



Full wwPDB EM Validation Report ⓘ

Mar 5, 2026 – 03:34 PM UTC

PDB ID : 7RQX / pdb_00007rqx
EMDB ID : EMD-24639
Title : Cryo-EM structure of the full-length TRPV1 with RTx at 25 degrees Celsius, in an intermediate-open state, class A
Authors : Kwon, D.H.; Suo, Y.; Lee, S.-Y.
Deposited on : 2021-08-08
Resolution : 3.36 Å(reported)
Based on initial model : 7LP9

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.dev132
Mogul : 2022.3.0, CSD as543be (2022)
MolProbity : 4-5-2 with Phenix2.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data in the EMDB archive up until May 2025)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

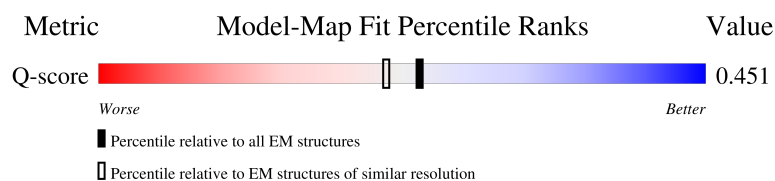
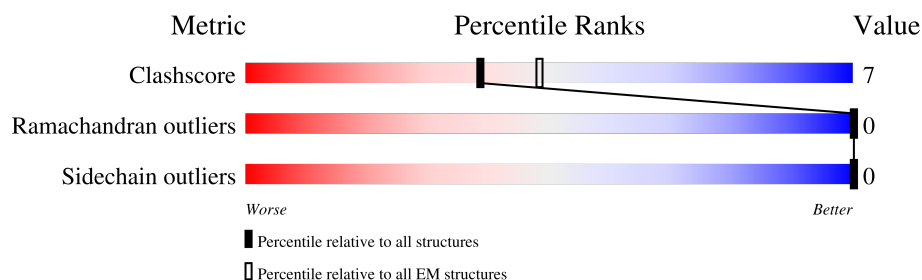
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 3.36 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)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
Q-score	-	25397	14332 (2.86 - 3.86)

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	20% 49% 9% 42%
1	B	868	20% 49% 9% 42%
1	C	868	20% 49% 9% 42%
1	D	868	20% 49% 9% 42%

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 31446 atoms, of which 15340 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	504	Total	C	H	N	O	S	0	0
			7413	2501	3586	624	679	23		
1	C	504	Total	C	H	N	O	S	0	0
			7413	2501	3586	624	679	23		
1	D	504	Total	C	H	N	O	S	0	0
			7413	2501	3586	624	679	23		
1	B	504	Total	C	H	N	O	S	0	0
			7413	2501	3586	624	679	23		

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
C	839	GLU	-	expression tag	UNP O35433
C	840	ASN	-	expression tag	UNP O35433
C	841	SER	-	expression tag	UNP O35433
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

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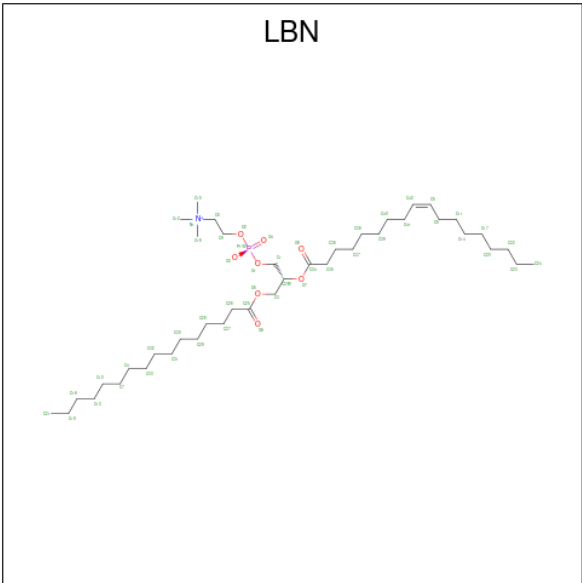
Chain	Residue	Modelled	Actual	Comment	Reference
D	842	LEU	-	expression tag	UNP O35433
D	843	GLU	-	expression tag	UNP O35433
D	844	VAL	-	expression tag	UNP O35433
D	845	LEU	-	expression tag	UNP O35433
D	846	PHE	-	expression tag	UNP O35433
D	847	GLN	-	expression tag	UNP O35433
D	848	GLY	-	expression tag	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
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
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

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Chain	Residue	Modelled	Actual	Comment	Reference
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

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



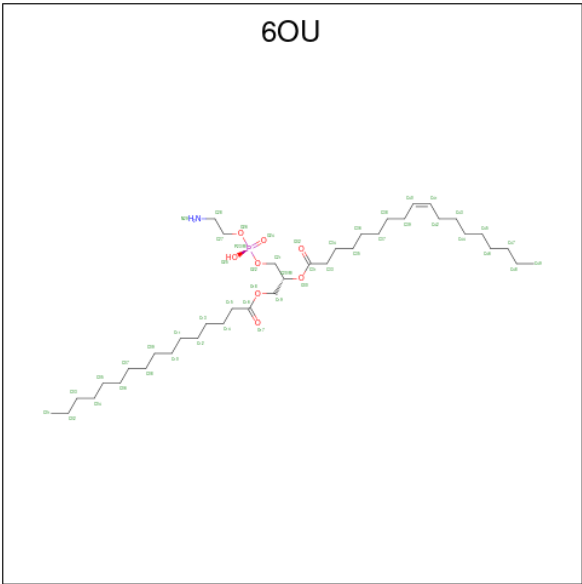
Mol	Chain	Residues	Atoms						AltConf
2	A	1	Total	C	H	N	O	P	0
			77	23	44	1	8	1	
2	A	1	Total	C	H	N	O	P	0
			102	32	60	1	8	1	
2	C	1	Total	C	H	N	O	P	0
			77	23	44	1	8	1	

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Mol	Chain	Residues	Atoms					AltConf
2	C	1	Total	C	H	N	O	P
			102	32	60	1	8	1
2	D	1	Total	C	H	N	O	P
			102	32	60	1	8	1
2	D	1	Total	C	H	N	O	P
			77	23	44	1	8	1
2	B	1	Total	C	H	N	O	P
			102	32	60	1	8	1
2	B	1	Total	C	H	N	O	P
			77	23	44	1	8	1

- Molecule 3 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
3	A	1	Total	C	H			
			29	10	19			0
3	A	1	Total	C	H	O	P	
			74	24	41	8	1	0
3	A	1	Total	C	H	O	P	
			80	26	45	8	1	0
3	C	1	Total	C	H	O	P	
			74	24	41	8	1	0
3	C	1	Total	C	H			
			29	10	19			0
3	C	1	Total	C	H	O	P	
			80	26	45	8	1	0

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Mol	Chain	Residues	Atoms					AltConf
3	D	1	Total 80	C 26	H 45	O 8	P 1	0
3	D	1	Total 29	C 10	H 19			0
3	B	1	Total 74	C 24	H 41	O 8	P 1	0
3	B	1	Total 80	C 26	H 45	O 8	P 1	0
3	B	1	Total 74	C 24	H 41	O 8	P 1	0
3	B	1	Total 29	C 10	H 19			0

- [illegible]

Mol	Chain	Residues	Atoms				AltConf
4	A	1	Total 86	C 37	H 40	O 9	0
4	C	1	Total 86	C 37	H 40	O 9	0
4	D	1	Total 86	C 37	H 40	O 9	0
4	B	1	Total 86	C 37	H 40	O 9	0

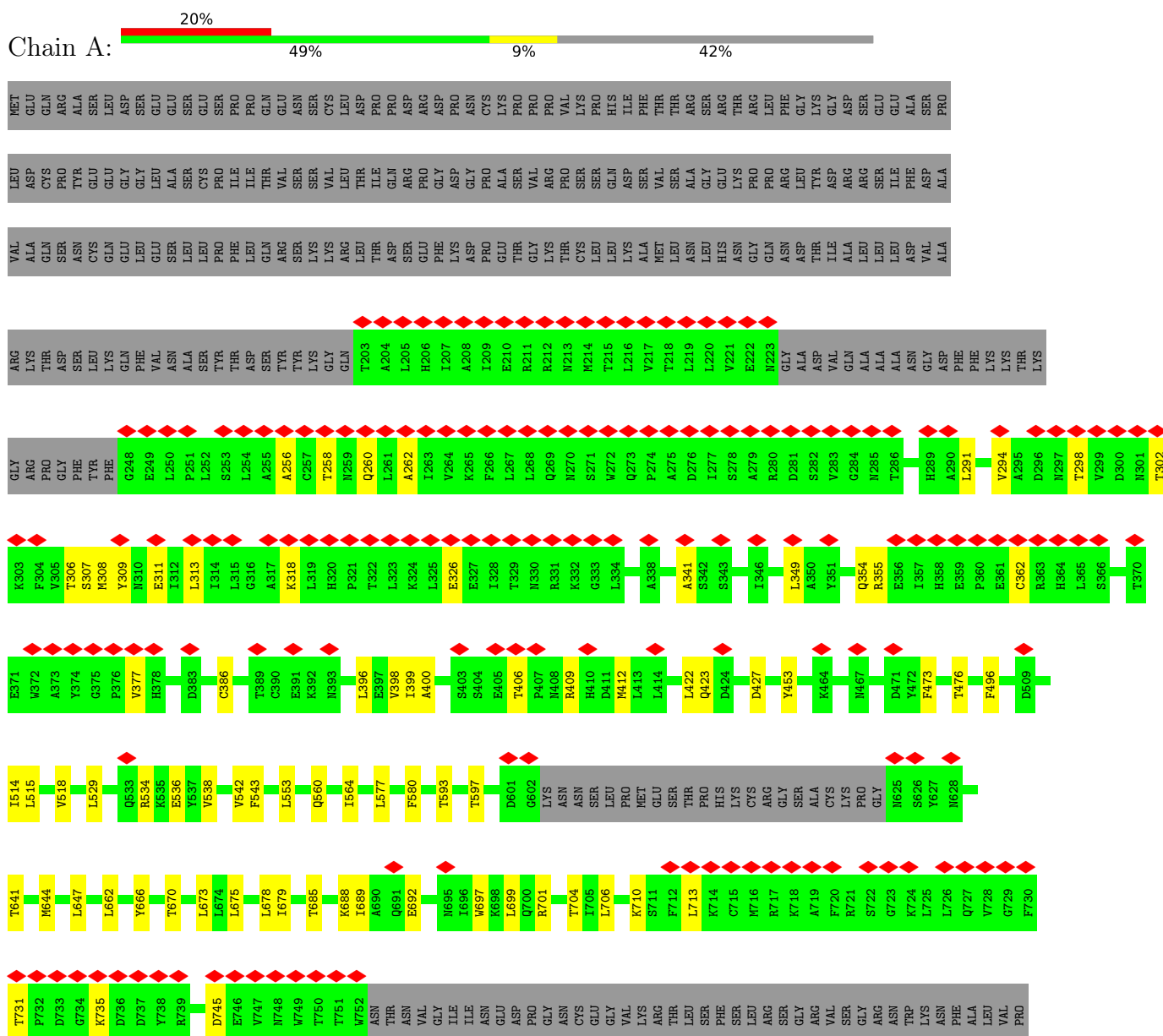
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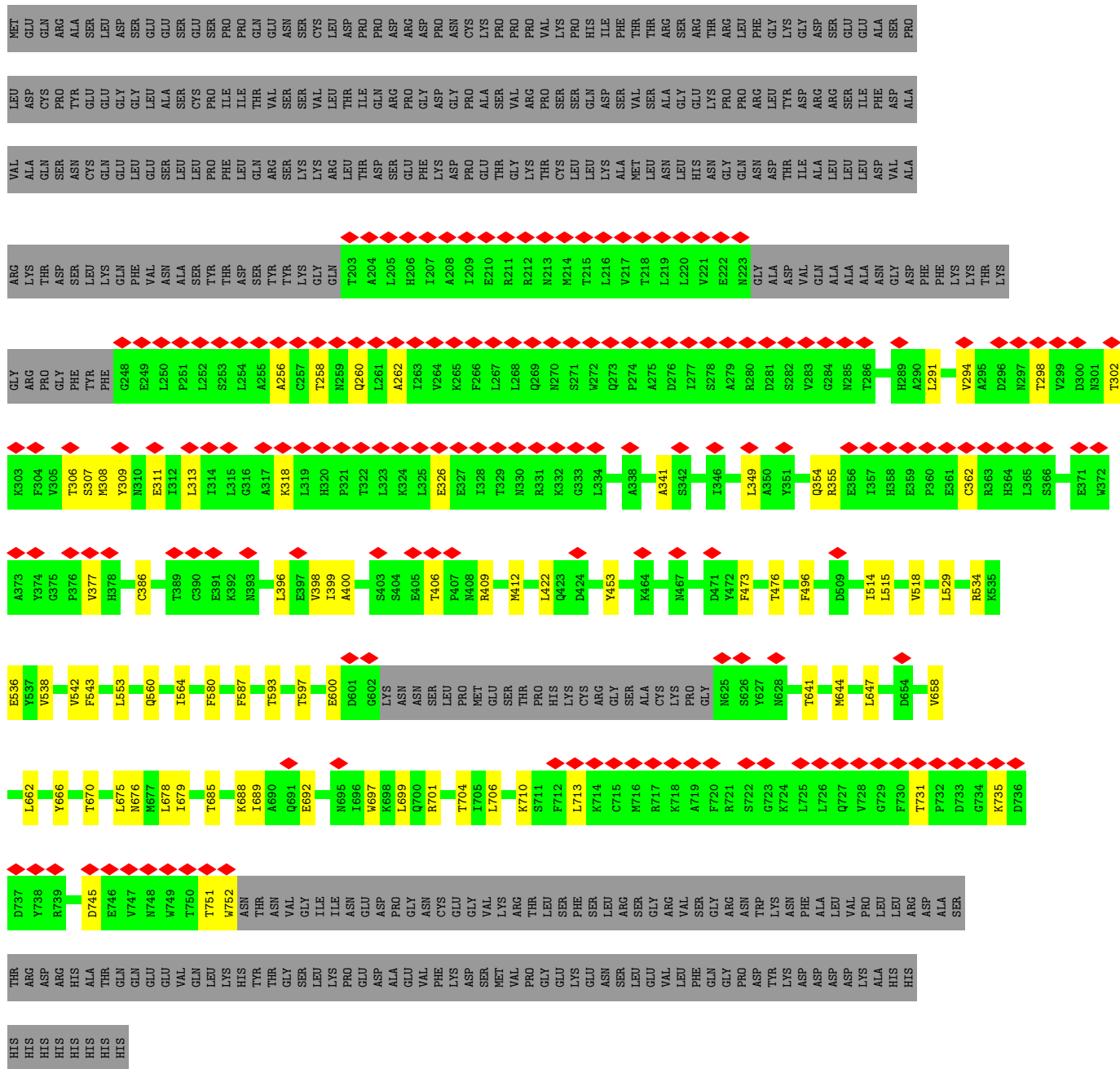
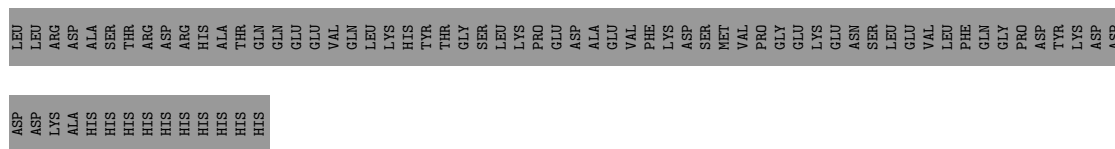
Mol	Chain	Residues	Atoms		AltConf
5	A	2	Total	Na	0
			2	2	

3 Residue-property plots

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion in map density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red diamond above a residue indicates a poor fit to the EM map for this residue (all-atom inclusion < 40%). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

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







4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	32121	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 ($e^-/\text{\AA}^2$)	44	Depositor
Minimum defocus (nm)	800	Depositor
Maximum defocus (nm)	1800	Depositor
Magnification	81000	Depositor
Image detector	GATAN K3 BIOQUANTUM (6k x 4k)	Depositor
Maximum map value	3.629	Depositor
Minimum map value	-2.296	Depositor
Average map value	0.010	Depositor
Map value standard deviation	0.099	Depositor
Recommended contour level	0.56	Depositor
Map size (Å)	263.424, 263.424, 263.424	wwPDB
Map dimensions	256, 256, 256	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.029, 1.029, 1.029	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: 6EU, LBN, NA, 6OU

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	0.20	0/3918	0.38	0/5337
1	B	0.20	0/3918	0.38	0/5337
1	C	0.20	0/3918	0.38	0/5337
1	D	0.20	0/3918	0.38	0/5337
All	All	0.20	0/15672	0.38	0/21348

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	3827	3586	3591	63	0
1	B	3827	3586	3591	62	0
1	C	3827	3586	3591	65	0
1	D	3827	3586	3591	68	0
2	A	75	104	0	0	0
2	B	75	104	0	0	0
2	C	75	104	0	0	0
2	D	75	104	0	0	0
3	A	78	105	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	B	111	146	0	0	0
3	C	78	105	0	0	0
3	D	45	64	0	0	0
4	A	46	40	0	2	0
4	B	46	40	0	2	0
4	C	46	40	0	2	0
4	D	46	40	0	2	0
5	A	2	0	0	0	0
All	All	16106	15340	14364	221	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 (221) 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:C:298:THR:O	1:C:302:THR:N	2.25	0.65
1:D:641:THR:O	1:D:675:LEU:HD11	1.98	0.64
1:A:641:THR:O	1:A:675:LEU:HD11	1.97	0.64
1:B:298:THR:O	1:B:302:THR:N	2.25	0.64
1:A:298:THR:O	1:A:302:THR:N	2.25	0.64
1:B:641:THR:O	1:B:675:LEU:HD11	1.97	0.64
1:C:641:THR:O	1:C:675:LEU:HD11	1.98	0.63
1:D:298:THR:O	1:D:302:THR:N	2.25	0.61
1:D:731:THR:HG22	1:D:735:LYS:O	2.01	0.61
1:C:731:THR:HG22	1:C:735:LYS:O	2.01	0.60
1:A:593:THR:O	1:A:597:THR:HG23	2.02	0.60
1:C:580:PHE:CE2	1:C:678:LEU:HD22	2.37	0.60
1:D:580:PHE:CE2	1:D:678:LEU:HD22	2.37	0.60
1:B:580:PHE:CE2	1:B:678:LEU:HD22	2.37	0.60
1:B:593:THR:O	1:B:597:THR:HG23	2.02	0.60
1:A:580:PHE:CE2	1:A:678:LEU:HD22	2.37	0.59
1:A:731:THR:HG22	1:A:735:LYS:O	2.01	0.59
1:D:593:THR:O	1:D:597:THR:HG23	2.02	0.59
1:B:731:THR:HG22	1:B:735:LYS:O	2.01	0.59
1:C:593:THR:O	1:C:597:THR:HG23	2.02	0.59
1:C:647:LEU:HD23	1:D:644:MET:HE3	1.85	0.58
1:B:399:ILE:HD11	1:B:412:MET:HG2	1.85	0.58
1:C:399:ILE:HD11	1:C:412:MET:HG2	1.85	0.58
1:C:318:LYS:NZ	1:C:362:CYS:SG	2.77	0.58
1:A:399:ILE:HD11	1:A:412:MET:HG2	1.85	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:307:SER:O	1:A:311:GLU:OE1	2.23	0.57
1:D:399:ILE:HD11	1:D:412:MET:HG2	1.85	0.56
1:C:647:LEU:CD2	1:D:644:MET:CE	2.82	0.56
1:B:307:SER:O	1:B:311:GLU:OE1	2.23	0.56
1:B:318:LYS:NZ	1:B:362:CYS:SG	2.77	0.56
1:A:318:LYS:NZ	1:A:362:CYS:SG	2.77	0.56
1:C:644:MET:CE	1:B:647:LEU:CD2	2.84	0.56
1:C:307:SER:O	1:C:311:GLU:OE1	2.23	0.56
1:D:307:SER:O	1:D:311:GLU:OE1	2.23	0.56
1:C:587:PHE:HE1	1:D:553:LEU:HD11	1.70	0.55
1:C:644:MET:HE3	1:B:647:LEU:HD23	1.87	0.55
1:A:256:ALA:HB1	1:A:308:MET:HE1	1.89	0.55
1:B:256:ALA:HB1	1:B:308:MET:HE1	1.89	0.55
1:D:318:LYS:NZ	1:D:362:CYS:SG	2.77	0.54
1:D:580:PHE:CD2	1:D:678:LEU:HD22	2.43	0.54
1:D:256:ALA:HB1	1:D:308:MET:HE1	1.89	0.54
1:C:580:PHE:CD2	1:C:678:LEU:HD22	2.43	0.54
1:C:256:ALA:HB1	1:C:308:MET:HE1	1.89	0.54
1:A:580:PHE:CD2	1:A:678:LEU:HD22	2.43	0.53
1:C:553:LEU:HD11	1:B:587:PHE:HE1	1.73	0.53
1:B:580:PHE:CD2	1:B:678:LEU:HD22	2.43	0.53
1:A:644:MET:HE3	1:D:647:LEU:HD23	1.91	0.53
1:A:473:PHE:O	1:A:476:THR:OG1	2.24	0.52
1:A:644:MET:CE	1:D:647:LEU:CD2	2.87	0.52
1:B:258:THR:O	1:B:258:THR:HG22	2.10	0.52
1:A:258:THR:HG22	1:A:258:THR:O	2.10	0.51
1:D:258:THR:HG22	1:D:258:THR:O	2.10	0.51
1:C:666:TYR:CE1	1:C:670:THR:HG21	2.46	0.51
1:C:258:THR:HG22	1:C:258:THR:O	2.10	0.51
1:C:473:PHE:O	1:C:476:THR:OG1	2.24	0.51
1:D:473:PHE:O	1:D:476:THR:OG1	2.24	0.51
1:C:587:PHE:CE1	1:D:553:LEU:HD11	2.46	0.51
1:B:666:TYR:CE1	1:B:670:THR:HG21	2.46	0.51
1:D:666:TYR:CE1	1:D:670:THR:HG21	2.46	0.51
1:B:349:LEU:HD13	1:B:412:MET:HE3	1.93	0.50
1:B:701:ARG:HA	1:B:704:THR:HG22	1.94	0.50
1:D:341:ALA:HB3	1:D:398:VAL:HG21	1.94	0.50
1:C:662:LEU:HD11	1:D:542:VAL:HG12	1.94	0.50
1:A:666:TYR:CE1	1:A:670:THR:HG21	2.46	0.50
1:A:701:ARG:HA	1:A:704:THR:HG22	1.94	0.50
1:A:341:ALA:HB3	1:A:398:VAL:HG21	1.94	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:349:LEU:HD13	1:C:412:MET:HE3	1.94	0.50
1:C:701:ARG:HA	1:C:704:THR:HG22	1.94	0.50
1:A:349:LEU:HD13	1:A:412:MET:HE3	1.93	0.49
1:A:647:LEU:HD23	1:B:644:MET:HE3	1.94	0.49
1:C:341:ALA:HB3	1:C:398:VAL:HG21	1.94	0.49
1:C:515:LEU:HD21	4:C:904:6EU:CBB	2.42	0.49
1:B:260:GLN:O	1:B:262:ALA:N	2.45	0.49
1:A:685:THR:O	1:A:689:ILE:HG12	2.13	0.49
1:D:515:LEU:HD21	4:D:905:6EU:CBB	2.42	0.49
1:C:685:THR:O	1:C:689:ILE:HG12	2.13	0.49
1:D:685:THR:O	1:D:689:ILE:HG12	2.13	0.49
1:D:701:ARG:HA	1:D:704:THR:HG22	1.94	0.49
1:B:515:LEU:HD21	4:B:907:6EU:CBB	2.42	0.49
1:A:647:LEU:CD2	1:B:644:MET:CE	2.90	0.49
1:C:260:GLN:O	1:C:262:ALA:N	2.45	0.49
1:A:515:LEU:HD21	4:A:903:6EU:CBB	2.42	0.49
1:C:542:VAL:HG12	1:B:662:LEU:HD11	1.95	0.48
1:D:260:GLN:O	1:D:262:ALA:N	2.45	0.48
1:A:260:GLN:O	1:A:262:ALA:N	2.45	0.48
1:D:349:LEU:HD13	1:D:412:MET:HE3	1.93	0.48
1:B:341:ALA:HB3	1:B:398:VAL:HG21	1.94	0.48
1:C:543:PHE:CE2	1:B:658:VAL:HG13	2.48	0.48
1:D:326:GLU:OE2	1:D:355:ARG:NH1	2.42	0.48
1:B:685:THR:O	1:B:689:ILE:HG12	2.13	0.48
1:A:542:VAL:HG12	1:D:662:LEU:HD11	1.96	0.48
1:C:514:ILE:O	1:C:518:VAL:HG23	2.14	0.48
1:C:710:LYS:O	1:C:713:LEU:HD22	2.14	0.48
1:A:710:LYS:O	1:A:713:LEU:HD22	2.14	0.47
1:B:473:PHE:O	1:B:476:THR:OG1	2.24	0.47
1:B:710:LYS:O	1:B:713:LEU:HD22	2.14	0.47
1:D:514:ILE:O	1:D:518:VAL:HG23	2.14	0.47
1:A:326:GLU:OE2	1:A:355:ARG:NH1	2.42	0.47
1:C:396:LEU:CD1	1:C:422:LEU:HD21	2.45	0.47
1:C:553:LEU:HD11	1:B:587:PHE:CE1	2.49	0.47
1:D:710:LYS:O	1:D:713:LEU:HD22	2.14	0.47
1:A:514:ILE:O	1:A:518:VAL:HG23	2.14	0.47
1:C:406:THR:OG1	1:C:409:ARG:HB2	2.15	0.47
1:C:658:VAL:HG13	1:D:543:PHE:CE2	2.49	0.47
1:D:309:TYR:CE2	1:D:313:LEU:HD11	2.50	0.47
1:D:396:LEU:CD1	1:D:422:LEU:HD21	2.45	0.47
1:B:396:LEU:CD1	1:B:422:LEU:HD21	2.44	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:396:LEU:CD1	1:A:422:LEU:HD21	2.45	0.47
1:A:309:TYR:CE2	1:A:313:LEU:HD11	2.50	0.47
1:C:647:LEU:CD2	1:D:644:MET:HE3	2.43	0.47
4:C:904:6EU:CAW	4:C:904:6EU:CAT	2.93	0.47
1:B:406:THR:OG1	1:B:409:ARG:HB2	2.15	0.47
1:B:514:ILE:O	1:B:518:VAL:HG23	2.14	0.47
1:D:302:THR:O	1:D:306:THR:HG22	2.15	0.47
4:D:905:6EU:CAW	4:D:905:6EU:CAT	2.93	0.47
1:D:406:THR:OG1	1:D:409:ARG:HB2	2.15	0.46
1:B:302:THR:O	1:B:306:THR:HG22	2.15	0.46
1:A:553:LEU:HD11	1:D:587:PHE:HE1	1.79	0.46
1:C:309:TYR:CE2	1:C:313:LEU:HD11	2.50	0.46
1:C:326:GLU:OE2	1:C:355:ARG:NH1	2.42	0.46
4:A:903:6EU:CAW	4:A:903:6EU:CAT	2.93	0.46
1:B:309:TYR:CE2	1:B:313:LEU:HD11	2.50	0.46
1:C:396:LEU:HD13	1:C:422:LEU:HD21	1.97	0.46
1:B:529:LEU:HD22	1:B:534:ARG:HG2	1.98	0.46
1:A:406:THR:OG1	1:A:409:ARG:HB2	2.15	0.46
1:B:396:LEU:HD13	1:B:422:LEU:HD21	1.97	0.46
4:B:907:6EU:CAW	4:B:907:6EU:CAT	2.93	0.46
1:A:400:ALA:HB3	1:A:706:LEU:HD12	1.99	0.46
1:D:396:LEU:HD13	1:D:422:LEU:HD21	1.97	0.46
1:A:302:THR:O	1:A:306:THR:HG22	2.15	0.45
1:C:676:ASN:CG	1:D:679:ILE:HG12	2.41	0.45
1:D:400:ALA:HB3	1:D:706:LEU:HD12	1.99	0.45
1:C:302:THR:O	1:C:306:THR:HG22	2.15	0.45
1:C:529:LEU:HD22	1:C:534:ARG:HG2	1.98	0.45
1:A:647:LEU:CD2	1:B:644:MET:HE3	2.46	0.45
1:A:396:LEU:HD13	1:A:422:LEU:HD21	1.97	0.45
1:C:644:MET:HE3	1:B:647:LEU:CD2	2.44	0.45
1:A:644:MET:HE3	1:D:647:LEU:CD2	2.45	0.45
1:A:529:LEU:HD22	1:A:534:ARG:HG2	1.98	0.45
1:B:400:ALA:HB3	1:B:706:LEU:HD12	1.98	0.45
1:C:400:ALA:HB3	1:C:706:LEU:HD12	1.99	0.45
1:A:538:VAL:O	1:A:542:VAL:HG23	2.18	0.44
1:A:577:LEU:HD13	1:D:673:LEU:HD12	1.99	0.44
1:B:377:VAL:HG23	1:B:745:ASP:OD1	2.17	0.44
1:C:291:LEU:O	1:C:294:VAL:HG12	2.18	0.44
1:A:662:LEU:HD11	1:B:542:VAL:HG12	1.99	0.44
1:C:699:LEU:O	1:C:699:LEU:HD23	2.18	0.44
1:D:529:LEU:HD22	1:D:534:ARG:HG2	1.98	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:538:VAL:O	1:B:542:VAL:HG23	2.18	0.44
1:B:699:LEU:HD23	1:B:699:LEU:O	2.18	0.44
1:A:377:VAL:HG23	1:A:745:ASP:OD1	2.17	0.44
1:A:534:ARG:HG3	1:A:536:GLU:H	1.83	0.44
1:D:377:VAL:HG23	1:D:745:ASP:OD1	2.17	0.44
1:A:679:ILE:HG12	1:D:676:ASN:CG	2.43	0.44
1:C:662:LEU:HD11	1:D:542:VAL:CG1	2.48	0.44
1:D:699:LEU:HD23	1:D:699:LEU:O	2.18	0.44
1:B:534:ARG:HG3	1:B:536:GLU:H	1.83	0.44
1:A:542:VAL:CG1	1:D:662:LEU:HD11	2.47	0.43
1:A:699:LEU:O	1:A:699:LEU:HD23	2.18	0.43
1:D:626:SER:O	1:D:626:SER:OG	2.34	0.43
1:C:600:GLU:OE2	1:D:455:ARG:NH2	2.34	0.43
1:B:291:LEU:O	1:B:294:VAL:HG12	2.18	0.43
1:C:377:VAL:HG23	1:C:745:ASP:OD1	2.17	0.43
1:C:538:VAL:O	1:C:542:VAL:HG23	2.18	0.43
1:C:542:VAL:CG1	1:B:662:LEU:HD11	2.49	0.43
1:C:309:TYR:CZ	1:C:313:LEU:HD11	2.54	0.43
1:D:291:LEU:O	1:D:294:VAL:HG12	2.18	0.43
1:D:534:ARG:HG3	1:D:536:GLU:H	1.83	0.43
1:B:309:TYR:CZ	1:B:313:LEU:HD11	2.54	0.43
1:A:291:LEU:O	1:A:294:VAL:HG12	2.18	0.42
1:D:538:VAL:O	1:D:542:VAL:HG23	2.18	0.42
1:A:673:LEU:HD12	1:B:577:LEU:HD13	2.01	0.42
1:C:534:ARG:HG3	1:C:536:GLU:H	1.83	0.42
1:C:560:GLN:HB2	1:C:697:TRP:CE2	2.54	0.42
1:B:560:GLN:HB2	1:B:697:TRP:CE2	2.54	0.42
1:A:256:ALA:HB1	1:A:308:MET:CE	2.50	0.42
1:C:354:GLN:O	1:C:354:GLN:HG3	2.20	0.42
1:A:560:GLN:HB2	1:A:697:TRP:CE2	2.54	0.42
1:A:309:TYR:CZ	1:A:313:LEU:HD11	2.54	0.42
1:A:354:GLN:O	1:A:354:GLN:HG3	2.20	0.42
1:A:688:LYS:O	1:A:692:GLU:HG3	2.20	0.42
1:D:560:GLN:HB2	1:D:697:TRP:CE2	2.54	0.42
1:B:688:LYS:O	1:B:692:GLU:HG3	2.20	0.42
1:A:309:TYR:OH	1:A:326:GLU:OE2	2.37	0.42
1:C:647:LEU:CD2	1:D:644:MET:HE1	2.48	0.42
1:B:256:ALA:HB1	1:B:308:MET:CE	2.50	0.42
1:D:309:TYR:CZ	1:D:313:LEU:HD11	2.54	0.41
1:D:354:GLN:HG3	1:D:354:GLN:O	2.20	0.41
1:A:597:THR:HG22	1:B:453:TYR:HA	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:564:ILE:O	1:B:564:ILE:HG22	2.20	0.41
1:C:679:ILE:HG12	1:B:676:ASN:CG	2.46	0.41
1:B:355:ARG:NH2	1:B:365:LEU:O	2.49	0.41
1:A:662:LEU:HD11	1:B:542:VAL:CG1	2.50	0.41
1:B:354:GLN:HG3	1:B:354:GLN:O	2.20	0.41
1:A:453:TYR:HA	1:D:597:THR:HG22	2.01	0.41
1:B:326:GLU:OE2	1:B:355:ARG:NH1	2.42	0.41
1:C:386:CYS:O	1:C:386:CYS:SG	2.79	0.41
1:D:688:LYS:O	1:D:692:GLU:HG3	2.20	0.41
1:A:553:LEU:HD11	1:D:587:PHE:CE1	2.56	0.41
1:D:256:ALA:HB1	1:D:308:MET:CE	2.50	0.41
1:B:386:CYS:SG	1:B:386:CYS:O	2.79	0.41
1:A:386:CYS:O	1:A:386:CYS:SG	2.79	0.41
1:A:423:GLN:NE2	1:A:427:ASP:OD2	2.54	0.41
1:B:675:LEU:O	1:B:679:ILE:HD12	2.21	0.41
1:A:675:LEU:O	1:A:679:ILE:HD12	2.21	0.41
1:C:496:PHE:CZ	1:C:514:ILE:HD13	2.56	0.41
1:C:644:MET:HE1	1:B:647:LEU:CD2	2.50	0.41
1:C:688:LYS:O	1:C:692:GLU:HG3	2.20	0.41
1:D:399:ILE:CD1	1:D:412:MET:HG2	2.51	0.41
1:A:564:ILE:O	1:A:564:ILE:HG22	2.20	0.40
1:C:453:TYR:HA	1:B:597:THR:HG22	2.03	0.40
1:B:496:PHE:CZ	1:B:514:ILE:HD13	2.56	0.40
1:D:386:CYS:SG	1:D:386:CYS:O	2.79	0.40
1:A:543:PHE:CE2	1:D:658:VAL:HG13	2.56	0.40
1:C:564:ILE:O	1:C:564:ILE:HG22	2.20	0.40
1:C:658:VAL:HG21	1:D:539:ALA:HB1	2.02	0.40
1:D:675:LEU:O	1:D:679:ILE:HD12	2.21	0.40
1:D:564:ILE:O	1:D:564:ILE:HG22	2.20	0.40
1:D:751:THR:HG23	1:D:752:TRP:N	2.37	0.40
1:A:496:PHE:CZ	1:A:514:ILE:HD13	2.56	0.40
1:C:751:THR:HG23	1:C:752:TRP:N	2.37	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	498/868 (57%)	481 (97%)	17 (3%)	0	100	100
1	B	498/868 (57%)	481 (97%)	17 (3%)	0	100	100
1	C	498/868 (57%)	482 (97%)	16 (3%)	0	100	100
1	D	498/868 (57%)	481 (97%)	17 (3%)	0	100	100
All	All	1992/3472 (57%)	1925 (97%)	67 (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	374/770 (49%)	374 (100%)	0	100	100
1	B	374/770 (49%)	374 (100%)	0	100	100
1	C	374/770 (49%)	374 (100%)	0	100	100
1	D	374/770 (49%)	374 (100%)	0	100	100
All	All	1496/3080 (49%)	1496 (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 [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](#)

Of 26 ligands modelled in this entry, 2 are monoatomic - leaving 24 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	LBN	B	902	-	41,41,51	1.34	4 (9%)	47,49,59	0.90	2 (4%)
2	LBN	C	901	-	32,32,51	1.42	3 (9%)	38,40,59	0.96	1 (2%)
3	6OU	C	905	-	34,34,48	1.71	3 (8%)	37,39,53	0.92	2 (5%)
3	6OU	D	904	-	9,9,48	0.76	0	8,8,53	0.35	0
3	6OU	B	901	-	32,32,48	1.55	3 (9%)	35,37,53	0.83	2 (5%)
3	6OU	A	902	-	9,9,48	0.76	0	8,8,53	0.35	0
3	6OU	B	906	-	9,9,48	0.77	0	8,8,53	0.35	0
3	6OU	D	901	-	34,34,48	1.71	4 (11%)	37,39,53	0.92	2 (5%)
2	LBN	B	904	-	32,32,51	1.42	3 (9%)	38,40,59	0.97	1 (2%)
3	6OU	B	905	-	32,32,48	1.55	3 (9%)	35,37,53	0.83	2 (5%)
2	LBN	A	901	-	32,32,51	1.42	3 (9%)	38,40,59	0.97	1 (2%)
3	6OU	A	906	-	34,34,48	1.71	4 (11%)	37,39,53	0.92	2 (5%)
4	6EU	C	904	-	45,52,52	4.47	18 (40%)	44,83,83	2.16	9 (20%)
3	6OU	C	902	-	32,32,48	1.55	4 (12%)	35,37,53	0.83	2 (5%)
3	6OU	A	904	-	32,32,48	1.55	3 (9%)	35,37,53	0.83	2 (5%)
2	LBN	D	902	-	41,41,51	1.34	4 (9%)	47,49,59	0.90	2 (4%)
4	6EU	D	905	-	45,52,52	4.48	18 (40%)	44,83,83	2.15	9 (20%)
2	LBN	C	906	-	41,41,51	1.34	4 (9%)	47,49,59	0.90	2 (4%)
2	LBN	A	905	-	41,41,51	1.34	4 (9%)	47,49,59	0.91	2 (4%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	LBN	D	903	-	32,32,51	1.42	3 (9%)	38,40,59	0.96	1 (2%)
4	6EU	B	907	-	45,52,52	4.47	17 (37%)	44,83,83	2.16	9 (20%)
4	6EU	A	903	-	45,52,52	4.47	18 (40%)	44,83,83	2.16	9 (20%)
3	6OU	C	903	-	9,9,48	0.77	0	8,8,53	0.35	0
3	6OU	B	903	-	34,34,48	1.71	4 (11%)	37,39,53	0.92	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
2	LBN	B	902	-	-	21/45/45/55	-
2	LBN	C	901	-	-	22/36/36/55	-
3	6OU	C	905	-	-	16/36/36/52	-
3	6OU	D	904	-	-	4/7/7/52	-
3	6OU	B	901	-	-	16/36/36/52	-
3	6OU	A	902	-	-	4/7/7/52	-
3	6OU	B	906	-	-	4/7/7/52	-
3	6OU	D	901	-	-	16/36/36/52	-
2	LBN	B	904	-	-	22/36/36/55	-
3	6OU	B	905	-	-	16/36/36/52	-
2	LBN	A	901	-	-	22/36/36/55	-
3	6OU	A	906	-	-	16/36/36/52	-
4	6EU	C	904	-	-	3/20/101/101	0/8/7/7
3	6OU	C	902	-	-	16/36/36/52	-
3	6OU	A	904	-	-	16/36/36/52	-
2	LBN	D	902	-	-	21/45/45/55	-
4	6EU	D	905	-	-	3/20/101/101	0/8/7/7
2	LBN	C	906	-	-	21/45/45/55	-
2	LBN	A	905	-	-	21/45/45/55	-
2	LBN	D	903	-	-	22/36/36/55	-
4	6EU	B	907	-	-	3/20/101/101	0/8/7/7
4	6EU	A	903	-	-	3/20/101/101	0/8/7/7
3	6OU	C	903	-	-	4/7/7/52	-
3	6OU	B	903	-	-	16/36/36/52	-

All (127) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	C	904	6EU	CAS-CAX	17.98	1.61	1.33
4	D	905	6EU	CAS-CAX	17.98	1.61	1.33
4	B	907	6EU	CAS-CAX	17.97	1.61	1.33
4	A	903	6EU	CAS-CAX	17.97	1.61	1.33
4	D	905	6EU	OAB-CAL	-11.31	1.27	1.43
4	C	904	6EU	OAB-CAL	-11.29	1.27	1.43
4	A	903	6EU	OAB-CAL	-11.27	1.27	1.43
4	B	907	6EU	OAB-CAL	-11.24	1.27	1.43
4	C	904	6EU	CAW-CBA	9.28	1.52	1.33
4	B	907	6EU	CAW-CBA	9.27	1.52	1.33
4	A	903	6EU	CAW-CBA	9.27	1.52	1.33
4	D	905	6EU	CAW-CBA	9.26	1.52	1.33
4	D	905	6EU	CAM-CAL	7.41	1.65	1.54
4	B	907	6EU	CAM-CAL	7.41	1.65	1.54
4	A	903	6EU	CAK-CAS	7.40	1.67	1.50
4	A	903	6EU	CAM-CAL	7.39	1.65	1.54
4	C	904	6EU	CAM-CAL	7.39	1.65	1.54
4	D	905	6EU	CAK-CAS	7.38	1.67	1.50
4	B	907	6EU	CAK-CAS	7.37	1.67	1.50
4	C	904	6EU	CAK-CAS	7.35	1.67	1.50
4	B	907	6EU	CAP-CAM	7.14	1.67	1.53
4	D	905	6EU	CAP-CAM	7.13	1.67	1.53
4	C	904	6EU	CAP-CAM	7.13	1.67	1.53
4	A	903	6EU	CAP-CAM	7.13	1.67	1.53
4	B	907	6EU	OAA-CAQ	6.45	1.50	1.42
4	D	905	6EU	OAA-CAQ	6.41	1.50	1.42
4	A	903	6EU	OAA-CAQ	6.41	1.50	1.42
4	C	904	6EU	OAA-CAQ	6.36	1.50	1.42
4	D	905	6EU	OAA-CAJ	6.33	1.58	1.44
4	A	903	6EU	OAA-CAJ	6.32	1.58	1.44
4	C	904	6EU	OAA-CAJ	6.32	1.58	1.44
4	B	907	6EU	OAA-CAJ	6.28	1.57	1.44
3	B	903	6OU	P23-O22	5.44	1.77	1.60
3	A	906	6OU	P23-O22	5.43	1.77	1.60
3	C	905	6OU	P23-O22	5.43	1.77	1.60
3	D	901	6OU	P23-O22	5.42	1.77	1.60
2	D	902	LBN	P1-O2	5.13	1.79	1.59
2	B	902	LBN	P1-O2	5.12	1.79	1.59
2	C	906	LBN	P1-O2	5.11	1.79	1.59
2	A	905	LBN	P1-O2	5.11	1.79	1.59
3	A	906	6OU	P23-O26	5.01	1.73	1.54
3	B	903	6OU	P23-O26	5.00	1.73	1.54

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	D	901	6OU	P23-O26	5.00	1.73	1.54
3	C	905	6OU	P23-O26	4.99	1.73	1.54
2	A	901	LBN	P1-O2	4.88	1.78	1.59
2	B	904	LBN	P1-O2	4.88	1.78	1.59
2	D	903	LBN	P1-O2	4.87	1.78	1.59
2	C	901	LBN	P1-O2	4.86	1.78	1.59
4	D	905	6EU	CAJ-CAO	4.82	1.62	1.54
4	C	904	6EU	CAJ-CAO	4.81	1.62	1.54
4	B	907	6EU	CAJ-CAO	4.79	1.62	1.54
4	A	903	6EU	CAJ-CAO	4.78	1.62	1.54
3	C	902	6OU	P23-O22	4.55	1.77	1.59
3	B	901	6OU	P23-O22	4.55	1.77	1.59
3	A	904	6OU	P23-O22	4.54	1.77	1.59
3	B	905	6OU	P23-O22	4.54	1.77	1.59
4	C	904	6EU	OAC-CAM	-4.17	1.38	1.44
4	A	903	6EU	OAC-CAM	-4.16	1.38	1.44
4	D	905	6EU	OAC-CAM	-4.16	1.38	1.44
4	B	907	6EU	OAC-CAM	-4.15	1.38	1.44
4	C	904	6EU	OAB-CAQ	-4.13	1.34	1.41
4	A	903	6EU	OAB-CAQ	-4.10	1.34	1.41
4	B	907	6EU	OAB-CAQ	-4.10	1.34	1.41
4	D	905	6EU	OAB-CAQ	-4.09	1.34	1.41
3	B	905	6OU	P23-O26	3.54	1.73	1.59
3	A	904	6OU	P23-O26	3.53	1.73	1.59
3	B	901	6OU	P23-O26	3.53	1.73	1.59
3	C	902	6OU	P23-O26	3.52	1.73	1.59
4	D	905	6EU	OAH-CBQ	2.95	1.42	1.37
4	C	904	6EU	OAF-CBK	2.94	1.41	1.33
4	A	903	6EU	OAF-CBK	2.93	1.41	1.33
4	B	907	6EU	OAF-CBK	2.93	1.41	1.33
4	A	903	6EU	OAH-CBQ	2.93	1.41	1.37
4	D	905	6EU	OAF-CBK	2.93	1.41	1.33
4	C	904	6EU	OAH-CBQ	2.92	1.41	1.37
4	B	907	6EU	OAH-CBQ	2.90	1.41	1.37
4	A	903	6EU	CAY-CBE	2.63	1.55	1.51
4	D	905	6EU	CAY-CBE	2.62	1.55	1.51
4	B	907	6EU	CAY-CBE	2.61	1.55	1.51
4	C	904	6EU	CAY-CBE	2.59	1.55	1.51
3	A	906	6OU	C21-C20	2.38	1.58	1.50
3	C	905	6OU	C21-C20	2.36	1.58	1.50
3	C	902	6OU	C21-C20	2.35	1.58	1.50
3	D	901	6OU	C21-C20	2.35	1.58	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	903	6OU	C21-C20	2.35	1.58	1.50
3	B	905	6OU	C21-C20	2.35	1.58	1.50
3	A	904	6OU	C21-C20	2.33	1.58	1.50
3	B	901	6OU	C21-C20	2.33	1.58	1.50
2	C	906	LBN	P1-O1	2.32	1.68	1.59
2	B	904	LBN	O2-C9	-2.32	1.35	1.44
2	A	905	LBN	P1-O1	2.31	1.68	1.59
2	D	902	LBN	P1-O1	2.31	1.68	1.59
2	B	902	LBN	P1-O1	2.31	1.68	1.59
2	C	901	LBN	O2-C9	-2.30	1.35	1.44
2	D	903	LBN	O2-C9	-2.29	1.35	1.44
2	A	901	LBN	O2-C9	-2.29	1.35	1.44
2	C	906	LBN	C1-C2	2.22	1.57	1.50
2	D	902	LBN	C1-C2	2.21	1.57	1.50
2	B	902	LBN	C1-C2	2.21	1.57	1.50
2	A	905	LBN	C1-C2	2.19	1.57	1.50
2	C	906	LBN	O2-C9	-2.19	1.36	1.44
2	D	902	LBN	O2-C9	-2.18	1.36	1.44
2	B	902	LBN	O2-C9	-2.18	1.36	1.44
2	A	905	LBN	O2-C9	-2.17	1.36	1.44
2	B	904	LBN	P1-O1	2.11	1.67	1.59
4	B	907	6EU	CBC-CAX	2.11	1.56	1.50
4	C	904	6EU	CBM-CBN	2.10	1.55	1.51
2	C	901	LBN	P1-O1	2.10	1.67	1.59
4	C	904	6EU	CBC-CAX	2.09	1.56	1.50
2	A	901	LBN	P1-O1	2.09	1.67	1.59
4	A	903	6EU	CBC-CAX	2.08	1.55	1.50
2	D	903	LBN	P1-O1	2.08	1.67	1.59
4	D	905	6EU	CBM-CBN	2.07	1.55	1.51
4	A	903	6EU	CBM-CBN	2.07	1.55	1.51
4	D	905	6EU	CBC-CAX	2.06	1.55	1.50
4	C	904	6EU	OAI-CBS	2.04	1.40	1.36
4	C	904	6EU	OAE-CAZ	-2.04	1.18	1.22
4	A	903	6EU	OAI-CBS	2.03	1.40	1.36
4	D	905	6EU	OAI-CBS	2.03	1.40	1.36
4	A	903	6EU	OAE-CAZ	-2.03	1.18	1.22
3	B	903	6OU	O30-C31	2.03	1.40	1.34
4	B	907	6EU	CBM-CBN	2.02	1.54	1.51
4	B	907	6EU	OAI-CBS	2.02	1.40	1.36
4	D	905	6EU	OAE-CAZ	-2.02	1.18	1.22
3	D	901	6OU	O30-C31	2.02	1.40	1.34
3	C	902	6OU	C19-C20	2.01	1.57	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	906	6OU	O30-C31	2.00	1.39	1.34

All (64) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	C	904	6EU	CBD-CAV-CAM	-7.34	98.85	116.79
4	B	907	6EU	CBD-CAV-CAM	-7.33	98.86	116.79
4	A	903	6EU	CBD-CAV-CAM	-7.33	98.86	116.79
4	D	905	6EU	CBD-CAV-CAM	-7.33	98.87	116.79
4	B	907	6EU	OAF-CBK-CBM	5.82	120.30	111.21
4	A	903	6EU	OAF-CBK-CBM	5.82	120.30	111.21
4	D	905	6EU	OAF-CBK-CBM	5.80	120.26	111.21
4	C	904	6EU	OAF-CBK-CBM	5.79	120.25	111.21
4	B	907	6EU	CAQ-CAY-CBE	-5.40	107.26	113.60
4	C	904	6EU	CAQ-CAY-CBE	-5.39	107.27	113.60
4	A	903	6EU	CAQ-CAY-CBE	-5.39	107.28	113.60
4	D	905	6EU	CAQ-CAY-CBE	-5.37	107.29	113.60
4	C	904	6EU	OAH-CBQ-CBS	3.70	120.10	114.55
4	A	903	6EU	OAH-CBQ-CBS	3.70	120.10	114.55
4	B	907	6EU	OAH-CBQ-CBS	3.69	120.08	114.55
4	A	903	6EU	CAJ-OAA-CAQ	3.67	119.64	113.53
4	B	907	6EU	CAJ-OAA-CAQ	3.67	119.63	113.53
4	D	905	6EU	CAJ-OAA-CAQ	3.67	119.62	113.53
4	C	904	6EU	CAJ-OAA-CAQ	3.66	119.62	113.53
4	D	905	6EU	OAH-CBQ-CBS	3.66	120.04	114.55
4	C	904	6EU	CAM-CAV-CBB	3.49	131.28	121.88
2	B	904	LBN	O3-P1-O4	3.48	128.64	112.44
2	A	901	LBN	O3-P1-O4	3.47	128.60	112.44
4	A	903	6EU	CAM-CAV-CBB	3.47	131.23	121.88
2	D	903	LBN	O3-P1-O4	3.47	128.58	112.44
4	B	907	6EU	CAM-CAV-CBB	3.47	131.22	121.88
2	C	901	LBN	O3-P1-O4	3.47	128.57	112.44
4	D	905	6EU	CAM-CAV-CBB	3.47	131.22	121.88
3	C	905	6OU	O25-P23-O24	3.43	124.20	110.83
3	D	901	6OU	O25-P23-O24	3.43	124.20	110.83
3	B	903	6OU	O25-P23-O24	3.43	124.19	110.83
3	A	906	6OU	O25-P23-O24	3.43	124.18	110.83
2	D	902	LBN	O3-P1-O4	3.42	128.37	112.44
2	C	906	LBN	O3-P1-O4	3.42	128.34	112.44
2	B	902	LBN	O3-P1-O4	3.41	128.33	112.44
2	A	905	LBN	O3-P1-O4	3.41	128.30	112.44
4	A	903	6EU	CBF-CBA-CAW	-2.84	124.96	130.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	C	904	6EU	CBF-CBA-CAW	-2.83	124.98	130.40
4	D	905	6EU	CBF-CBA-CAW	-2.83	124.98	130.40
4	B	907	6EU	CBF-CBA-CAW	-2.82	125.00	130.40
3	B	905	6OU	O25-P23-O24	2.54	124.26	112.44
3	A	904	6OU	O25-P23-O24	2.54	124.25	112.44
3	B	901	6OU	O25-P23-O24	2.54	124.25	112.44
3	C	902	6OU	O25-P23-O24	2.53	124.23	112.44
4	D	905	6EU	CBD-CAV-CBB	2.44	129.92	121.12
4	B	907	6EU	CBD-CAV-CBB	2.44	129.91	121.12
4	A	903	6EU	CBD-CAV-CBB	2.43	129.91	121.12
4	C	904	6EU	CBD-CAV-CBB	2.42	129.87	121.12
3	B	905	6OU	O30-C31-C33	2.39	116.64	111.48
3	B	901	6OU	O30-C31-C33	2.38	116.63	111.48
3	C	902	6OU	O30-C31-C33	2.38	116.63	111.48
3	A	904	6OU	O30-C31-C33	2.37	116.62	111.48
3	C	905	6OU	O30-C31-C33	2.30	116.46	111.48
3	A	906	6OU	O30-C31-C33	2.30	116.45	111.48
3	D	901	6OU	O30-C31-C33	2.29	116.44	111.48
3	B	903	6OU	O30-C31-C33	2.29	116.44	111.48
4	D	905	6EU	OAC-CAQ-CAY	2.04	114.12	111.18
4	B	907	6EU	OAC-CAQ-CAY	2.04	114.11	111.18
4	A	903	6EU	OAC-CAQ-CAY	2.03	114.09	111.18
2	D	902	LBN	O2-P1-O4	-2.03	100.91	108.94
2	A	905	LBN	O2-P1-O4	-2.02	100.91	108.94
2	B	902	LBN	O2-P1-O4	-2.02	100.92	108.94
2	C	906	LBN	O2-P1-O4	-2.02	100.93	108.94
4	C	904	6EU	OAC-CAQ-CAY	2.01	114.07	111.18

There are no chirality outliers.

All (328) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	901	LBN	C1-O1-P1-O2
2	A	901	LBN	C1-O1-P1-O3
2	A	901	LBN	C9-O2-P1-O3
2	A	901	LBN	N1-C6-C9-O2
2	A	905	LBN	C2-C1-O1-P1
2	A	905	LBN	C9-O2-P1-O1
2	A	905	LBN	C9-O2-P1-O4
2	A	905	LBN	N1-C6-C9-O2
2	A	905	LBN	C35-C34-O7-C2
2	C	901	LBN	C1-O1-P1-O2

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Mol	Chain	Res	Type	Atoms
2	C	901	LBN	C1-O1-P1-O3
2	C	901	LBN	C9-O2-P1-O3
2	C	901	LBN	N1-C6-C9-O2
2	C	906	LBN	C2-C1-O1-P1
2	C	906	LBN	C9-O2-P1-O1
2	C	906	LBN	C9-O2-P1-O4
2	C	906	LBN	N1-C6-C9-O2
2	C	906	LBN	C35-C34-O7-C2
2	D	902	LBN	C2-C1-O1-P1
2	D	902	LBN	C9-O2-P1-O1
2	D	902	LBN	C9-O2-P1-O4
2	D	902	LBN	N1-C6-C9-O2
2	D	902	LBN	C35-C34-O7-C2
2	D	903	LBN	C1-O1-P1-O2
2	D	903	LBN	C1-O1-P1-O3
2	D	903	LBN	C9-O2-P1-O3
2	D	903	LBN	N1-C6-C9-O2
2	B	902	LBN	C2-C1-O1-P1
2	B	902	LBN	C9-O2-P1-O1
2	B	902	LBN	C9-O2-P1-O4
2	B	902	LBN	N1-C6-C9-O2
2	B	902	LBN	C35-C34-O7-C2
2	B	904	LBN	C1-O1-P1-O2
2	B	904	LBN	C1-O1-P1-O3
2	B	904	LBN	C9-O2-P1-O3
2	B	904	LBN	N1-C6-C9-O2
3	A	904	6OU	C21-O22-P23-O24
3	A	906	6OU	C21-O22-P23-O25
3	A	906	6OU	C21-O22-P23-O26
3	C	902	6OU	C21-O22-P23-O24
3	C	905	6OU	C21-O22-P23-O25
3	C	905	6OU	C21-O22-P23-O26
3	D	901	6OU	C21-O22-P23-O25
3	D	901	6OU	C21-O22-P23-O26
3	B	901	6OU	C21-O22-P23-O24
3	B	903	6OU	C21-O22-P23-O25
3	B	903	6OU	C21-O22-P23-O26
3	B	905	6OU	C21-O22-P23-O24
4	A	903	6EU	OAA-CAQ-CAY-CBE
4	A	903	6EU	OAC-CAQ-CAY-CBE
4	A	903	6EU	OAB-CAQ-CAY-CBE
4	C	904	6EU	OAA-CAQ-CAY-CBE

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Mol	Chain	Res	Type	Atoms
4	C	904	6EU	OAC-CAQ-CAY-CBE
4	C	904	6EU	OAB-CAQ-CAY-CBE
4	D	905	6EU	OAA-CAQ-CAY-CBE
4	D	905	6EU	OAC-CAQ-CAY-CBE
4	D	905	6EU	OAB-CAQ-CAY-CBE
4	B	907	6EU	OAA-CAQ-CAY-CBE
4	B	907	6EU	OAC-CAQ-CAY-CBE
4	B	907	6EU	OAB-CAQ-CAY-CBE
3	A	904	6OU	O17-C16-O18-C19
3	C	902	6OU	O17-C16-O18-C19
3	B	901	6OU	O17-C16-O18-C19
3	B	905	6OU	O17-C16-O18-C19
3	A	904	6OU	C15-C16-O18-C19
3	C	902	6OU	C15-C16-O18-C19
3	B	901	6OU	C15-C16-O18-C19
3	B	905	6OU	C15-C16-O18-C19
2	A	905	LBN	O8-C34-O7-C2
2	C	906	LBN	O8-C34-O7-C2
2	D	902	LBN	O8-C34-O7-C2
2	B	902	LBN	O8-C34-O7-C2
2	A	901	LBN	C34-C35-C36-C37
2	C	901	LBN	C34-C35-C36-C37
2	D	903	LBN	C34-C35-C36-C37
2	B	904	LBN	C34-C35-C36-C37
2	A	905	LBN	C25-C26-C27-C28
2	C	906	LBN	C25-C26-C27-C28
2	D	902	LBN	C25-C26-C27-C28
2	B	902	LBN	C25-C26-C27-C28
2	A	905	LBN	C26-C25-O5-C3
2	C	906	LBN	C26-C25-O5-C3
2	D	902	LBN	C26-C25-O5-C3
2	B	902	LBN	C26-C25-O5-C3
3	A	906	6OU	C12-C13-C14-C15
3	C	905	6OU	C12-C13-C14-C15
3	D	901	6OU	C12-C13-C14-C15
3	B	903	6OU	C12-C13-C14-C15
3	A	902	6OU	C44-C45-C46-C47
3	C	903	6OU	C44-C45-C46-C47
3	D	904	6OU	C44-C45-C46-C47
3	B	906	6OU	C44-C45-C46-C47
3	C	905	6OU	C09-C10-C11-C12
3	B	903	6OU	C09-C10-C11-C12

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Mol	Chain	Res	Type	Atoms
3	A	906	6OU	C09-C10-C11-C12
2	A	905	LBN	C26-C27-C28-C29
2	C	906	LBN	C26-C27-C28-C29
2	D	902	LBN	C26-C27-C28-C29
2	B	902	LBN	C26-C27-C28-C29
3	D	901	6OU	C09-C10-C11-C12
2	A	901	LBN	C35-C36-C37-C38
2	C	901	LBN	C35-C36-C37-C38
2	B	904	LBN	C35-C36-C37-C38
2	A	905	LBN	O6-C25-O5-C3
2	C	906	LBN	O6-C25-O5-C3
2	D	902	LBN	O6-C25-O5-C3
2	B	902	LBN	O6-C25-O5-C3
2	D	903	LBN	C35-C36-C37-C38
3	A	906	6OU	C11-C12-C13-C14
3	C	905	6OU	C11-C12-C13-C14
3	D	901	6OU	C11-C12-C13-C14
3	B	903	6OU	C11-C12-C13-C14
3	A	904	6OU	C33-C34-C35-C36
3	B	901	6OU	C33-C34-C35-C36
3	B	905	6OU	C33-C34-C35-C36
3	C	902	6OU	C33-C34-C35-C36
3	A	906	6OU	C10-C11-C12-C13
3	C	905	6OU	C10-C11-C12-C13
3	D	901	6OU	C10-C11-C12-C13
3	B	903	6OU	C10-C11-C12-C13
3	A	906	6OU	C34-C35-C36-C37
3	C	905	6OU	C34-C35-C36-C37
3	D	901	6OU	C34-C35-C36-C37
3	B	903	6OU	C34-C35-C36-C37
3	A	906	6OU	C07-C08-C09-C10
3	C	905	6OU	C07-C08-C09-C10
3	D	901	6OU	C07-C08-C09-C10
3	B	903	6OU	C07-C08-C09-C10
2	A	901	LBN	C26-C25-O5-C3
2	D	903	LBN	C26-C25-O5-C3
2	B	904	LBN	C26-C25-O5-C3
3	A	906	6OU	C31-C33-C34-C35
3	C	905	6OU	C31-C33-C34-C35
3	D	901	6OU	C31-C33-C34-C35
3	B	903	6OU	C31-C33-C34-C35
2	C	901	LBN	C26-C25-O5-C3

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Mol	Chain	Res	Type	Atoms
2	A	901	LBN	C2-C1-O1-P1
2	C	901	LBN	C2-C1-O1-P1
2	D	903	LBN	C2-C1-O1-P1
2	B	904	LBN	C2-C1-O1-P1
2	A	905	LBN	C14-C11-C8-C5
2	C	906	LBN	C14-C11-C8-C5
2	D	902	LBN	C14-C11-C8-C5
2	B	902	LBN	C14-C11-C8-C5
2	A	905	LBN	C34-C35-C36-C37
2	C	906	LBN	C34-C35-C36-C37
2	D	902	LBN	C34-C35-C36-C37
2	B	902	LBN	C34-C35-C36-C37
3	A	904	6OU	C12-C13-C14-C15
3	C	902	6OU	C12-C13-C14-C15
3	B	901	6OU	C12-C13-C14-C15
3	B	905	6OU	C12-C13-C14-C15
2	A	901	LBN	C1-C2-C3-O5
2	A	905	LBN	C1-C2-C3-O5
2	C	901	LBN	C1-C2-C3-O5
2	C	906	LBN	C1-C2-C3-O5
2	D	902	LBN	C1-C2-C3-O5
2	D	903	LBN	C1-C2-C3-O5
2	B	902	LBN	C1-C2-C3-O5
2	B	904	LBN	C1-C2-C3-O5
2	A	905	LBN	C30-C31-C32-C33
2	C	906	LBN	C30-C31-C32-C33
2	D	902	LBN	C30-C31-C32-C33
2	B	902	LBN	C30-C31-C32-C33
2	A	901	LBN	O6-C25-O5-C3
2	C	901	LBN	O6-C25-O5-C3
2	D	903	LBN	O6-C25-O5-C3
2	B	904	LBN	O6-C25-O5-C3
3	C	902	6OU	C36-C37-C38-C39
3	A	904	6OU	C36-C37-C38-C39
3	B	901	6OU	C36-C37-C38-C39
3	B	905	6OU	C36-C37-C38-C39
2	A	905	LBN	C37-C38-C39-C40
2	C	906	LBN	C37-C38-C39-C40
2	B	902	LBN	C37-C38-C39-C40
2	D	902	LBN	C37-C38-C39-C40
3	A	904	6OU	C10-C11-C12-C13
2	C	901	LBN	C30-C31-C32-C33

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Mol	Chain	Res	Type	Atoms
3	B	905	6OU	C10-C11-C12-C13
2	A	901	LBN	C30-C31-C32-C33
2	D	903	LBN	C30-C31-C32-C33
2	B	904	LBN	C30-C31-C32-C33
3	C	902	6OU	C10-C11-C12-C13
3	B	901	6OU	C10-C11-C12-C13
3	A	904	6OU	O30-C20-C21-O22
3	C	902	6OU	O30-C20-C21-O22
3	B	901	6OU	O30-C20-C21-O22
3	B	905	6OU	O30-C20-C21-O22
2	A	901	LBN	O7-C2-C3-O5
2	A	905	LBN	O7-C2-C3-O5
2	C	901	LBN	O7-C2-C3-O5
2	C	906	LBN	O7-C2-C3-O5
2	D	902	LBN	O7-C2-C3-O5
2	D	903	LBN	O7-C2-C3-O5
2	B	902	LBN	O7-C2-C3-O5
2	B	904	LBN	O7-C2-C3-O5
3	A	904	6OU	C40-C41-C42-C43
3	C	902	6OU	C40-C41-C42-C43
3	B	901	6OU	C40-C41-C42-C43
3	B	905	6OU	C40-C41-C42-C43
3	A	904	6OU	C19-C20-C21-O22
3	B	901	6OU	C19-C20-C21-O22
3	B	905	6OU	C19-C20-C21-O22
2	C	906	LBN	C28-C29-C30-C31
2	B	902	LBN	C28-C29-C30-C31
3	A	902	6OU	C45-C46-C47-C48
3	C	903	6OU	C45-C46-C47-C48
3	D	904	6OU	C45-C46-C47-C48
3	B	906	6OU	C45-C46-C47-C48
2	D	902	LBN	C28-C29-C30-C31
2	A	905	LBN	C28-C29-C30-C31
2	A	901	LBN	C28-C29-C30-C31
2	C	901	LBN	C28-C29-C30-C31
2	D	903	LBN	C28-C29-C30-C31
2	B	904	LBN	C28-C29-C30-C31
3	C	902	6OU	C19-C20-C21-O22
3	A	904	6OU	C20-C21-O22-P23
3	C	902	6OU	C20-C21-O22-P23
3	B	901	6OU	C20-C21-O22-P23
3	B	905	6OU	C20-C21-O22-P23

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Mol	Chain	Res	Type	Atoms
2	A	905	LBN	C31-C32-C33-C4
2	C	906	LBN	C31-C32-C33-C4
2	D	902	LBN	C31-C32-C33-C4
2	B	902	LBN	C31-C32-C33-C4
3	A	902	6OU	C40-C41-C42-C43
3	C	903	6OU	C40-C41-C42-C43
3	D	904	6OU	C40-C41-C42-C43
3	B	906	6OU	C40-C41-C42-C43
3	A	906	6OU	C36-C37-C38-C39
3	C	905	6OU	C36-C37-C38-C39
3	D	901	6OU	C36-C37-C38-C39
3	B	903	6OU	C36-C37-C38-C39
2	A	901	LBN	C9-O2-P1-O1
2	A	901	LBN	C9-O2-P1-O4
2	C	901	LBN	C9-O2-P1-O1
2	C	901	LBN	C9-O2-P1-O4
2	D	903	LBN	C9-O2-P1-O1
2	D	903	LBN	C9-O2-P1-O4
2	B	904	LBN	C9-O2-P1-O1
2	B	904	LBN	C9-O2-P1-O4
3	A	904	6OU	C21-O22-P23-O26
3	C	902	6OU	C21-O22-P23-O26
3	B	901	6OU	C21-O22-P23-O26
3	B	905	6OU	C21-O22-P23-O26
3	A	906	6OU	C20-C21-O22-P23
3	C	905	6OU	C20-C21-O22-P23
3	D	901	6OU	C20-C21-O22-P23
3	B	903	6OU	C20-C21-O22-P23
2	A	901	LBN	C9-C6-N1-C12
2	C	901	LBN	C9-C6-N1-C12
2	D	903	LBN	C9-C6-N1-C12
2	B	904	LBN	C9-C6-N1-C12
3	A	904	6OU	C37-C38-C39-C40
3	C	902	6OU	C37-C38-C39-C40
3	B	901	6OU	C37-C38-C39-C40
3	B	905	6OU	C37-C38-C39-C40
3	A	906	6OU	C40-C41-C42-C43
3	C	905	6OU	C40-C41-C42-C43
3	D	901	6OU	C40-C41-C42-C43
3	B	903	6OU	C40-C41-C42-C43
2	A	905	LBN	C39-C40-C41-C42
2	C	906	LBN	C39-C40-C41-C42

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Mol	Chain	Res	Type	Atoms
2	D	902	LBN	C39-C40-C41-C42
2	B	902	LBN	C39-C40-C41-C42
2	A	901	LBN	C9-C6-N1-C18
2	C	901	LBN	C9-C6-N1-C18
2	D	903	LBN	C9-C6-N1-C18
2	B	904	LBN	C9-C6-N1-C18
2	C	901	LBN	C26-C27-C28-C29
2	A	901	LBN	C26-C27-C28-C29
2	D	903	LBN	C26-C27-C28-C29
2	B	904	LBN	C26-C27-C28-C29
3	B	905	6OU	C34-C35-C36-C37
3	A	904	6OU	C34-C35-C36-C37
3	C	902	6OU	C34-C35-C36-C37
3	B	901	6OU	C34-C35-C36-C37
2	A	901	LBN	C9-C6-N1-C15
2	C	901	LBN	C9-C6-N1-C15
2	D	903	LBN	C9-C6-N1-C15
2	B	904	LBN	C9-C6-N1-C15
3	A	906	6OU	O30-C20-C21-O22
3	C	905	6OU	O30-C20-C21-O22
3	D	901	6OU	O30-C20-C21-O22
3	B	903	6OU	O30-C20-C21-O22
3	A	906	6OU	C14-C15-C16-O18
3	C	905	6OU	C14-C15-C16-O18
3	D	901	6OU	C14-C15-C16-O18
3	B	903	6OU	C14-C15-C16-O18
2	A	901	LBN	O1-C1-C2-C3
2	C	901	LBN	O1-C1-C2-C3
2	D	903	LBN	O1-C1-C2-C3
2	B	904	LBN	O1-C1-C2-C3
3	A	904	6OU	C31-C33-C34-C35
3	B	905	6OU	C31-C33-C34-C35
3	C	902	6OU	C31-C33-C34-C35
3	B	901	6OU	C31-C33-C34-C35
2	C	901	LBN	O7-C34-C35-C36
2	A	901	LBN	O7-C34-C35-C36
2	B	904	LBN	O7-C34-C35-C36
3	A	906	6OU	C19-C20-C21-O22
3	C	905	6OU	C19-C20-C21-O22
3	D	901	6OU	C19-C20-C21-O22
3	B	903	6OU	C19-C20-C21-O22
2	D	903	LBN	O7-C34-C35-C36

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Mol	Chain	Res	Type	Atoms
2	A	905	LBN	C42-C5-C8-C11
2	C	906	LBN	C42-C5-C8-C11
2	D	902	LBN	C42-C5-C8-C11
2	B	902	LBN	C42-C5-C8-C11
2	B	904	LBN	O8-C34-C35-C36
2	D	903	LBN	O8-C34-C35-C36
3	D	904	6OU	C46-C47-C48-C49
3	A	902	6OU	C46-C47-C48-C49
3	B	906	6OU	C46-C47-C48-C49
2	A	901	LBN	O8-C34-C35-C36
2	C	901	LBN	O8-C34-C35-C36
3	C	903	6OU	C46-C47-C48-C49
2	A	905	LBN	O5-C25-C26-C27
2	C	906	LBN	O5-C25-C26-C27
2	D	902	LBN	O5-C25-C26-C27
2	B	902	LBN	O5-C25-C26-C27
3	A	904	6OU	O30-C31-C33-C34
3	A	906	6OU	O30-C31-C33-C34
3	C	902	6OU	O30-C31-C33-C34
3	C	905	6OU	O30-C31-C33-C34
3	D	901	6OU	O30-C31-C33-C34
3	B	901	6OU	O30-C31-C33-C34
3	B	903	6OU	O30-C31-C33-C34
3	B	905	6OU	O30-C31-C33-C34

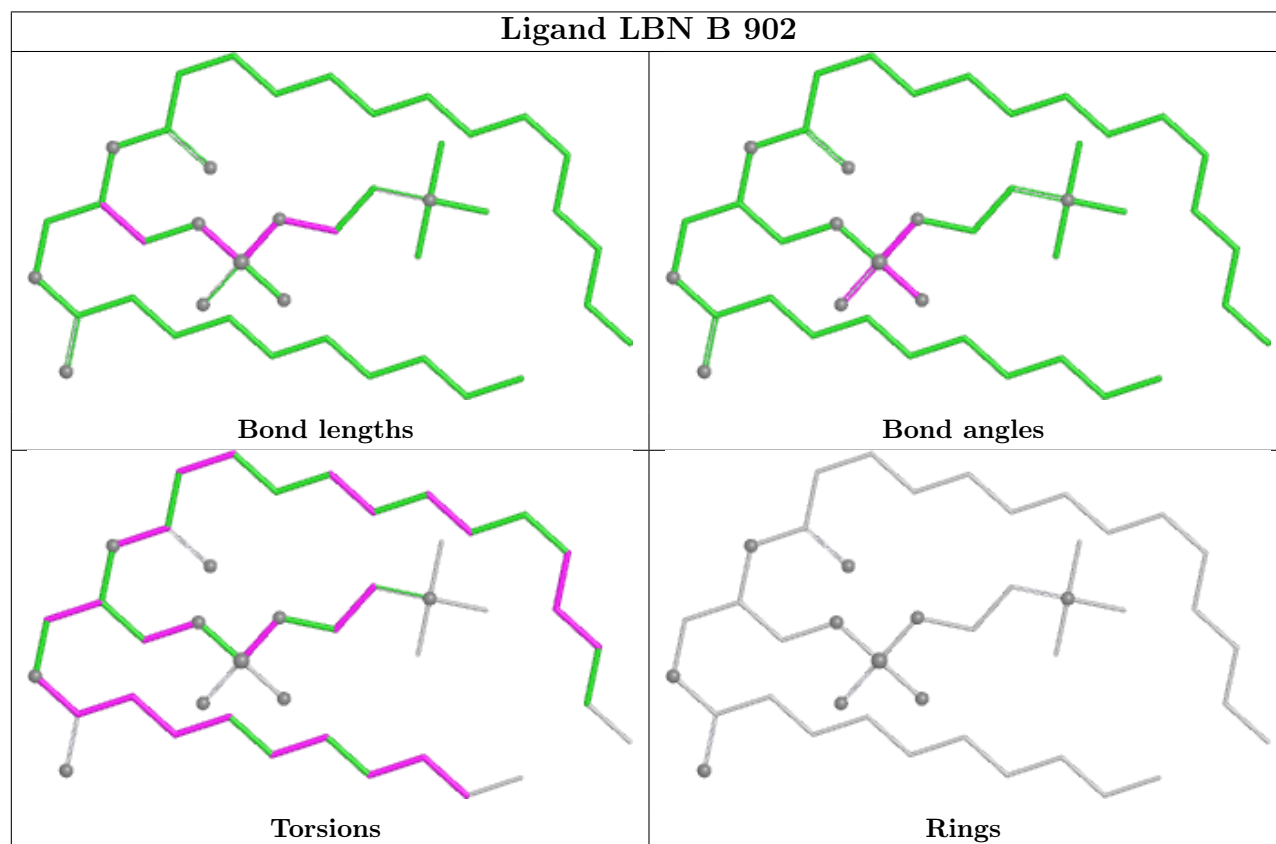
There are no ring outliers.

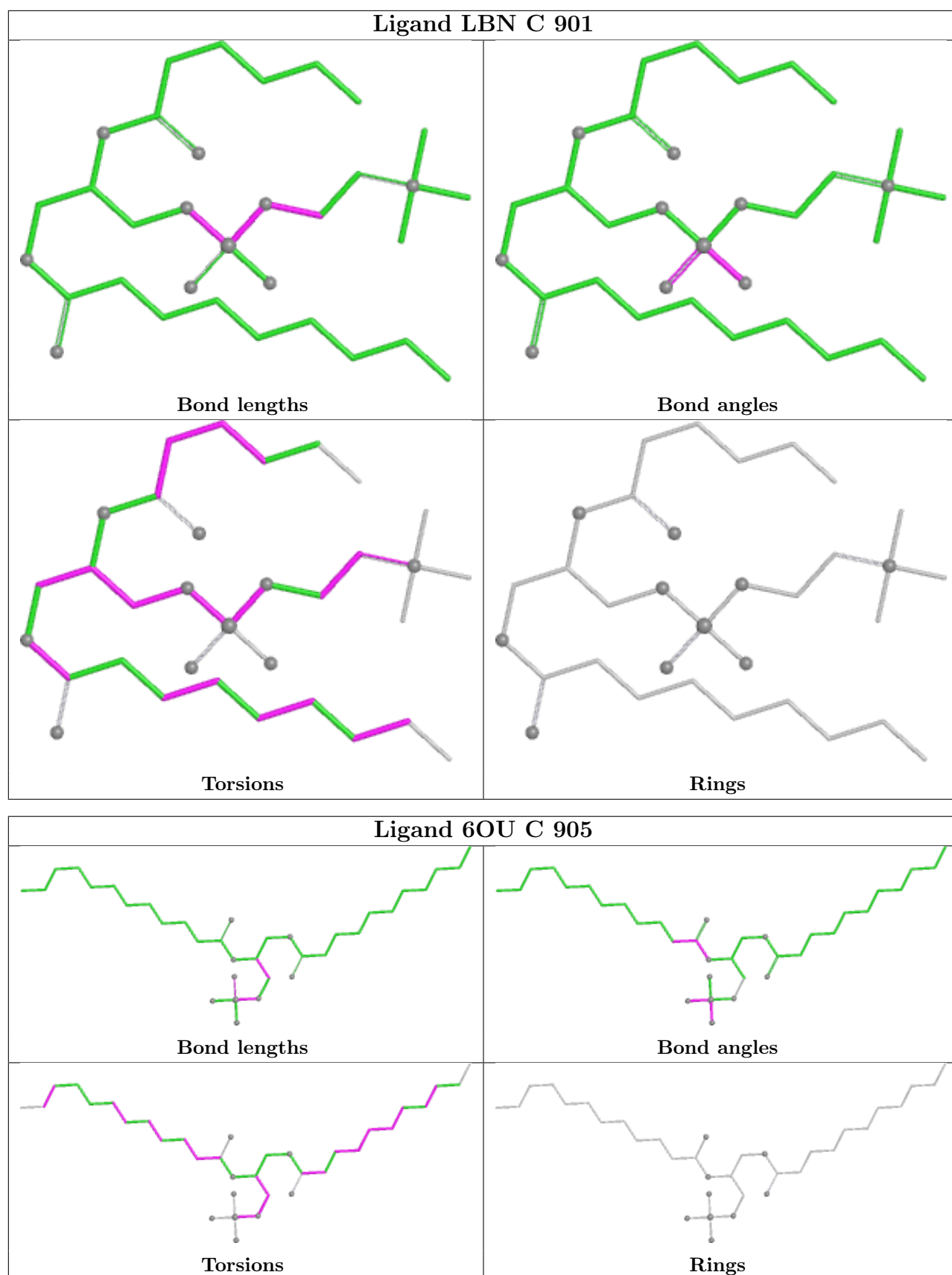
4 monomers are involved in 8 short contacts:

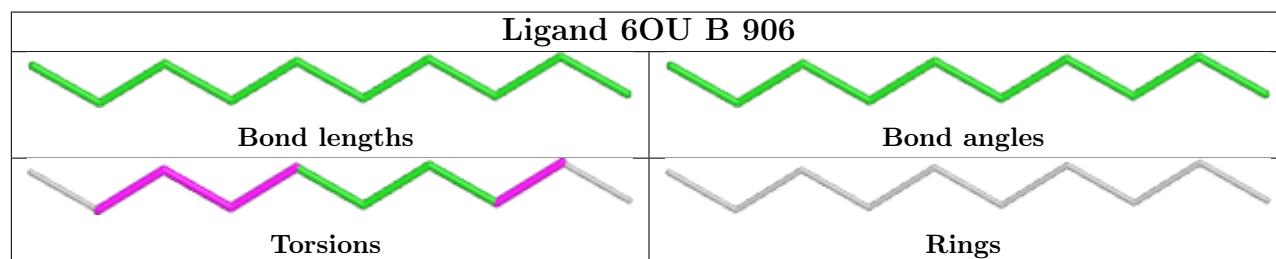
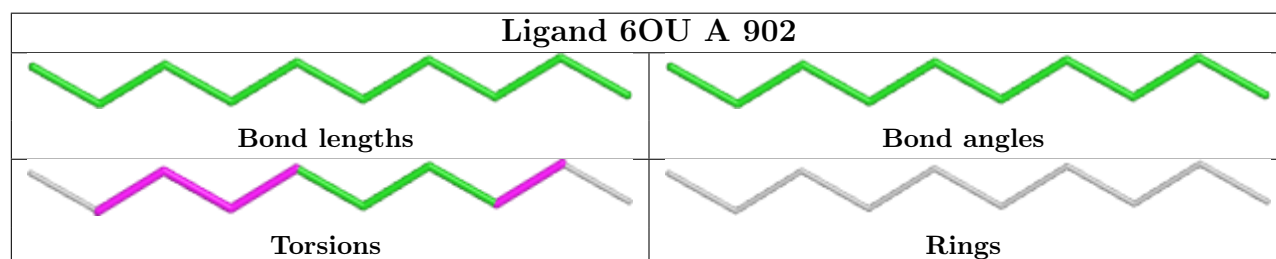
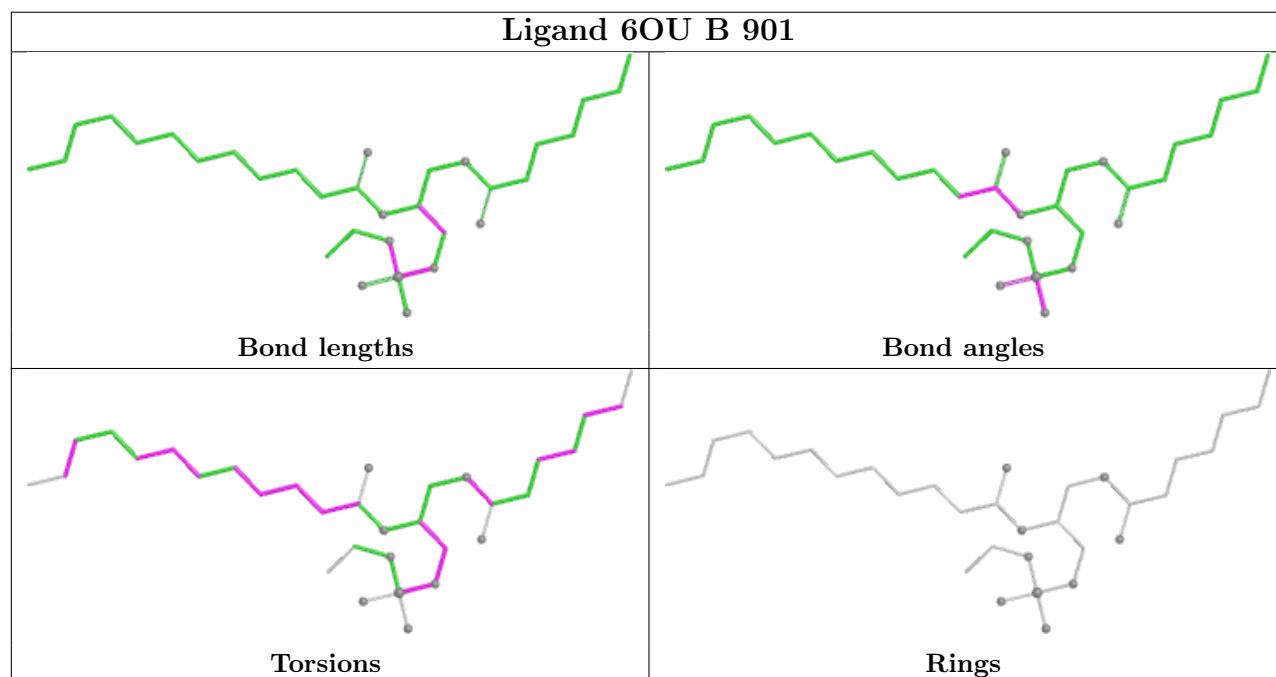
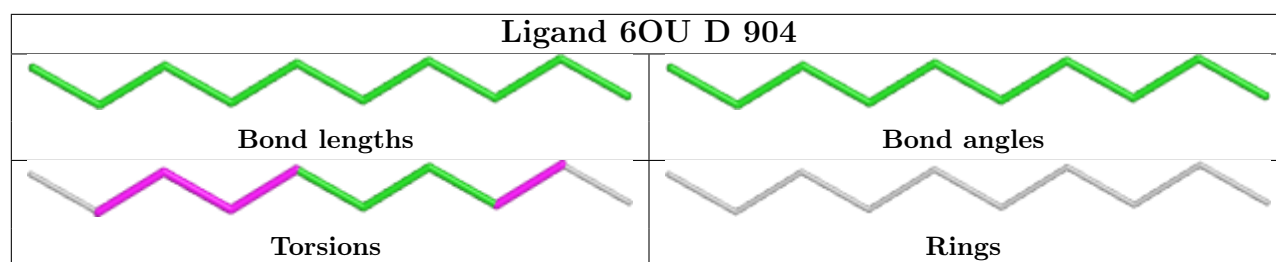
Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	C	904	6EU	2	0
4	D	905	6EU	2	0
4	B	907	6EU	2	0
4	A	903	6EU	2	0

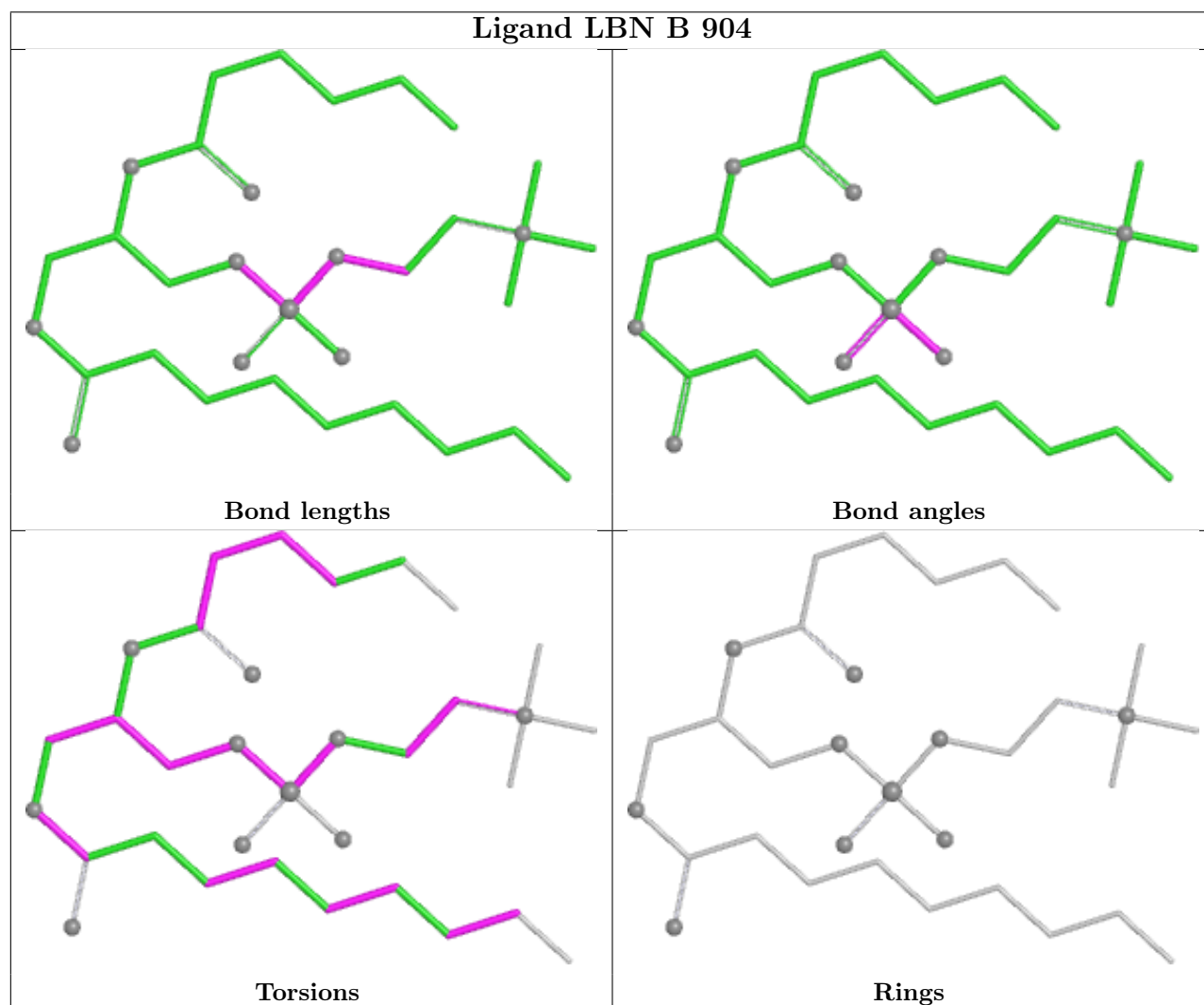
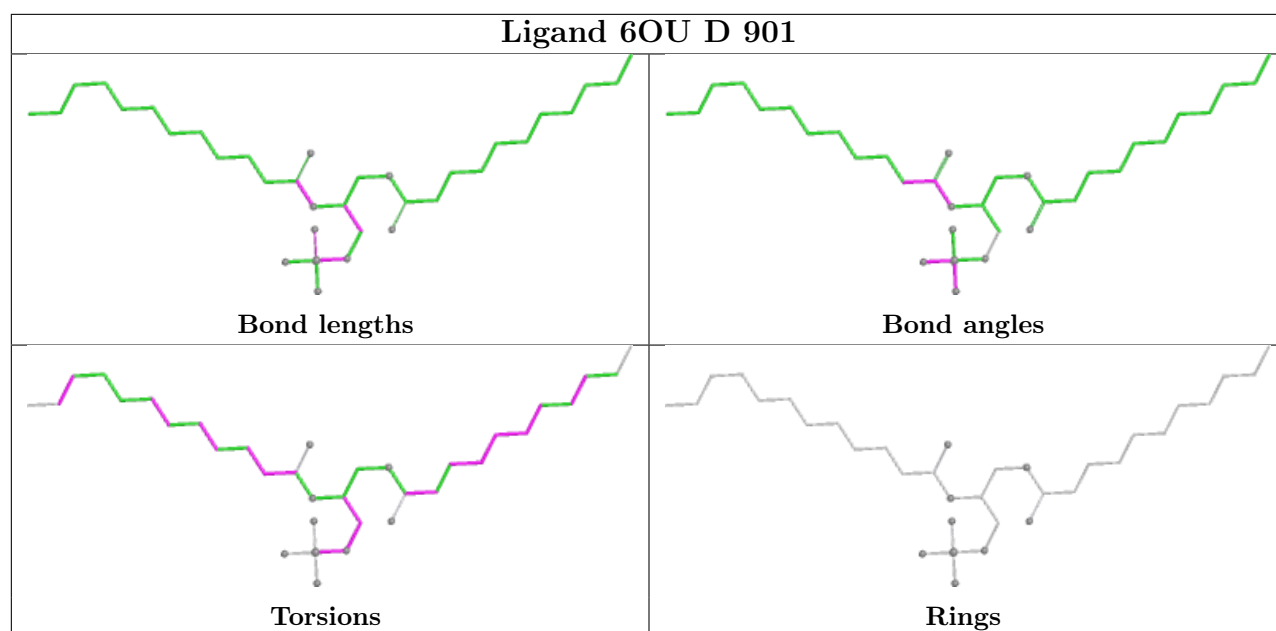
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the

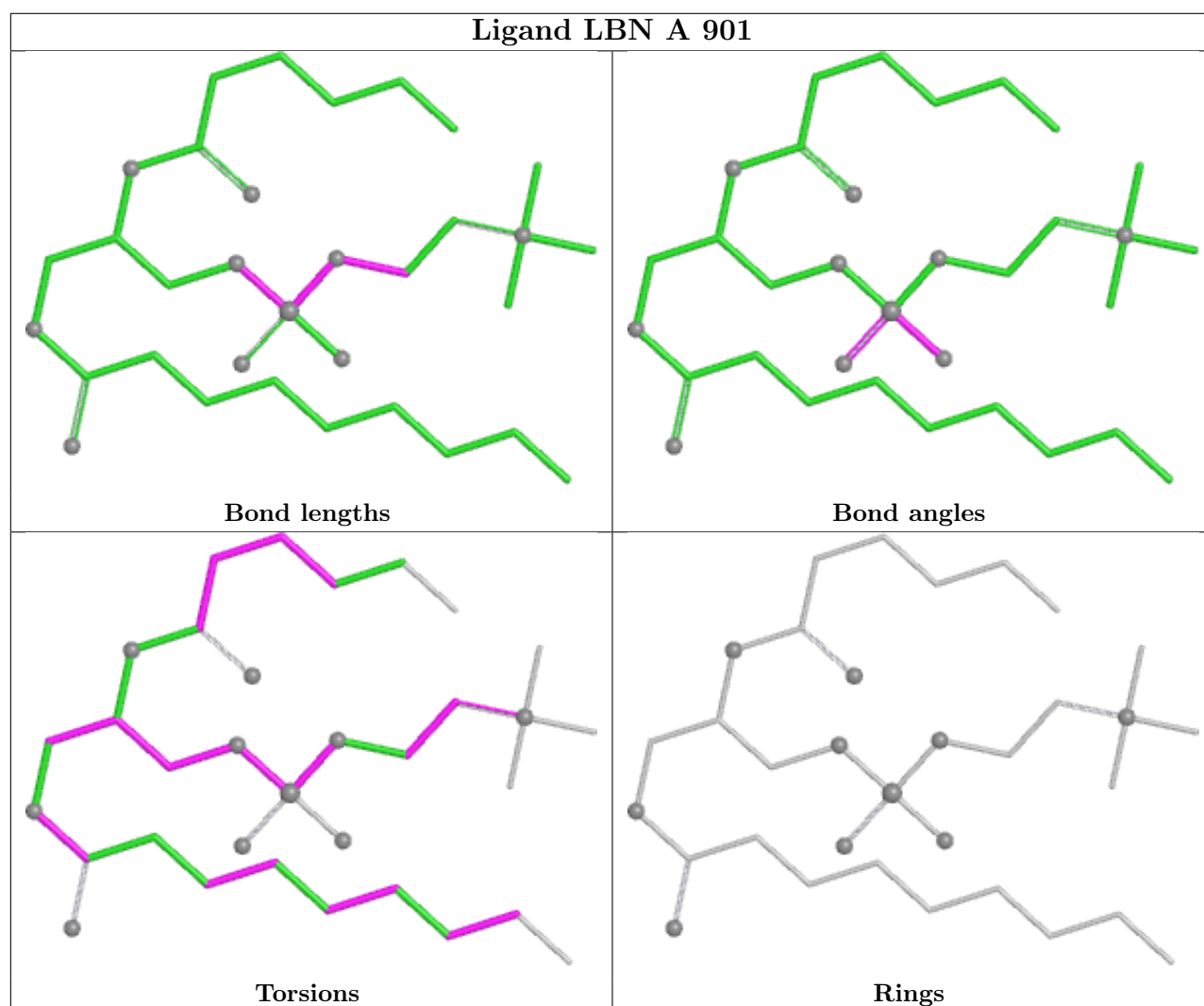
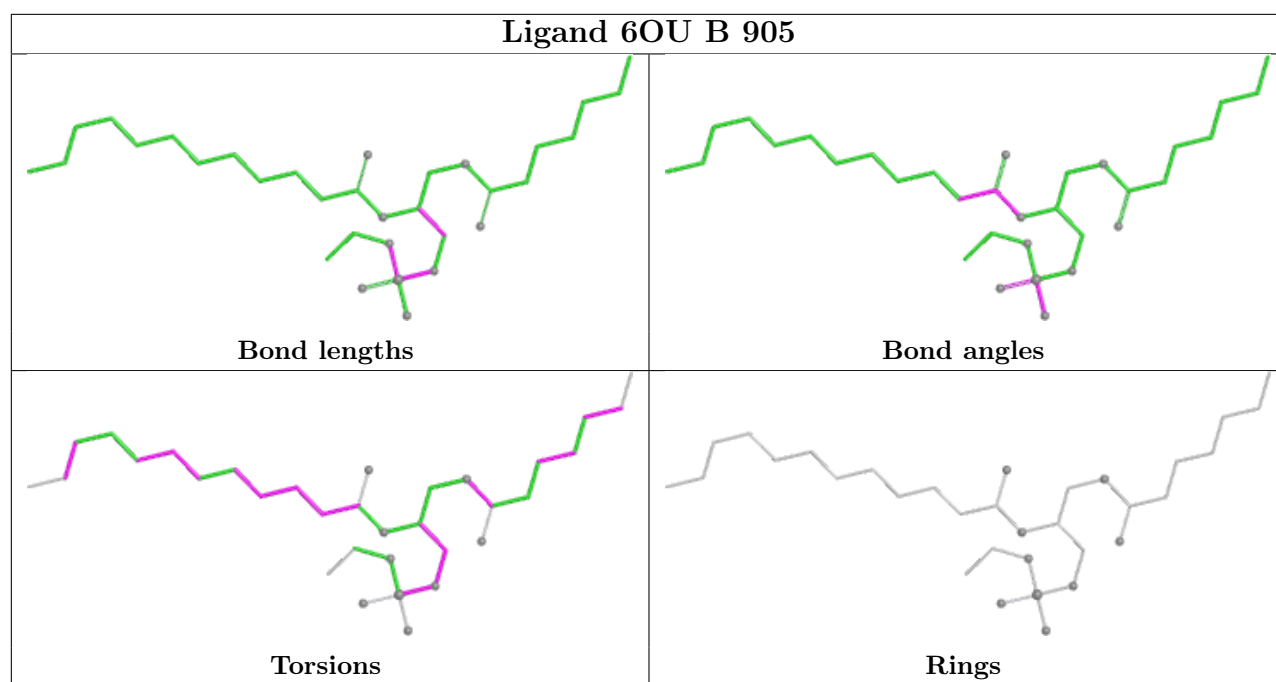
average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

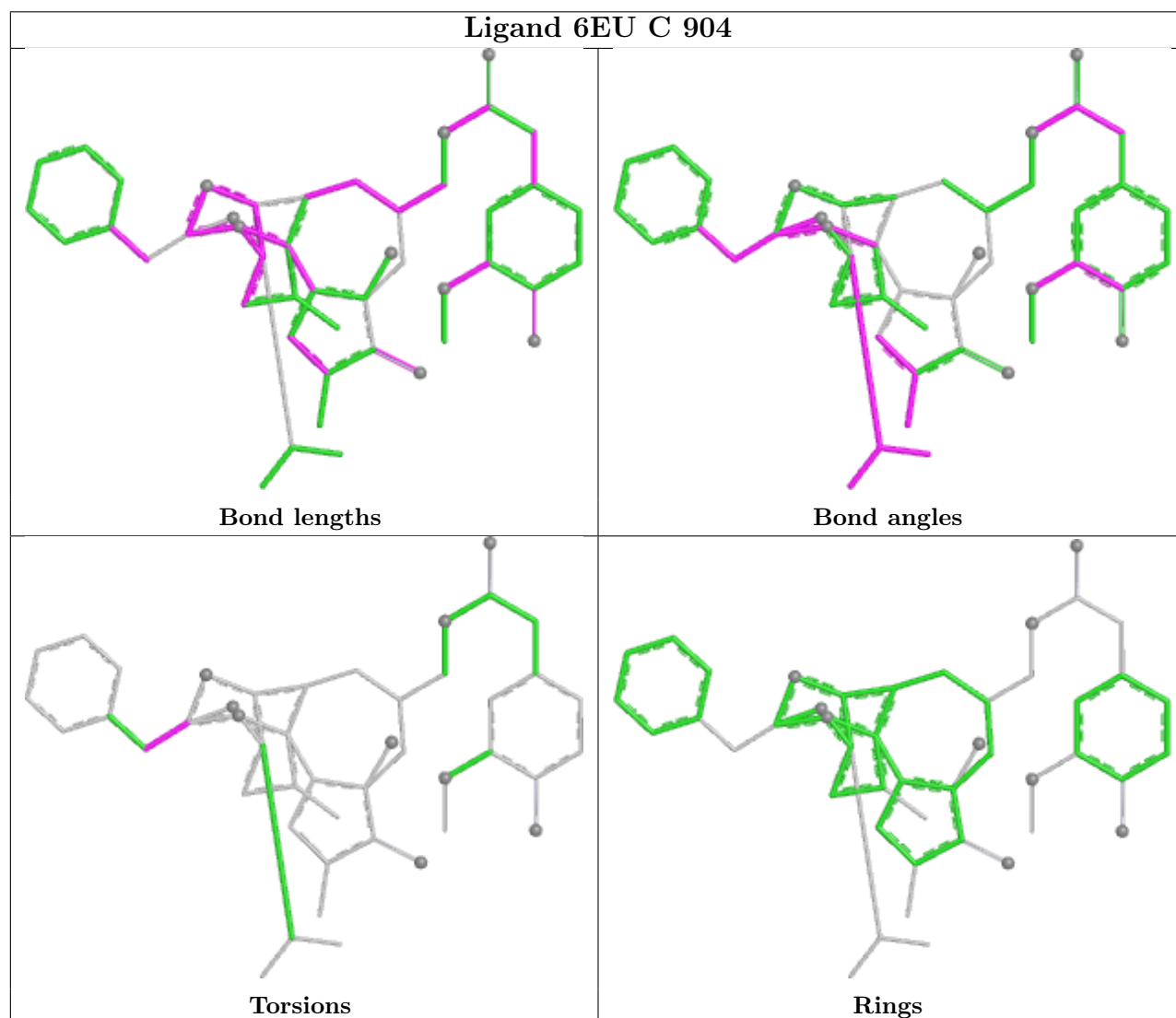
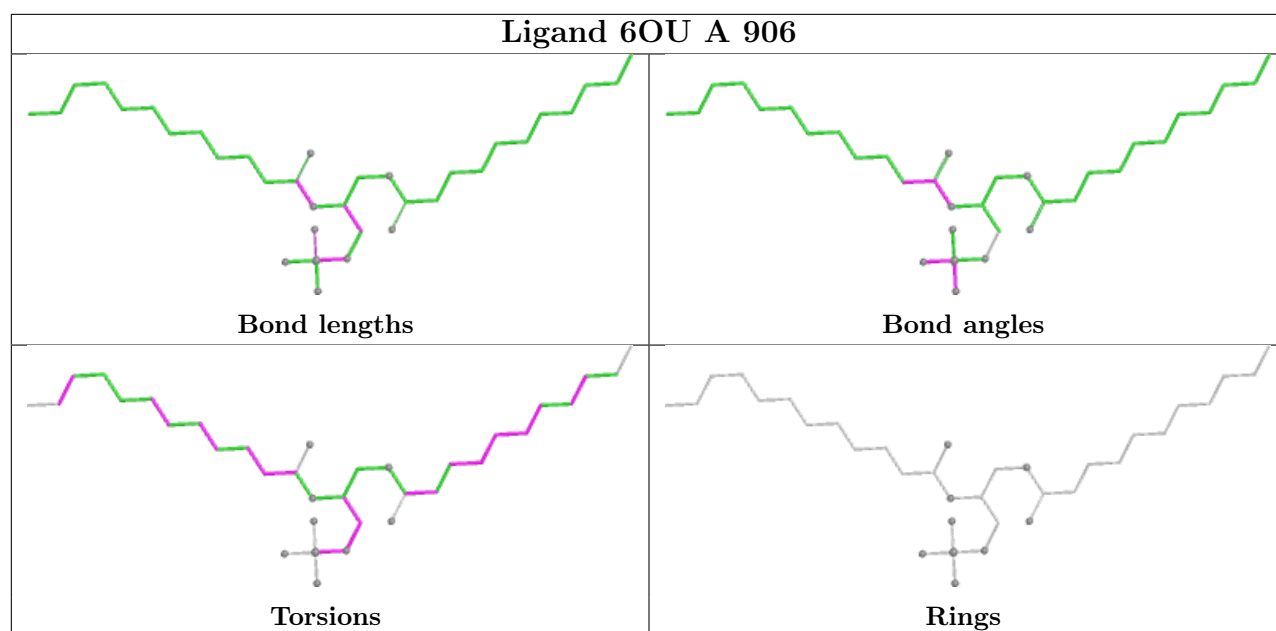


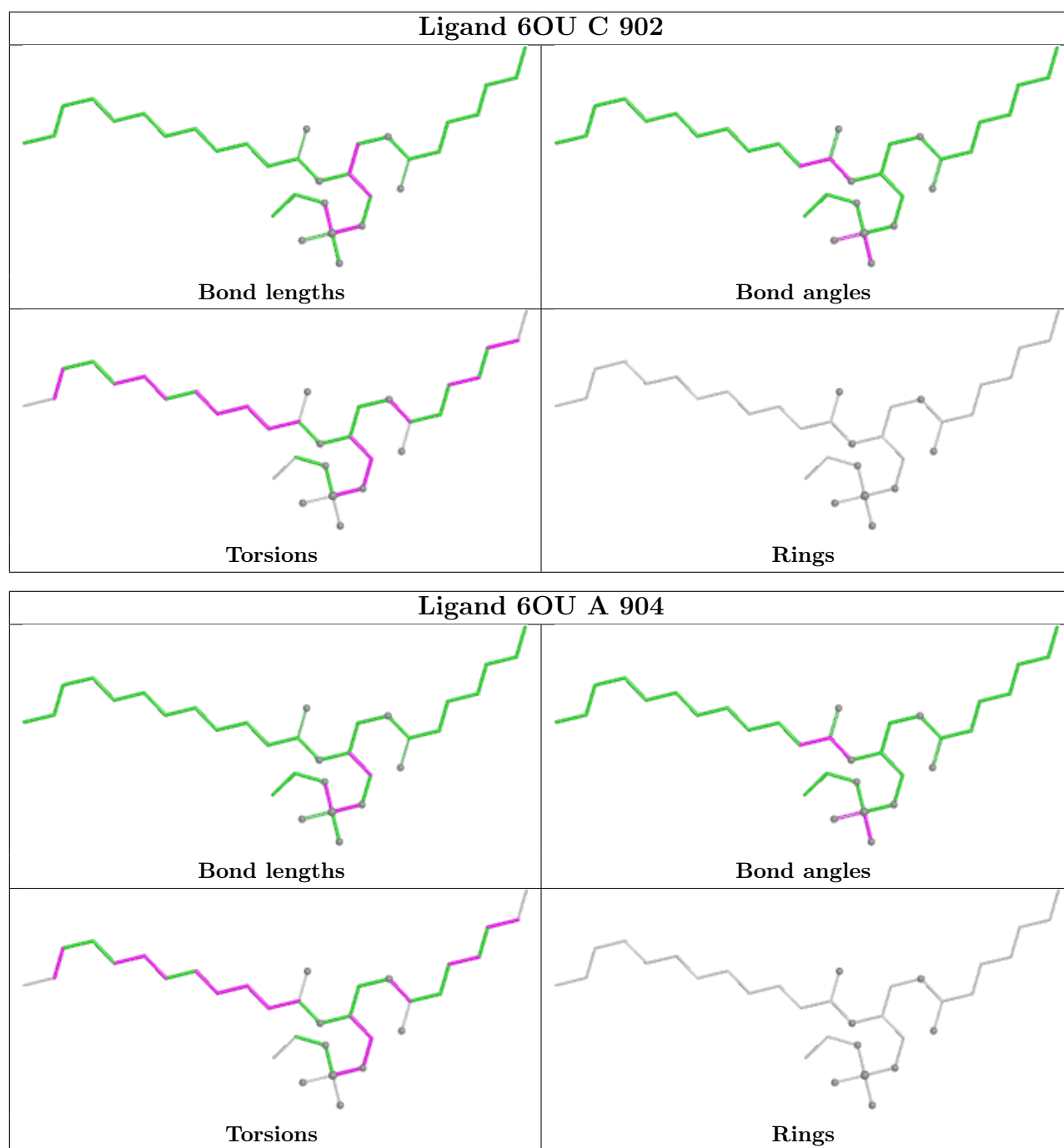


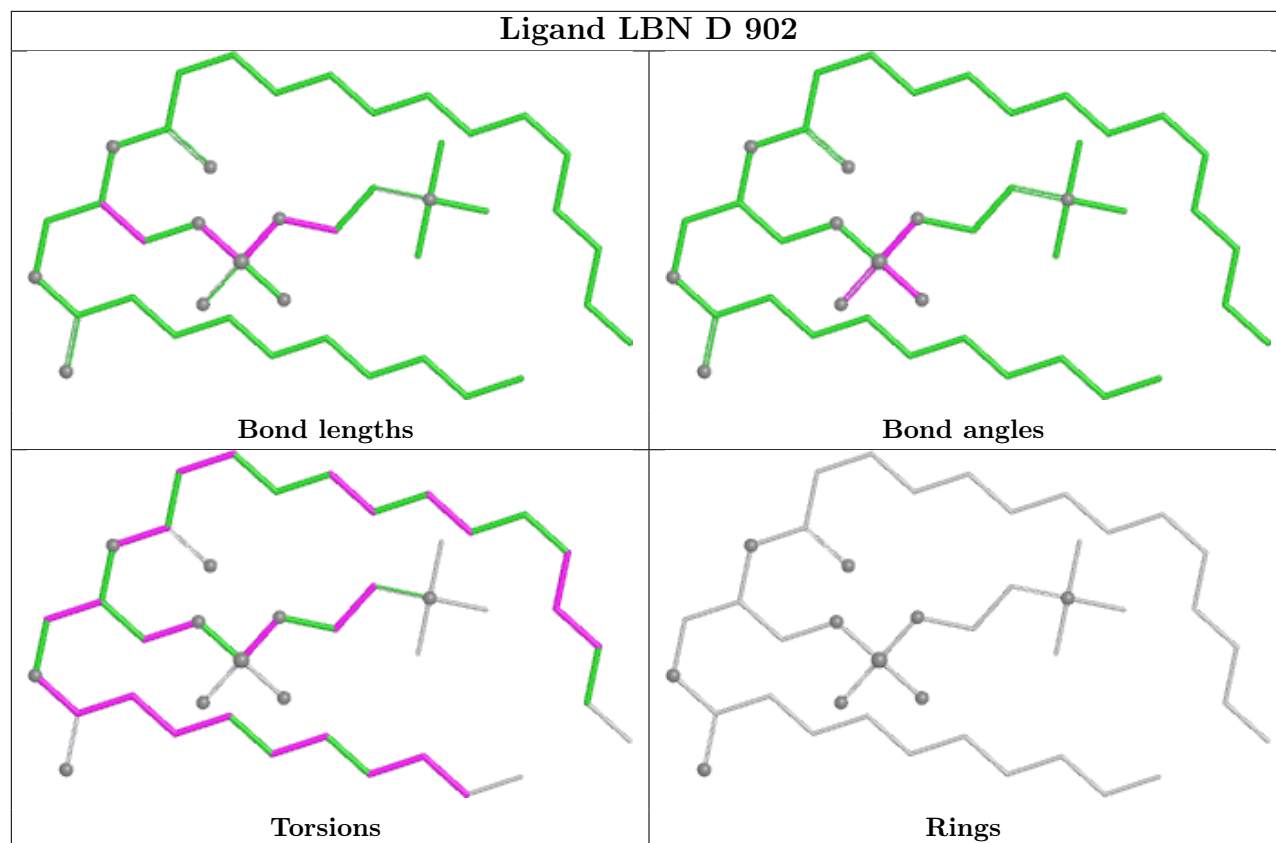


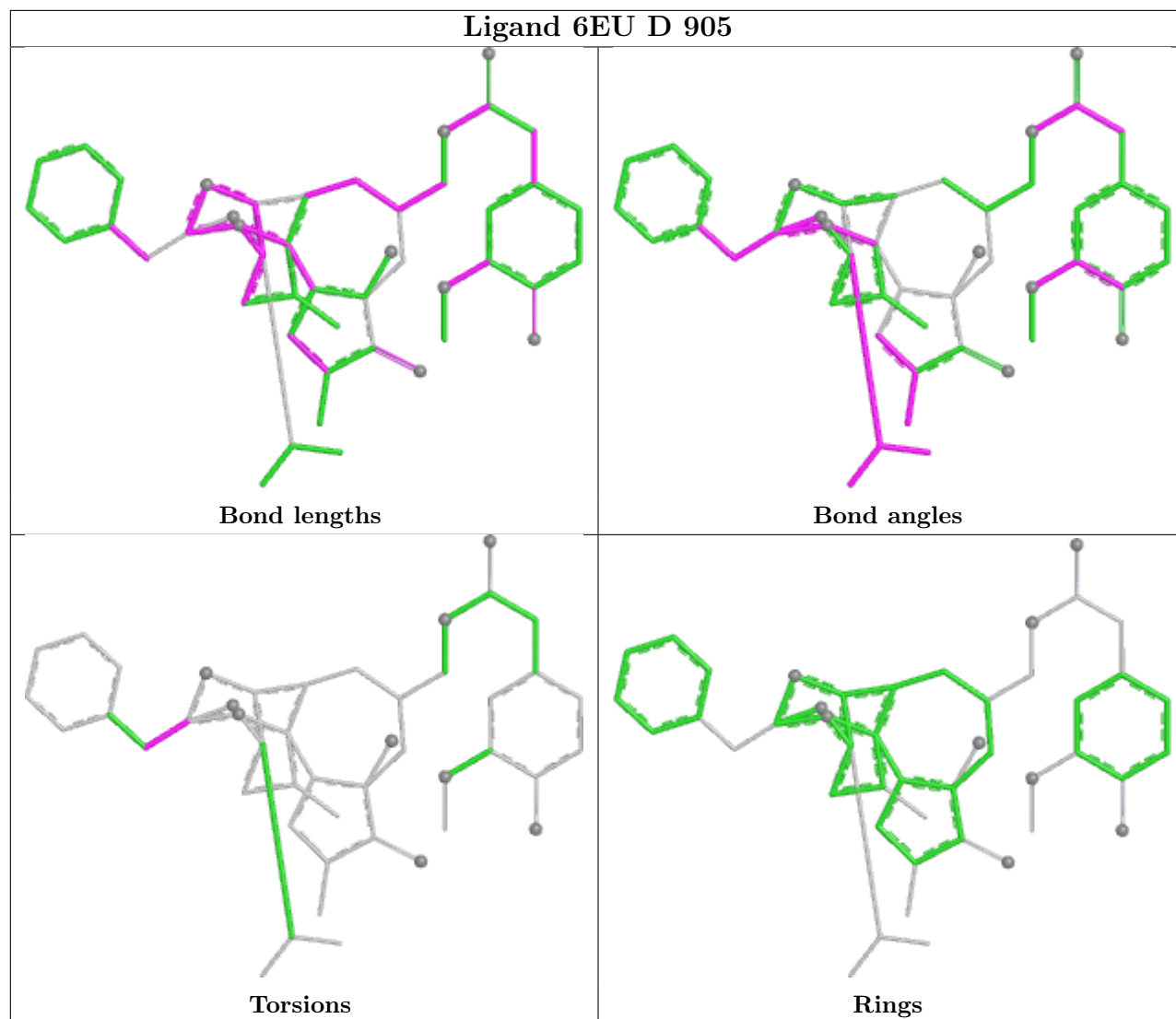




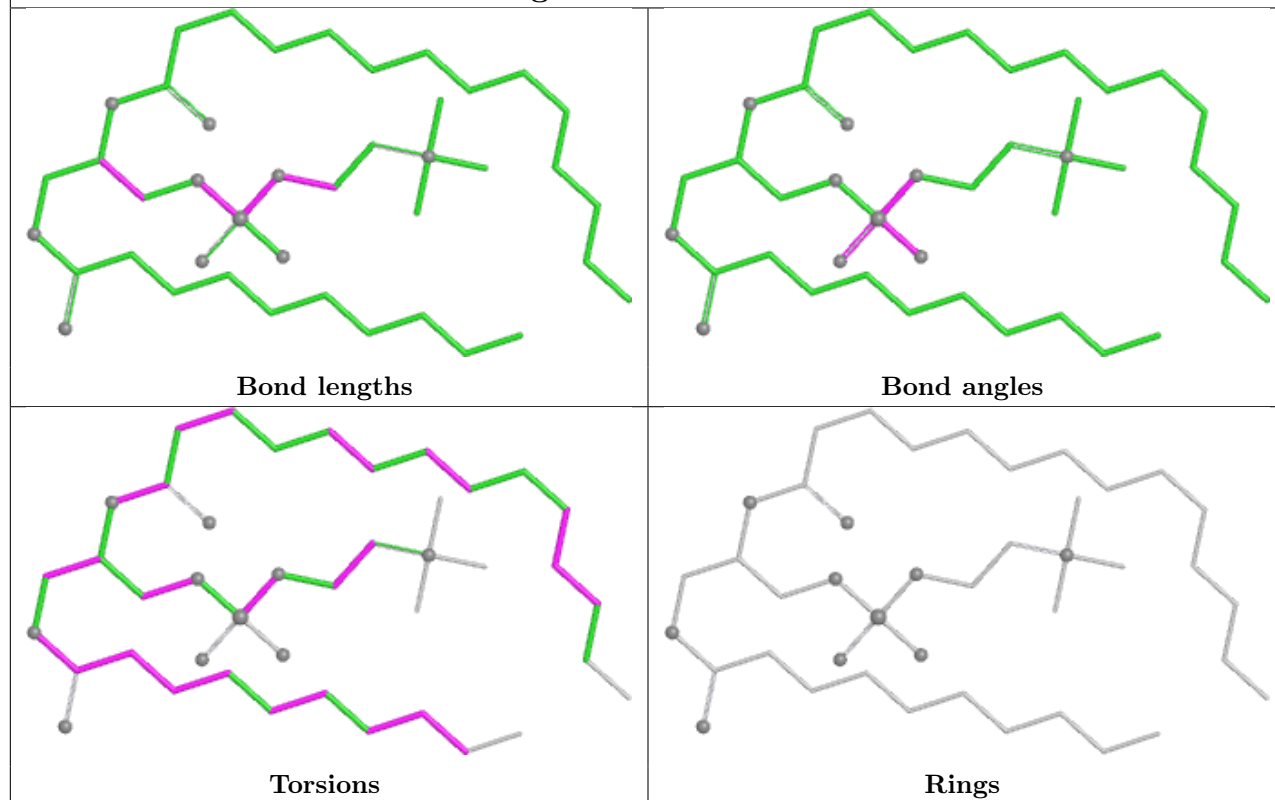




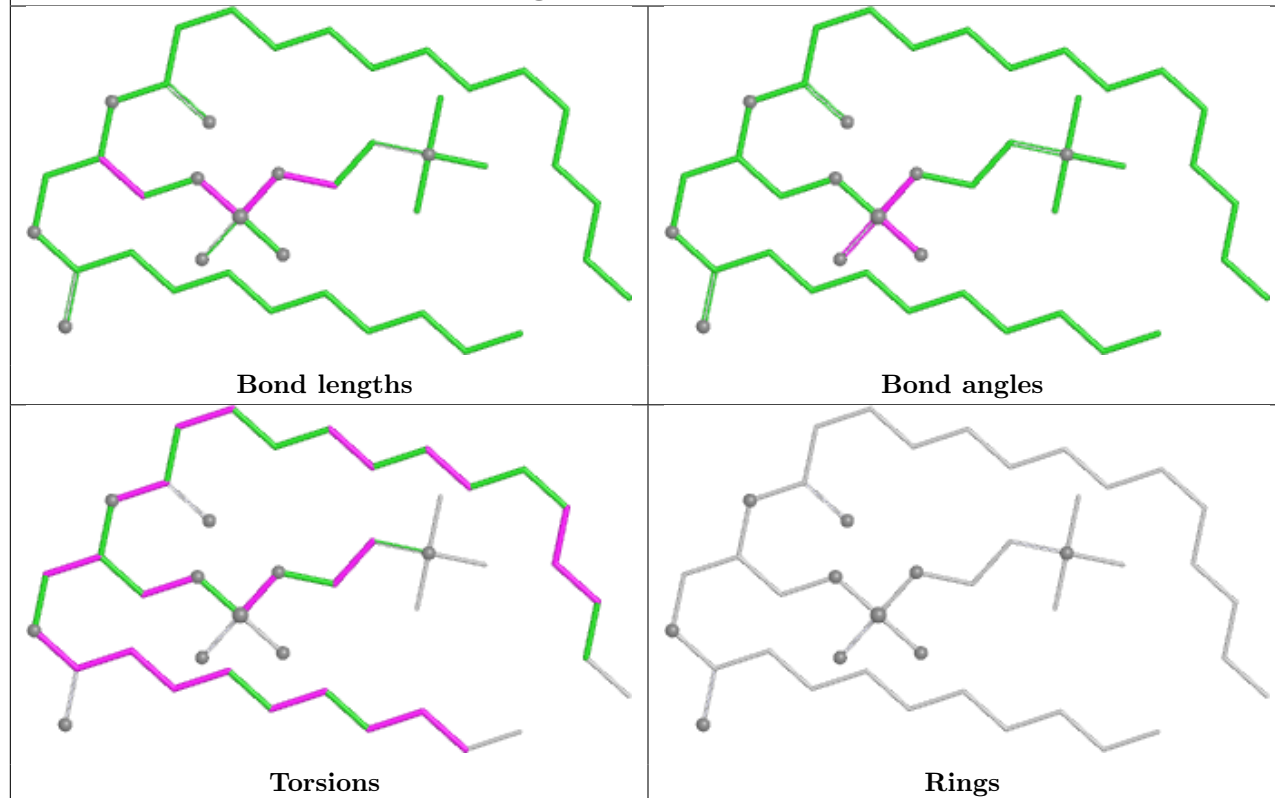


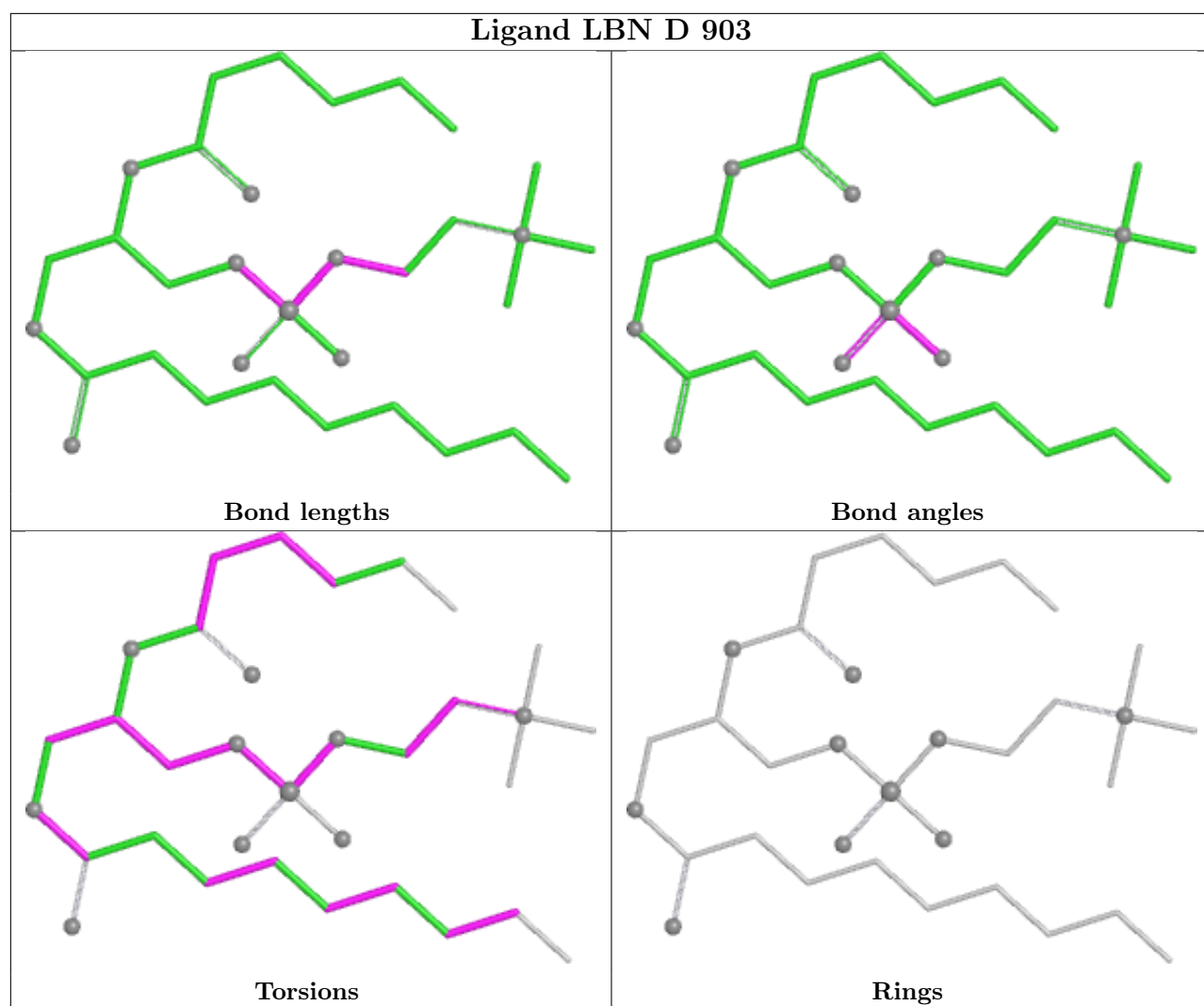


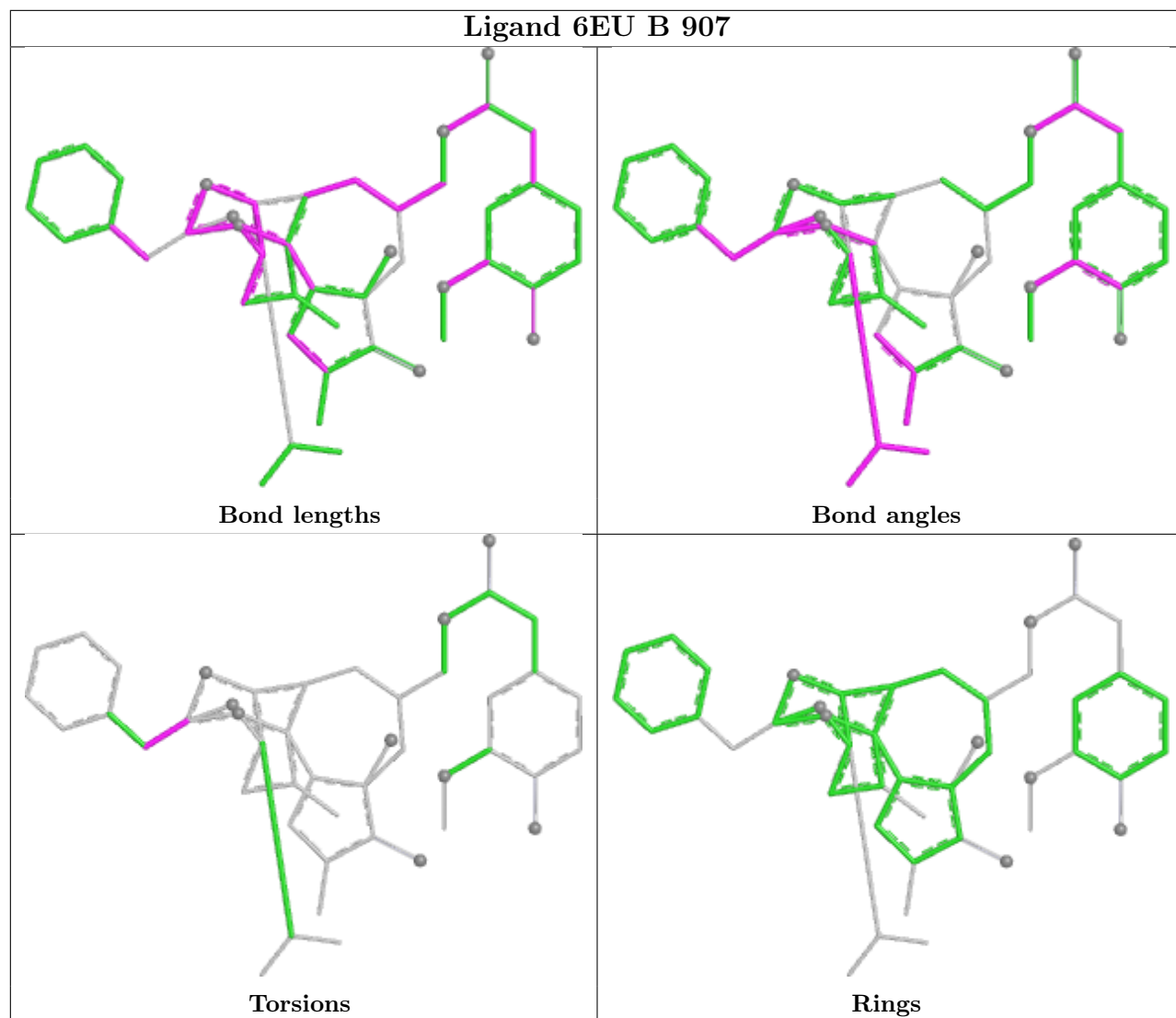
Ligand LBN C 906

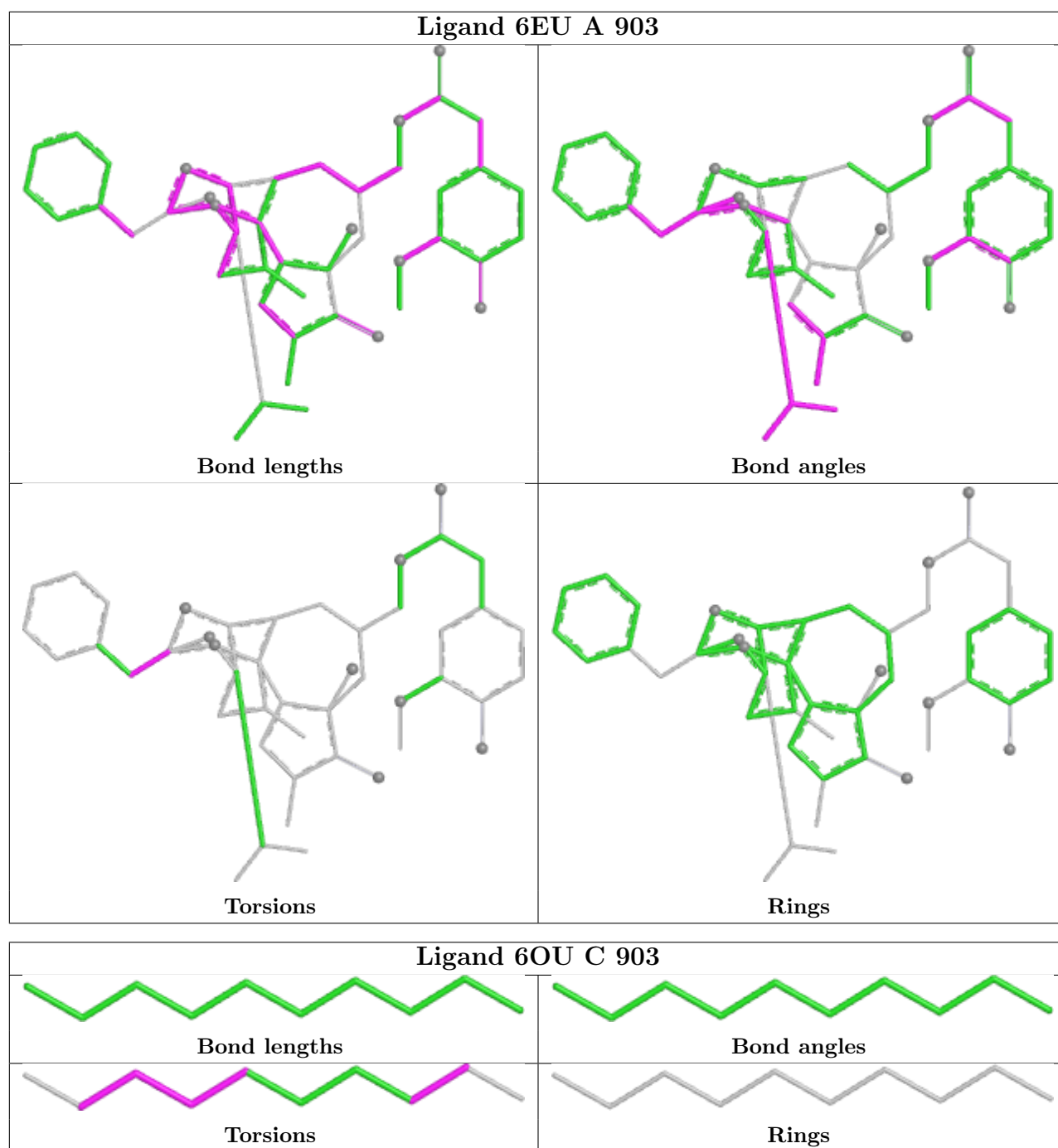


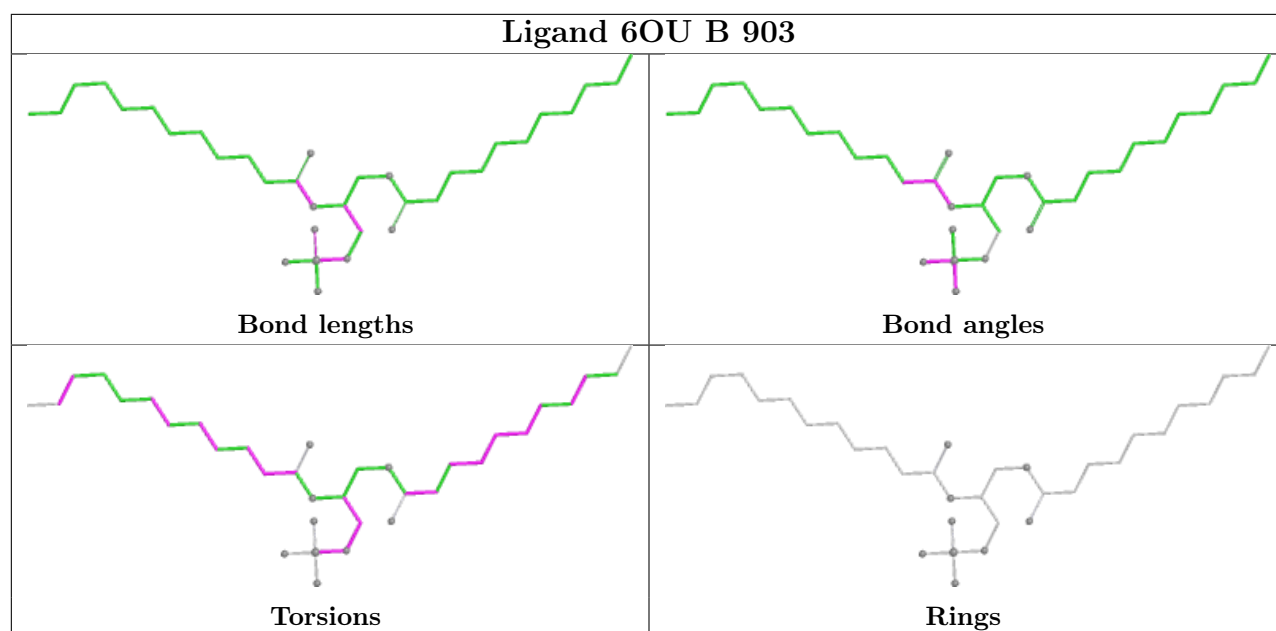
Ligand LBN A 905











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.

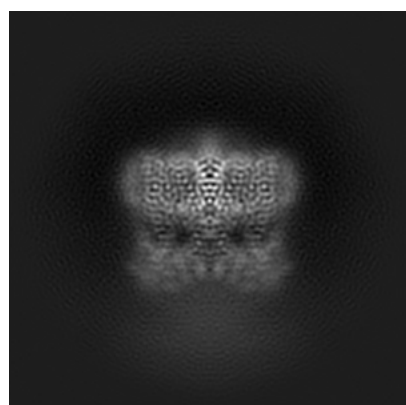
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-24639. These allow visual inspection of the internal detail of the map and identification of artifacts.

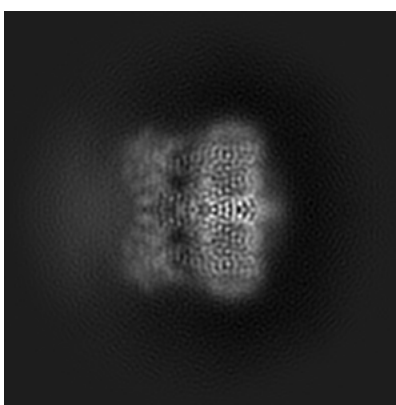
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

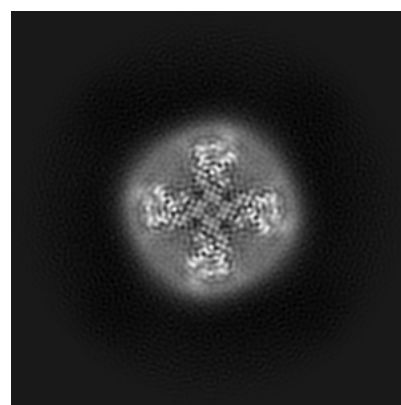
6.1.1 Primary map



X



Y

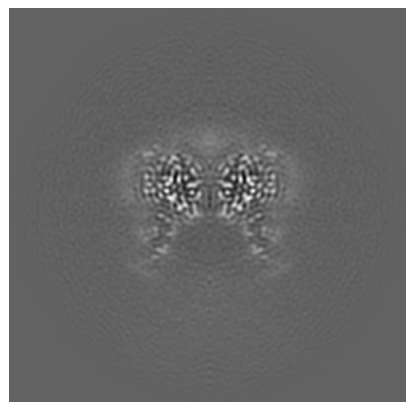


Z

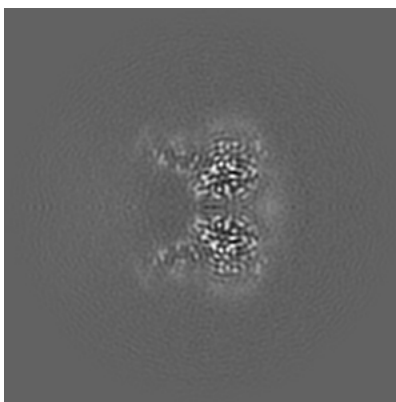
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

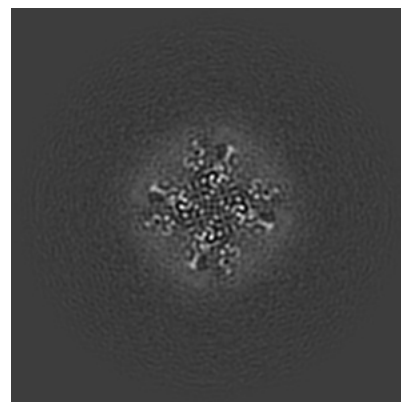
6.2.1 Primary map



X Index: 128



Y Index: 128

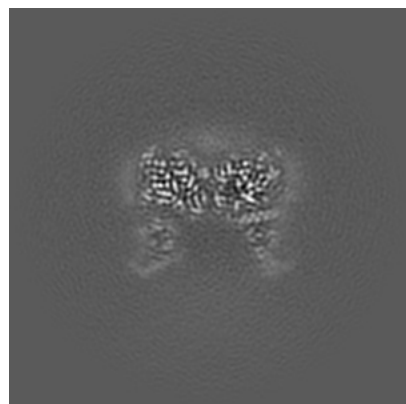


Z Index: 128

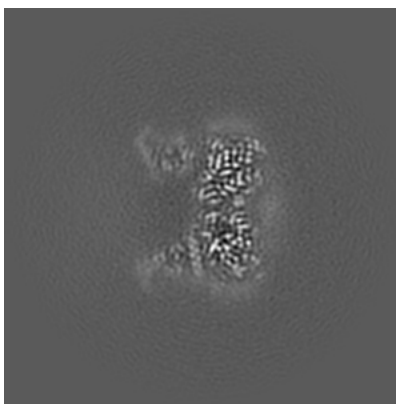
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

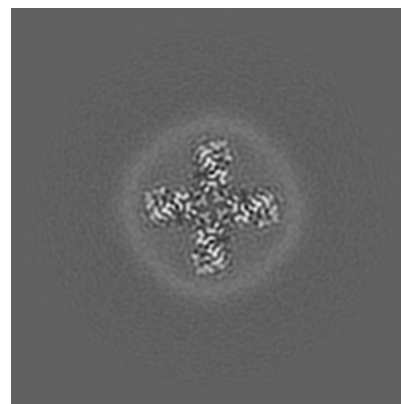
6.3.1 Primary map



X Index: 132



Y Index: 132

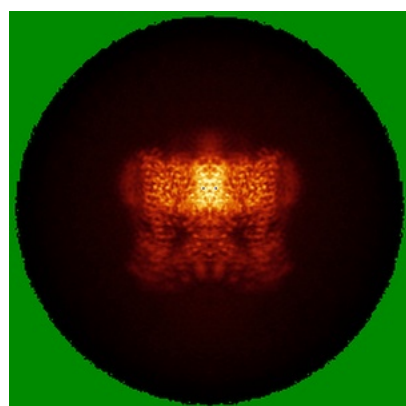


Z Index: 147

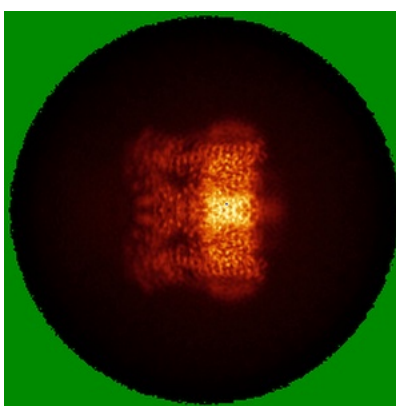
The images above show the largest variance slices of the map in three orthogonal directions.

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

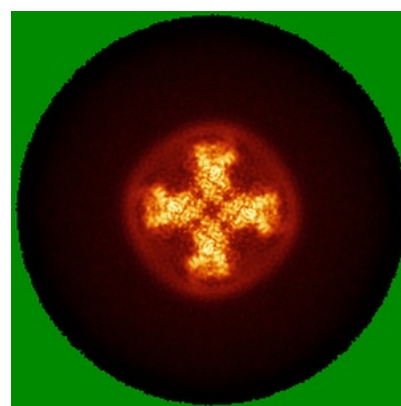
6.4.1 Primary map



X



Y

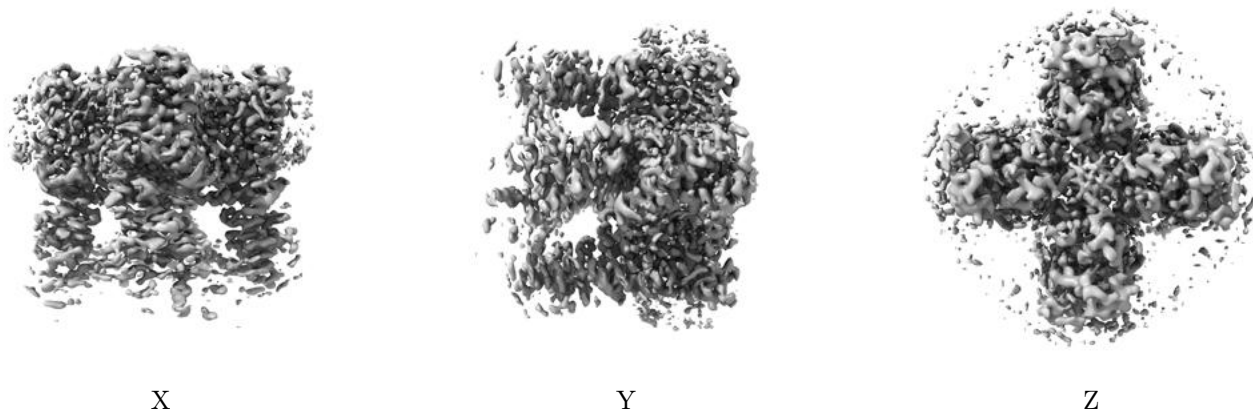


Z

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 0.56. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

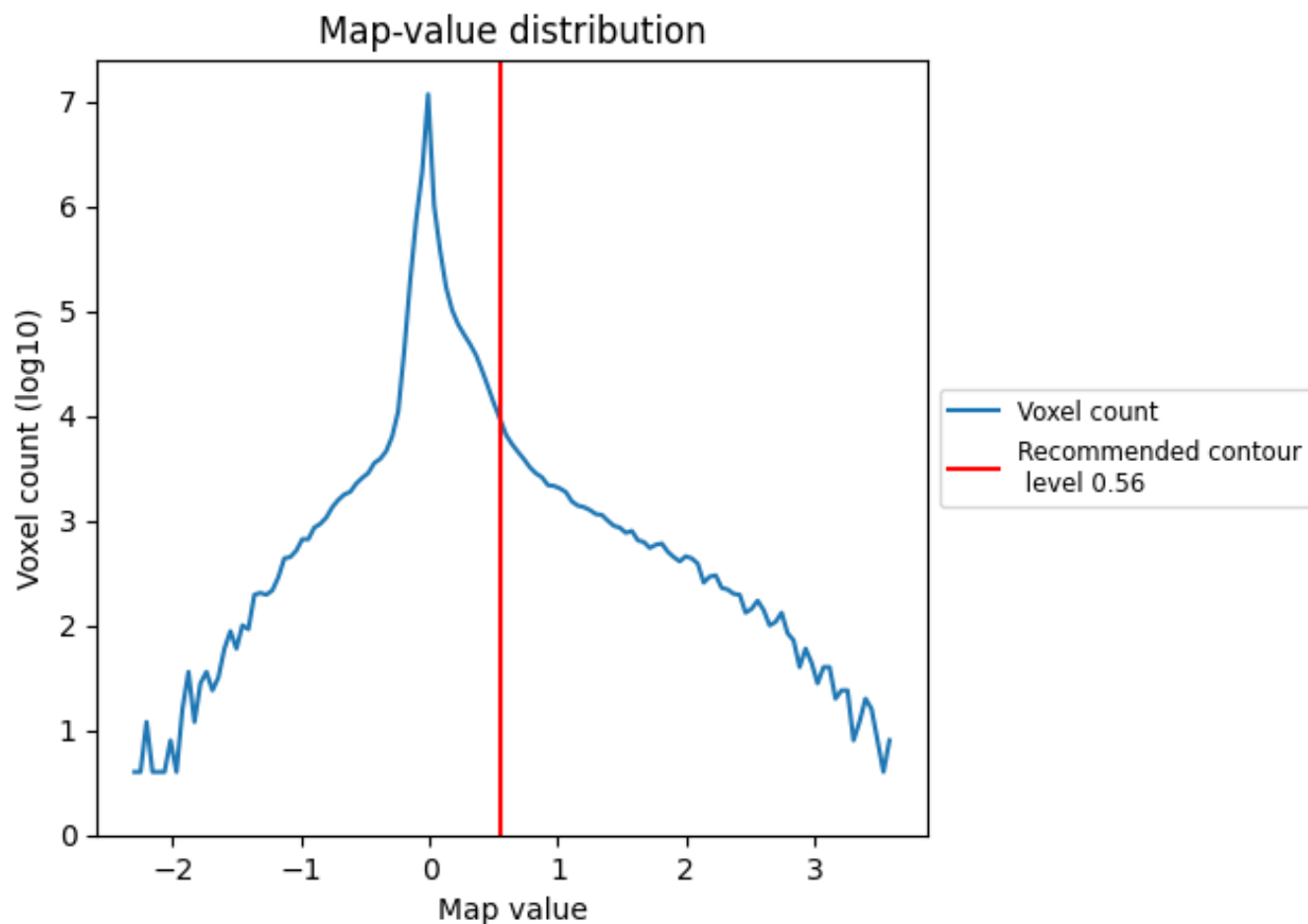
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

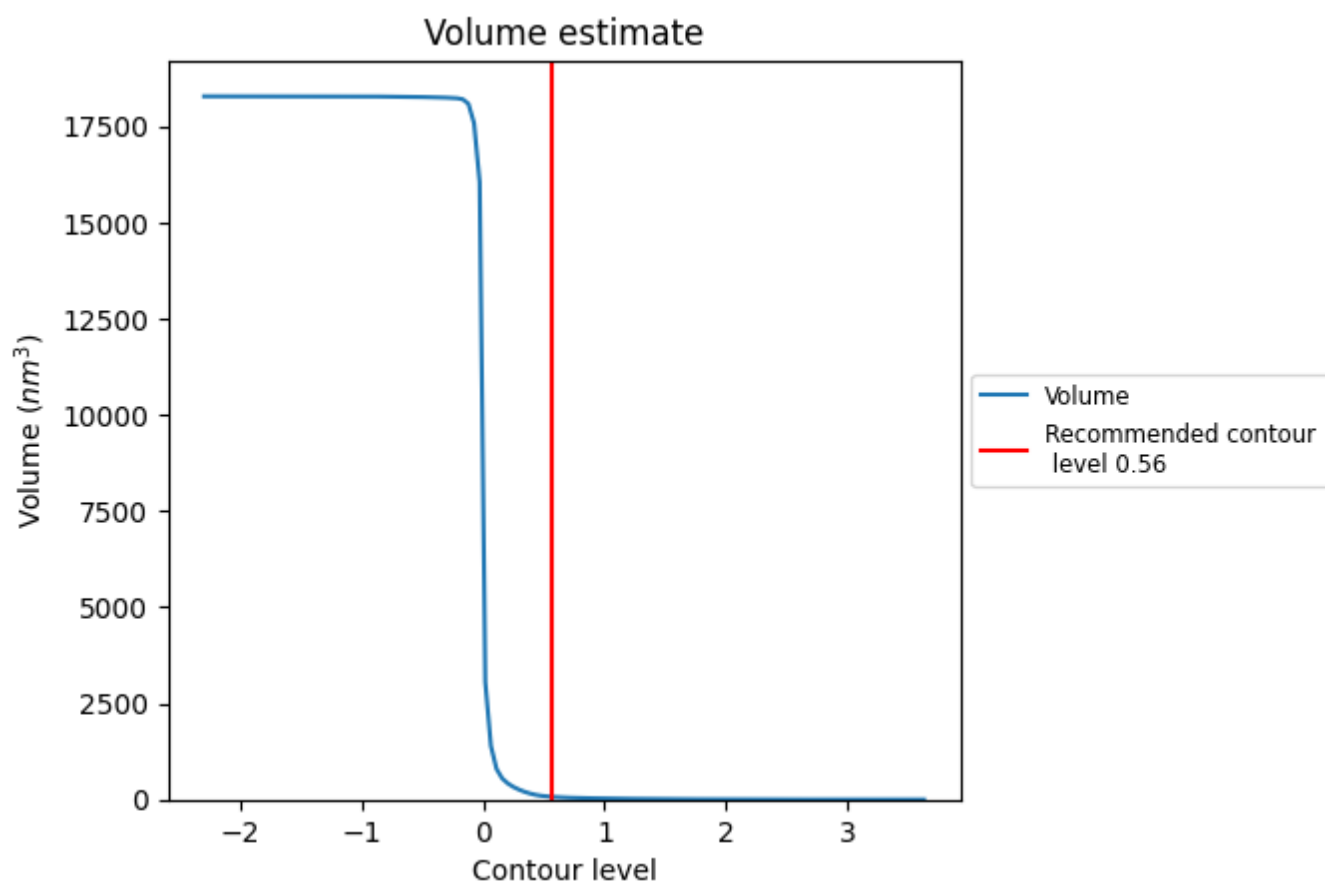
This section contains the results of statistical analysis of the map.

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.

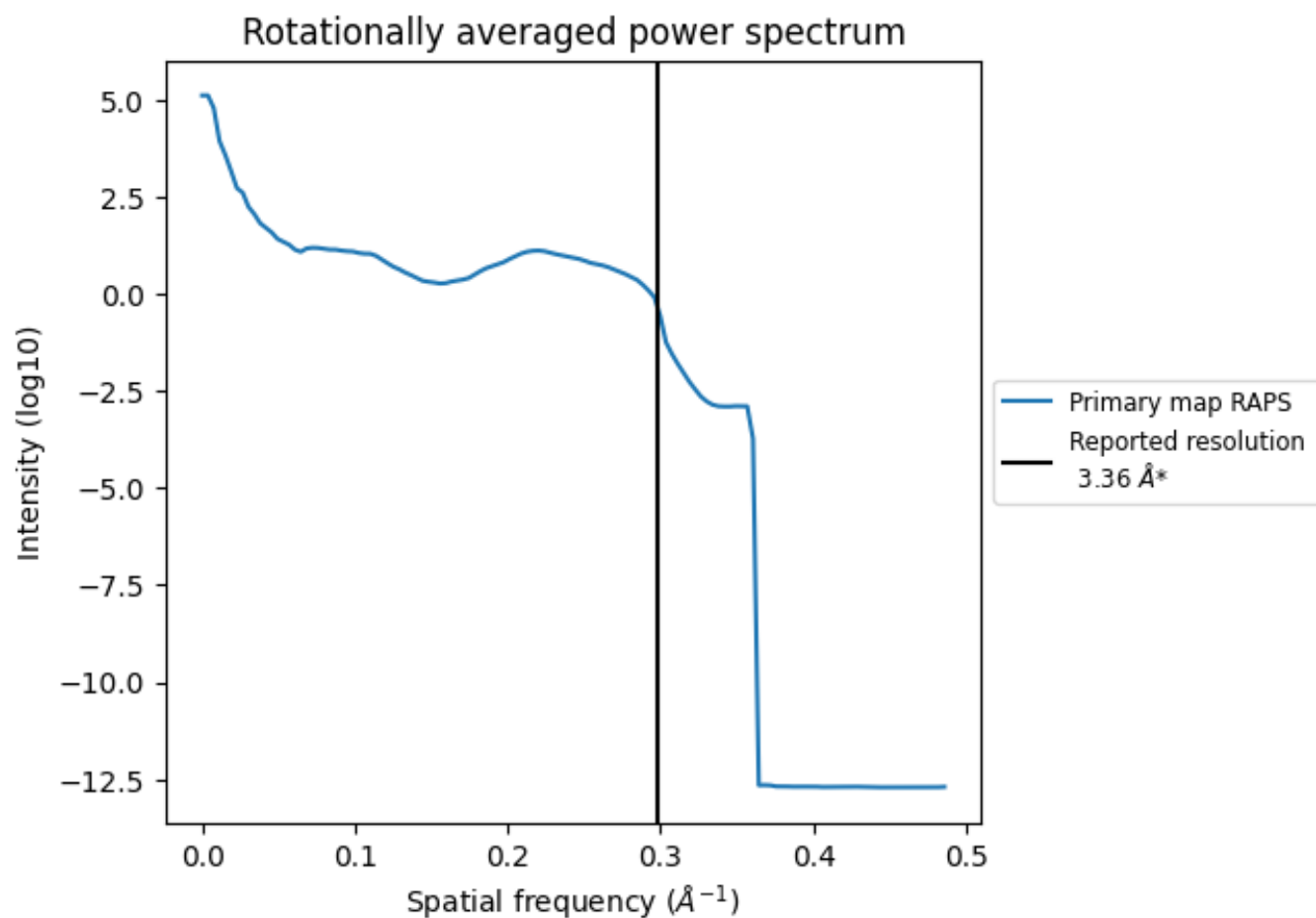
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 71 nm³; this corresponds to an approximate mass of 64 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 0.298 Å⁻¹

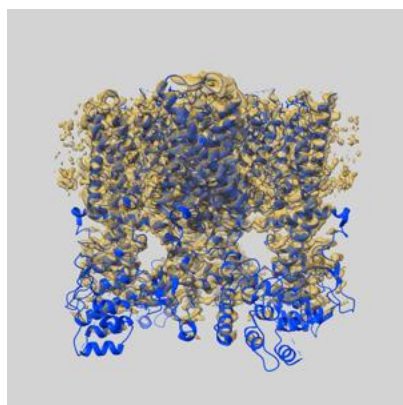
8 Fourier-Shell correlation ⓘ

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

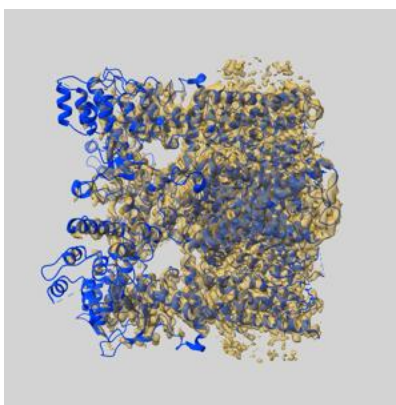
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-24639 and PDB model 7RQX. Per-residue inclusion information can be found in section [3](#) on page [10](#).

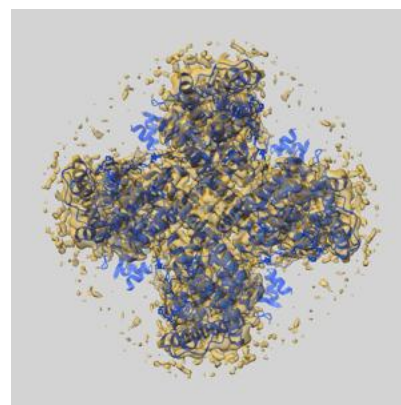
9.1 Map-model overlay [i](#)



X



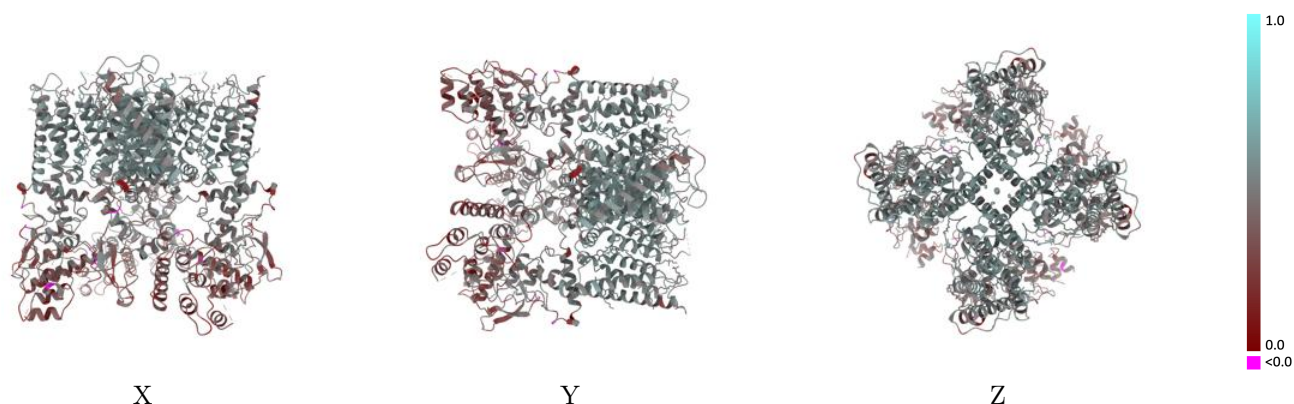
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.56 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](#)

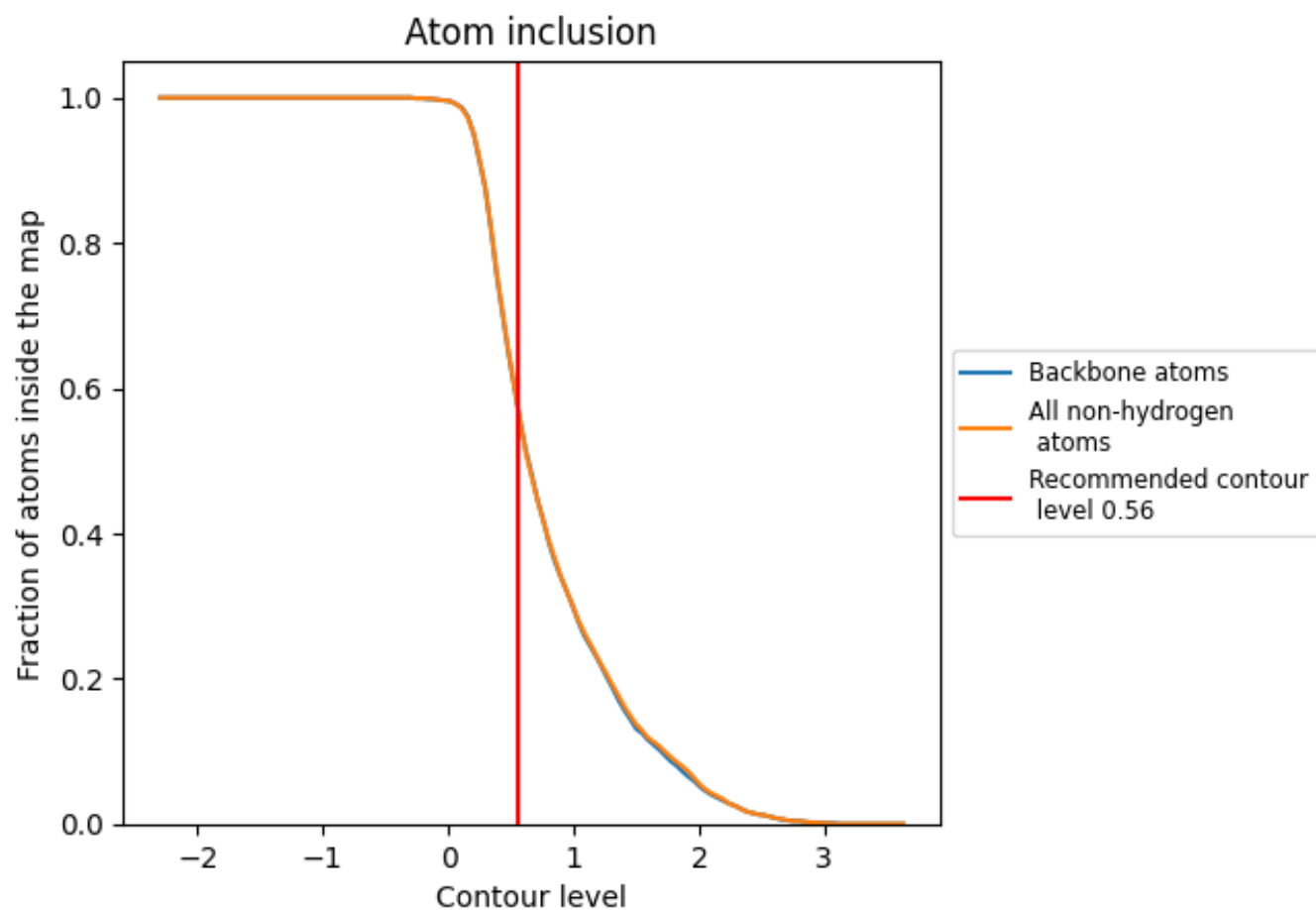


The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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

This section was not generated.

9.4 Atom inclusion [i](#)



At the recommended contour level, 57% of all backbone atoms, 57% 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 (0.56) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.5690	0.4510
A	0.5680	0.4560
B	0.5700	0.4510
C	0.5670	0.4480
D	0.5700	0.4520

