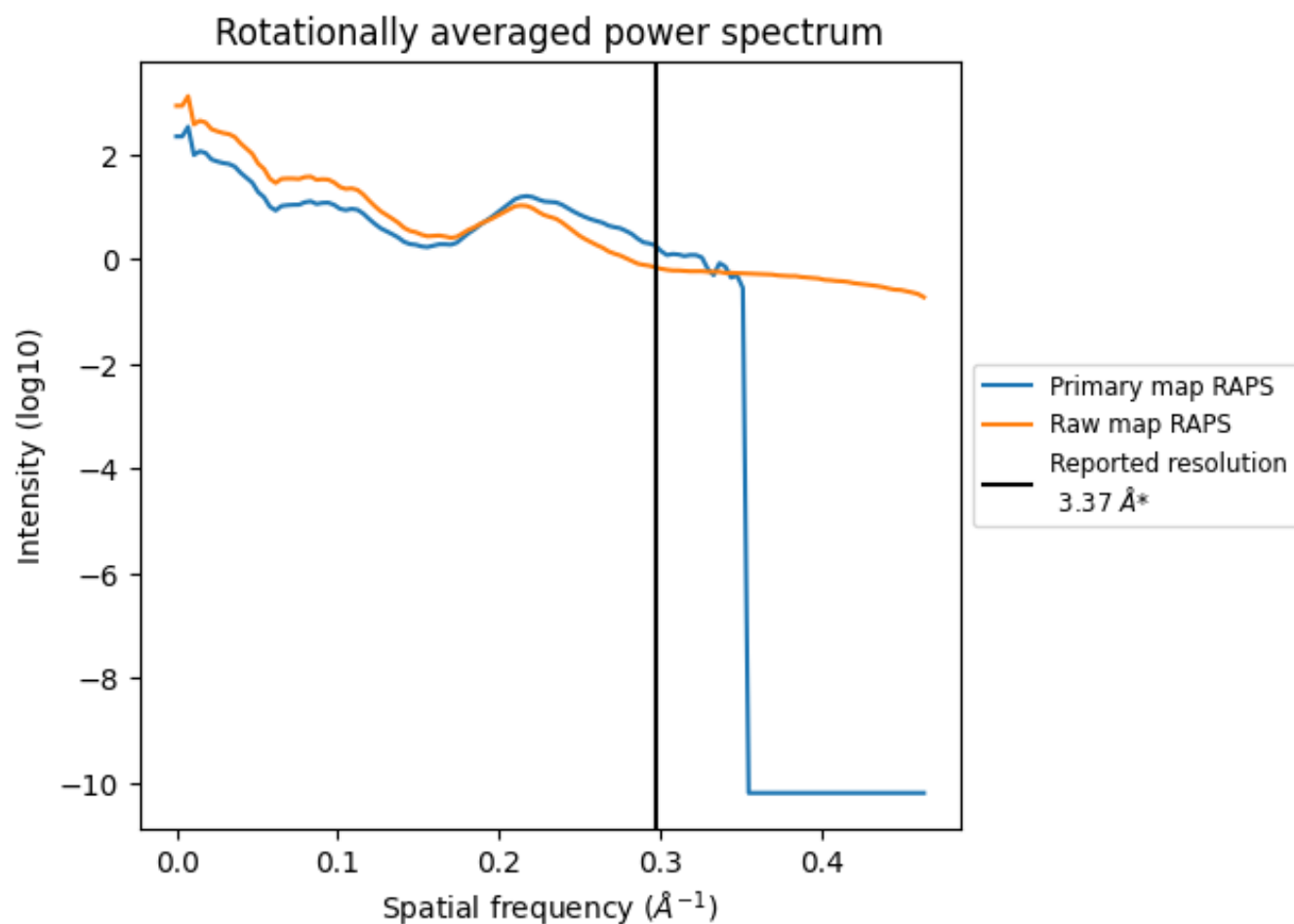
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 98 nm³; this corresponds to an approximate mass of 89 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 ⓘ

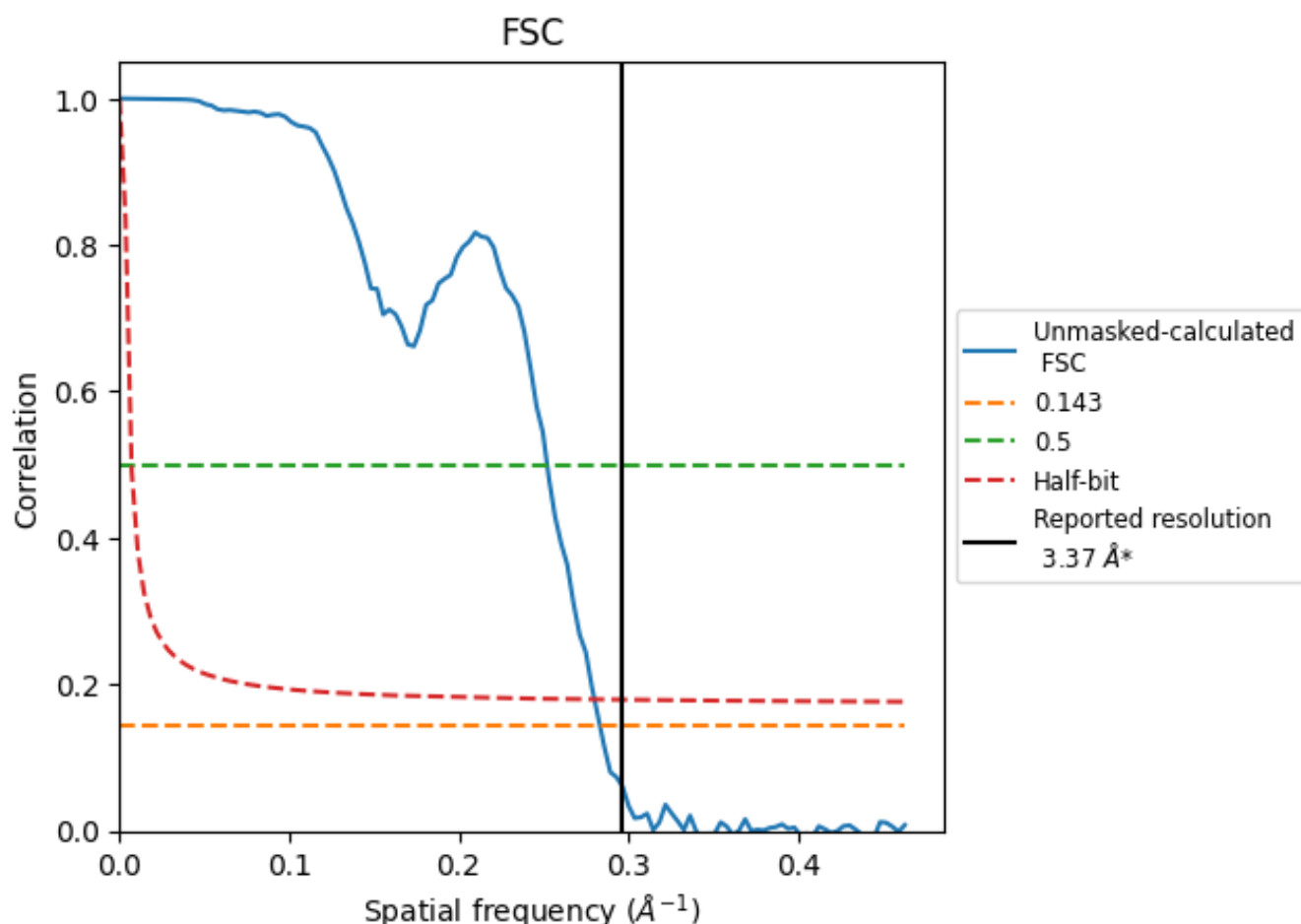


*Reported resolution corresponds to spatial frequency of 0.297 Å⁻¹

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 0.297 \AA^{-1}

8.2 Resolution estimates [i](#)

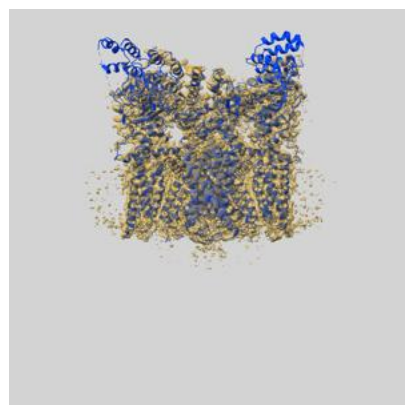
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.37	-	-
Author-provided FSC curve	-	-	-
Unmasked-calculated*	3.53	3.97	3.57

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps.

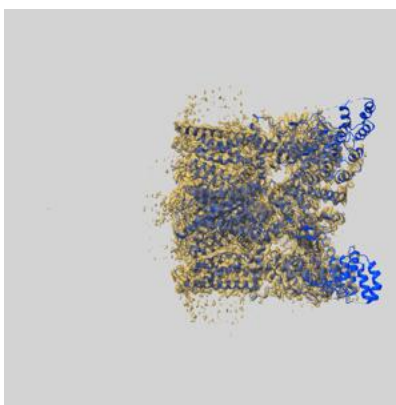
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-23474 and PDB model 7LPA. Per-residue inclusion information can be found in [section 3](#) on [page 10](#).

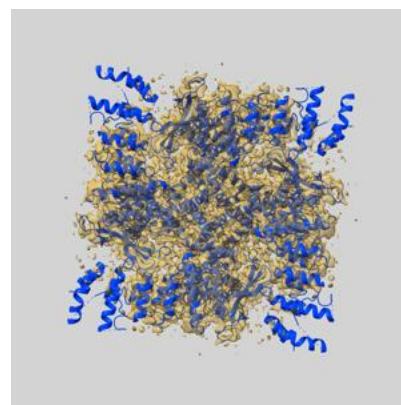
9.1 Map-model overlay [i](#)



X



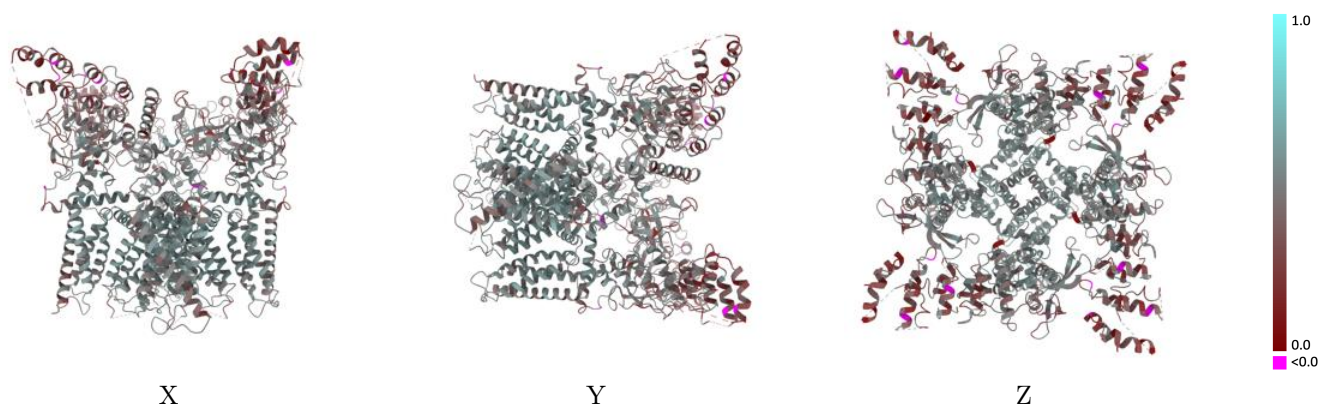
Y



Z

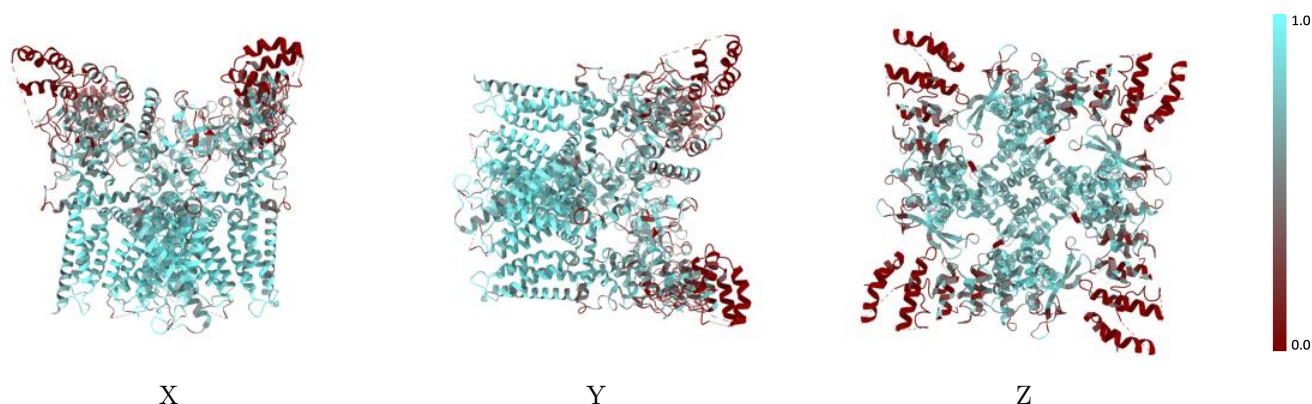
The images above show the 3D surface view of the map at the recommended contour level 0.014 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



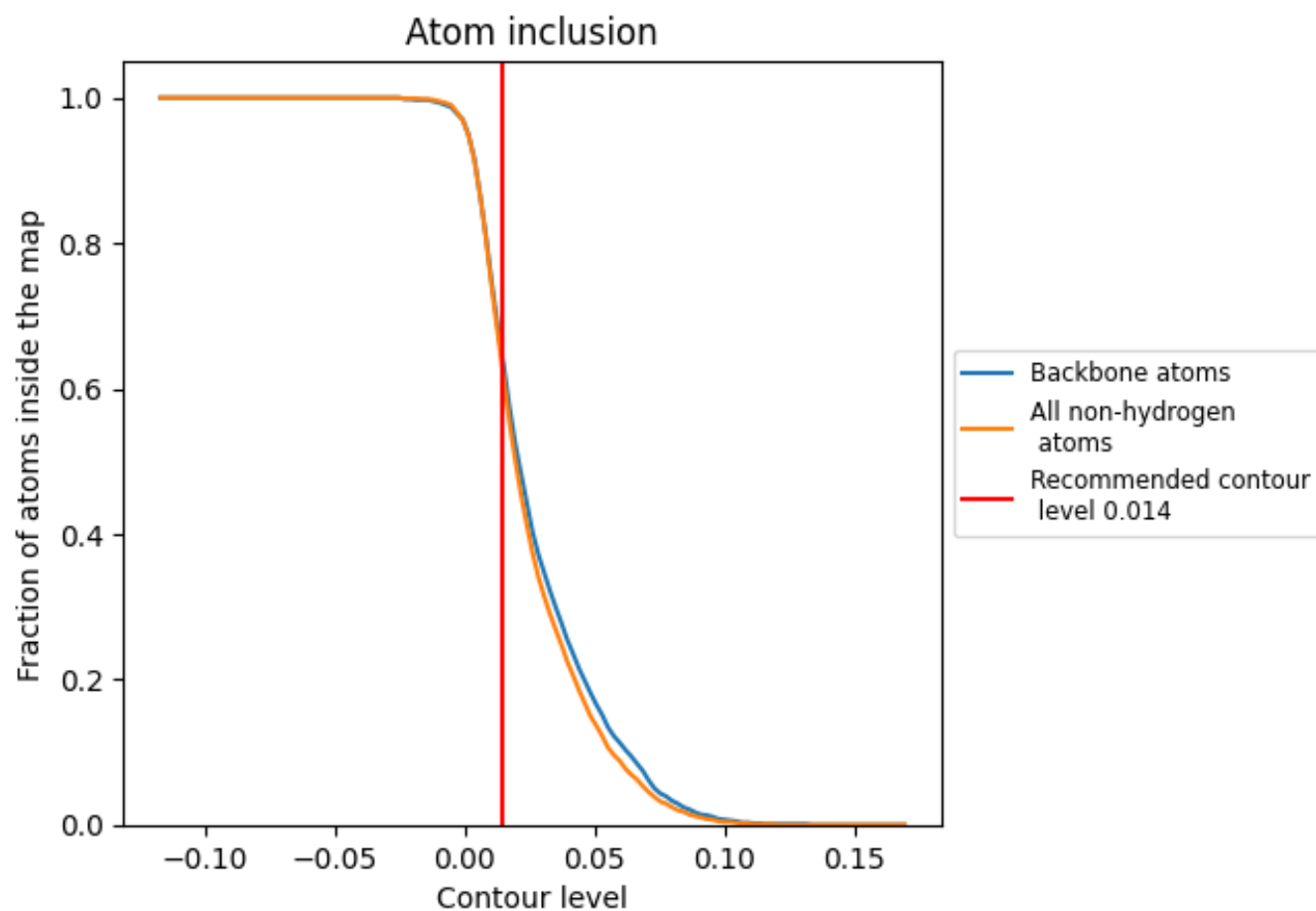
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.014).

9.4 Atom inclusion [i](#)



At the recommended contour level, 65% of all backbone atoms, 64% 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 (0.014) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	<div></div> 0.6380	<div></div> 0.4640
A	<div></div> 0.6380	<div></div> 0.4650
B	<div></div> 0.6380	<div></div> 0.4640
C	<div></div> 0.6380	<div></div> 0.4630
D	<div></div> 0.6380	<div></div> 0.4640

