



Full wwPDB EM Validation Report ⓘ

Nov 19, 2022 – 02:04 PM EST

PDB ID : 7LP9
EMDB ID : EMD-23473
Title : Cryo-EM structure of full-length TRPV1 at 4 degrees Celsius
Authors : Kwon, D.H.; Zhang, F.; Suo, Y.; Lee, S.-Y.
Deposited on : 2021-02-11
Resolution : 2.63 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.dev43
Mogul : 1.8.5 (274361), CSD as541be (2020)
MolProbity : 4.02b-467
buster-report : 1.1.7 (2018)
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ : 1.9.9
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.31.2

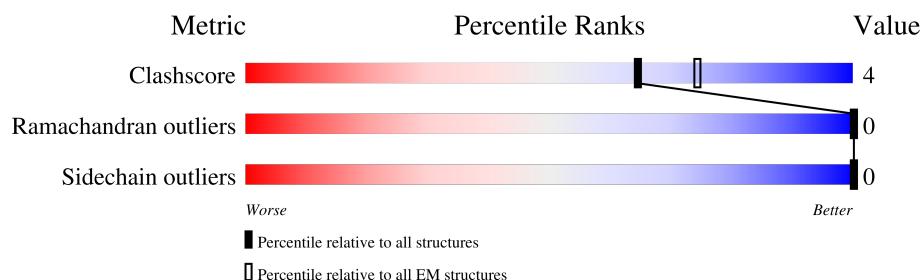
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 2.63 Å.

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



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

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

Mol	Chain	Length	Quality of chain
1	A	868	
1	B	868	
1	C	868	
1	D	868	

2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 20977 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	634	Total	C	N	O	S	0	0
			4906	3198	803	877	28		
1	B	634	Total	C	N	O	S	0	0
			4906	3198	803	877	28		
1	C	634	Total	C	N	O	S	0	0
			4906	3198	803	877	28		
1	D	634	Total	C	N	O	S	0	0
			4906	3198	803	877	28		

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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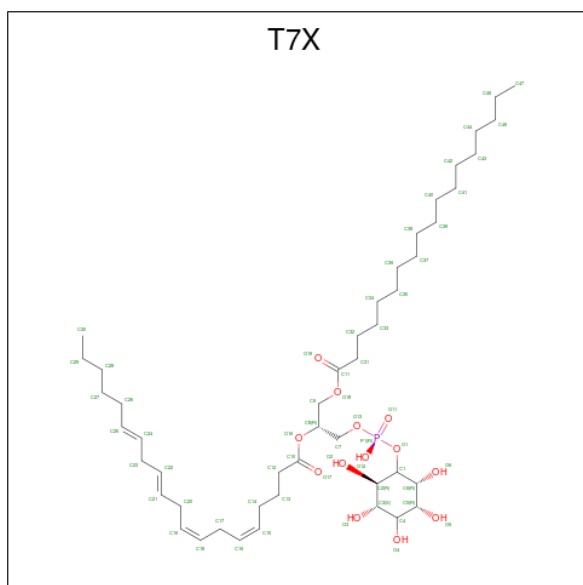
Chain	Residue	Modelled	Actual	Comment	Reference
C	842	LEU	-	expression tag	UNP O35433
C	843	GLU	-	expression tag	UNP O35433
C	844	VAL	-	expression tag	UNP O35433
C	845	LEU	-	expression tag	UNP O35433
C	846	PHE	-	expression tag	UNP O35433
C	847	GLN	-	expression tag	UNP O35433
C	848	GLY	-	expression tag	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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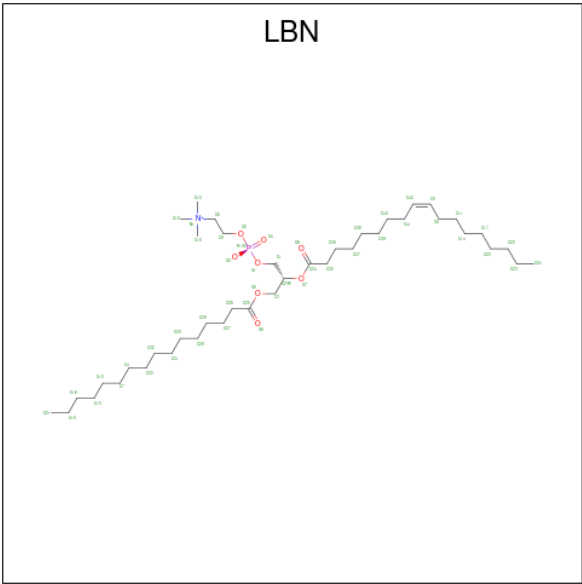
Chain	Residue	Modelled	Actual	Comment	Reference
D	854	ASP	-	expression tag	UNP O35433
D	855	ASP	-	expression tag	UNP O35433
D	856	ASP	-	expression tag	UNP O35433
D	857	LYS	-	expression tag	UNP O35433
D	858	ALA	-	expression tag	UNP O35433
D	859	HIS	-	expression tag	UNP O35433
D	860	HIS	-	expression tag	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 Phosphatidylinositol (three-letter code: T7X) (formula: $C_{47}H_{83}O_{13}P$).



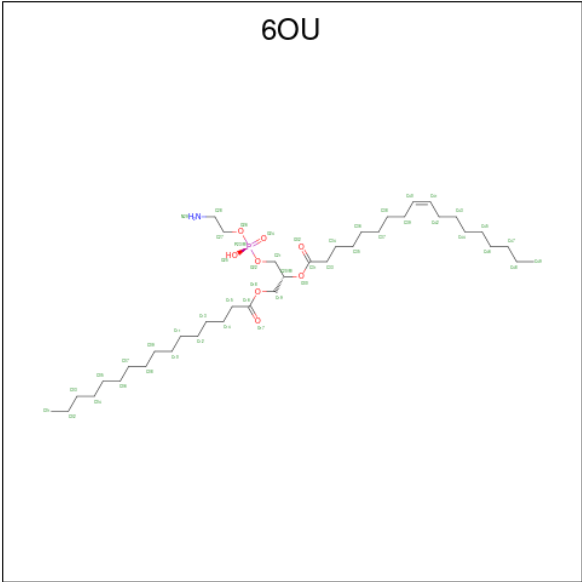
Mol	Chain	Residues	Atoms				AltConf
2	A	1	Total	C	O	P	0
			43	29	13	1	
2	B	1	Total	C	O	P	0
			43	29	13	1	
2	C	1	Total	C	O	P	0
			43	29	13	1	
2	D	1	Total	C	O	P	0
			43	29	13	1	

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



Mol	Chain	Residues	Atoms					AltConf
3	A	1	Total	C	N	O	P	0
			75	55	2	16	2	
3	A	1	Total	C	N	O	P	0
			75	55	2	16	2	
3	B	1	Total	C	N	O	P	0
			75	55	2	16	2	
3	B	1	Total	C	N	O	P	0
			75	55	2	16	2	
3	C	1	Total	C	N	O	P	0
			75	55	2	16	2	
3	C	1	Total	C	N	O	P	0
			75	55	2	16	2	
3	D	1	Total	C	N	O	P	0
			75	55	2	16	2	
3	D	1	Total	C	N	O	P	0
			75	55	2	16	2	

- Molecule 4 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
4	A	1	Total	C	N	O	P	0
			189	139	1	44	5	
4	A	1	Total	C	N	O	P	0
			189	139	1	44	5	
4	A	1	Total	C	N	O	P	0
			189	139	1	44	5	
4	A	1	Total	C	N	O	P	0
			189	139	1	44	5	
4	A	1	Total	C	N	O	P	0
			189	139	1	44	5	
4	A	1	Total	C	N	O	P	0
			189	139	1	44	5	
4	B	1	Total	C	N	O	P	0
			189	139	1	44	5	
4	B	1	Total	C	N	O	P	0
			189	139	1	44	5	
4	B	1	Total	C	N	O	P	0
			189	139	1	44	5	
4	B	1	Total	C	N	O	P	0
			189	139	1	44	5	
4	B	1	Total	C	N	O	P	0
			189	139	1	44	5	
4	B	1	Total	C	N	O	P	0
			189	139	1	44	5	

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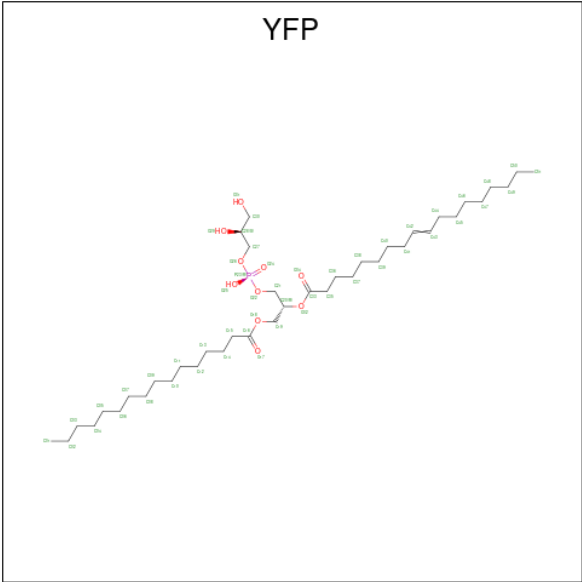
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Mol	Chain	Residues	Atoms					AltConf
4	C	1	Total	C	N	O	P	0
			189	139	1	44	5	
4	C	1	Total	C	N	O	P	0
			189	139	1	44	5	
4	C	1	Total	C	N	O	P	0
			189	139	1	44	5	
4	C	1	Total	C	N	O	P	0
			189	139	1	44	5	
4	C	1	Total	C	N	O	P	0
			189	139	1	44	5	
4	C	1	Total	C	N	O	P	0
			189	139	1	44	5	
4	D	1	Total	C	N	O	P	0
			189	139	1	44	5	
4	D	1	Total	C	N	O	P	0
			189	139	1	44	5	
4	D	1	Total	C	N	O	P	0
			189	139	1	44	5	
4	D	1	Total	C	N	O	P	0
			189	139	1	44	5	
4	D	1	Total	C	N	O	P	0
			189	139	1	44	5	
4	D	1	Total	C	N	O	P	0
			189	139	1	44	5	

- Molecule 5 is SODIUM ION (three-letter code: NA) (formula: Na).

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

- Molecule 6 is 1-palmitoyl-2-oleoyl-sn-glycero-3-phosphoglycerol (three-letter code: YFP) (formula: C₄₀H₇₇O₁₀P).

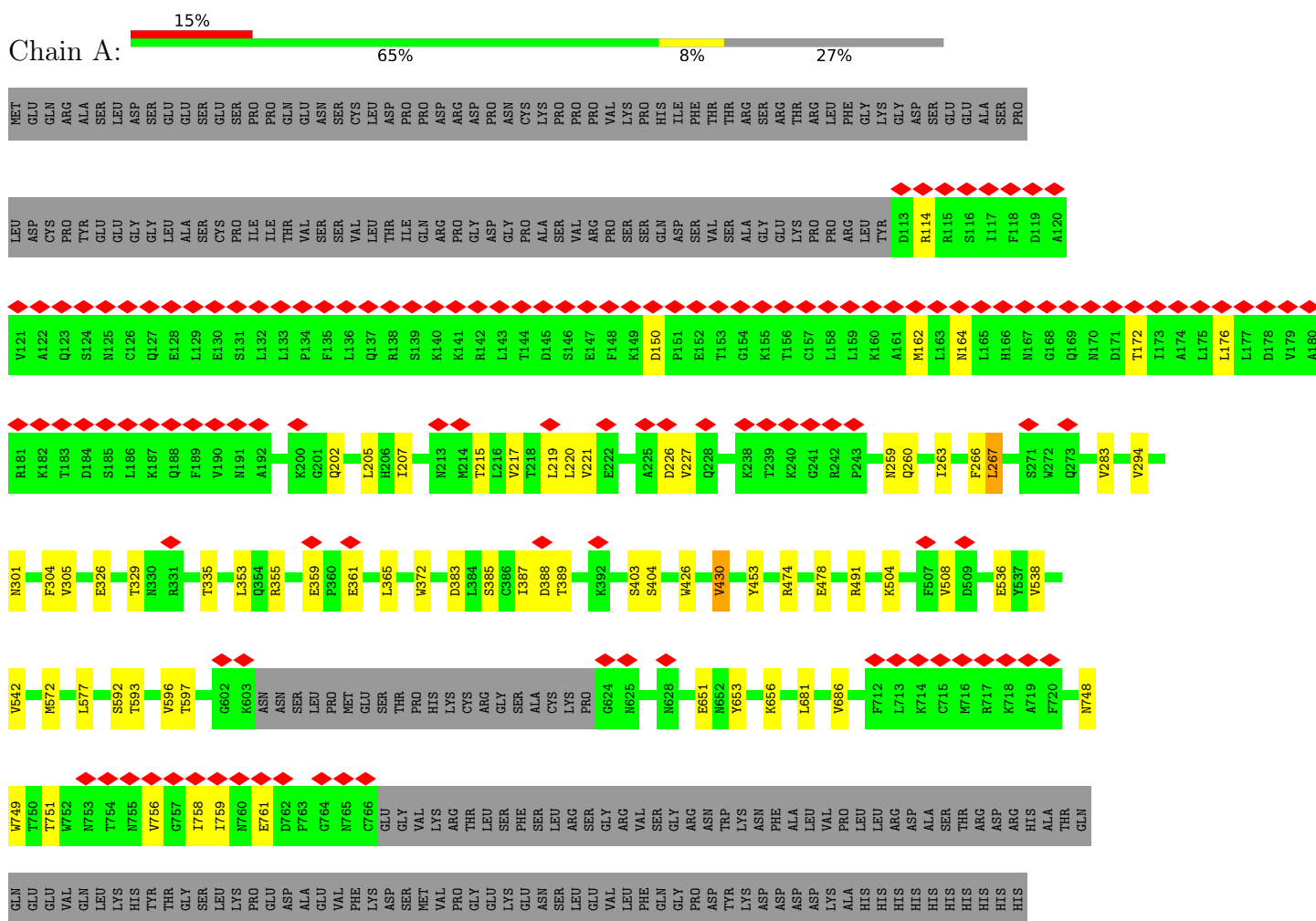


Mol	Chain	Residues	Atoms				AltConf
6	B	1	Total	C	O	P	0
			28	19	8	1	
6	C	1	Total	C	O	P	0
			62	40	20	2	
6	C	1	Total	C	O	P	0
			62	40	20	2	
6	D	1	Total	C	O	P	0
			33	22	10	1	

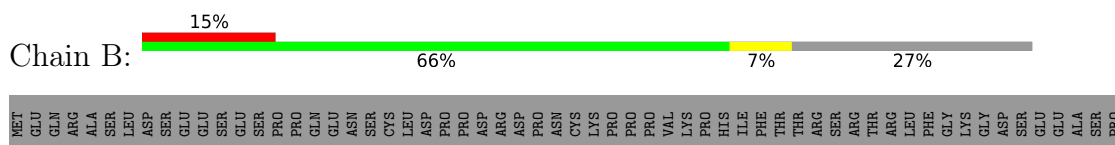
3 Residue-property plots

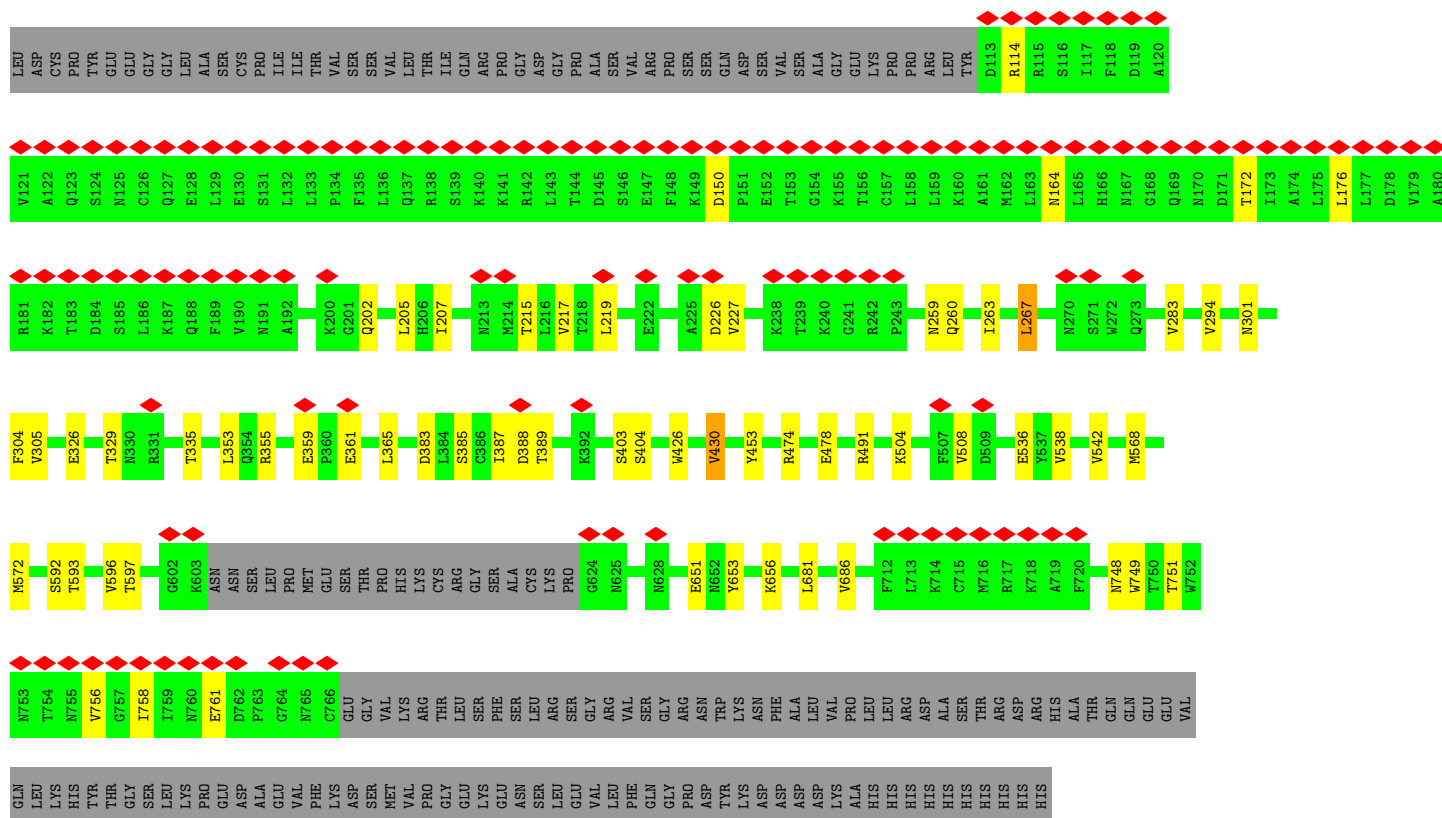
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion 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

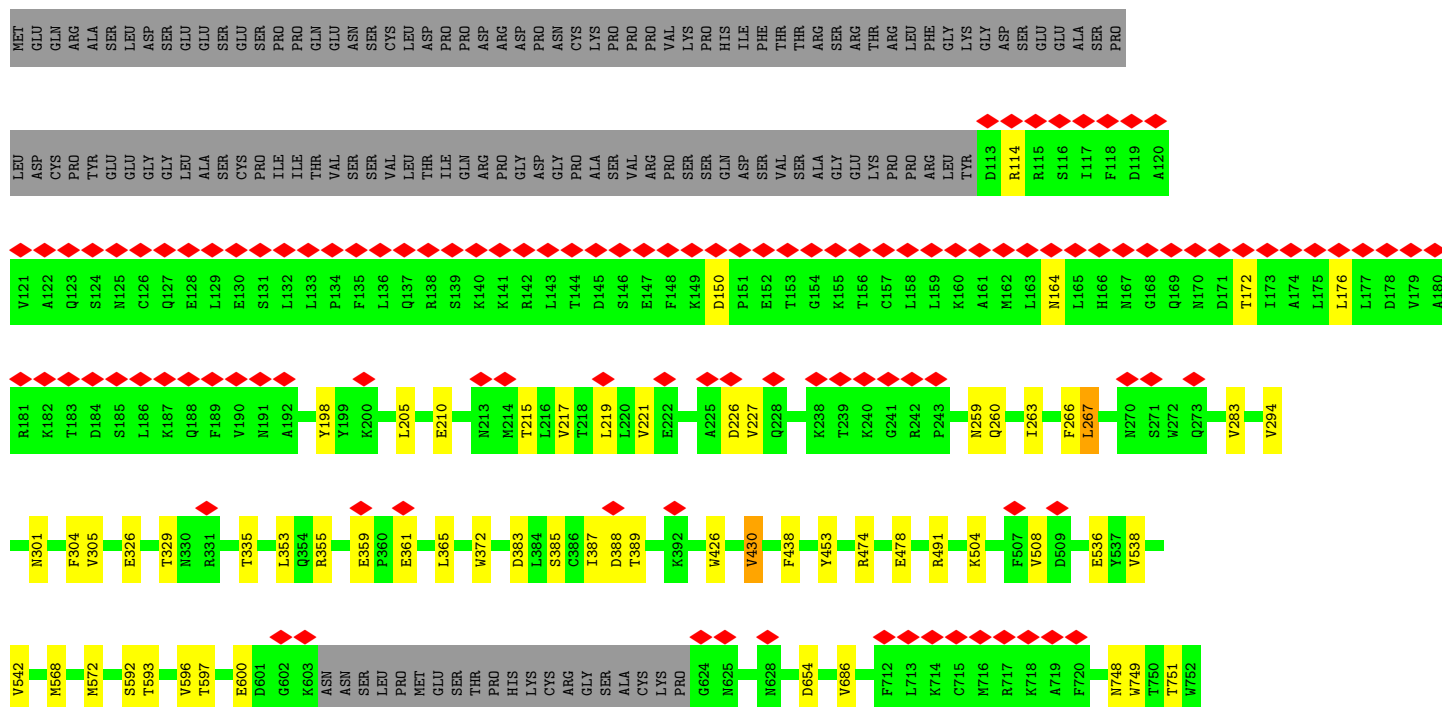


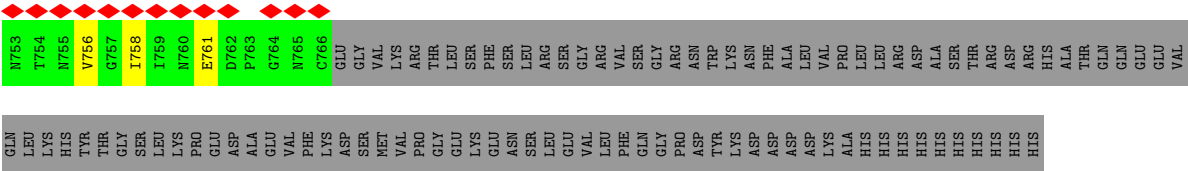
- Molecule 1: Transient receptor potential cation channel subfamily V member 1



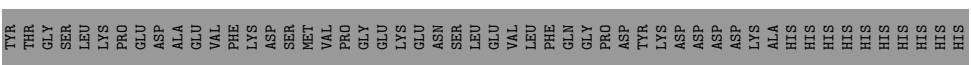
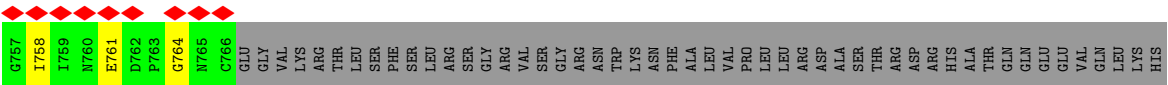
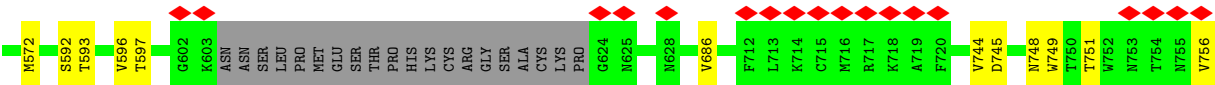
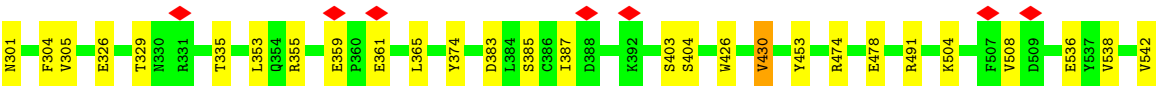
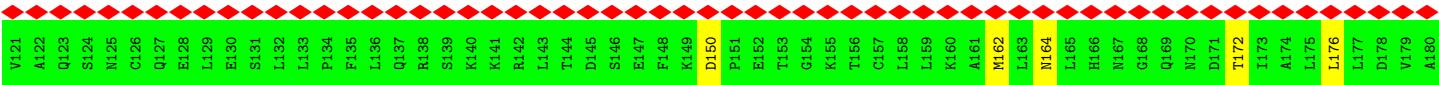
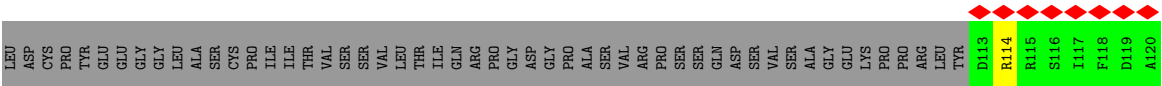
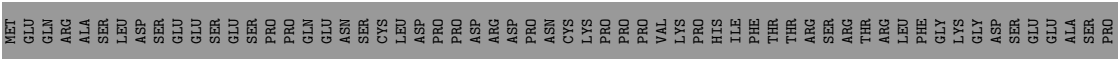


- Molecule 1: Transient receptor potential cation channel subfamily V member 1





● 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, C4	Depositor
Number of particles used	191327	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 ($e^-/\text{\AA}^2$)	60	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	0.092	Depositor
Minimum map value	-0.028	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.003	Depositor
Recommended contour level	0.02	Depositor
Map size (Å)	276.224, 276.224, 276.224	wwPDB
Map dimensions	256, 256, 256	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.079, 1.079, 1.079	Depositor

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: T7X, LBN, YFP, 6OU, NA

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	0.26	0/5019	0.43	3/6823 (0.0%)
1	B	0.26	0/5019	0.43	3/6823 (0.0%)
1	C	0.26	0/5019	0.43	3/6823 (0.0%)
1	D	0.26	0/5019	0.43	3/6823 (0.0%)
All	All	0.26	0/20076	0.43	12/27292 (0.0%)

There are no bond length outliers.

All (12) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	430	VAL	CG1-CB-CG2	7.15	122.34	110.90
1	B	430	VAL	CG1-CB-CG2	7.15	122.34	110.90
1	D	430	VAL	CG1-CB-CG2	7.14	122.32	110.90
1	A	430	VAL	CG1-CB-CG2	7.12	122.29	110.90
1	B	267	LEU	CB-CG-CD1	6.24	121.61	111.00
1	A	267	LEU	CB-CG-CD1	6.22	121.58	111.00
1	C	267	LEU	CB-CG-CD1	6.20	121.54	111.00
1	D	267	LEU	CB-CG-CD1	5.88	121.00	111.00
1	D	267	LEU	CB-CG-CD2	5.37	120.14	111.00
1	C	267	LEU	CB-CG-CD2	5.17	119.78	111.00
1	A	267	LEU	CB-CG-CD2	5.17	119.78	111.00
1	B	267	LEU	CB-CG-CD2	5.12	119.70	111.00

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts ⓘ

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	4906	0	4757	48	0
1	B	4906	0	4757	43	0
1	C	4906	0	4757	49	0
1	D	4906	0	4757	41	0
2	A	43	0	0	0	0
2	B	43	0	0	0	0
2	C	43	0	0	0	0
2	D	43	0	0	0	0
3	A	75	0	0	1	0
3	B	75	0	0	1	0
3	C	75	0	0	1	0
3	D	75	0	0	1	0
4	A	189	0	0	1	0
4	B	189	0	0	0	0
4	C	189	0	0	0	0
4	D	189	0	0	0	0
5	A	2	0	0	0	0
6	B	28	0	0	0	0
6	C	62	0	0	4	0
6	D	33	0	0	1	0
All	All	20977	0	19028	167	0

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

All (167) 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:438:PHE:CE2	6:C:903:YFP:C09	2.37	1.07
1:C:438:PHE:CZ	6:C:903:YFP:C09	2.39	1.04
1:B:355:ARG:NH1	1:B:365:LEU:O	2.10	0.85
1:C:355:ARG:NH1	1:C:365:LEU:O	2.10	0.85
1:A:355:ARG:NH1	1:A:365:LEU:O	2.10	0.83
1:D:355:ARG:NH1	1:D:365:LEU:O	2.10	0.83
1:D:748:ASN:ND2	1:D:751:THR:OG1	2.16	0.79

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:748:ASN:ND2	1:A:751:THR:OG1	2.16	0.78
1:C:748:ASN:ND2	1:C:751:THR:OG1	2.17	0.77
1:B:748:ASN:ND2	1:B:751:THR:OG1	2.16	0.77
1:D:593:THR:O	1:D:597:THR:HG23	1.87	0.75
1:C:383:ASP:OD1	1:C:385:SER:OG	2.04	0.75
1:A:593:THR:O	1:A:597:THR:HG23	1.87	0.75
1:A:383:ASP:OD1	1:A:385:SER:OG	2.04	0.75
1:D:383:ASP:OD1	1:D:385:SER:OG	2.04	0.74
1:B:593:THR:O	1:B:597:THR:HG23	1.87	0.74
1:C:593:THR:O	1:C:597:THR:HG23	1.87	0.74
1:B:383:ASP:OD1	1:B:385:SER:OG	2.04	0.72
1:D:491:ARG:NH2	3:D:905:LBN:O4	2.26	0.69
1:D:536:GLU:N	1:D:536:GLU:OE1	2.26	0.69
1:C:491:ARG:NH2	3:C:905:LBN:O4	2.26	0.69
1:A:491:ARG:NH2	3:A:902:LBN:O4	2.26	0.68
1:B:491:ARG:NH2	3:B:905:LBN:O4	2.26	0.68
1:B:536:GLU:N	1:B:536:GLU:OE1	2.26	0.68
1:A:536:GLU:N	1:A:536:GLU:OE1	2.26	0.68
1:C:536:GLU:N	1:C:536:GLU:OE1	2.26	0.68
1:D:172:THR:HG22	1:D:176:LEU:CD1	2.24	0.67
1:B:205:LEU:HD11	1:B:217:VAL:HG23	1.75	0.67
1:A:260:GLN:HG2	1:A:263:ILE:HD12	1.77	0.67
1:B:260:GLN:HG2	1:B:263:ILE:HD12	1.77	0.66
1:C:260:GLN:HG2	1:C:263:ILE:HD12	1.77	0.66
1:A:172:THR:HG22	1:A:176:LEU:CD1	2.25	0.66
1:B:172:THR:HG22	1:B:176:LEU:CD1	2.26	0.66
1:C:172:THR:HG22	1:C:176:LEU:CD1	2.26	0.65
1:A:205:LEU:HD11	1:A:217:VAL:HG23	1.78	0.64
1:D:205:LEU:HD11	1:D:217:VAL:HG23	1.79	0.64
1:D:260:GLN:HG2	1:D:263:ILE:HD12	1.80	0.63
1:B:114:ARG:NH1	1:B:150:ASP:OD1	2.32	0.62
1:C:205:LEU:HD11	1:C:217:VAL:HG23	1.80	0.62
1:C:438:PHE:HE2	6:C:903:YFP:C09	2.07	0.62
1:D:114:ARG:NH1	1:D:150:ASP:OD1	2.33	0.62
1:A:114:ARG:NH1	1:A:150:ASP:OD1	2.33	0.61
1:C:114:ARG:NH1	1:C:150:ASP:OD1	2.32	0.60
1:B:205:LEU:CD1	1:B:217:VAL:HG23	2.32	0.60
1:C:438:PHE:HZ	6:C:903:YFP:C09	2.11	0.60
1:B:681:LEU:HD21	1:C:568:MET:SD	2.43	0.58
1:A:205:LEU:CD1	1:A:217:VAL:HG23	2.34	0.57
1:A:681:LEU:HD21	1:B:568:MET:SD	2.44	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:205:LEU:CD1	1:D:217:VAL:HG23	2.34	0.57
1:D:215:THR:O	1:D:219:LEU:HD23	2.05	0.56
1:C:215:THR:O	1:C:219:LEU:HD23	2.06	0.56
1:A:215:THR:O	1:A:219:LEU:HD23	2.05	0.56
1:C:205:LEU:CD1	1:C:217:VAL:HG23	2.35	0.56
1:A:504:LYS:O	1:A:508:VAL:HG22	2.06	0.55
1:D:359:GLU:OE1	1:D:361:GLU:N	2.40	0.55
1:B:504:LYS:O	1:B:508:VAL:HG22	2.08	0.54
1:D:504:LYS:O	1:D:508:VAL:HG22	2.06	0.54
6:D:908:YFP:C19	6:D:908:YFP:C14	2.86	0.54
1:A:359:GLU:OE1	1:A:361:GLU:N	2.40	0.54
1:B:359:GLU:OE1	1:B:361:GLU:N	2.40	0.54
1:C:426:TRP:HA	1:C:430:VAL:HG22	1.90	0.54
1:C:359:GLU:OE1	1:C:361:GLU:N	2.40	0.53
1:C:504:LYS:O	1:C:508:VAL:HG22	2.08	0.53
1:B:426:TRP:HA	1:B:430:VAL:HG22	1.90	0.53
1:D:426:TRP:HA	1:D:430:VAL:HG22	1.90	0.53
1:A:426:TRP:HA	1:A:430:VAL:HG22	1.90	0.52
1:C:283:VAL:HG22	1:C:283:VAL:O	2.11	0.51
1:D:172:THR:HG22	1:D:176:LEU:HD13	1.93	0.50
1:A:388:ASP:O	1:A:389:THR:OG1	2.22	0.50
1:D:538:VAL:O	1:D:542:VAL:HG23	2.12	0.50
1:A:538:VAL:O	1:A:542:VAL:HG23	2.12	0.50
1:B:283:VAL:O	1:B:283:VAL:HG22	2.11	0.50
1:D:283:VAL:HG22	1:D:283:VAL:O	2.11	0.50
1:C:538:VAL:O	1:C:542:VAL:HG23	2.12	0.50
1:B:538:VAL:O	1:B:542:VAL:HG23	2.12	0.50
1:A:283:VAL:O	1:A:283:VAL:HG22	2.11	0.49
1:A:226:ASP:OD1	1:A:227:VAL:N	2.46	0.49
1:A:172:THR:HG22	1:A:176:LEU:HD13	1.94	0.49
4:A:908:6OU:C19	4:A:908:6OU:C14	2.91	0.49
1:B:226:ASP:OD1	1:B:227:VAL:N	2.46	0.48
1:C:226:ASP:OD1	1:C:227:VAL:N	2.46	0.48
1:D:226:ASP:OD1	1:D:227:VAL:N	2.46	0.48
1:D:259:ASN:HA	1:D:304:PHE:CZ	2.50	0.47
1:C:259:ASN:HA	1:C:304:PHE:CZ	2.50	0.47
1:B:259:ASN:HA	1:B:304:PHE:CZ	2.50	0.47
1:A:259:ASN:HA	1:A:304:PHE:CZ	2.50	0.47
1:C:572:MET:CE	1:C:686:VAL:HG23	2.44	0.47
1:B:329:THR:HG22	1:B:335:THR:HG22	1.96	0.47
1:C:326:GLU:OE1	1:C:355:ARG:NH2	2.48	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:326:GLU:OE1	1:D:355:ARG:NH2	2.48	0.47
1:B:172:THR:HG22	1:B:176:LEU:HD13	1.96	0.46
1:C:388:ASP:O	1:C:389:THR:OG1	2.24	0.46
1:D:329:THR:HG22	1:D:335:THR:HG22	1.97	0.46
1:A:329:THR:HG22	1:A:335:THR:HG22	1.96	0.46
1:C:572:MET:HE2	1:C:686:VAL:HG23	1.98	0.46
1:B:215:THR:O	1:B:219:LEU:HD13	2.16	0.45
1:C:329:THR:HG22	1:C:335:THR:HG22	1.98	0.45
1:C:172:THR:HG22	1:C:176:LEU:HD13	1.98	0.45
1:B:164:ASN:ND2	1:C:761:GLU:OE2	2.49	0.45
1:C:592:SER:O	1:C:596:VAL:HG23	2.17	0.45
1:A:326:GLU:OE1	1:A:355:ARG:NH2	2.49	0.45
1:D:592:SER:O	1:D:596:VAL:HG23	2.17	0.45
1:D:572:MET:CE	1:D:686:VAL:HG23	2.47	0.44
1:A:761:GLU:OE2	1:D:164:ASN:ND2	2.49	0.44
1:A:592:SER:O	1:A:596:VAL:HG23	2.18	0.44
1:C:596:VAL:HG11	1:D:453:TYR:HE1	1.83	0.44
1:B:326:GLU:OE1	1:B:355:ARG:NH2	2.49	0.44
1:B:592:SER:O	1:B:596:VAL:HG23	2.18	0.44
1:C:263:ILE:HG22	1:C:267:LEU:HD13	2.00	0.44
1:C:600:GLU:OE2	1:C:654:ASP:OD2	2.36	0.44
1:A:453:TYR:HE1	1:D:596:VAL:HG11	1.83	0.43
1:C:221:VAL:HG11	1:C:266:PHE:HE1	1.83	0.43
1:C:353:LEU:HD22	1:C:387:ILE:HD11	2.01	0.43
1:A:263:ILE:HG22	1:A:267:LEU:HD13	2.00	0.43
1:A:353:LEU:HD22	1:A:387:ILE:HD11	2.01	0.43
1:A:756:VAL:HG23	1:A:758:ILE:HD11	2.01	0.43
1:B:596:VAL:HG11	1:C:453:TYR:HE1	1.83	0.43
1:B:263:ILE:HG22	1:B:267:LEU:HD13	2.00	0.43
1:D:756:VAL:HG23	1:D:758:ILE:HD11	2.01	0.43
1:B:353:LEU:HD22	1:B:387:ILE:HD11	2.01	0.43
1:C:217:VAL:O	1:C:221:VAL:HG12	2.19	0.43
1:C:294:VAL:HG13	1:D:749:TRP:CH2	2.54	0.43
1:D:353:LEU:HD22	1:D:387:ILE:HD11	2.01	0.43
1:A:164:ASN:ND2	1:B:761:GLU:OE2	2.50	0.43
1:A:474:ARG:NH2	1:A:478:GLU:OE2	2.52	0.43
1:B:294:VAL:HG13	1:C:749:TRP:CH2	2.54	0.43
1:C:164:ASN:ND2	1:D:761:GLU:OE2	2.51	0.42
1:C:756:VAL:HG23	1:C:758:ILE:HD11	2.01	0.42
1:D:263:ILE:HG22	1:D:267:LEU:HD13	2.00	0.42
1:D:474:ARG:NH2	1:D:478:GLU:OE2	2.52	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:474:ARG:NH2	1:C:478:GLU:OE2	2.52	0.42
1:A:572:MET:CE	1:A:686:VAL:HG23	2.49	0.42
1:B:756:VAL:HG23	1:B:758:ILE:HD11	2.01	0.42
1:C:198:TYR:HE2	1:D:764:GLY:HA3	1.84	0.42
1:A:653:TYR:CE1	1:A:656:LYS:HA	2.54	0.42
1:A:749:TRP:CH2	1:D:294:VAL:HG13	2.54	0.42
1:B:572:MET:CE	1:B:686:VAL:HG23	2.50	0.42
1:D:162:MET:CE	1:D:220:LEU:HD11	2.50	0.42
1:A:294:VAL:HG13	1:B:749:TRP:CH2	2.54	0.42
1:B:172:THR:HG22	1:B:176:LEU:HD11	2.02	0.42
1:B:388:ASP:O	1:B:389:THR:OG1	2.22	0.42
1:B:653:TYR:CE1	1:B:656:LYS:HA	2.54	0.42
1:A:301:ASN:O	1:A:305:VAL:HG23	2.20	0.42
1:B:474:ARG:NH2	1:B:478:GLU:OE2	2.52	0.42
1:C:210:GLU:OE2	1:D:374:TYR:O	2.38	0.42
1:A:651:GLU:HA	1:A:653:TYR:CE2	2.55	0.42
1:A:596:VAL:HG11	1:B:453:TYR:HE1	1.83	0.41
1:B:202:GLN:HE22	1:B:207:ILE:HG13	1.85	0.41
1:B:651:GLU:HA	1:B:653:TYR:CE2	2.55	0.41
1:D:202:GLN:HE22	1:D:207:ILE:HG13	1.85	0.41
1:A:572:MET:HE1	1:A:686:VAL:HG23	2.03	0.41
1:A:577:LEU:HD23	1:A:577:LEU:HA	1.97	0.41
1:B:301:ASN:O	1:B:305:VAL:HG23	2.21	0.41
1:A:162:MET:CE	1:A:220:LEU:HD11	2.50	0.41
1:A:221:VAL:HG11	1:A:266:PHE:CE1	2.56	0.41
1:A:202:GLN:HE22	1:A:207:ILE:HG13	1.85	0.41
1:C:372:TRP:HA	1:C:758:ILE:HG23	2.03	0.41
1:C:221:VAL:HG11	1:C:266:PHE:CE1	2.54	0.41
1:C:301:ASN:O	1:C:305:VAL:HG23	2.21	0.41
1:A:221:VAL:HG11	1:A:266:PHE:HE1	1.86	0.40
1:A:403:SER:O	1:A:404:SER:HB3	2.22	0.40
1:A:758:ILE:HG22	1:A:759:ILE:N	2.36	0.40
1:B:403:SER:O	1:B:404:SER:HB3	2.22	0.40
1:A:372:TRP:HA	1:A:758:ILE:HG23	2.03	0.40
1:D:301:ASN:O	1:D:305:VAL:HG23	2.20	0.40
1:D:403:SER:O	1:D:404:SER:HB3	2.22	0.40
1:D:744:VAL:HG12	1:D:745:ASP:N	2.36	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	630/868 (73%)	612 (97%)	18 (3%)	0	100	100
1	B	630/868 (73%)	612 (97%)	18 (3%)	0	100	100
1	C	630/868 (73%)	613 (97%)	17 (3%)	0	100	100
1	D	630/868 (73%)	614 (98%)	16 (2%)	0	100	100
All	All	2520/3472 (73%)	2451 (97%)	69 (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	503/770 (65%)	503 (100%)	0	100	100
1	B	503/770 (65%)	503 (100%)	0	100	100
1	C	503/770 (65%)	503 (100%)	0	100	100
1	D	503/770 (65%)	503 (100%)	0	100	100
All	All	2012/3080 (65%)	2012 (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. All (12) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	202	GLN
1	A	700	GLN
1	A	748	ASN
1	B	202	GLN
1	B	700	GLN
1	B	748	ASN
1	C	202	GLN
1	C	700	GLN
1	C	748	ASN
1	D	202	GLN
1	D	700	GLN
1	D	748	ASN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no monosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 46 ligands modelled in this entry, 2 are monoatomic - leaving 44 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	$\# Z > 2$
4	6OU	A	909	-	32,32,48	1.49	3 (9%)	34,37,53	0.82	2 (5%)
4	6OU	D	907	-	34,34,48	1.67	4 (11%)	37,39,53	0.92	2 (5%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
3	LBN	D	903	-	41,41,51	1.31	4 (9%)	47,49,59	0.89	2 (4%)
4	6OU	B	906	-	29,29,48	1.62	4 (13%)	32,34,53	0.84	2 (6%)
4	6OU	D	911	-	9,9,48	0.73	0	8,8,53	0.38	0
3	LBN	C	902	-	41,41,51	1.31	4 (9%)	47,49,59	0.89	2 (4%)
4	6OU	B	909	-	24,24,48	1.24	1 (4%)	25,26,53	0.85	1 (4%)
4	6OU	C	901	-	32,32,48	1.49	3 (9%)	34,37,53	0.83	2 (5%)
4	6OU	B	908	-	24,24,48	1.92	4 (16%)	28,29,53	0.98	2 (7%)
4	6OU	A	907	-	9,9,48	0.73	0	8,8,53	0.38	0
3	LBN	D	905	-	32,32,51	1.38	3 (9%)	38,40,59	0.95	2 (5%)
4	6OU	C	907	-	34,34,48	1.67	4 (11%)	37,39,53	0.92	2 (5%)
6	YFP	B	903	-	27,27,50	1.59	5 (18%)	30,32,56	1.45	4 (13%)
6	YFP	C	903	-	31,31,50	1.54	6 (19%)	34,37,56	1.38	4 (11%)
4	6OU	B	910	-	9,9,48	0.73	0	8,8,53	0.38	0
3	LBN	A	910	-	41,41,51	1.31	4 (9%)	47,49,59	0.89	2 (4%)
4	6OU	B	911	-	30,30,48	1.75	4 (13%)	34,35,53	0.92	2 (5%)
4	6OU	D	902	-	32,32,48	1.49	3 (9%)	34,37,53	0.82	2 (5%)
4	6OU	D	909	-	24,24,48	1.92	4 (16%)	28,29,53	0.97	2 (7%)
3	LBN	A	902	-	32,32,51	1.38	3 (9%)	38,40,59	0.95	2 (5%)
4	6OU	A	904	-	34,34,48	1.67	4 (11%)	37,39,53	0.92	2 (5%)
6	YFP	C	908	-	29,29,50	1.57	6 (20%)	32,35,56	1.43	4 (12%)
4	6OU	C	906	-	29,29,48	1.62	4 (13%)	32,34,53	0.84	2 (6%)
6	YFP	D	908	-	32,32,50	1.53	6 (18%)	35,38,56	1.37	4 (11%)
2	T7X	B	904	-	43,43,61	0.99	4 (9%)	53,55,73	1.20	6 (11%)
3	LBN	C	905	-	32,32,51	1.38	3 (9%)	38,40,59	0.94	1 (2%)
4	6OU	D	906	-	29,29,48	1.62	4 (13%)	32,34,53	0.84	2 (6%)
3	LBN	B	902	-	41,41,51	1.31	4 (9%)	47,49,59	0.89	2 (4%)
4	6OU	C	909	-	24,24,48	1.93	4 (16%)	28,29,53	0.98	2 (7%)
4	6OU	B	907	-	34,34,48	1.67	4 (11%)	37,39,53	0.92	2 (5%)
2	T7X	C	904	-	43,43,61	0.99	4 (9%)	53,55,73	1.20	6 (11%)
4	6OU	B	901	-	32,32,48	1.50	3 (9%)	34,37,53	0.83	2 (5%)
4	6OU	A	906	-	24,24,48	1.24	1 (4%)	25,26,53	0.85	1 (4%)
4	6OU	C	910	-	24,24,48	1.24	1 (4%)	25,26,53	0.86	1 (4%)
4	6OU	A	905	-	24,24,48	1.92	4 (16%)	28,29,53	0.98	2 (7%)
4	6OU	C	911	-	9,9,48	0.73	0	8,8,53	0.38	0
2	T7X	D	904	-	43,43,61	1.00	4 (9%)	53,55,73	1.19	6 (11%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
4	6OU	A	903	-	29,29,48	1.62	4 (13%)	32,34,53	0.84	2 (6%)
4	6OU	D	910	-	24,24,48	1.24	1 (4%)	25,26,53	0.85	1 (4%)
2	T7X	A	901	-	43,43,61	0.99	4 (9%)	53,55,73	1.20	6 (11%)
3	LBN	B	905	-	32,32,51	1.38	3 (9%)	38,40,59	0.95	1 (2%)
4	6OU	A	908	-	30,30,48	1.75	4 (13%)	34,35,53	0.92	2 (5%)
4	6OU	D	901	-	30,30,48	1.75	4 (13%)	34,35,53	0.92	2 (5%)
4	6OU	C	912	-	30,30,48	1.75	4 (13%)	34,35,53	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
4	6OU	A	909	-	-	19/36/36/52	-
4	6OU	D	907	-	-	16/36/36/52	-
3	LBN	D	903	-	-	24/45/45/55	-
4	6OU	B	906	-	-	18/33/33/52	-
4	6OU	D	911	-	-	5/7/7/52	-
3	LBN	C	902	-	-	24/45/45/55	-
4	6OU	B	909	-	-	12/25/25/52	-
4	6OU	C	901	-	-	18/36/36/52	-
4	6OU	B	908	-	-	11/26/26/52	-
4	6OU	A	907	-	-	5/7/7/52	-
3	LBN	D	905	-	-	13/36/36/55	-
4	6OU	C	907	-	-	16/36/36/52	-
6	YFP	B	903	-	-	18/31/31/55	-
6	YFP	C	903	-	-	22/36/36/55	-
4	6OU	B	910	-	-	5/7/7/52	-
3	LBN	A	910	-	-	24/45/45/55	-
4	6OU	B	911	-	-	18/32/32/52	-
4	6OU	D	902	-	-	19/36/36/52	-
4	6OU	D	909	-	-	11/26/26/52	-
3	LBN	A	902	-	-	13/36/36/55	-
4	6OU	A	904	-	-	16/36/36/52	-
6	YFP	C	908	-	-	20/34/34/55	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	6OU	C	906	-	-	18/33/33/52	-
6	YFP	D	908	-	-	21/37/37/55	-
2	T7X	B	904	-	-	17/38/62/80	0/1/1/1
3	LBN	C	905	-	-	13/36/36/55	-
4	6OU	D	906	-	-	18/33/33/52	-
3	LBN	B	902	-	-	24/45/45/55	-
4	6OU	C	909	-	-	11/26/26/52	-
4	6OU	B	907	-	-	16/36/36/52	-
2	T7X	C	904	-	-	17/38/62/80	0/1/1/1
4	6OU	B	901	-	-	19/36/36/52	-
4	6OU	A	906	-	-	12/25/25/52	-
4	6OU	C	910	-	-	12/25/25/52	-
4	6OU	A	905	-	-	11/26/26/52	-
4	6OU	C	911	-	-	5/7/7/52	-
2	T7X	D	904	-	-	17/38/62/80	0/1/1/1
4	6OU	A	903	-	-	18/33/33/52	-
4	6OU	D	910	-	-	12/25/25/52	-
2	T7X	A	901	-	-	17/38/62/80	0/1/1/1
3	LBN	B	905	-	-	13/36/36/55	-
4	6OU	A	908	-	-	20/32/32/52	-
4	6OU	D	901	-	-	20/32/32/52	-
4	6OU	C	912	-	-	15/32/32/52	-

All (147) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	904	6OU	P23-O22	5.27	1.77	1.60
4	B	911	6OU	P23-O22	5.26	1.77	1.60
4	A	905	6OU	P23-O22	5.26	1.77	1.60
4	D	907	6OU	P23-O22	5.26	1.77	1.60
4	C	909	6OU	P23-O22	5.26	1.77	1.60
4	B	908	6OU	P23-O22	5.25	1.77	1.60
4	D	909	6OU	P23-O22	5.24	1.77	1.60
4	C	907	6OU	P23-O22	5.24	1.77	1.60
4	A	908	6OU	P23-O22	5.24	1.77	1.60
4	B	907	6OU	P23-O22	5.22	1.77	1.60
4	C	912	6OU	P23-O22	5.20	1.77	1.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	D	901	6OU	P23-O22	5.20	1.76	1.60
3	C	902	LBN	P1-O2	5.00	1.79	1.59
3	A	910	LBN	P1-O2	4.99	1.79	1.59
3	D	903	LBN	P1-O2	4.99	1.79	1.59
3	B	902	LBN	P1-O2	4.99	1.79	1.59
3	D	905	LBN	P1-O2	4.92	1.79	1.59
3	A	902	LBN	P1-O2	4.90	1.79	1.59
3	B	905	LBN	P1-O2	4.90	1.79	1.59
3	C	905	LBN	P1-O2	4.89	1.79	1.59
4	A	904	6OU	P23-O26	4.81	1.73	1.54
4	C	909	6OU	P23-O26	4.81	1.73	1.54
4	C	912	6OU	P23-O26	4.80	1.73	1.54
4	B	908	6OU	P23-O26	4.80	1.73	1.54
4	D	907	6OU	P23-O26	4.80	1.73	1.54
4	A	908	6OU	P23-O26	4.80	1.73	1.54
4	C	907	6OU	P23-O26	4.80	1.73	1.54
4	D	909	6OU	P23-O26	4.79	1.73	1.54
4	D	901	6OU	P23-O26	4.79	1.73	1.54
4	A	905	6OU	P23-O26	4.79	1.73	1.54
4	B	907	6OU	P23-O26	4.79	1.73	1.54
4	B	911	6OU	P23-O26	4.77	1.73	1.54
4	A	903	6OU	P23-O22	4.43	1.77	1.59
4	B	906	6OU	P23-O22	4.42	1.77	1.59
4	C	906	6OU	P23-O22	4.41	1.77	1.59
4	D	906	6OU	P23-O22	4.41	1.77	1.59
4	B	901	6OU	P23-O22	4.35	1.76	1.59
4	D	902	6OU	P23-O22	4.33	1.76	1.59
4	C	901	6OU	P23-O22	4.32	1.76	1.59
4	A	909	6OU	P23-O22	4.32	1.76	1.59
6	B	903	YFP	C19-C20	3.62	1.61	1.50
6	C	903	YFP	C19-C20	3.59	1.61	1.50
6	C	908	YFP	C19-C20	3.59	1.61	1.50
6	D	908	YFP	C19-C20	3.55	1.61	1.50
4	B	901	6OU	P23-O26	3.49	1.73	1.59
4	D	902	6OU	P23-O26	3.47	1.73	1.59
4	A	909	6OU	P23-O26	3.47	1.73	1.59
4	C	901	6OU	P23-O26	3.46	1.73	1.59
4	D	906	6OU	P23-O26	3.45	1.73	1.59
4	B	906	6OU	P23-O26	3.45	1.73	1.59
4	A	903	6OU	P23-O26	3.44	1.73	1.59
4	C	906	6OU	P23-O26	3.43	1.73	1.59
6	B	903	YFP	P23-O26	2.93	1.71	1.59

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	D	908	YFP	P23-O26	2.93	1.71	1.59
6	C	903	YFP	P23-O26	2.92	1.71	1.59
6	C	908	YFP	P23-O26	2.91	1.71	1.59
4	C	910	6OU	C19-C20	2.77	1.57	1.50
4	A	906	6OU	C19-C20	2.76	1.57	1.50
4	B	909	6OU	C19-C20	2.76	1.57	1.50
4	D	910	6OU	C19-C20	2.73	1.57	1.50
6	B	903	YFP	P23-O22	2.66	1.70	1.59
6	D	908	YFP	P23-O22	2.64	1.70	1.59
2	D	904	T7X	O16-C8	-2.57	1.40	1.46
2	A	901	T7X	O16-C8	-2.57	1.40	1.46
6	C	903	YFP	P23-O22	2.57	1.69	1.59
6	C	908	YFP	P23-O22	2.57	1.69	1.59
2	C	904	T7X	O16-C8	-2.53	1.40	1.46
4	C	906	6OU	C21-C20	2.50	1.58	1.50
2	B	904	T7X	O16-C8	-2.50	1.40	1.46
4	B	906	6OU	C21-C20	2.48	1.58	1.50
4	D	906	6OU	C21-C20	2.48	1.58	1.50
4	D	901	6OU	C21-C20	2.48	1.58	1.50
4	B	911	6OU	C21-C20	2.47	1.58	1.50
6	D	908	YFP	C21-C20	2.47	1.58	1.50
4	A	903	6OU	C21-C20	2.46	1.58	1.50
4	C	907	6OU	C21-C20	2.44	1.58	1.50
4	A	908	6OU	C21-C20	2.43	1.58	1.50
4	D	907	6OU	C21-C20	2.41	1.58	1.50
4	A	904	6OU	C21-C20	2.41	1.58	1.50
4	B	907	6OU	C21-C20	2.41	1.58	1.50
4	C	909	6OU	C21-C20	2.40	1.58	1.50
4	D	909	6OU	C21-C20	2.40	1.58	1.50
4	C	912	6OU	C21-C20	2.39	1.58	1.50
3	C	902	LBN	C1-C2	2.39	1.58	1.50
6	B	903	YFP	C21-C20	2.39	1.58	1.50
3	B	902	LBN	C1-C2	2.39	1.58	1.50
3	D	903	LBN	C1-C2	2.37	1.58	1.50
4	A	905	6OU	C21-C20	2.37	1.58	1.50
4	B	908	6OU	C21-C20	2.36	1.57	1.50
3	A	910	LBN	C1-C2	2.36	1.57	1.50
2	B	904	T7X	O18-C11	2.34	1.40	1.33
2	C	904	T7X	O18-C11	2.34	1.40	1.33
6	C	903	YFP	C21-C20	2.33	1.57	1.50
6	C	908	YFP	C21-C20	2.33	1.57	1.50
2	A	901	T7X	O18-C11	2.31	1.40	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	904	T7X	O18-C11	2.31	1.40	1.33
4	B	908	6OU	C19-C20	2.26	1.57	1.50
3	D	903	LBN	P1-O1	2.25	1.68	1.59
3	A	910	LBN	P1-O1	2.25	1.68	1.59
4	A	905	6OU	C19-C20	2.24	1.57	1.50
2	C	904	T7X	O18-C9	-2.23	1.40	1.45
3	C	902	LBN	P1-O1	2.23	1.68	1.59
3	B	902	LBN	P1-O1	2.23	1.68	1.59
4	D	909	6OU	C19-C20	2.23	1.57	1.50
4	A	909	6OU	C21-C20	2.22	1.57	1.50
4	B	901	6OU	C21-C20	2.21	1.57	1.50
2	A	901	T7X	O18-C9	-2.21	1.40	1.45
2	B	904	T7X	O18-C9	-2.21	1.40	1.45
2	D	904	T7X	O18-C9	-2.21	1.40	1.45
4	C	909	6OU	C19-C20	2.21	1.57	1.50
3	D	905	LBN	O2-C9	-2.21	1.35	1.44
4	C	901	6OU	C21-C20	2.20	1.57	1.50
4	D	902	6OU	C21-C20	2.20	1.57	1.50
3	A	902	LBN	O2-C9	-2.20	1.35	1.44
3	B	905	LBN	O2-C9	-2.19	1.35	1.44
3	C	905	LBN	O2-C9	-2.19	1.35	1.44
6	D	908	YFP	C27-C28	2.19	1.58	1.51
2	C	904	T7X	O16-C10	2.18	1.40	1.34
2	D	904	T7X	O16-C10	2.18	1.40	1.34
6	C	908	YFP	O18-C16	2.18	1.39	1.33
2	A	901	T7X	O16-C10	2.18	1.40	1.34
6	B	903	YFP	O18-C16	2.17	1.39	1.33
2	B	904	T7X	O16-C10	2.17	1.40	1.34
6	D	908	YFP	O18-C16	2.17	1.39	1.33
4	B	907	6OU	C19-C20	2.16	1.57	1.50
6	C	903	YFP	C27-C28	2.15	1.58	1.51
4	C	912	6OU	C19-C20	2.15	1.57	1.50
6	C	903	YFP	O18-C16	2.15	1.39	1.33
4	D	907	6OU	C19-C20	2.15	1.57	1.50
4	C	906	6OU	C19-C20	2.14	1.57	1.50
4	A	903	6OU	C19-C20	2.14	1.57	1.50
6	C	908	YFP	C27-C28	2.14	1.58	1.51
4	A	904	6OU	C19-C20	2.12	1.57	1.50
4	B	906	6OU	C19-C20	2.12	1.57	1.50
4	D	906	6OU	C19-C20	2.11	1.57	1.50
4	D	901	6OU	C19-C20	2.10	1.57	1.50
3	D	903	LBN	O2-C9	-2.09	1.36	1.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	910	LBN	O2-C9	-2.09	1.36	1.44
3	C	902	LBN	O2-C9	-2.08	1.36	1.44
4	C	907	6OU	C19-C20	2.08	1.57	1.50
3	B	902	LBN	O2-C9	-2.08	1.36	1.44
4	B	911	6OU	C19-C20	2.05	1.57	1.50
4	A	908	6OU	C19-C20	2.05	1.57	1.50
3	B	905	LBN	P1-O1	2.01	1.67	1.59
3	A	902	LBN	P1-O1	2.01	1.67	1.59
3	D	905	LBN	P1-O1	2.01	1.67	1.59
3	C	905	LBN	P1-O1	2.01	1.67	1.59

All (98) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	D	908	YFP	O32-C33-C35	5.42	123.19	111.50
6	C	908	YFP	O32-C33-C35	5.40	123.15	111.50
6	C	903	YFP	O32-C33-C35	5.39	123.12	111.50
6	B	903	YFP	O32-C33-C35	5.36	123.06	111.50
2	C	904	T7X	O16-C10-C12	3.78	119.65	111.50
2	A	901	T7X	O16-C10-C12	3.76	119.61	111.50
2	B	904	T7X	O16-C10-C12	3.75	119.59	111.50
2	D	904	T7X	O16-C10-C12	3.74	119.56	111.50
4	D	907	6OU	O25-P23-O24	3.49	124.36	110.68
4	A	904	6OU	O25-P23-O24	3.48	124.32	110.68
4	C	907	6OU	O25-P23-O24	3.48	124.31	110.68
4	B	907	6OU	O25-P23-O24	3.48	124.30	110.68
4	C	912	6OU	O25-P23-O24	3.45	124.17	110.68
4	B	911	6OU	O25-P23-O24	3.44	124.14	110.68
4	A	905	6OU	O25-P23-O24	3.43	124.12	110.68
4	D	901	6OU	O25-P23-O24	3.43	124.12	110.68
4	C	909	6OU	O25-P23-O24	3.43	124.12	110.68
4	A	908	6OU	O25-P23-O24	3.43	124.12	110.68
4	D	909	6OU	O25-P23-O24	3.42	124.06	110.68
4	B	908	6OU	O25-P23-O24	3.41	124.05	110.68
2	C	904	T7X	C6-C1-C2	3.40	115.75	110.85
2	A	901	T7X	C6-C1-C2	3.35	115.69	110.85
3	A	902	LBN	O3-P1-O4	3.34	128.77	112.24
3	B	905	LBN	O3-P1-O4	3.34	128.76	112.24
3	D	905	LBN	O3-P1-O4	3.34	128.75	112.24
2	B	904	T7X	C6-C1-C2	3.33	115.66	110.85
2	D	904	T7X	C6-C1-C2	3.33	115.65	110.85
3	C	905	LBN	O3-P1-O4	3.33	128.69	112.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	C	903	YFP	O18-C16-C15	3.28	122.21	111.91
6	C	908	YFP	O18-C16-C15	3.28	122.21	111.91
3	A	910	LBN	O3-P1-O4	3.27	128.42	112.24
3	D	903	LBN	O3-P1-O4	3.27	128.42	112.24
3	B	902	LBN	O3-P1-O4	3.27	128.39	112.24
3	C	902	LBN	O3-P1-O4	3.27	128.39	112.24
6	B	903	YFP	O18-C16-C15	3.26	122.14	111.91
6	D	908	YFP	O18-C16-C15	3.25	122.11	111.91
6	C	903	YFP	O18-C16-O17	-2.80	116.52	123.59
6	C	908	YFP	O18-C16-O17	-2.79	116.54	123.59
6	B	903	YFP	O18-C16-O17	-2.79	116.55	123.59
6	D	908	YFP	O18-C16-O17	-2.77	116.61	123.59
6	D	908	YFP	O32-C33-O34	-2.71	117.16	123.70
6	C	908	YFP	O32-C33-O34	-2.70	117.17	123.70
6	C	903	YFP	O32-C33-O34	-2.69	117.21	123.70
6	B	903	YFP	O32-C33-O34	-2.68	117.22	123.70
2	A	901	T7X	O18-C11-C31	2.63	120.17	111.91
2	C	904	T7X	O18-C11-C31	2.62	120.13	111.91
2	B	904	T7X	O18-C11-C31	2.61	120.10	111.91
2	D	904	T7X	O18-C11-C31	2.61	120.09	111.91
4	A	908	6OU	O30-C31-C33	2.49	116.86	111.50
4	D	901	6OU	O30-C31-C33	2.48	116.85	111.50
2	D	904	T7X	C12-C13-C14	-2.47	108.82	113.23
4	B	911	6OU	O30-C31-C33	2.46	116.81	111.50
2	A	901	T7X	C12-C13-C14	-2.46	108.84	113.23
4	B	901	6OU	O25-P23-O24	2.44	124.32	112.24
2	C	904	T7X	C12-C13-C14	-2.44	108.88	113.23
4	C	901	6OU	O25-P23-O24	2.44	124.28	112.24
4	A	909	6OU	O25-P23-O24	2.43	124.27	112.24
4	D	906	6OU	O25-P23-O24	2.43	124.27	112.24
4	B	906	6OU	O25-P23-O24	2.43	124.25	112.24
4	A	903	6OU	O30-C31-C33	2.43	116.74	111.50
4	D	902	6OU	O25-P23-O24	2.43	124.25	112.24
4	C	906	6OU	O25-P23-O24	2.43	124.24	112.24
4	A	903	6OU	O25-P23-O24	2.43	124.23	112.24
4	C	906	6OU	O30-C31-C33	2.42	116.72	111.50
2	B	904	T7X	C12-C13-C14	-2.42	108.91	113.23
4	D	906	6OU	O30-C31-C33	2.42	116.71	111.50
4	B	906	6OU	O30-C31-C33	2.41	116.70	111.50
4	B	907	6OU	O30-C31-C33	2.39	116.66	111.50
4	D	907	6OU	O30-C31-C33	2.39	116.65	111.50
4	A	909	6OU	O30-C31-C33	2.39	116.65	111.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	C	907	6OU	O30-C31-C33	2.39	116.65	111.50
4	B	909	6OU	O30-C31-C33	2.39	116.65	111.50
4	C	912	6OU	O30-C31-C33	2.39	116.64	111.50
4	C	910	6OU	O30-C31-C33	2.39	116.64	111.50
4	B	901	6OU	O30-C31-C33	2.38	116.63	111.50
4	A	904	6OU	O30-C31-C33	2.38	116.62	111.50
4	C	901	6OU	O30-C31-C33	2.38	116.62	111.50
4	D	902	6OU	O30-C31-C33	2.37	116.60	111.50
4	A	906	6OU	O30-C31-C33	2.37	116.60	111.50
4	D	910	6OU	O30-C31-C33	2.36	116.60	111.50
4	B	908	6OU	O30-C31-C33	2.28	116.42	111.50
4	A	905	6OU	O30-C31-C33	2.28	116.42	111.50
4	C	909	6OU	O30-C31-C33	2.28	116.42	111.50
4	D	909	6OU	O30-C31-C33	2.25	116.34	111.50
2	C	904	T7X	C5-C6-C1	2.22	114.76	109.68
2	B	904	T7X	C5-C6-C1	2.21	114.72	109.68
2	B	904	T7X	C3-C2-C1	2.19	114.69	109.68
2	A	901	T7X	C3-C2-C1	2.19	114.68	109.68
2	A	901	T7X	C5-C6-C1	2.19	114.68	109.68
2	D	904	T7X	C5-C6-C1	2.18	114.66	109.68
2	D	904	T7X	C3-C2-C1	2.17	114.64	109.68
2	C	904	T7X	C3-C2-C1	2.16	114.62	109.68
3	C	902	LBN	O2-P1-O4	-2.09	100.89	109.07
3	B	902	LBN	O2-P1-O4	-2.09	100.89	109.07
3	A	910	LBN	O2-P1-O4	-2.08	100.93	109.07
3	D	903	LBN	O2-P1-O4	-2.08	100.94	109.07
3	A	902	LBN	O2-P1-O4	-2.00	101.23	109.07
3	D	905	LBN	O2-P1-O4	-2.00	101.24	109.07

There are no chirality outliers.

All (693) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	902	LBN	N1-C6-C9-O2
3	A	910	LBN	C1-O1-P1-O4
3	A	910	LBN	C9-O2-P1-O1
3	A	910	LBN	C9-O2-P1-O4
3	A	910	LBN	N1-C6-C9-O2
3	A	910	LBN	C35-C34-O7-C2
3	B	902	LBN	C1-O1-P1-O4
3	B	902	LBN	C9-O2-P1-O1
3	B	902	LBN	C9-O2-P1-O4

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Mol	Chain	Res	Type	Atoms
3	B	902	LBN	N1-C6-C9-O2
3	B	902	LBN	C35-C34-O7-C2
3	B	905	LBN	N1-C6-C9-O2
3	C	902	LBN	C1-O1-P1-O4
3	C	902	LBN	C9-O2-P1-O1
3	C	902	LBN	C9-O2-P1-O4
3	C	902	LBN	N1-C6-C9-O2
3	C	902	LBN	C35-C34-O7-C2
3	C	905	LBN	N1-C6-C9-O2
3	D	903	LBN	C1-O1-P1-O4
3	D	903	LBN	C9-O2-P1-O1
3	D	903	LBN	C9-O2-P1-O4
3	D	903	LBN	N1-C6-C9-O2
3	D	903	LBN	C35-C34-O7-C2
3	D	905	LBN	N1-C6-C9-O2
4	A	903	6OU	C21-O22-P23-O24
4	A	903	6OU	C27-O26-P23-O24
4	A	903	6OU	O26-C27-C28-N29
4	A	904	6OU	C21-O22-P23-O24
4	A	904	6OU	C21-O22-P23-O25
4	A	904	6OU	C21-O22-P23-O26
4	A	904	6OU	C40-C41-C42-C43
4	A	908	6OU	C21-O22-P23-O24
4	A	908	6OU	C33-C31-O30-C20
4	A	909	6OU	C21-O22-P23-O24
4	A	909	6OU	C40-C41-C42-C43
4	B	901	6OU	C21-O22-P23-O24
4	B	901	6OU	C40-C41-C42-C43
4	B	906	6OU	C21-O22-P23-O24
4	B	906	6OU	C27-O26-P23-O24
4	B	906	6OU	O26-C27-C28-N29
4	B	907	6OU	C21-O22-P23-O24
4	B	907	6OU	C21-O22-P23-O25
4	B	907	6OU	C21-O22-P23-O26
4	B	907	6OU	C40-C41-C42-C43
4	B	911	6OU	C15-C16-O18-C19
4	B	911	6OU	O17-C16-O18-C19
4	B	911	6OU	C20-C21-O22-P23
4	B	911	6OU	C21-O22-P23-O25
4	B	911	6OU	C33-C31-O30-C20
4	C	901	6OU	C21-O22-P23-O24
4	C	901	6OU	C40-C41-C42-C43

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Mol	Chain	Res	Type	Atoms
4	C	906	6OU	C21-O22-P23-O24
4	C	906	6OU	C27-O26-P23-O24
4	C	906	6OU	O26-C27-C28-N29
4	C	907	6OU	C21-O22-P23-O24
4	C	907	6OU	C21-O22-P23-O25
4	C	907	6OU	C21-O22-P23-O26
4	C	907	6OU	C40-C41-C42-C43
4	C	912	6OU	C21-O22-P23-O24
4	C	912	6OU	C21-O22-P23-O25
4	C	912	6OU	C21-O22-P23-O26
4	C	912	6OU	O32-C31-O30-C20
4	C	912	6OU	C33-C31-O30-C20
4	D	901	6OU	C21-O22-P23-O24
4	D	901	6OU	C21-O22-P23-O25
4	D	901	6OU	C21-O22-P23-O26
4	D	902	6OU	C21-O22-P23-O24
4	D	906	6OU	C21-O22-P23-O24
4	D	906	6OU	C27-O26-P23-O24
4	D	906	6OU	O26-C27-C28-N29
4	D	907	6OU	C21-O22-P23-O24
4	D	907	6OU	C21-O22-P23-O25
4	D	907	6OU	C21-O22-P23-O26
4	D	907	6OU	C40-C41-C42-C43
6	B	903	YFP	C35-C33-O32-C20
6	B	903	YFP	C21-O22-P23-O25
6	B	903	YFP	C27-O26-P23-O25
6	C	903	YFP	C35-C33-O32-C20
6	C	903	YFP	C27-O26-P23-O24
6	C	908	YFP	C27-O26-P23-O24
6	C	908	YFP	C27-O26-P23-O25
6	D	908	YFP	O34-C33-O32-C20
6	D	908	YFP	C21-O22-P23-O24
4	A	908	6OU	O17-C16-O18-C19
6	D	908	YFP	O17-C16-O18-C19
4	A	908	6OU	C15-C16-O18-C19
6	D	908	YFP	C15-C16-O18-C19
2	A	901	T7X	O19-C11-O18-C9
2	B	904	T7X	O19-C11-O18-C9
2	C	904	T7X	O19-C11-O18-C9
2	D	904	T7X	O19-C11-O18-C9
4	A	903	6OU	O17-C16-O18-C19
4	A	909	6OU	O17-C16-O18-C19

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Mol	Chain	Res	Type	Atoms
4	B	901	6OU	O17-C16-O18-C19
4	B	906	6OU	O17-C16-O18-C19
4	C	901	6OU	O17-C16-O18-C19
4	C	906	6OU	O17-C16-O18-C19
4	D	902	6OU	O17-C16-O18-C19
4	D	906	6OU	O17-C16-O18-C19
4	A	908	6OU	O32-C31-O30-C20
4	B	911	6OU	O32-C31-O30-C20
6	C	903	YFP	O34-C33-O32-C20
2	A	901	T7X	C31-C11-O18-C9
2	B	904	T7X	C31-C11-O18-C9
2	C	904	T7X	C31-C11-O18-C9
2	D	904	T7X	C31-C11-O18-C9
4	A	903	6OU	C15-C16-O18-C19
4	A	909	6OU	C15-C16-O18-C19
4	B	901	6OU	C15-C16-O18-C19
4	B	906	6OU	C15-C16-O18-C19
4	C	901	6OU	C15-C16-O18-C19
4	C	906	6OU	C15-C16-O18-C19
4	D	902	6OU	C15-C16-O18-C19
4	D	906	6OU	C15-C16-O18-C19
6	D	908	YFP	C35-C33-O32-C20
6	C	908	YFP	C15-C16-O18-C19
3	A	910	LBN	O8-C34-O7-C2
3	B	902	LBN	O8-C34-O7-C2
3	C	902	LBN	O8-C34-O7-C2
3	D	903	LBN	O8-C34-O7-C2
6	B	903	YFP	O34-C33-O32-C20
6	C	908	YFP	C20-C19-O18-C16
4	A	908	6OU	C33-C34-C35-C36
3	A	910	LBN	C2-C1-O1-P1
3	B	902	LBN	C2-C1-O1-P1
3	C	902	LBN	C2-C1-O1-P1
3	D	903	LBN	C2-C1-O1-P1
6	D	908	YFP	C28-C27-O26-P23
6	C	908	YFP	O17-C16-O18-C19
4	C	909	6OU	C15-C16-O18-C19
4	D	909	6OU	C15-C16-O18-C19
4	D	901	6OU	C33-C34-C35-C36
6	C	908	YFP	O26-C27-C28-C30
4	A	905	6OU	C15-C16-O18-C19
4	B	908	6OU	C15-C16-O18-C19

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Mol	Chain	Res	Type	Atoms
6	B	903	YFP	C15-C16-O18-C19
3	B	902	LBN	C25-C26-C27-C28
3	C	902	LBN	C25-C26-C27-C28
6	D	908	YFP	O26-C27-C28-O29
3	A	910	LBN	C25-C26-C27-C28
3	D	903	LBN	C25-C26-C27-C28
4	A	903	6OU	C13-C14-C15-C16
4	B	906	6OU	C13-C14-C15-C16
4	C	906	6OU	C13-C14-C15-C16
4	D	906	6OU	C13-C14-C15-C16
2	A	901	T7X	C11-C31-C32-C33
2	B	904	T7X	C11-C31-C32-C33
2	C	904	T7X	C11-C31-C32-C33
2	D	904	T7X	C11-C31-C32-C33
3	D	905	LBN	C34-C35-C36-C37
3	A	902	LBN	C34-C35-C36-C37
3	B	905	LBN	C34-C35-C36-C37
3	C	905	LBN	C34-C35-C36-C37
4	A	904	6OU	C31-C33-C34-C35
4	B	907	6OU	C31-C33-C34-C35
4	B	911	6OU	C13-C14-C15-C16
4	C	907	6OU	C31-C33-C34-C35
4	D	907	6OU	C31-C33-C34-C35
6	C	908	YFP	C13-C14-C15-C16
6	D	908	YFP	C13-C14-C15-C16
4	A	905	6OU	O17-C16-O18-C19
4	B	908	6OU	O17-C16-O18-C19
4	C	909	6OU	O17-C16-O18-C19
4	D	909	6OU	O17-C16-O18-C19
6	B	903	YFP	O17-C16-O18-C19
3	A	910	LBN	C34-C35-C36-C37
3	C	902	LBN	C34-C35-C36-C37
6	C	903	YFP	C13-C14-C15-C16
6	C	908	YFP	C35-C33-O32-C20
3	A	910	LBN	C1-O1-P1-O2
3	B	902	LBN	C1-O1-P1-O2
3	C	902	LBN	C1-O1-P1-O2
3	D	903	LBN	C1-O1-P1-O2
6	B	903	YFP	C21-O22-P23-O26
6	C	903	YFP	C21-O22-P23-O26
6	C	903	YFP	C27-O26-P23-O22
6	C	908	YFP	C27-O26-P23-O22

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Mol	Chain	Res	Type	Atoms
4	A	906	6OU	C15-C16-O18-C19
4	B	909	6OU	C15-C16-O18-C19
4	C	910	6OU	C15-C16-O18-C19
4	D	910	6OU	C15-C16-O18-C19
3	B	902	LBN	C34-C35-C36-C37
3	D	903	LBN	C34-C35-C36-C37
6	C	908	YFP	O34-C33-O32-C20
3	A	910	LBN	C14-C11-C8-C5
3	B	902	LBN	C14-C11-C8-C5
3	C	902	LBN	C14-C11-C8-C5
3	D	903	LBN	C14-C11-C8-C5
4	A	908	6OU	C12-C13-C14-C15
2	A	901	T7X	C34-C35-C36-C37
2	B	904	T7X	C34-C35-C36-C37
2	C	904	T7X	C34-C35-C36-C37
2	D	904	T7X	C34-C35-C36-C37
4	B	910	6OU	C44-C45-C46-C47
4	B	911	6OU	C10-C11-C12-C13
4	C	911	6OU	C44-C45-C46-C47
4	D	911	6OU	C44-C45-C46-C47
4	A	907	6OU	C44-C45-C46-C47
4	B	911	6OU	C21-C20-O30-C31
4	A	908	6OU	C11-C12-C13-C14
4	A	906	6OU	C34-C35-C36-C37
4	B	909	6OU	C34-C35-C36-C37
4	C	910	6OU	C34-C35-C36-C37
4	D	910	6OU	C34-C35-C36-C37
6	C	903	YFP	O26-C27-C28-O29
6	C	908	YFP	O26-C27-C28-O29
4	A	904	6OU	C36-C37-C38-C39
4	B	907	6OU	C36-C37-C38-C39
4	C	912	6OU	C33-C34-C35-C36
4	C	912	6OU	C36-C37-C38-C39
4	A	906	6OU	O17-C16-O18-C19
4	B	909	6OU	O17-C16-O18-C19
4	C	910	6OU	O17-C16-O18-C19
4	D	910	6OU	O17-C16-O18-C19
3	A	910	LBN	C28-C29-C30-C31
3	D	903	LBN	C28-C29-C30-C31
4	C	907	6OU	C36-C37-C38-C39
4	D	907	6OU	C36-C37-C38-C39
3	B	902	LBN	C28-C29-C30-C31

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Mol	Chain	Res	Type	Atoms
3	C	902	LBN	C28-C29-C30-C31
4	A	909	6OU	C33-C34-C35-C36
4	B	901	6OU	C33-C34-C35-C36
4	C	901	6OU	C33-C34-C35-C36
6	C	908	YFP	C12-C13-C14-C15
4	B	906	6OU	C12-C13-C14-C15
6	D	908	YFP	C35-C36-C37-C38
4	A	903	6OU	C12-C13-C14-C15
4	D	901	6OU	C35-C36-C37-C38
4	D	902	6OU	C33-C34-C35-C36
4	D	906	6OU	C12-C13-C14-C15
6	D	908	YFP	C36-C37-C38-C39
6	C	903	YFP	C33-C35-C36-C37
3	C	902	LBN	C26-C27-C28-C29
4	A	904	6OU	C07-C08-C09-C10
4	A	906	6OU	C12-C13-C14-C15
4	B	907	6OU	C07-C08-C09-C10
4	B	909	6OU	C12-C13-C14-C15
4	C	906	6OU	C12-C13-C14-C15
4	C	907	6OU	C07-C08-C09-C10
4	D	901	6OU	C11-C12-C13-C14
4	D	907	6OU	C07-C08-C09-C10
4	D	910	6OU	C12-C13-C14-C15
3	B	902	LBN	C26-C27-C28-C29
4	C	910	6OU	C12-C13-C14-C15
3	A	910	LBN	C26-C27-C28-C29
6	C	903	YFP	C12-C13-C14-C15
3	D	903	LBN	C26-C27-C28-C29
4	A	908	6OU	C35-C36-C37-C38
4	C	907	6OU	C35-C36-C37-C38
4	D	907	6OU	C35-C36-C37-C38
4	A	904	6OU	C35-C36-C37-C38
4	B	907	6OU	C35-C36-C37-C38
4	B	910	6OU	C45-C46-C47-C48
4	A	907	6OU	C45-C46-C47-C48
4	D	901	6OU	C36-C37-C38-C39
4	D	911	6OU	C45-C46-C47-C48
4	A	908	6OU	C37-C38-C39-C40
4	C	911	6OU	C45-C46-C47-C48
4	B	901	6OU	C36-C37-C38-C39
4	C	901	6OU	C36-C37-C38-C39
4	C	912	6OU	C09-C10-C11-C12

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Mol	Chain	Res	Type	Atoms
4	A	909	6OU	C36-C37-C38-C39
4	B	906	6OU	C09-C10-C11-C12
4	D	906	6OU	C09-C10-C11-C12
4	A	903	6OU	C09-C10-C11-C12
4	C	906	6OU	C09-C10-C11-C12
4	D	902	6OU	C36-C37-C38-C39
4	A	906	6OU	C40-C41-C42-C43
4	B	909	6OU	C40-C41-C42-C43
4	C	910	6OU	C40-C41-C42-C43
4	D	910	6OU	C40-C41-C42-C43
4	B	906	6OU	C34-C35-C36-C37
4	D	906	6OU	C34-C35-C36-C37
4	A	903	6OU	C34-C35-C36-C37
4	C	906	6OU	C34-C35-C36-C37
4	A	903	6OU	C31-C33-C34-C35
4	B	906	6OU	C31-C33-C34-C35
4	D	901	6OU	C13-C14-C15-C16
4	D	906	6OU	C31-C33-C34-C35
4	C	906	6OU	C31-C33-C34-C35
4	B	911	6OU	C11-C12-C13-C14
4	A	906	6OU	C33-C31-O30-C20
4	A	909	6OU	C33-C31-O30-C20
4	B	901	6OU	C33-C31-O30-C20
4	B	909	6OU	C33-C31-O30-C20
4	C	901	6OU	C33-C31-O30-C20
4	D	910	6OU	C33-C31-O30-C20
2	A	901	T7X	O13-C7-C8-O16
2	B	904	T7X	O13-C7-C8-O16
2	C	904	T7X	O13-C7-C8-O16
2	D	904	T7X	O13-C7-C8-O16
6	C	903	YFP	C35-C36-C37-C38
4	D	901	6OU	C37-C38-C39-C40
4	A	904	6OU	C12-C13-C14-C15
4	B	907	6OU	C12-C13-C14-C15
4	C	907	6OU	C12-C13-C14-C15
4	D	907	6OU	C12-C13-C14-C15
4	C	910	6OU	C36-C37-C38-C39
4	D	910	6OU	C36-C37-C38-C39
4	C	910	6OU	C33-C31-O30-C20
4	A	906	6OU	C36-C37-C38-C39
4	B	909	6OU	C36-C37-C38-C39
4	D	901	6OU	C34-C35-C36-C37

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Mol	Chain	Res	Type	Atoms
4	A	903	6OU	C27-O26-P23-O22
4	B	906	6OU	C27-O26-P23-O22
4	C	906	6OU	C27-O26-P23-O22
4	D	906	6OU	C27-O26-P23-O22
6	B	903	YFP	C27-O26-P23-O22
6	D	908	YFP	C21-O22-P23-O26
6	D	908	YFP	C27-O26-P23-O22
4	A	906	6OU	C35-C36-C37-C38
4	B	909	6OU	C35-C36-C37-C38
4	C	910	6OU	C35-C36-C37-C38
4	D	910	6OU	C35-C36-C37-C38
4	A	905	6OU	C13-C14-C15-C16
4	D	909	6OU	C13-C14-C15-C16
4	A	903	6OU	C19-C20-C21-O22
4	B	906	6OU	C19-C20-C21-O22
4	D	902	6OU	C19-C20-C21-O22
4	D	906	6OU	C19-C20-C21-O22
6	C	908	YFP	C19-C20-C21-O22
4	B	908	6OU	C13-C14-C15-C16
4	C	909	6OU	C13-C14-C15-C16
4	C	912	6OU	C11-C12-C13-C14
4	D	901	6OU	C12-C13-C14-C15
4	A	909	6OU	C12-C13-C14-C15
4	C	901	6OU	C12-C13-C14-C15
4	D	902	6OU	C12-C13-C14-C15
4	B	901	6OU	C12-C13-C14-C15
4	D	902	6OU	C33-C31-O30-C20
3	B	902	LBN	C1-C2-C3-O5
3	C	902	LBN	C1-C2-C3-O5
6	C	903	YFP	O18-C19-C20-C21
6	D	908	YFP	O18-C19-C20-C21
3	D	905	LBN	C28-C29-C30-C31
6	C	903	YFP	C09-C10-C11-C12
2	A	901	T7X	C40-C41-C42-C43
2	B	904	T7X	C40-C41-C42-C43
2	C	904	T7X	C40-C41-C42-C43
2	D	904	T7X	C40-C41-C42-C43
3	A	902	LBN	C28-C29-C30-C31
4	A	908	6OU	C10-C11-C12-C13
4	A	904	6OU	C37-C38-C39-C40
4	B	907	6OU	C37-C38-C39-C40
4	C	907	6OU	C37-C38-C39-C40

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Mol	Chain	Res	Type	Atoms
4	D	907	6OU	C37-C38-C39-C40
3	C	905	LBN	C28-C29-C30-C31
3	B	905	LBN	C28-C29-C30-C31
4	A	908	6OU	C08-C09-C10-C11
4	D	901	6OU	C21-C20-O30-C31
6	B	903	YFP	C20-C21-O22-P23
6	C	903	YFP	C36-C37-C38-C39
4	A	909	6OU	O32-C31-O30-C20
4	B	901	6OU	O32-C31-O30-C20
4	B	909	6OU	O32-C31-O30-C20
4	C	901	6OU	O32-C31-O30-C20
6	D	908	YFP	C10-C11-C12-C13
4	A	906	6OU	O32-C31-O30-C20
4	B	907	6OU	C11-C12-C13-C14
2	A	901	T7X	O13-C7-C8-C9
2	B	904	T7X	O13-C7-C8-C9
2	C	904	T7X	O13-C7-C8-C9
2	D	904	T7X	O13-C7-C8-C9
3	A	910	LBN	O1-C1-C2-C3
3	B	902	LBN	O1-C1-C2-C3
3	C	902	LBN	O1-C1-C2-C3
3	D	903	LBN	O1-C1-C2-C3
4	A	905	6OU	C19-C20-C21-O22
4	B	908	6OU	C19-C20-C21-O22
4	C	906	6OU	C19-C20-C21-O22
4	C	909	6OU	C19-C20-C21-O22
4	D	909	6OU	C19-C20-C21-O22
4	A	904	6OU	C11-C12-C13-C14
4	C	907	6OU	C11-C12-C13-C14
4	D	907	6OU	C11-C12-C13-C14
4	D	910	6OU	O32-C31-O30-C20
4	A	908	6OU	C36-C37-C38-C39
4	B	910	6OU	C42-C43-C44-C45
6	D	908	YFP	C37-C38-C39-C40
4	D	901	6OU	C15-C16-O18-C19
4	C	912	6OU	C34-C35-C36-C37
4	D	911	6OU	C42-C43-C44-C45
4	D	901	6OU	C20-C21-O22-P23
6	C	903	YFP	C28-C27-O26-P23
6	C	908	YFP	C28-C27-O26-P23
4	A	907	6OU	C42-C43-C44-C45
4	C	911	6OU	C42-C43-C44-C45

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Mol	Chain	Res	Type	Atoms
4	A	908	6OU	C34-C35-C36-C37
3	A	910	LBN	C1-C2-C3-O5
3	D	903	LBN	C1-C2-C3-O5
3	A	910	LBN	O1-C1-C2-O7
3	B	902	LBN	O1-C1-C2-O7
3	C	902	LBN	O1-C1-C2-O7
4	A	908	6OU	O30-C20-C21-O22
4	D	902	6OU	O30-C20-C21-O22
6	C	908	YFP	O32-C20-C21-O22
4	C	910	6OU	O32-C31-O30-C20
4	A	908	6OU	O18-C19-C20-O30
4	C	912	6OU	O18-C19-C20-O30
6	B	903	YFP	O18-C19-C20-O32
6	C	903	YFP	O18-C19-C20-O32
4	D	907	6OU	C09-C10-C11-C12
4	D	901	6OU	C33-C31-O30-C20
4	A	904	6OU	C09-C10-C11-C12
4	C	910	6OU	C33-C34-C35-C36
6	C	903	YFP	O26-C27-C28-C30
6	D	908	YFP	O26-C27-C28-C30
4	D	902	6OU	O32-C31-O30-C20
3	D	903	LBN	C30-C31-C32-C33
4	D	910	6OU	C33-C34-C35-C36
4	A	906	6OU	C33-C34-C35-C36
4	C	907	6OU	C09-C10-C11-C12
4	B	907	6OU	C09-C10-C11-C12
4	B	909	6OU	C33-C34-C35-C36
4	A	909	6OU	C20-C21-O22-P23
4	B	901	6OU	C20-C21-O22-P23
4	C	901	6OU	C20-C21-O22-P23
4	C	906	6OU	C20-C21-O22-P23
4	D	902	6OU	C20-C21-O22-P23
6	C	903	YFP	C20-C21-O22-P23
4	A	905	6OU	C33-C31-O30-C20
4	D	902	6OU	C40-C41-C42-C43
3	A	910	LBN	C30-C31-C32-C33
4	A	908	6OU	C19-C20-C21-O22
4	A	909	6OU	C19-C20-C21-O22
4	B	901	6OU	C19-C20-C21-O22
4	C	901	6OU	C19-C20-C21-O22
6	D	908	YFP	C14-C15-C16-O18
4	B	908	6OU	C33-C31-O30-C20

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Mol	Chain	Res	Type	Atoms
4	C	909	6OU	C33-C31-O30-C20
4	D	909	6OU	C33-C31-O30-C20
3	C	902	LBN	C30-C31-C32-C33
3	B	902	LBN	C30-C31-C32-C33
4	D	901	6OU	O32-C31-O30-C20
4	A	903	6OU	C20-C21-O22-P23
4	B	906	6OU	C20-C21-O22-P23
4	D	906	6OU	C20-C21-O22-P23
6	C	903	YFP	C20-C19-O18-C16
3	D	903	LBN	O1-C1-C2-O7
4	A	905	6OU	O30-C20-C21-O22
4	A	909	6OU	O30-C20-C21-O22
4	B	901	6OU	O30-C20-C21-O22
4	B	908	6OU	O30-C20-C21-O22
4	C	901	6OU	O30-C20-C21-O22
4	C	909	6OU	O30-C20-C21-O22
4	D	909	6OU	O30-C20-C21-O22
6	B	903	YFP	O32-C20-C21-O22
4	D	901	6OU	C38-C39-C40-C41
4	A	905	6OU	O32-C31-O30-C20
4	D	909	6OU	O32-C31-O30-C20
3	A	910	LBN	O7-C2-C3-O5
3	B	902	LBN	O7-C2-C3-O5
3	C	902	LBN	O7-C2-C3-O5
3	D	903	LBN	O7-C2-C3-O5
6	C	908	YFP	O18-C19-C20-O32
4	C	909	6OU	C10-C11-C12-C13
4	B	908	6OU	C10-C11-C12-C13
4	D	909	6OU	C10-C11-C12-C13
4	D	901	6OU	O17-C16-O18-C19
4	A	905	6OU	C10-C11-C12-C13
6	B	903	YFP	C10-C11-C12-C13
4	B	908	6OU	O32-C31-O30-C20
4	C	909	6OU	O32-C31-O30-C20
3	B	905	LBN	C29-C30-C31-C32
2	B	904	T7X	C10-C12-C13-C14
2	C	904	T7X	C10-C12-C13-C14
2	D	904	T7X	C12-C13-C14-C15
2	A	901	T7X	C7-O13-P1-O1
2	B	904	T7X	C7-O13-P1-O1
2	C	904	T7X	C7-O13-P1-O1
2	D	904	T7X	C7-O13-P1-O1

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Mol	Chain	Res	Type	Atoms
4	D	902	6OU	C21-O22-P23-O26
3	C	905	LBN	C29-C30-C31-C32
2	A	901	T7X	C10-C12-C13-C14
3	A	902	LBN	C29-C30-C31-C32
3	D	905	LBN	C29-C30-C31-C32
4	A	904	6OU	C20-C21-O22-P23
4	B	907	6OU	C20-C21-O22-P23
4	C	907	6OU	C20-C21-O22-P23
4	D	907	6OU	C20-C21-O22-P23
3	A	910	LBN	C1-O1-P1-O3
3	B	902	LBN	C1-O1-P1-O3
3	C	902	LBN	C1-O1-P1-O3
3	D	903	LBN	C1-O1-P1-O3
4	A	903	6OU	C27-O26-P23-O25
4	B	906	6OU	C27-O26-P23-O25
4	C	906	6OU	C27-O26-P23-O25
4	D	906	6OU	C27-O26-P23-O25
6	B	903	YFP	C27-O26-P23-O24
6	C	903	YFP	C21-O22-P23-O25
6	C	903	YFP	C27-O26-P23-O25
2	D	904	T7X	C10-C12-C13-C14
2	A	901	T7X	C12-C13-C14-C15
2	B	904	T7X	C12-C13-C14-C15
2	C	904	T7X	C12-C13-C14-C15
4	B	911	6OU	C31-C33-C34-C35
4	C	906	6OU	O30-C20-C21-O22
4	D	902	6OU	C10-C11-C12-C13
4	A	908	6OU	O18-C19-C20-C21
4	C	912	6OU	O18-C19-C20-C21
6	D	908	YFP	O18-C19-C20-O32
4	A	909	6OU	C10-C11-C12-C13
4	B	901	6OU	C10-C11-C12-C13
4	C	901	6OU	C10-C11-C12-C13
2	B	904	T7X	C36-C37-C38-C39
2	D	904	T7X	C36-C37-C38-C39
2	A	901	T7X	C36-C37-C38-C39
2	C	904	T7X	C36-C37-C38-C39
6	C	908	YFP	C36-C37-C38-C39
2	A	901	T7X	C7-C8-O16-C10
2	B	904	T7X	C7-C8-O16-C10
2	C	904	T7X	C7-C8-O16-C10
2	D	904	T7X	C7-C8-O16-C10

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Mol	Chain	Res	Type	Atoms
6	B	903	YFP	C19-C20-O32-C33
4	A	903	6OU	O30-C20-C21-O22
4	B	906	6OU	O30-C20-C21-O22
4	D	906	6OU	O30-C20-C21-O22
4	C	912	6OU	C38-C39-C40-C41
4	B	911	6OU	C35-C36-C37-C38
3	A	902	LBN	C1-O1-P1-O2
3	B	905	LBN	C1-O1-P1-O2
3	C	905	LBN	C1-O1-P1-O2
3	D	905	LBN	C1-O1-P1-O2
4	A	909	6OU	C21-O22-P23-O26
4	B	901	6OU	C21-O22-P23-O26
4	C	901	6OU	C21-O22-P23-O26
6	B	903	YFP	O18-C19-C20-C21
4	C	909	6OU	C20-C21-O22-P23
4	A	907	6OU	C40-C41-C42-C43
4	B	910	6OU	C40-C41-C42-C43
4	C	911	6OU	C40-C41-C42-C43
4	D	911	6OU	C40-C41-C42-C43
4	D	901	6OU	C14-C15-C16-O18
6	B	903	YFP	C13-C14-C15-C16
3	A	902	LBN	C2-C1-O1-P1
3	B	905	LBN	C2-C1-O1-P1
3	C	905	LBN	C2-C1-O1-P1
3	D	905	LBN	C2-C1-O1-P1
4	A	905	6OU	C20-C21-O22-P23
4	B	908	6OU	C20-C21-O22-P23
4	D	909	6OU	C20-C21-O22-P23
3	A	910	LBN	C42-C5-C8-C11
3	B	902	LBN	C42-C5-C8-C11
3	C	902	LBN	C42-C5-C8-C11
3	D	903	LBN	C42-C5-C8-C11
4	B	911	6OU	C38-C39-C40-C41
3	C	902	LBN	C31-C32-C33-C4
4	D	902	6OU	C37-C38-C39-C40
2	A	901	T7X	C9-C8-O16-C10
2	B	904	T7X	C9-C8-O16-C10
2	C	904	T7X	C9-C8-O16-C10
2	D	904	T7X	C9-C8-O16-C10
6	C	908	YFP	C19-C20-O32-C33
6	C	908	YFP	C21-C20-O32-C33
3	B	902	LBN	C31-C32-C33-C4

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Mol	Chain	Res	Type	Atoms
3	D	905	LBN	C26-C27-C28-C29
4	A	904	6OU	C10-C11-C12-C13
4	B	907	6OU	C10-C11-C12-C13
2	A	901	T7X	O17-C10-O16-C8
4	C	907	6OU	C10-C11-C12-C13
4	D	907	6OU	C10-C11-C12-C13
3	A	902	LBN	C26-C27-C28-C29
3	D	905	LBN	C27-C28-C29-C30
4	D	901	6OU	C09-C10-C11-C12
6	B	903	YFP	C11-C12-C13-C14
6	D	908	YFP	C09-C10-C11-C12
4	A	909	6OU	C37-C38-C39-C40
4	B	901	6OU	C37-C38-C39-C40
4	C	901	6OU	C37-C38-C39-C40
3	C	905	LBN	C26-C27-C28-C29
3	A	910	LBN	C31-C32-C33-C4
2	B	904	T7X	O17-C10-O16-C8
2	C	904	T7X	O17-C10-O16-C8
2	D	904	T7X	O17-C10-O16-C8
3	B	905	LBN	C26-C27-C28-C29
3	A	902	LBN	C27-C28-C29-C30
6	C	903	YFP	C11-C12-C13-C14
4	A	904	6OU	C14-C15-C16-O18
4	B	907	6OU	C14-C15-C16-O18
4	C	907	6OU	C14-C15-C16-O18
4	D	907	6OU	C14-C15-C16-O18
3	D	903	LBN	C31-C32-C33-C4
4	A	907	6OU	C46-C47-C48-C49
4	D	911	6OU	C46-C47-C48-C49
3	C	905	LBN	C27-C28-C29-C30
4	C	911	6OU	C46-C47-C48-C49
6	B	903	YFP	C19-C20-C21-O22
4	B	910	6OU	C46-C47-C48-C49
4	A	905	6OU	O30-C31-C33-C34
4	B	908	6OU	O30-C31-C33-C34
4	A	908	6OU	C20-C21-O22-P23
4	C	912	6OU	O17-C16-O18-C19
4	C	909	6OU	O30-C31-C33-C34
4	D	909	6OU	O30-C31-C33-C34
4	A	908	6OU	C38-C39-C40-C41
4	C	912	6OU	C15-C16-O18-C19
4	B	911	6OU	C21-O22-P23-O26

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Mol	Chain	Res	Type	Atoms
3	B	905	LBN	C27-C28-C29-C30
4	A	909	6OU	C38-C39-C40-C41
4	B	901	6OU	C38-C39-C40-C41
4	C	901	6OU	C38-C39-C40-C41
4	D	902	6OU	C38-C39-C40-C41
2	A	901	T7X	O18-C11-C31-C32
2	B	904	T7X	O18-C11-C31-C32
2	C	904	T7X	O18-C11-C31-C32
2	D	904	T7X	O18-C11-C31-C32
3	B	905	LBN	O5-C25-C26-C27
3	C	905	LBN	O5-C25-C26-C27
3	A	902	LBN	O5-C25-C26-C27
4	B	906	6OU	C14-C15-C16-O18
4	C	906	6OU	C14-C15-C16-O18
4	B	907	6OU	C08-C09-C10-C11
3	D	905	LBN	O5-C25-C26-C27
4	D	906	6OU	C14-C15-C16-O18
4	A	904	6OU	C08-C09-C10-C11
4	A	903	6OU	C14-C15-C16-O18
4	B	911	6OU	C12-C13-C14-C15
4	C	907	6OU	C08-C09-C10-C11
4	B	901	6OU	O30-C31-C33-C34
4	C	901	6OU	O30-C31-C33-C34
6	D	908	YFP	C08-C09-C10-C11
4	A	906	6OU	C14-C15-C16-O18
4	A	909	6OU	O30-C31-C33-C34
4	B	909	6OU	C14-C15-C16-O18
4	C	910	6OU	C14-C15-C16-O18
4	D	902	6OU	O30-C31-C33-C34
4	D	910	6OU	C14-C15-C16-O18
2	A	901	T7X	C12-C10-O16-C8
2	D	904	T7X	C12-C10-O16-C8
4	D	907	6OU	C08-C09-C10-C11
3	D	903	LBN	C26-C25-O5-C3
2	B	904	T7X	C12-C10-O16-C8
2	C	904	T7X	C12-C10-O16-C8
3	C	902	LBN	C26-C25-O5-C3
4	C	909	6OU	O32-C31-C33-C34
3	A	910	LBN	C26-C25-O5-C3
3	B	902	LBN	C26-C25-O5-C3
2	A	901	T7X	O19-C11-C31-C32
4	A	905	6OU	O32-C31-C33-C34

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Mol	Chain	Res	Type	Atoms
4	B	908	6OU	O32-C31-C33-C34
4	A	909	6OU	O32-C31-C33-C34
4	B	901	6OU	O32-C31-C33-C34
4	D	909	6OU	O32-C31-C33-C34
3	D	903	LBN	O6-C25-O5-C3
4	C	906	6OU	C11-C12-C13-C14
2	B	904	T7X	O19-C11-C31-C32
2	C	904	T7X	O19-C11-C31-C32
2	D	904	T7X	O19-C11-C31-C32
4	C	901	6OU	O32-C31-C33-C34
4	D	902	6OU	O32-C31-C33-C34
3	C	902	LBN	O6-C25-O5-C3
3	A	902	LBN	C1-O1-P1-O4
3	B	905	LBN	C1-O1-P1-O4
3	C	905	LBN	C1-O1-P1-O4
3	D	905	LBN	C1-O1-P1-O4
4	A	909	6OU	C21-O22-P23-O25
4	B	901	6OU	C21-O22-P23-O25
4	D	902	6OU	C21-O22-P23-O25
6	C	903	YFP	C21-O22-P23-O24
6	C	908	YFP	C21-O22-P23-O24
3	A	910	LBN	O6-C25-O5-C3
4	B	911	6OU	C19-C20-C21-O22
3	D	903	LBN	C36-C37-C38-C39
4	B	906	6OU	C11-C12-C13-C14
3	B	902	LBN	O6-C25-O5-C3
4	A	903	6OU	O30-C31-C33-C34
4	B	906	6OU	O30-C31-C33-C34
4	D	906	6OU	O30-C31-C33-C34
3	A	902	LBN	O6-C25-C26-C27
6	D	908	YFP	C14-C15-C16-O17
4	C	906	6OU	O30-C31-C33-C34
4	B	911	6OU	C09-C10-C11-C12
3	D	905	LBN	O6-C25-C26-C27
4	A	903	6OU	C11-C12-C13-C14
3	B	905	LBN	O6-C25-O5-C3
3	B	905	LBN	O6-C25-C26-C27
3	C	905	LBN	O6-C25-C26-C27
4	A	906	6OU	C14-C15-C16-O17
4	B	909	6OU	C14-C15-C16-O17
4	C	910	6OU	C14-C15-C16-O17
4	D	910	6OU	C14-C15-C16-O17

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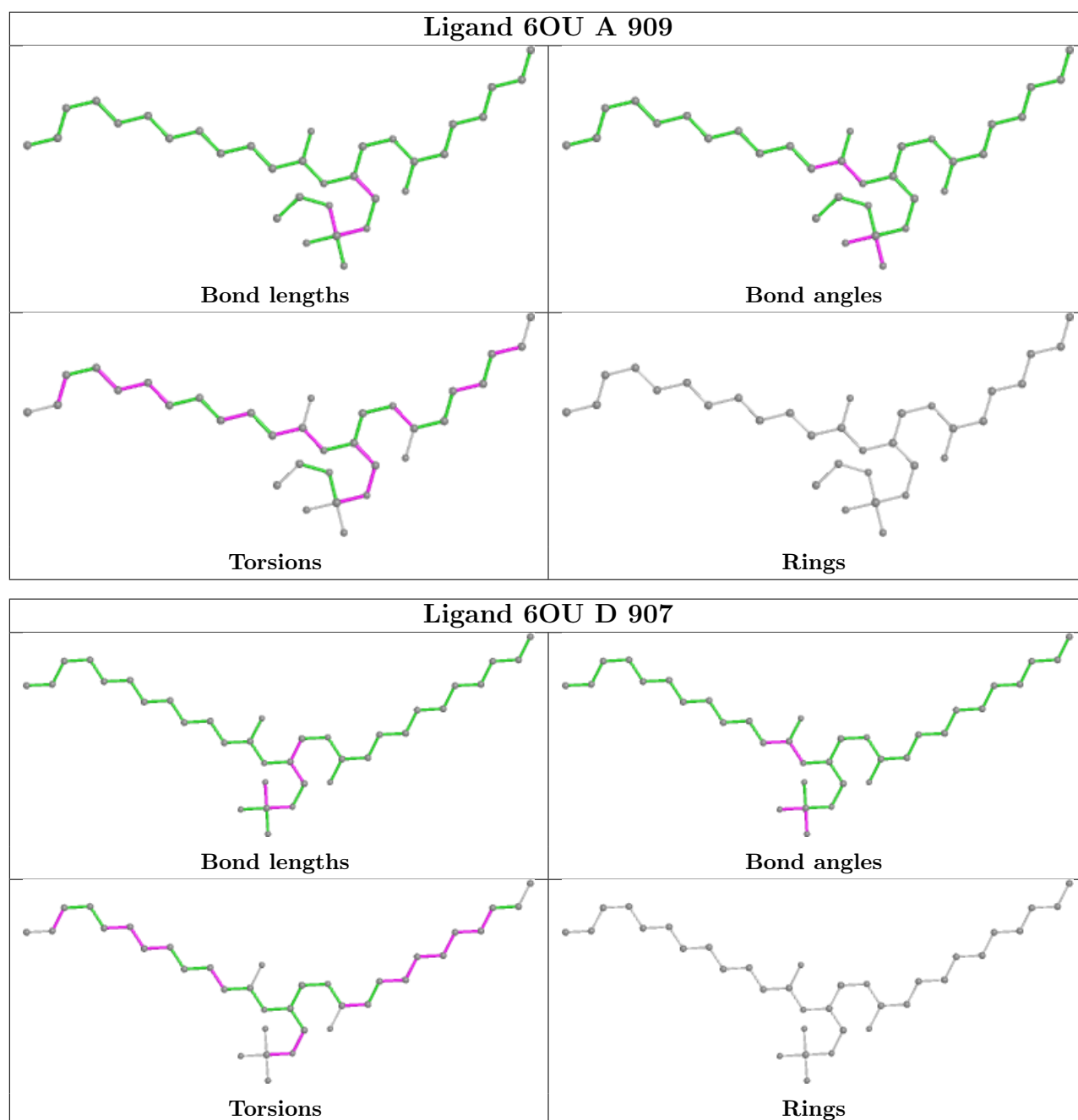
Mol	Chain	Res	Type	Atoms
4	D	906	6OU	C11-C12-C13-C14
3	A	902	LBN	O6-C25-O5-C3
3	C	905	LBN	O6-C25-O5-C3
3	A	910	LBN	C36-C37-C38-C39
3	D	905	LBN	O6-C25-O5-C3
3	B	902	LBN	C36-C37-C38-C39
4	B	911	6OU	C34-C35-C36-C37
3	C	902	LBN	C36-C37-C38-C39
3	A	902	LBN	O7-C34-C35-C36
3	B	905	LBN	O7-C34-C35-C36
3	C	905	LBN	O7-C34-C35-C36
3	D	905	LBN	O7-C34-C35-C36

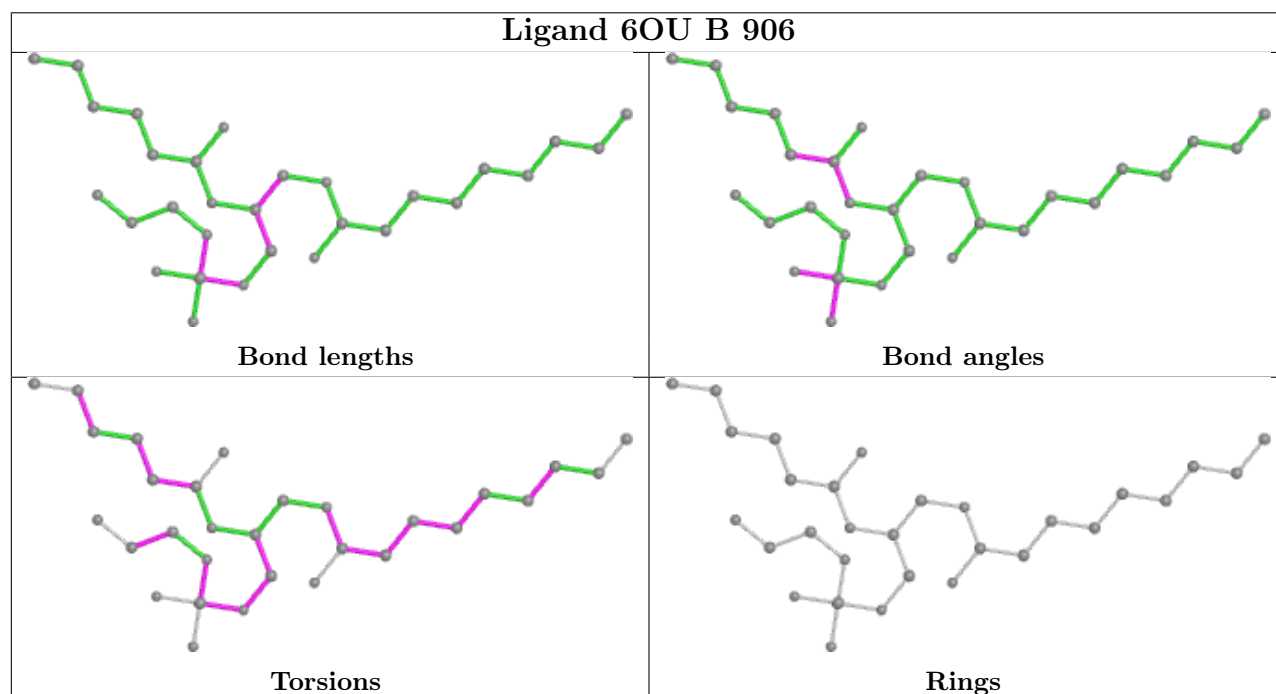
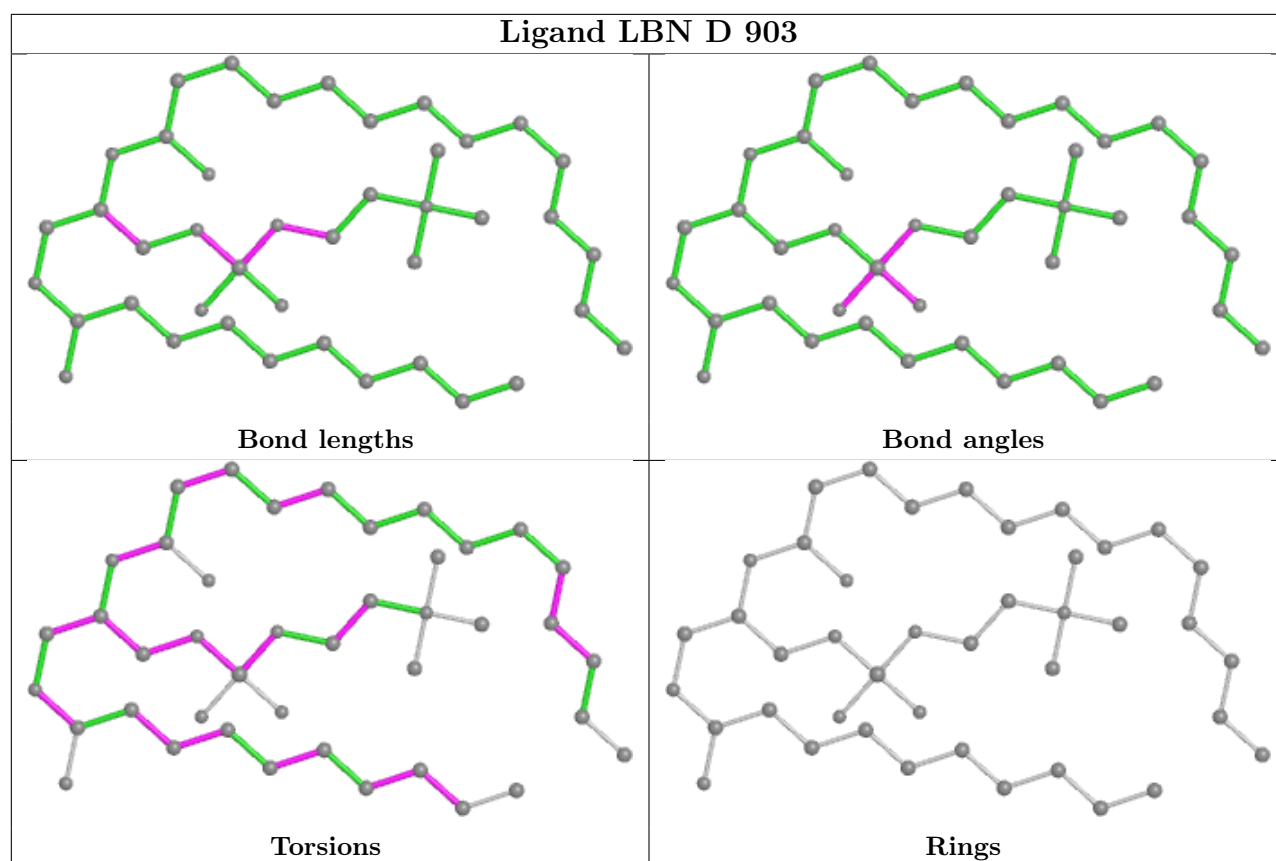
There are no ring outliers.

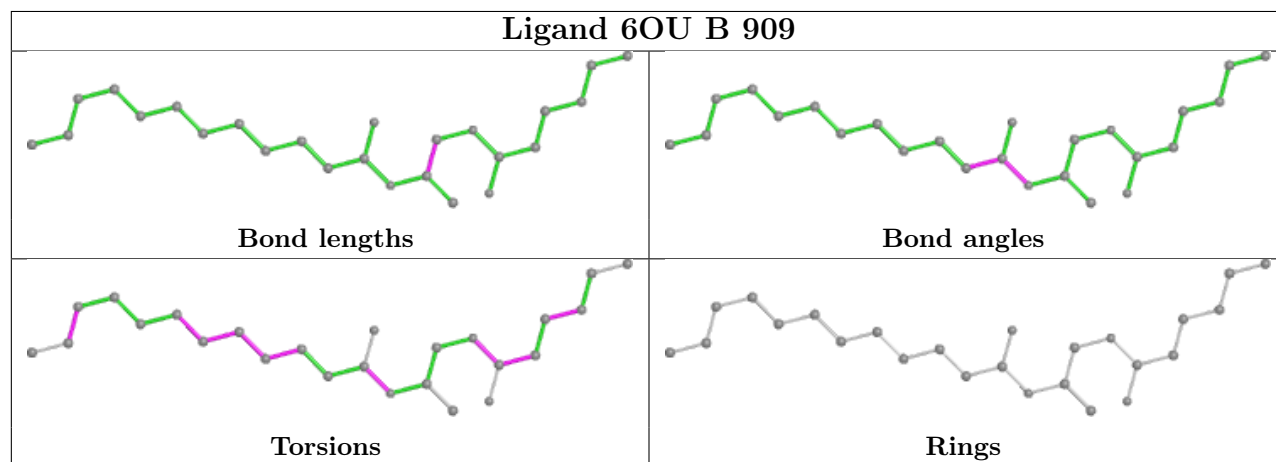
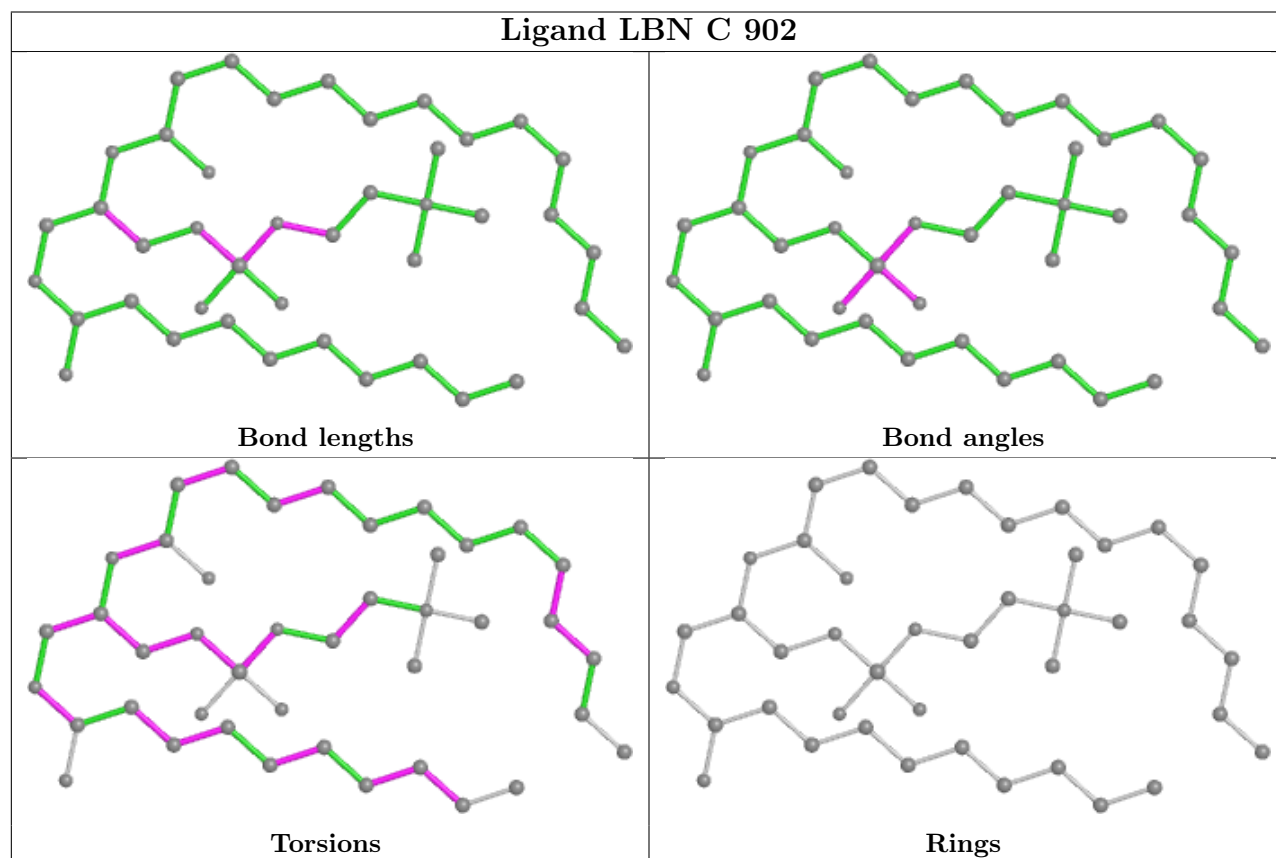
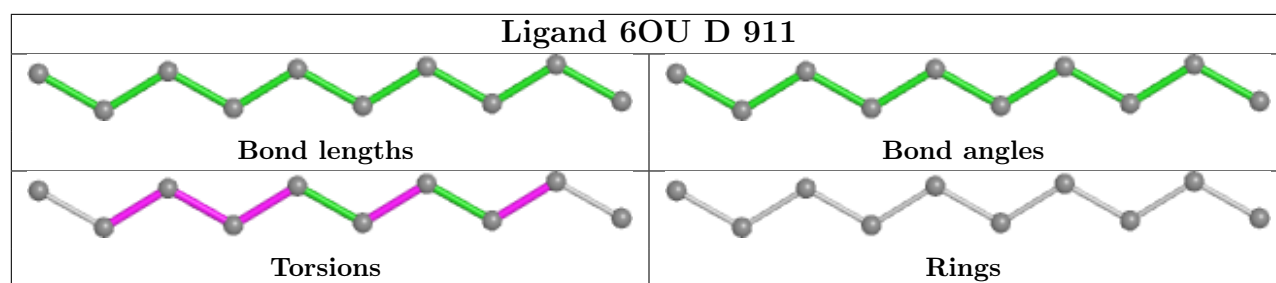
7 monomers are involved in 10 short contacts:

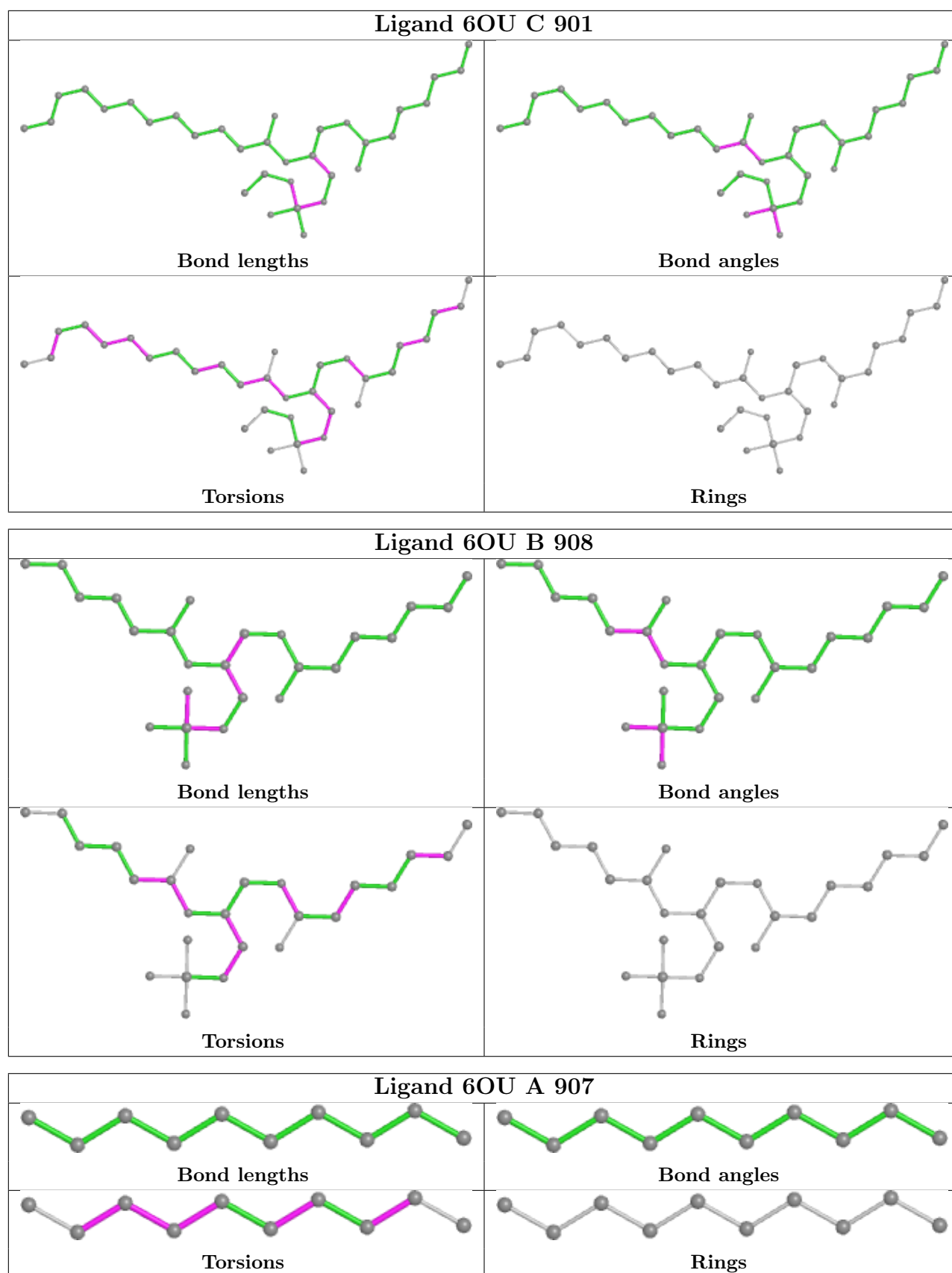
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	D	905	LBN	1	0
6	C	903	YFP	4	0
3	A	902	LBN	1	0
6	D	908	YFP	1	0
3	C	905	LBN	1	0
3	B	905	LBN	1	0
4	A	908	6OU	1	0

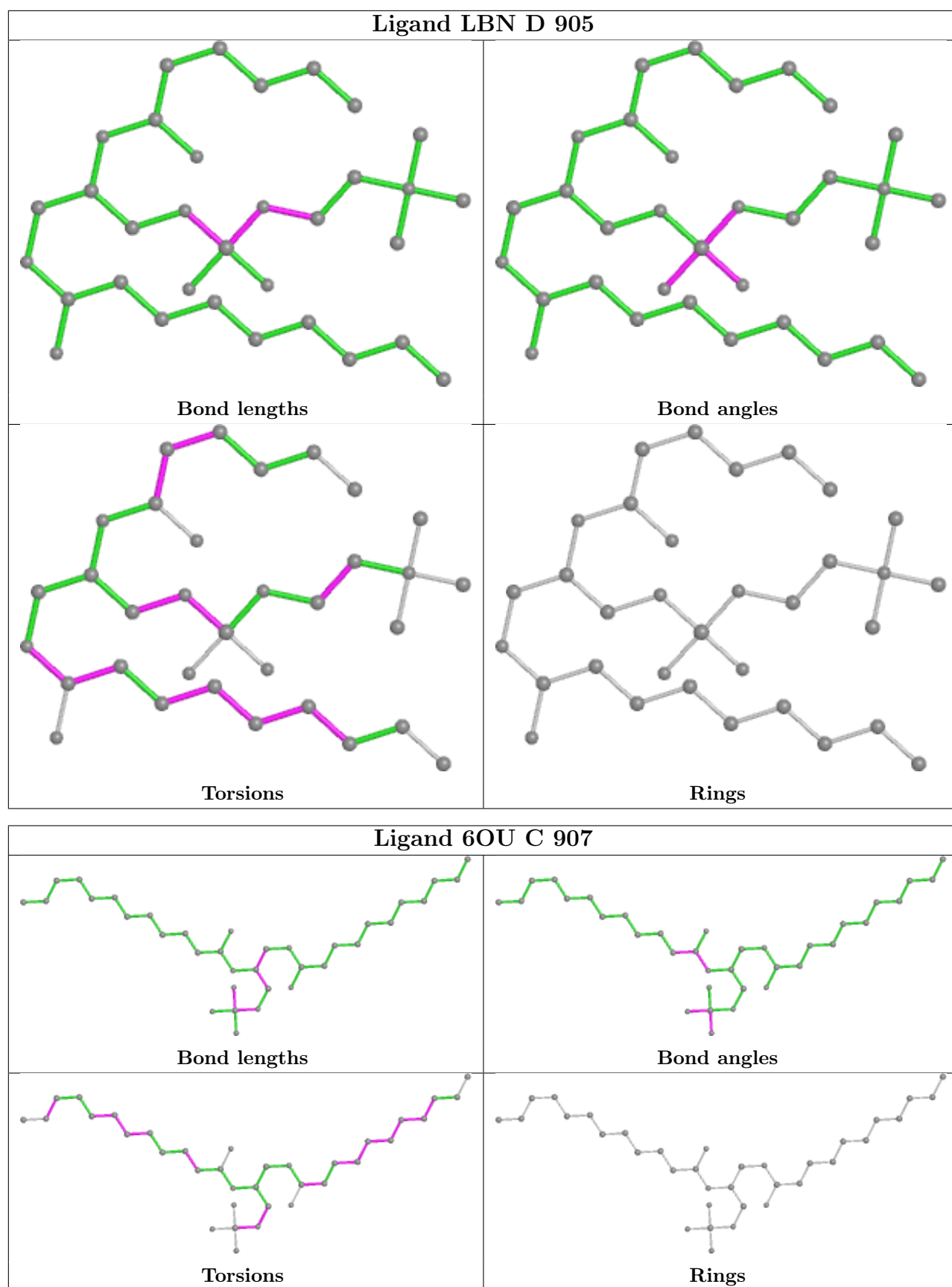
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

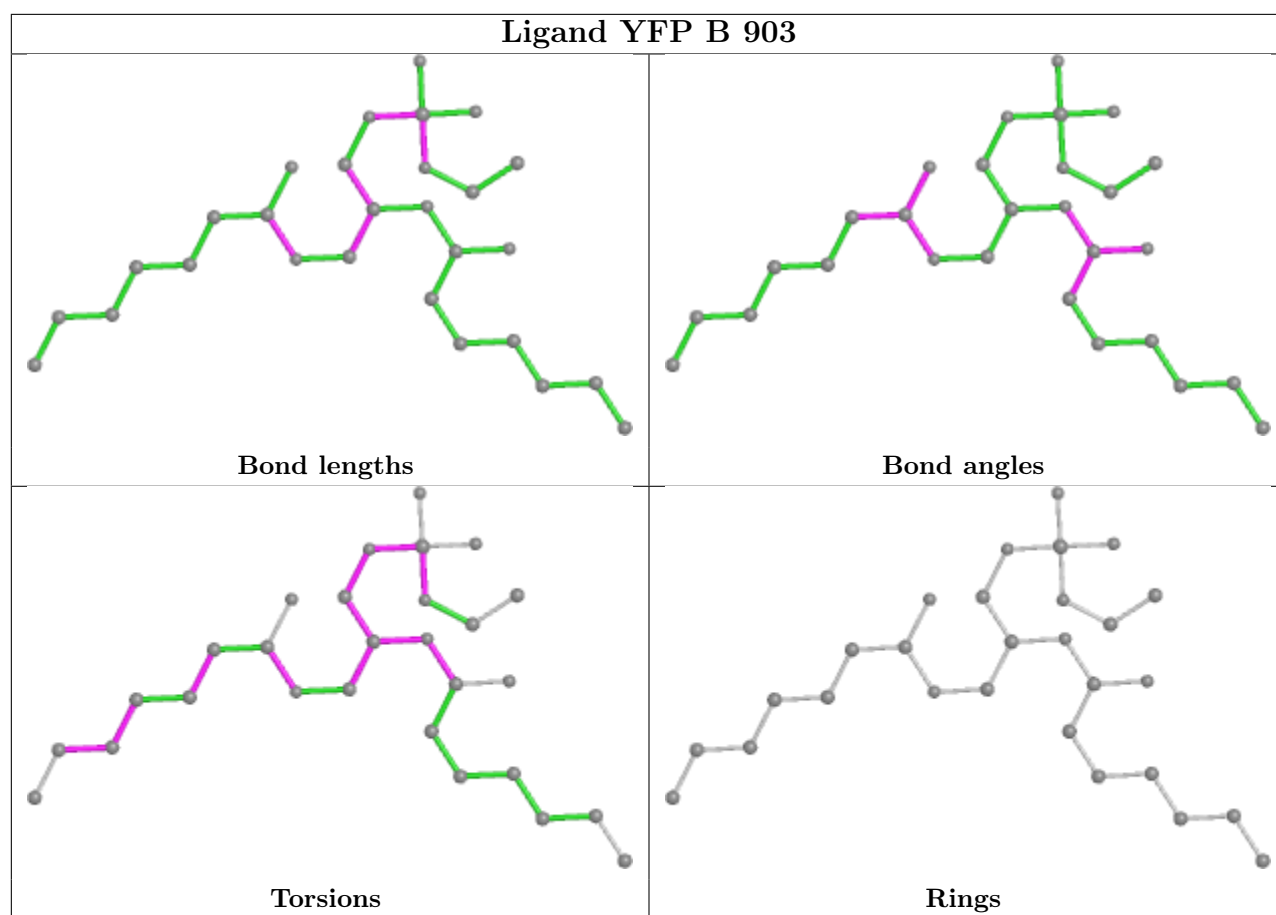


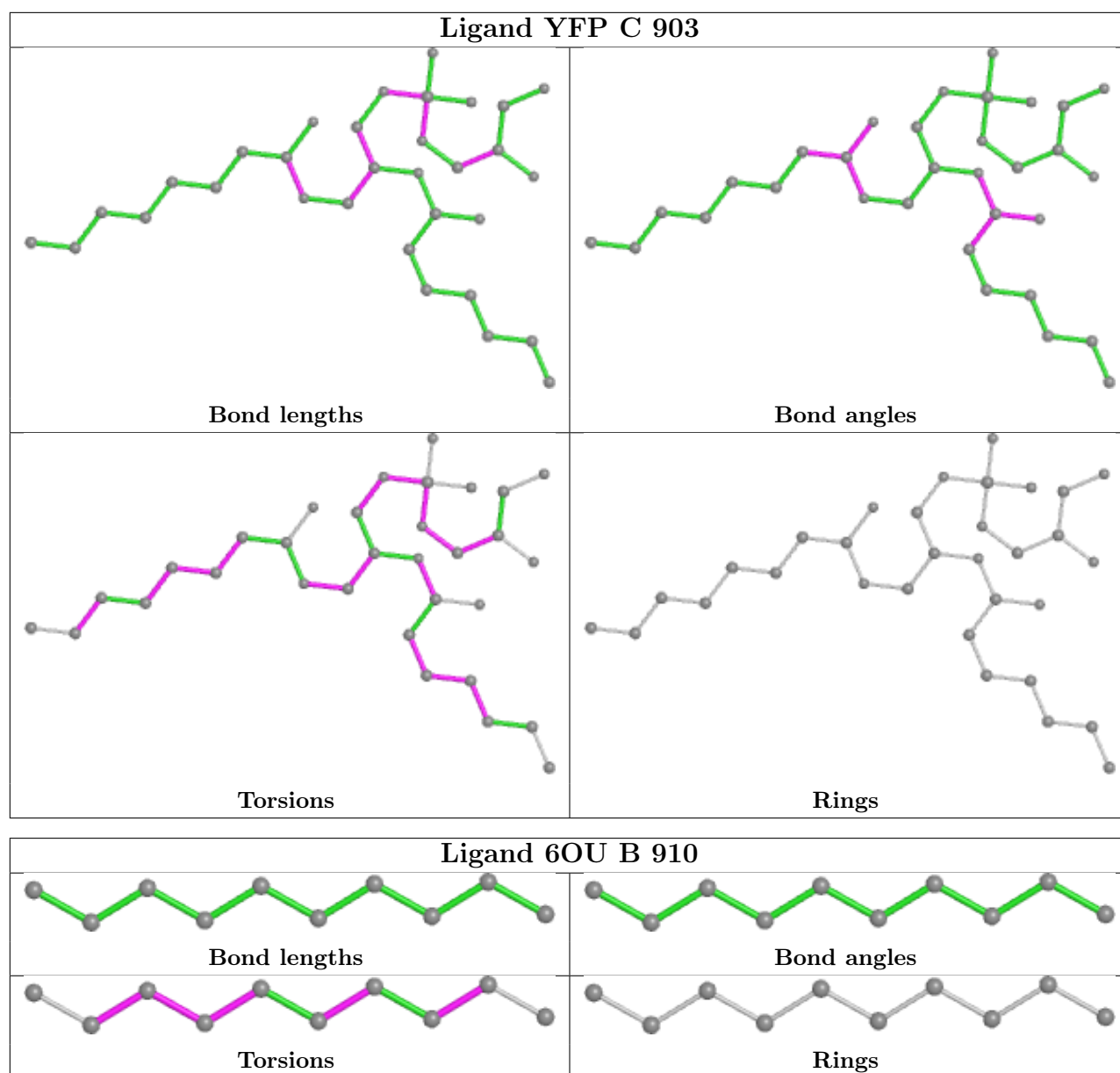


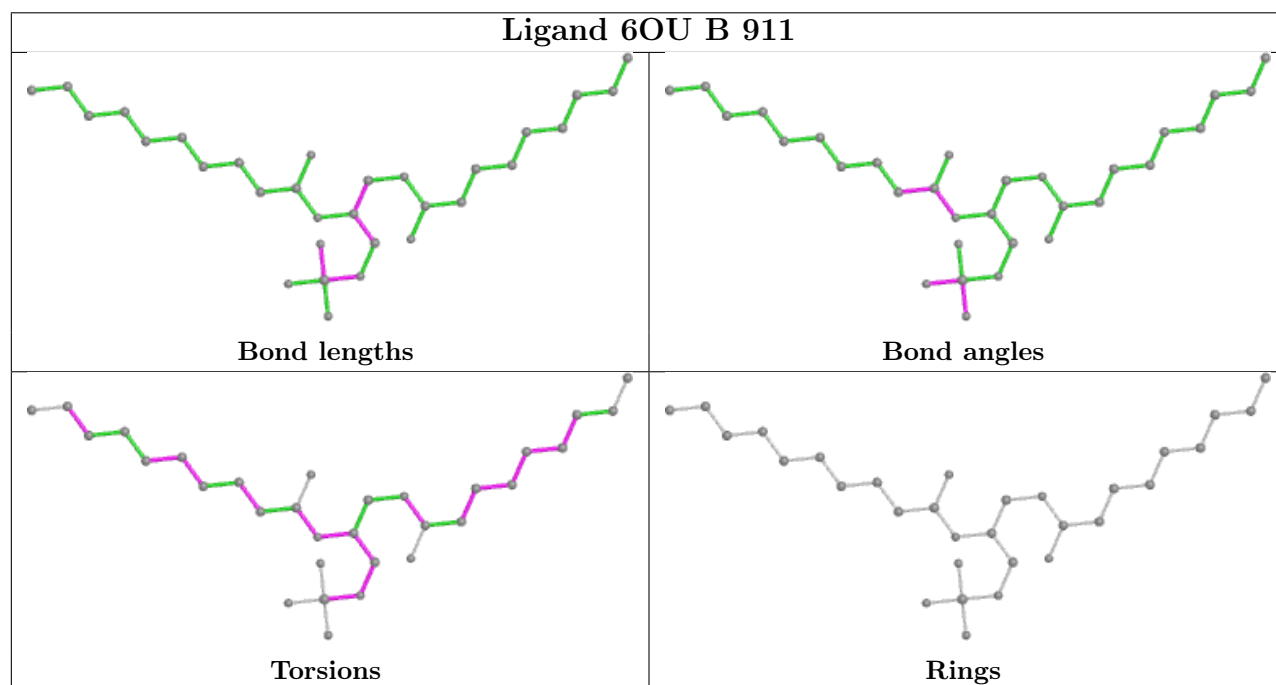
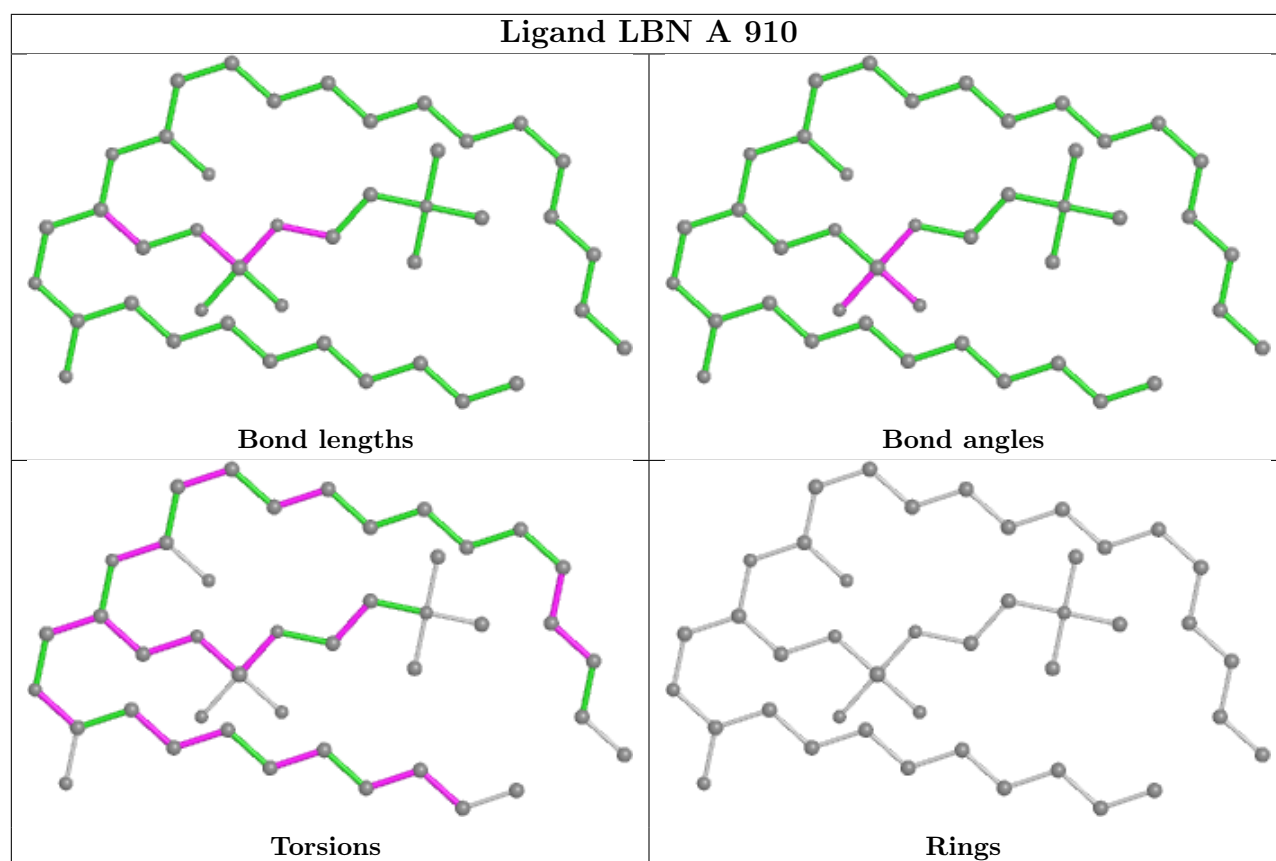


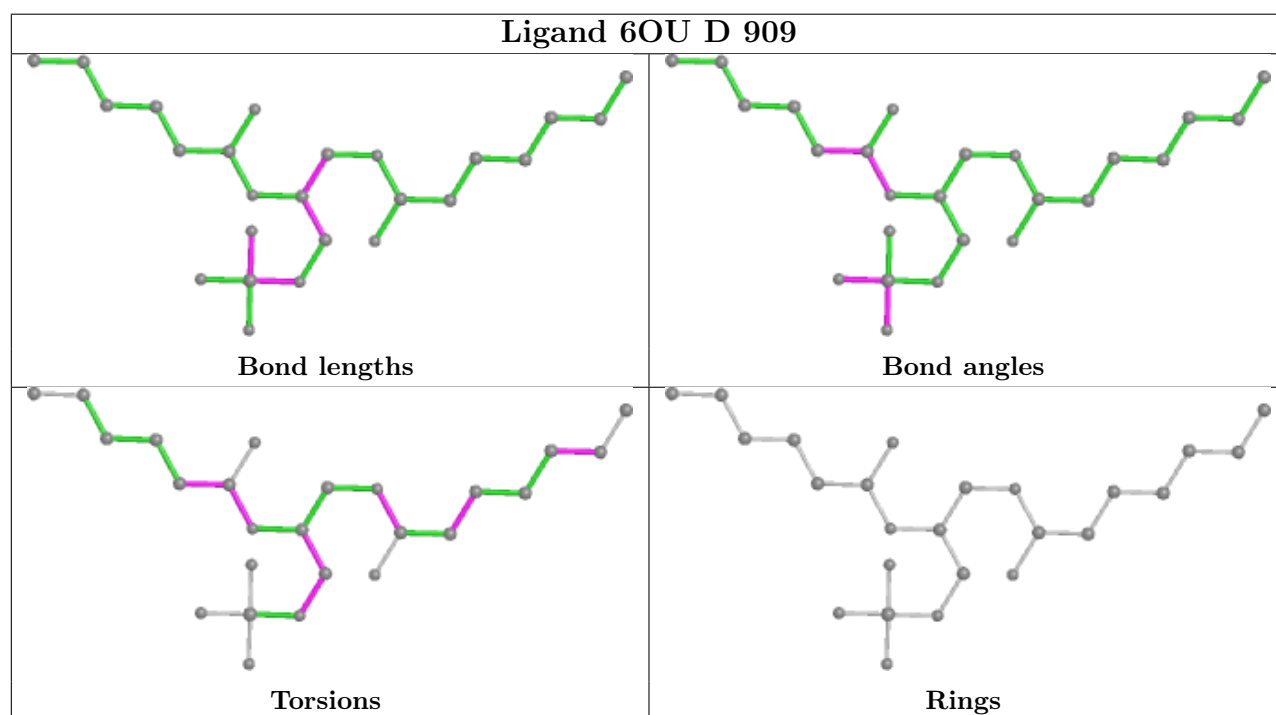
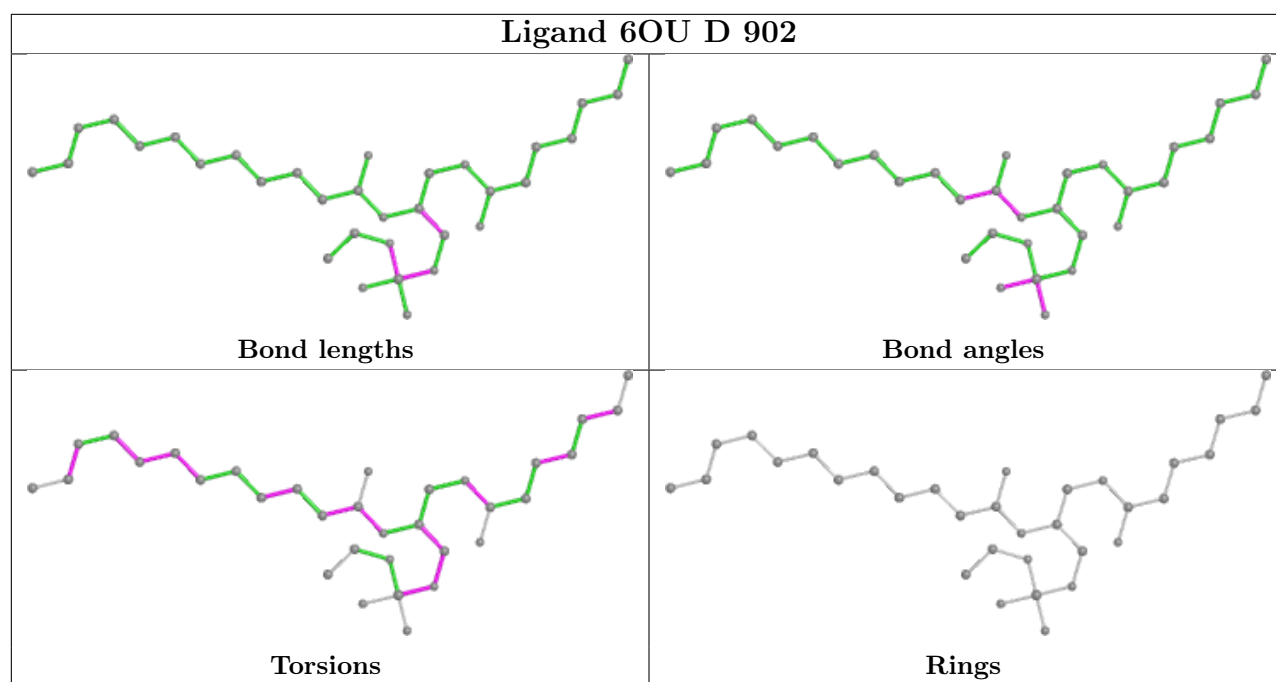


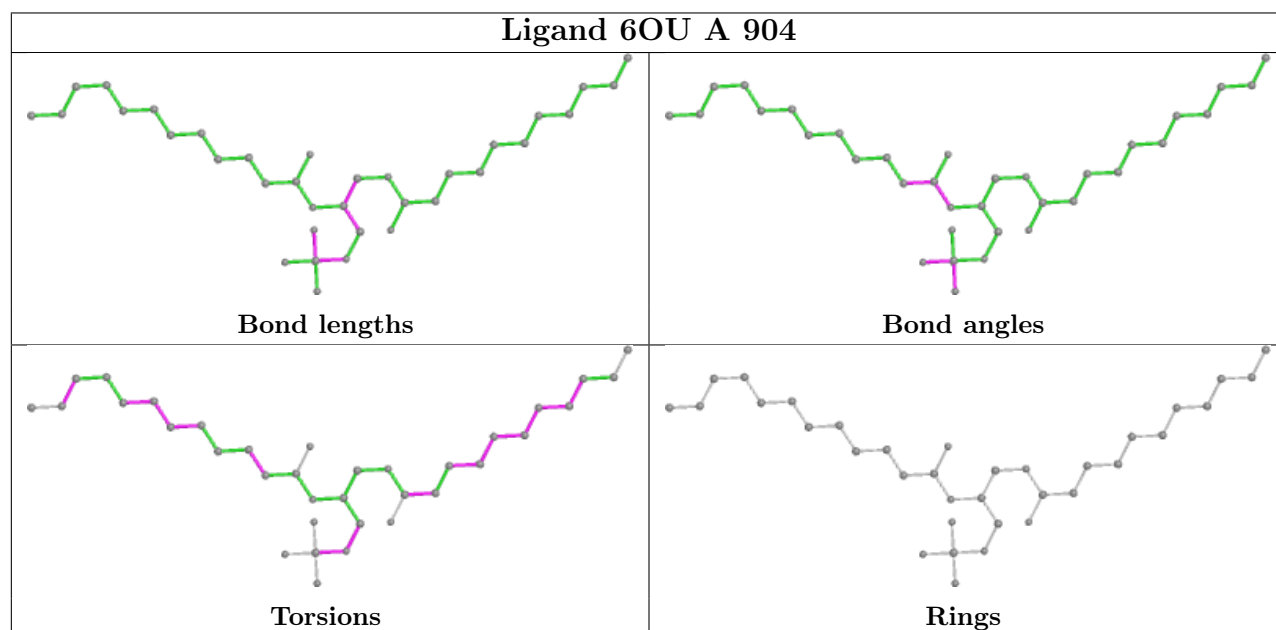
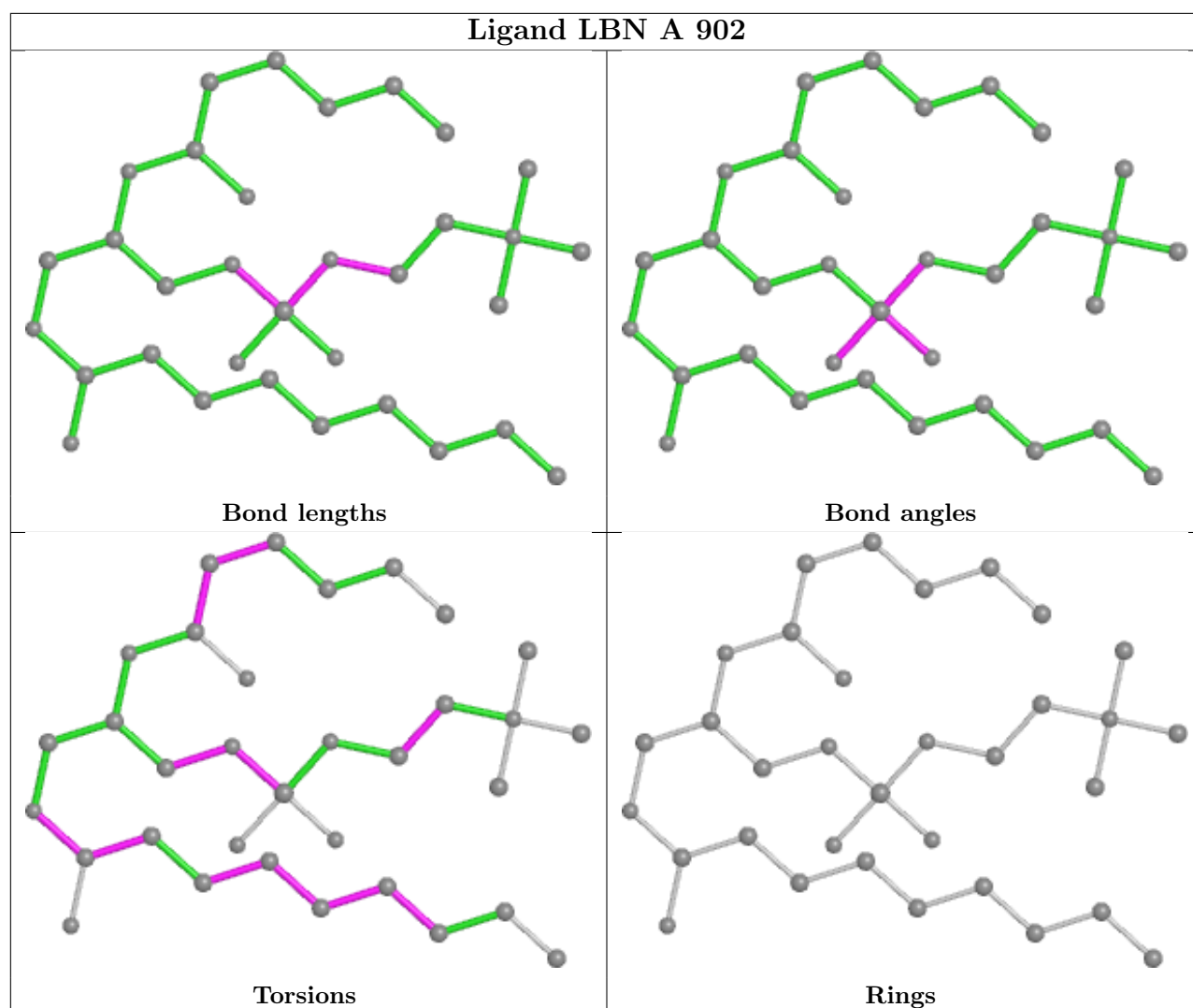


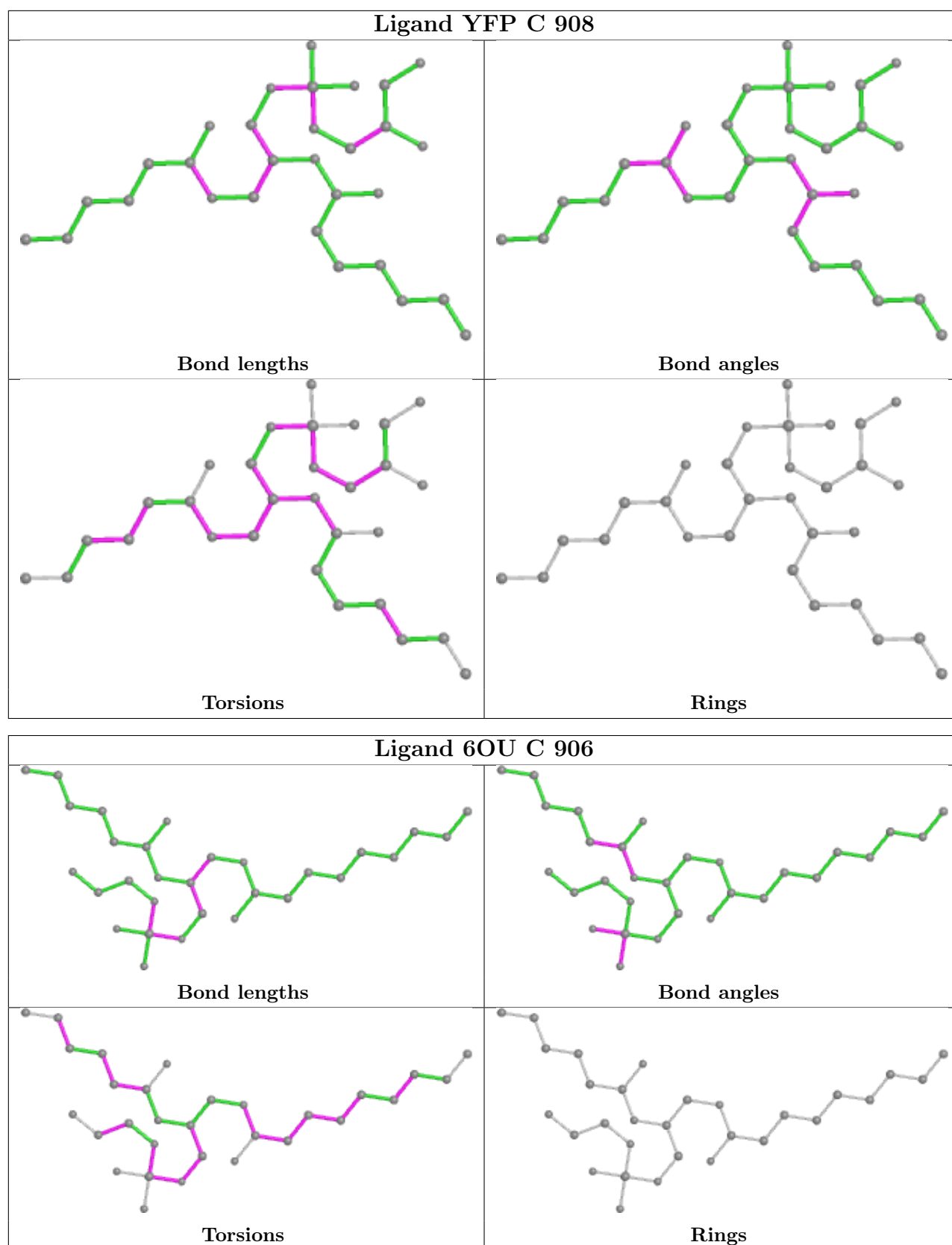


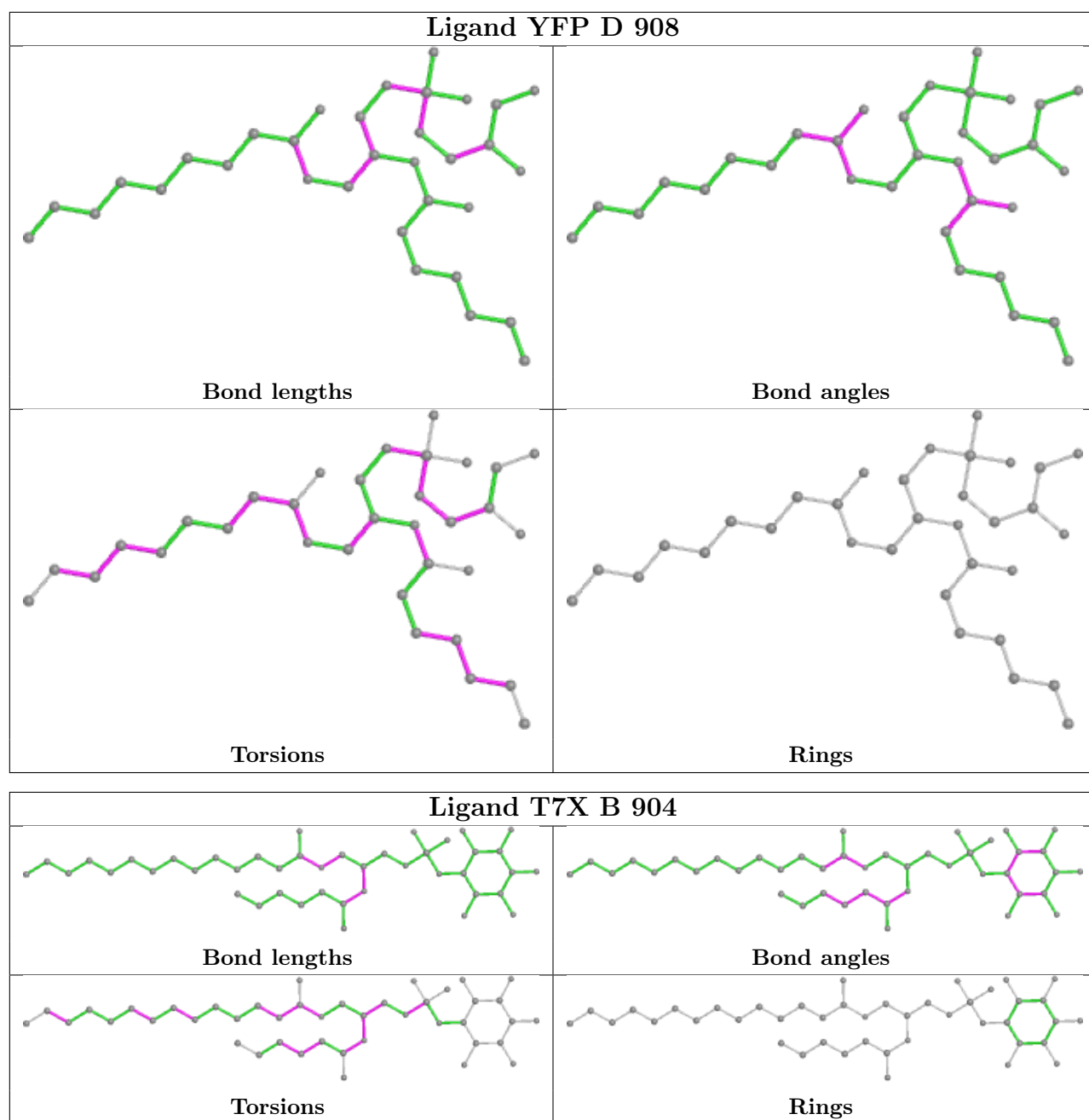


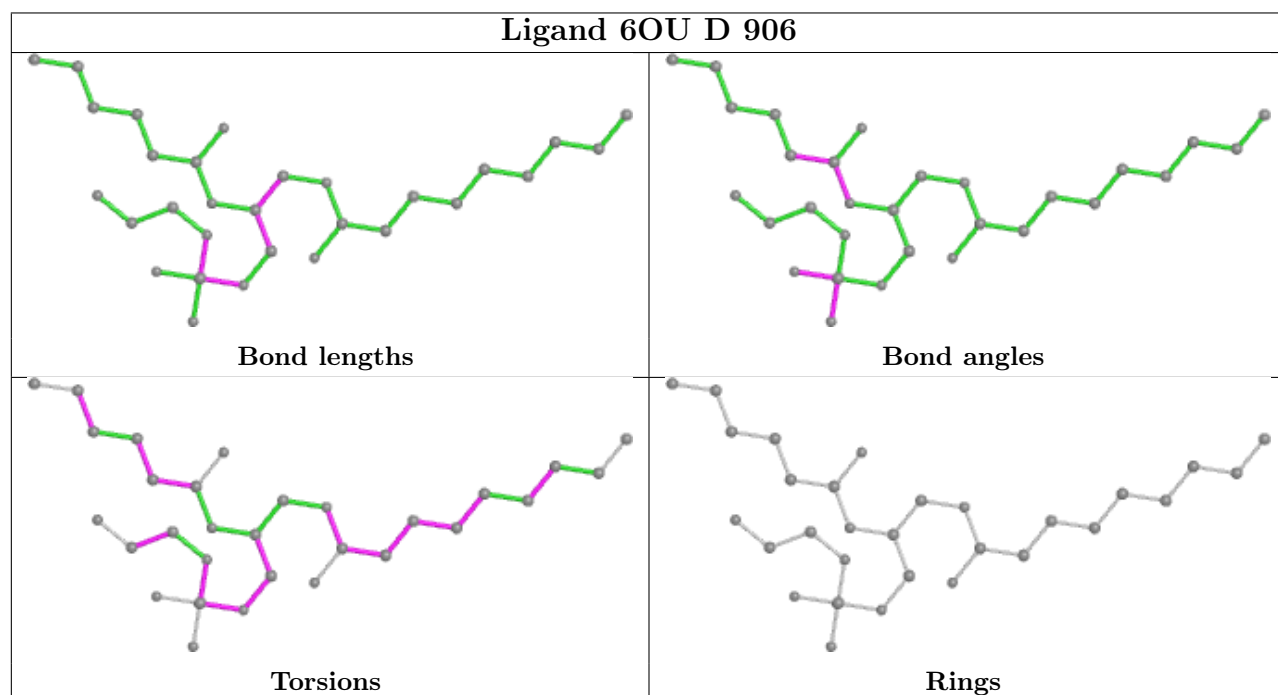
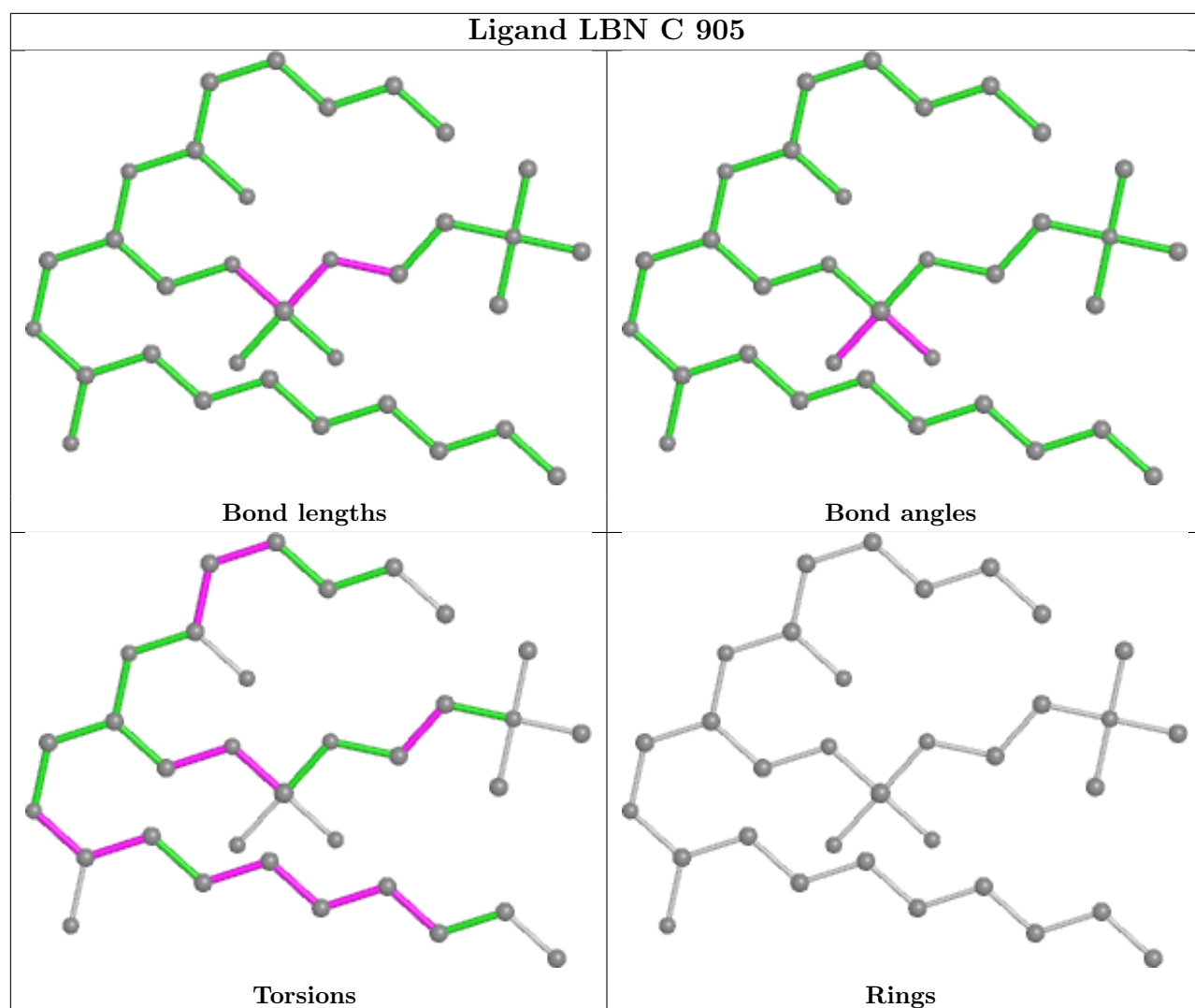


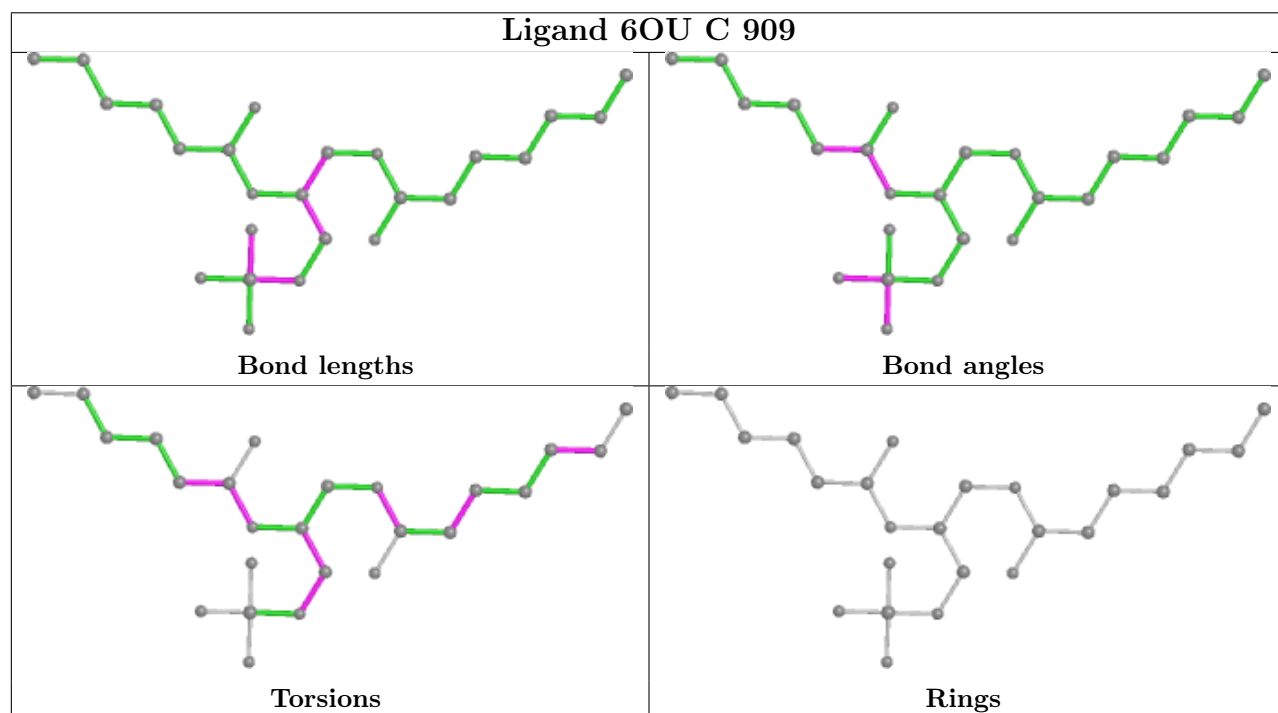
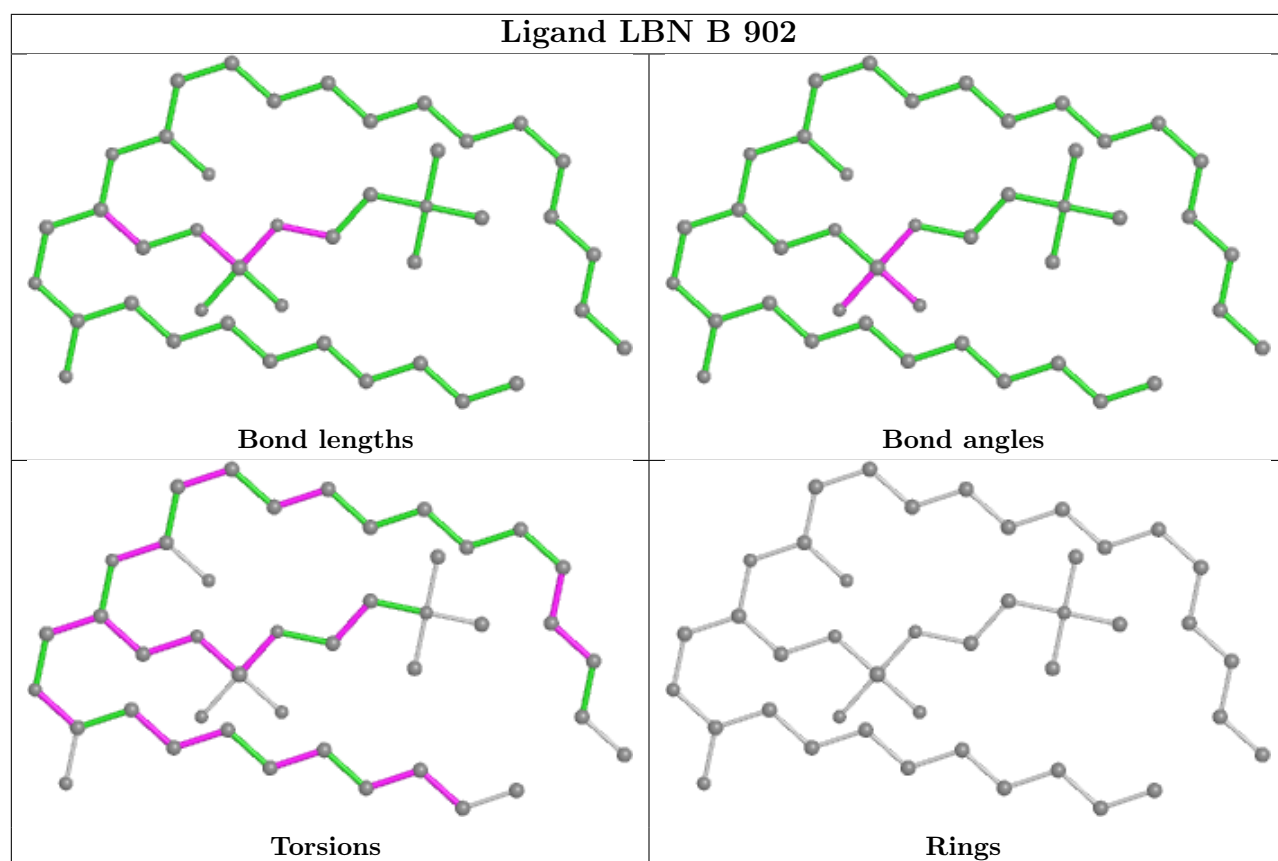


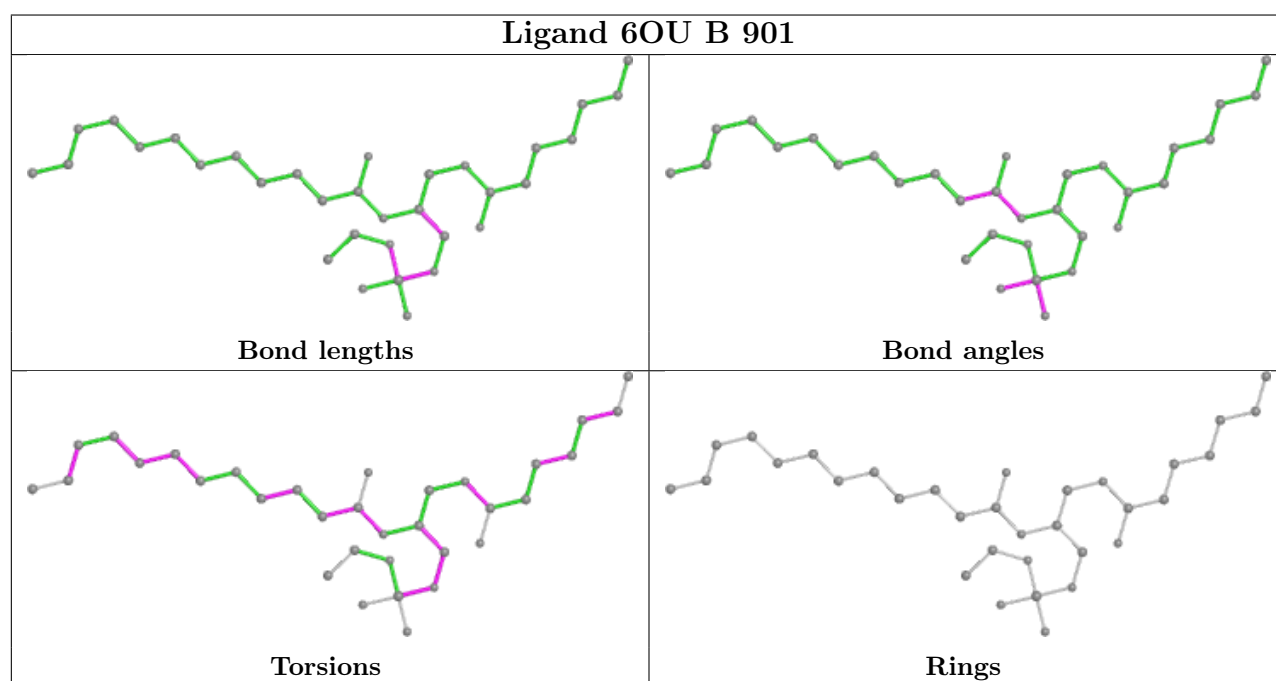
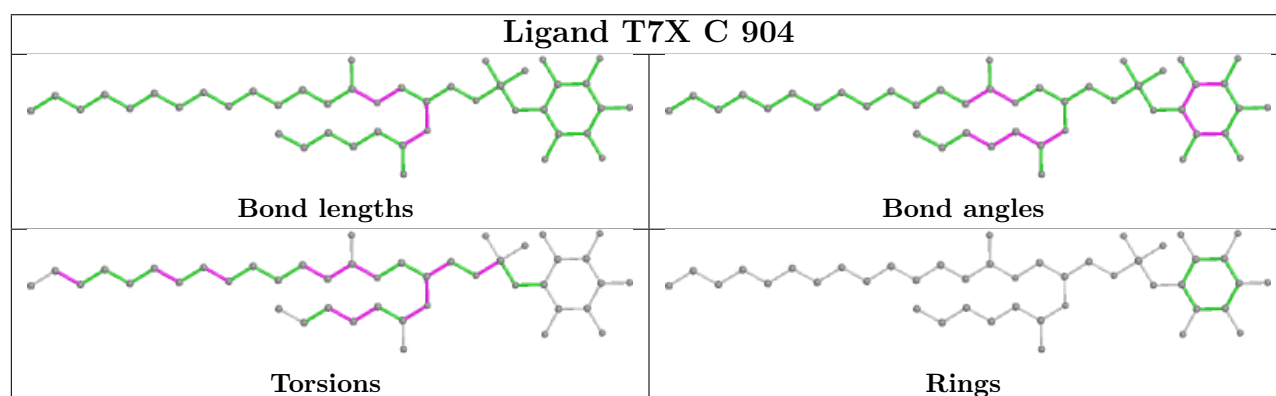
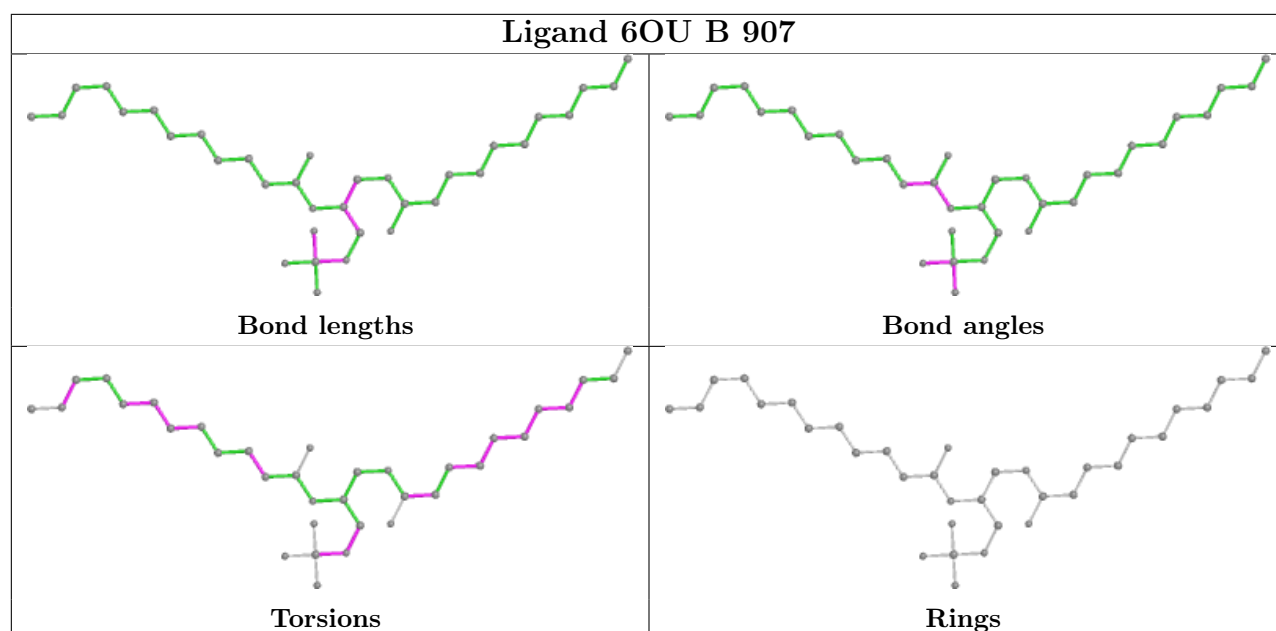


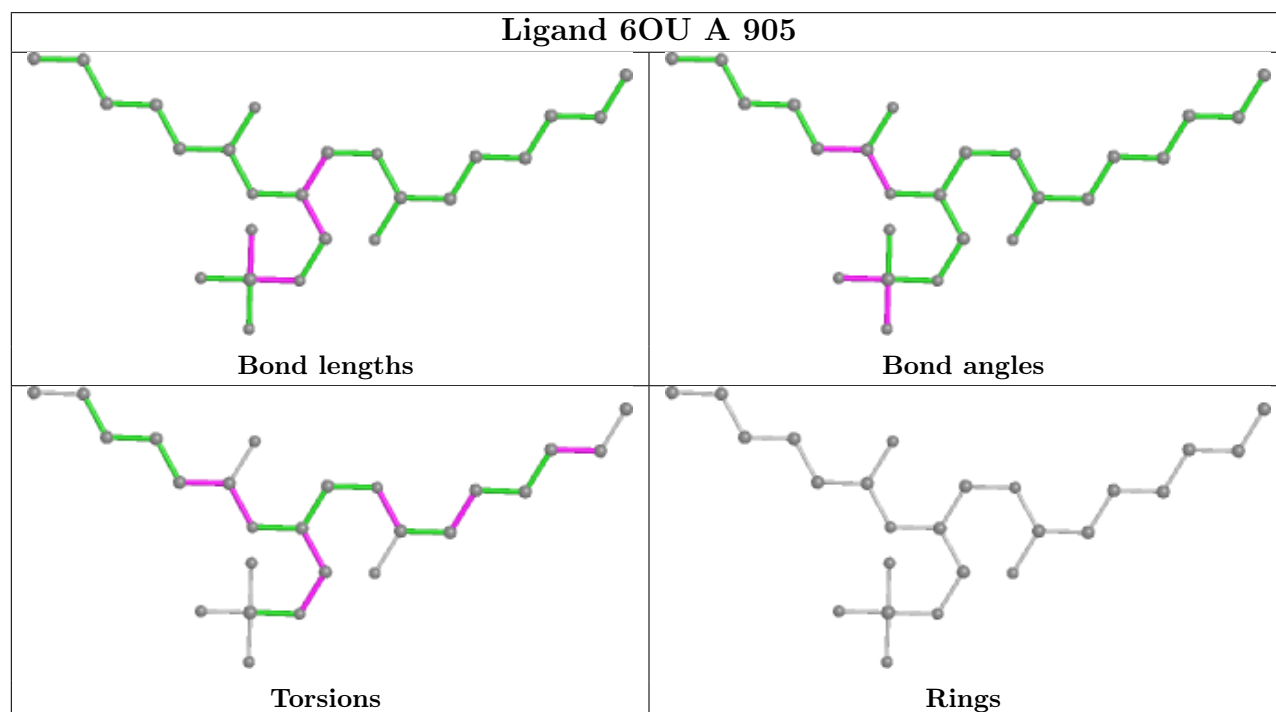
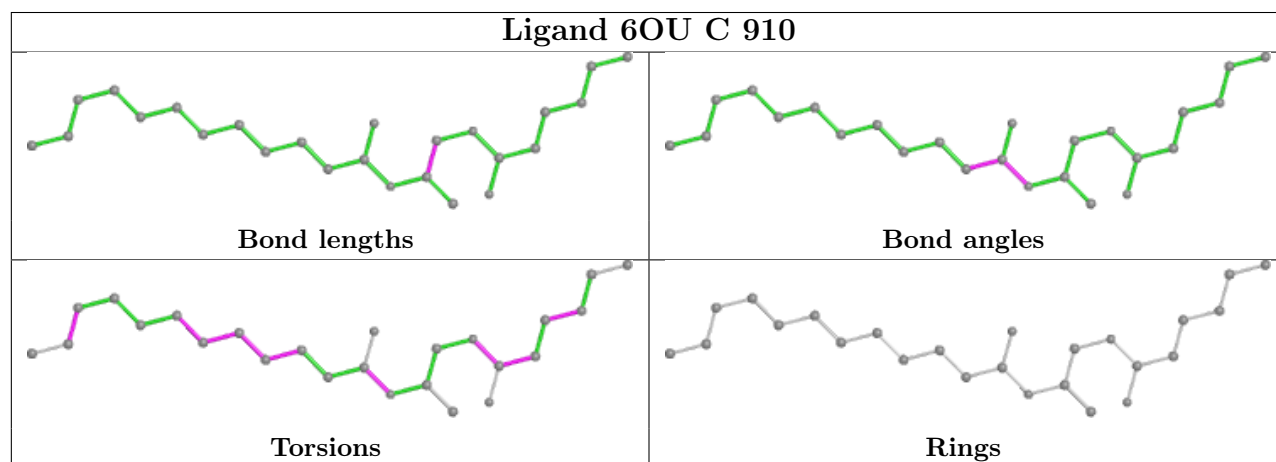
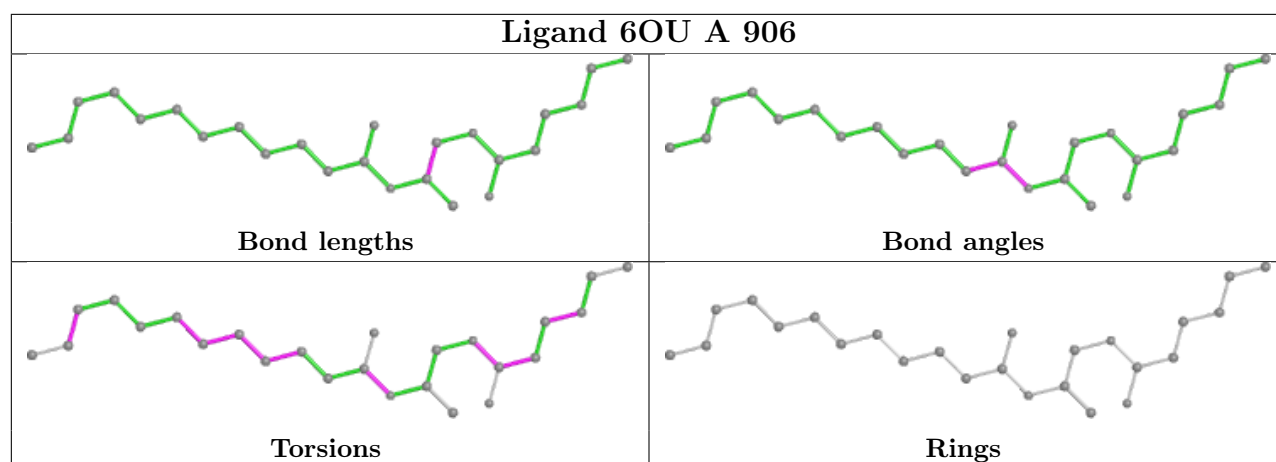


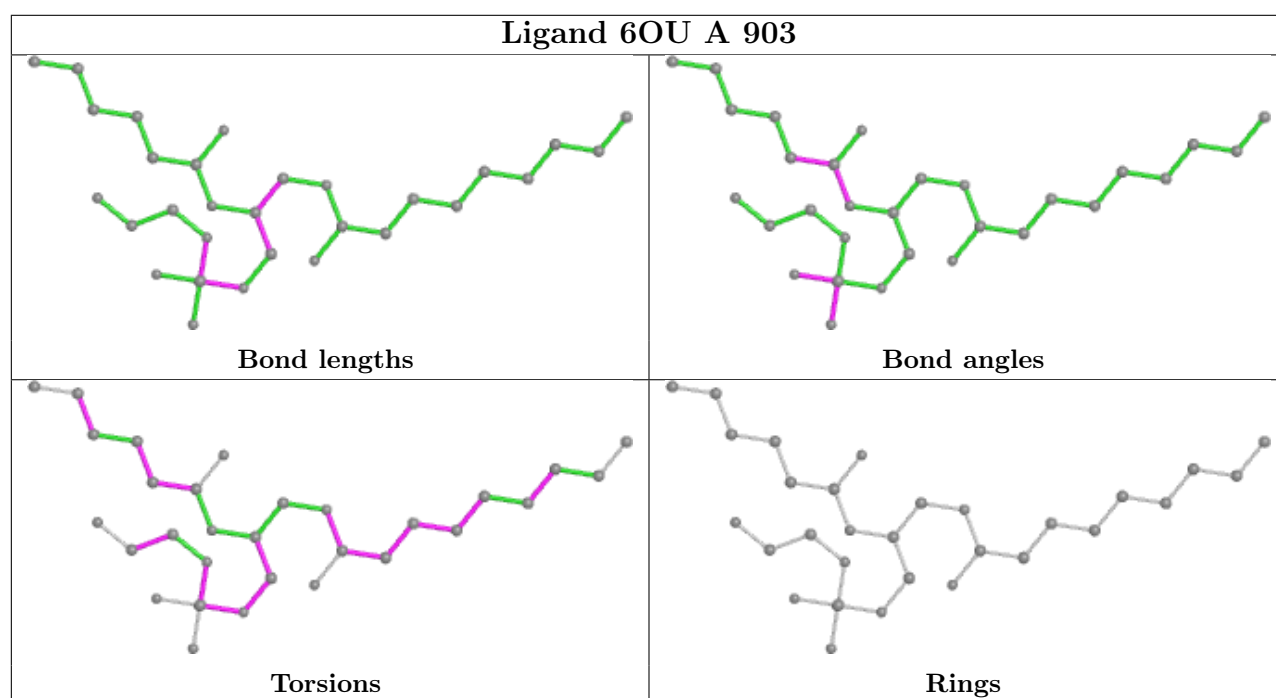
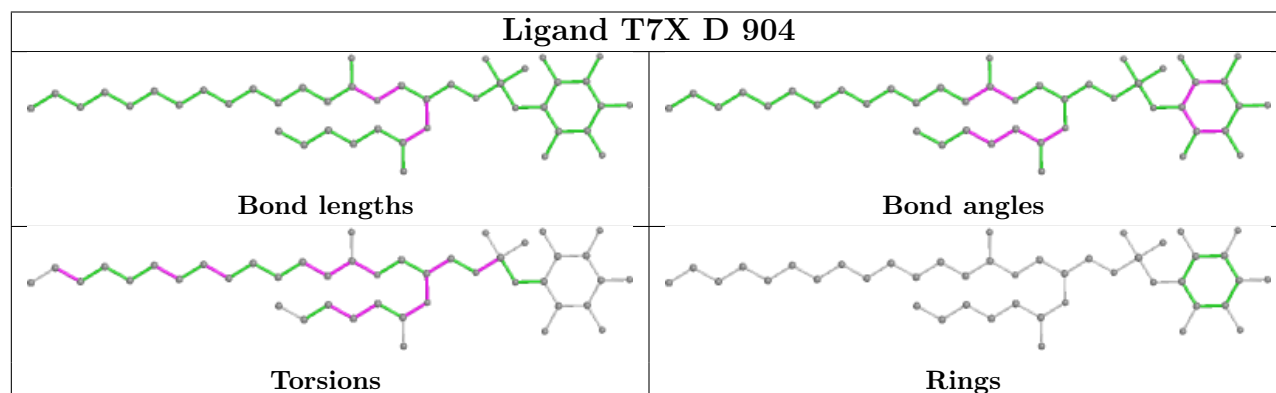
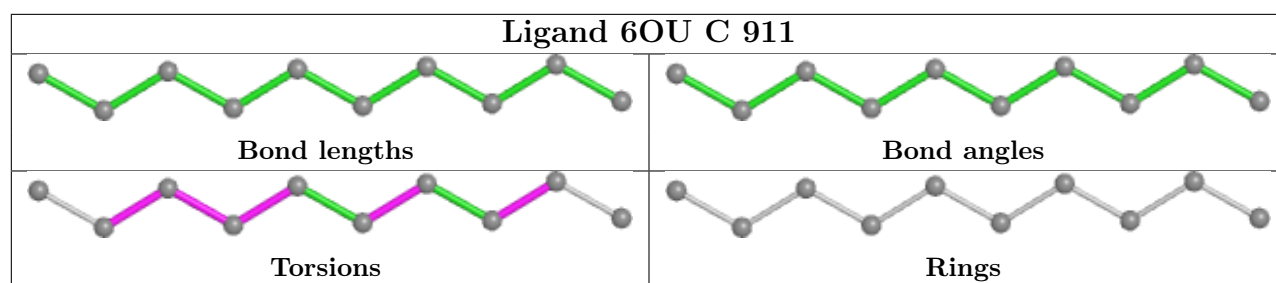


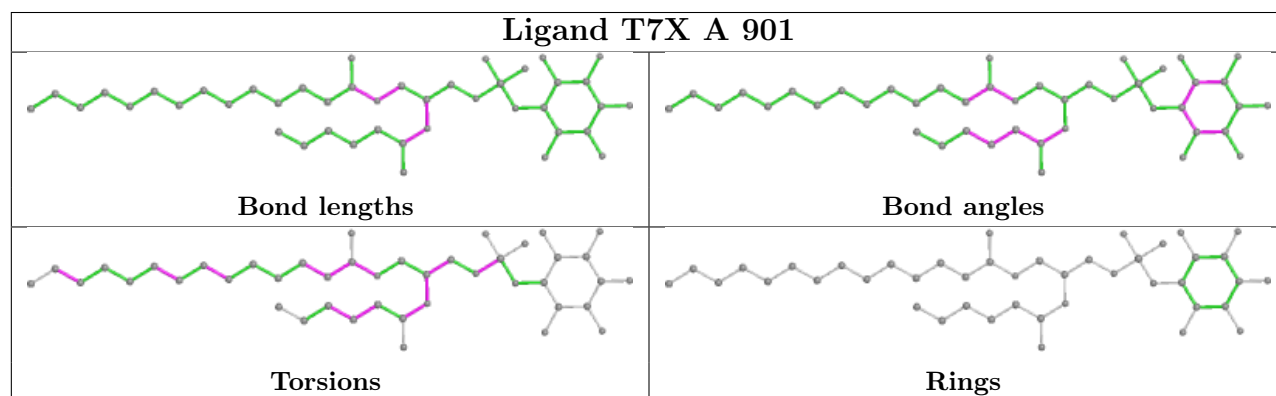
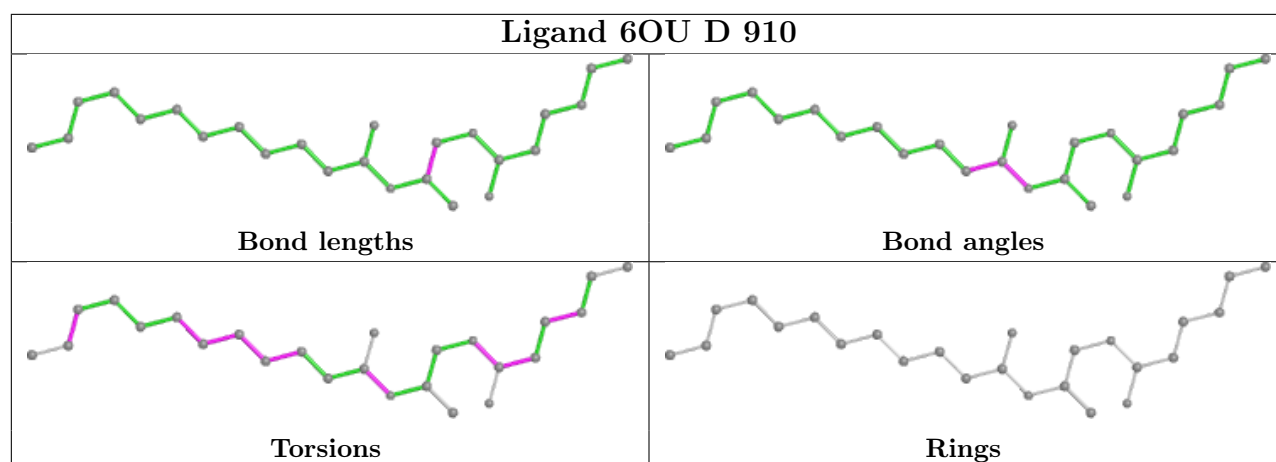




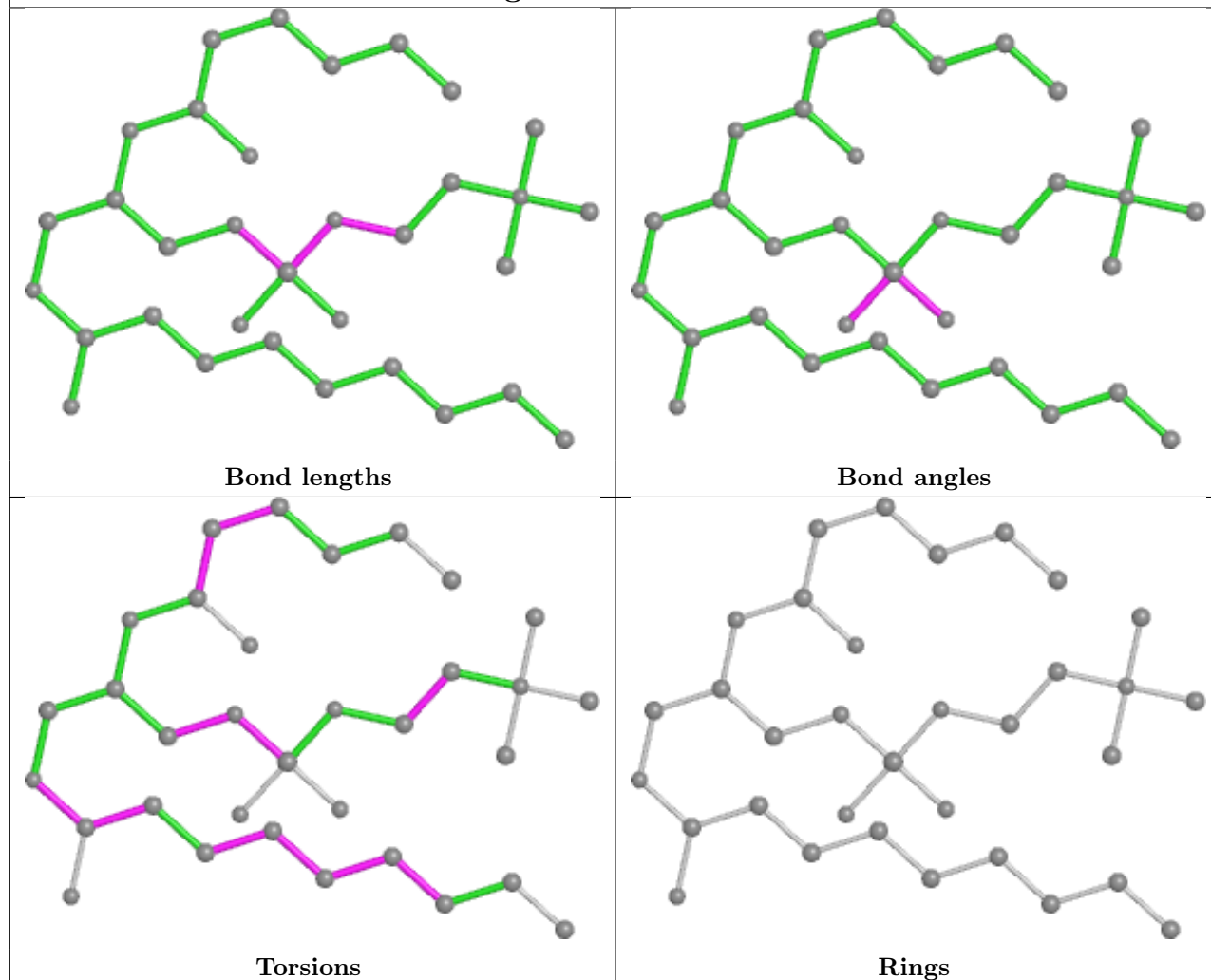




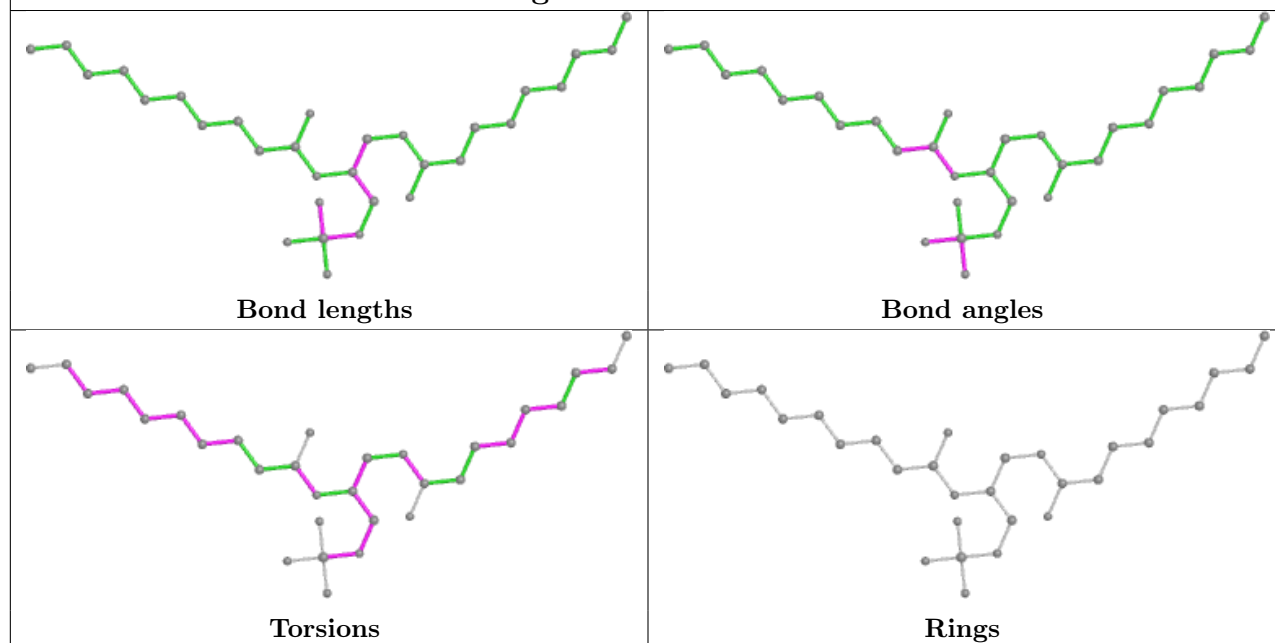


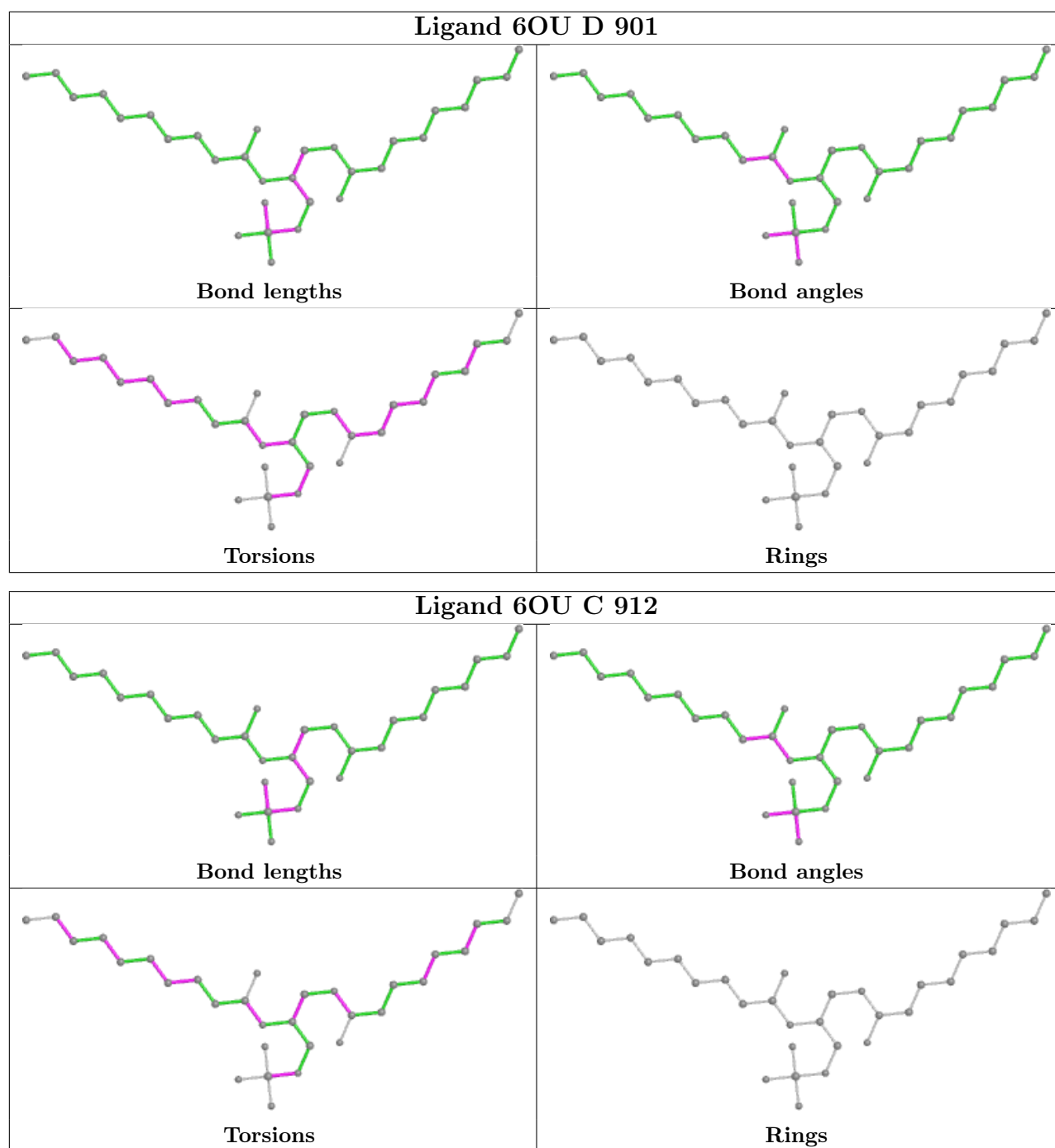


Ligand LBN B 905



Ligand 6OU A 908





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.

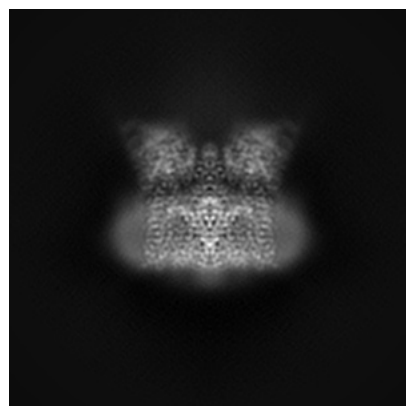
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-23473. These allow visual inspection of the internal detail of the map and identification of artifacts.

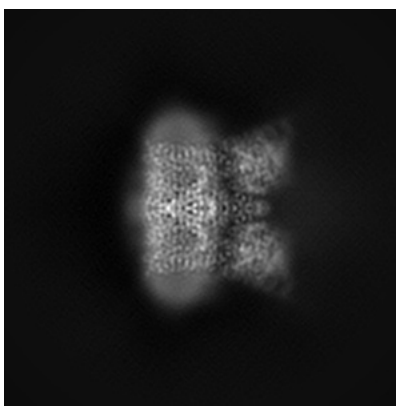
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

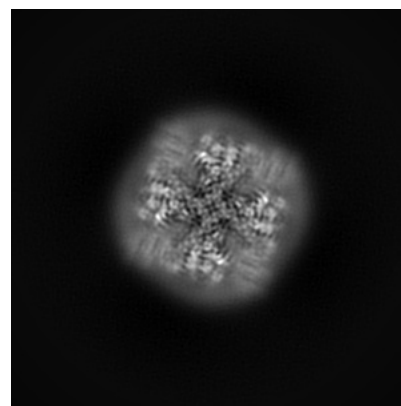
6.1.1 Primary map



X

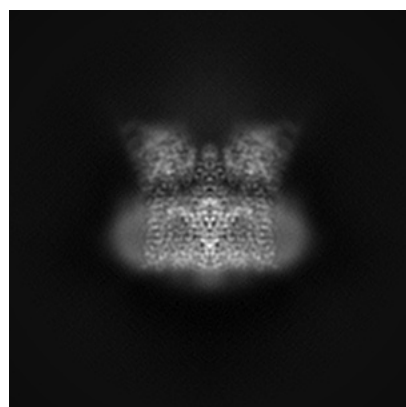


Y

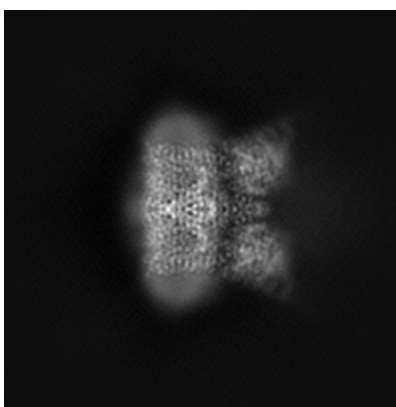


Z

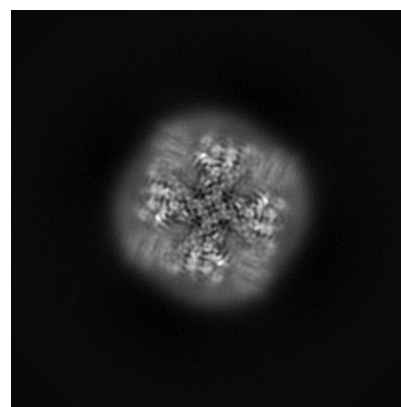
6.1.2 Raw map



X



Y

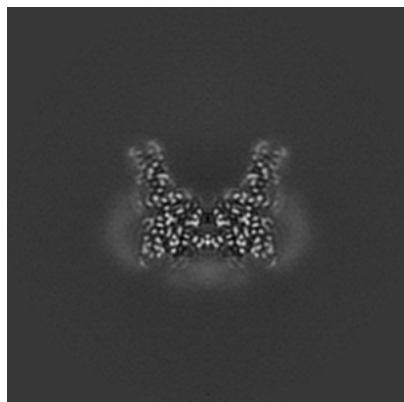


Z

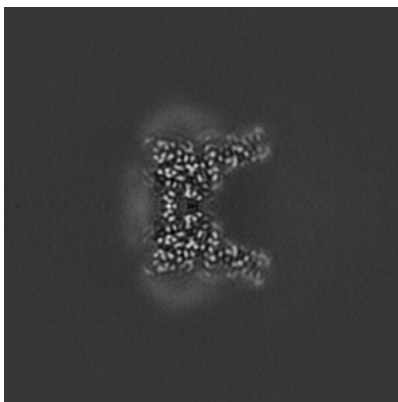
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

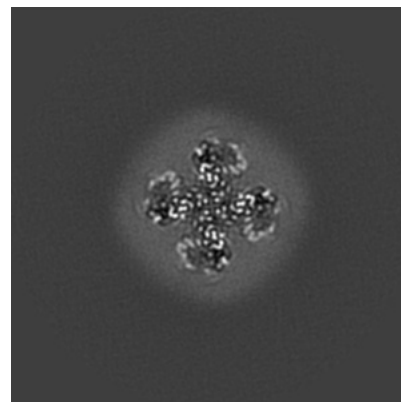
6.2.1 Primary map



X Index: 128

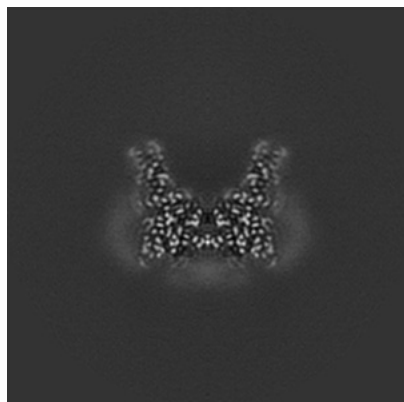


Y Index: 128

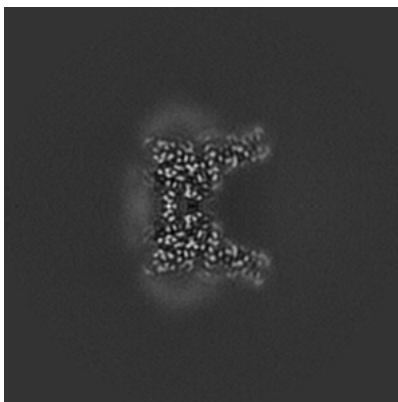


Z Index: 128

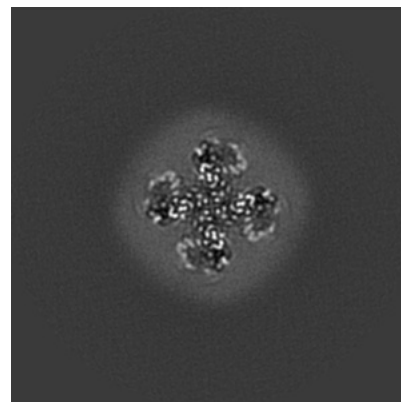
6.2.2 Raw map



X Index: 128



Y Index: 128

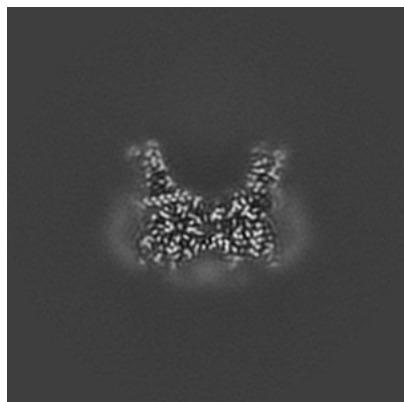


Z Index: 128

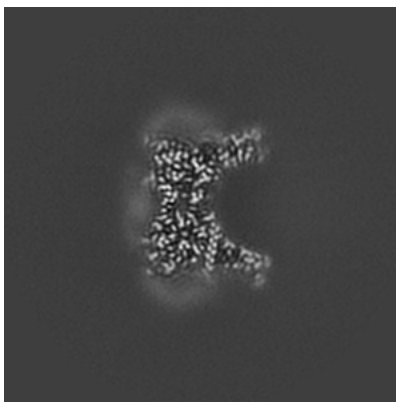
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

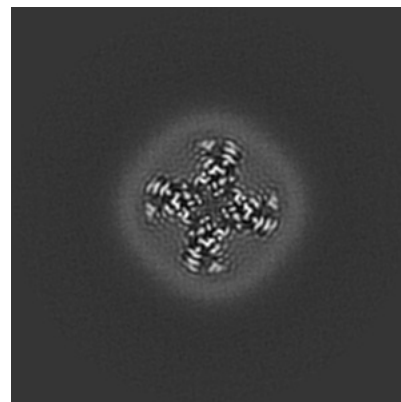
6.3.1 Primary map



X Index: 126

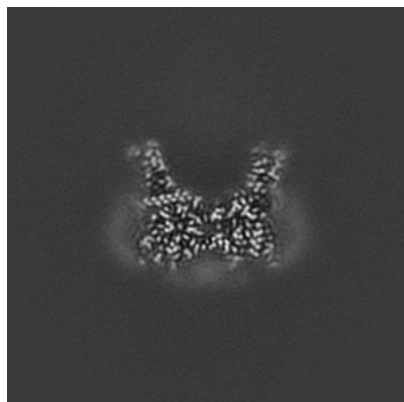


Y Index: 130

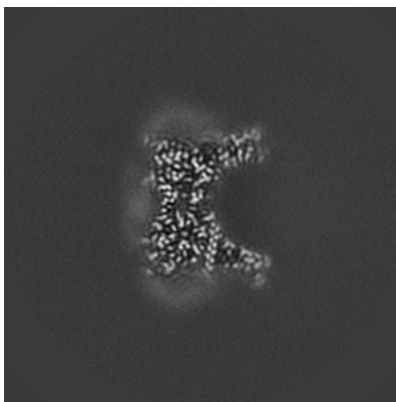


Z Index: 99

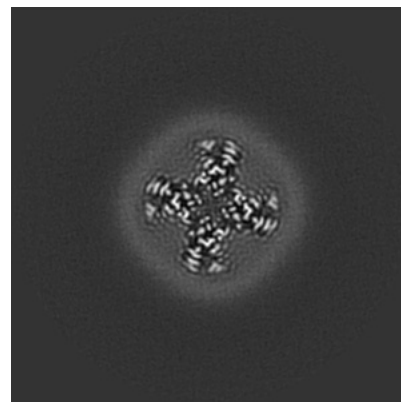
6.3.2 Raw map



X Index: 126



Y Index: 130

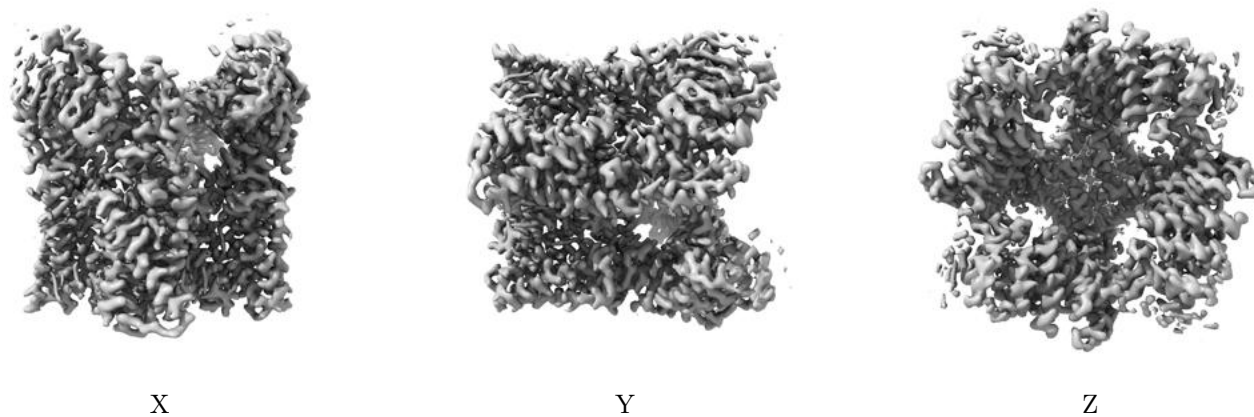


Z Index: 99

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

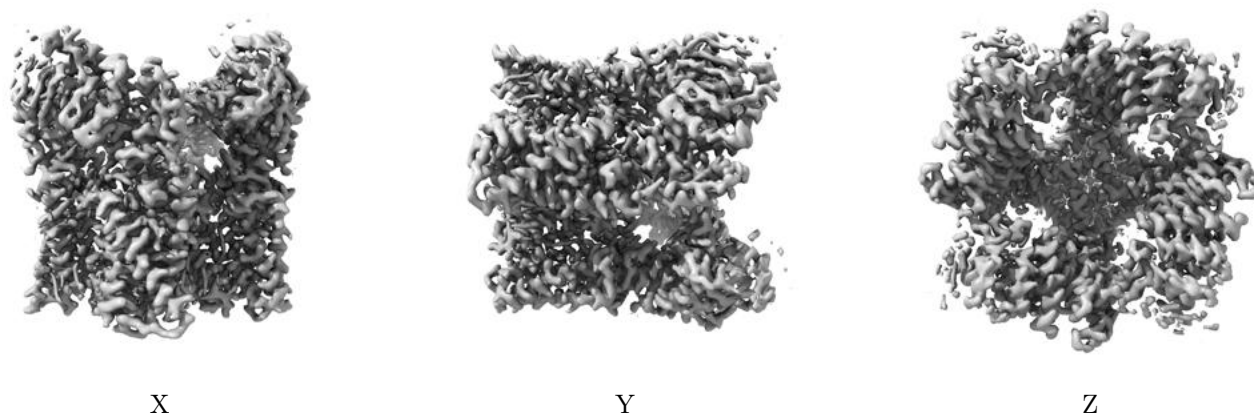
6.4 Orthogonal surface views [i](#)

6.4.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.02. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

6.4.2 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.

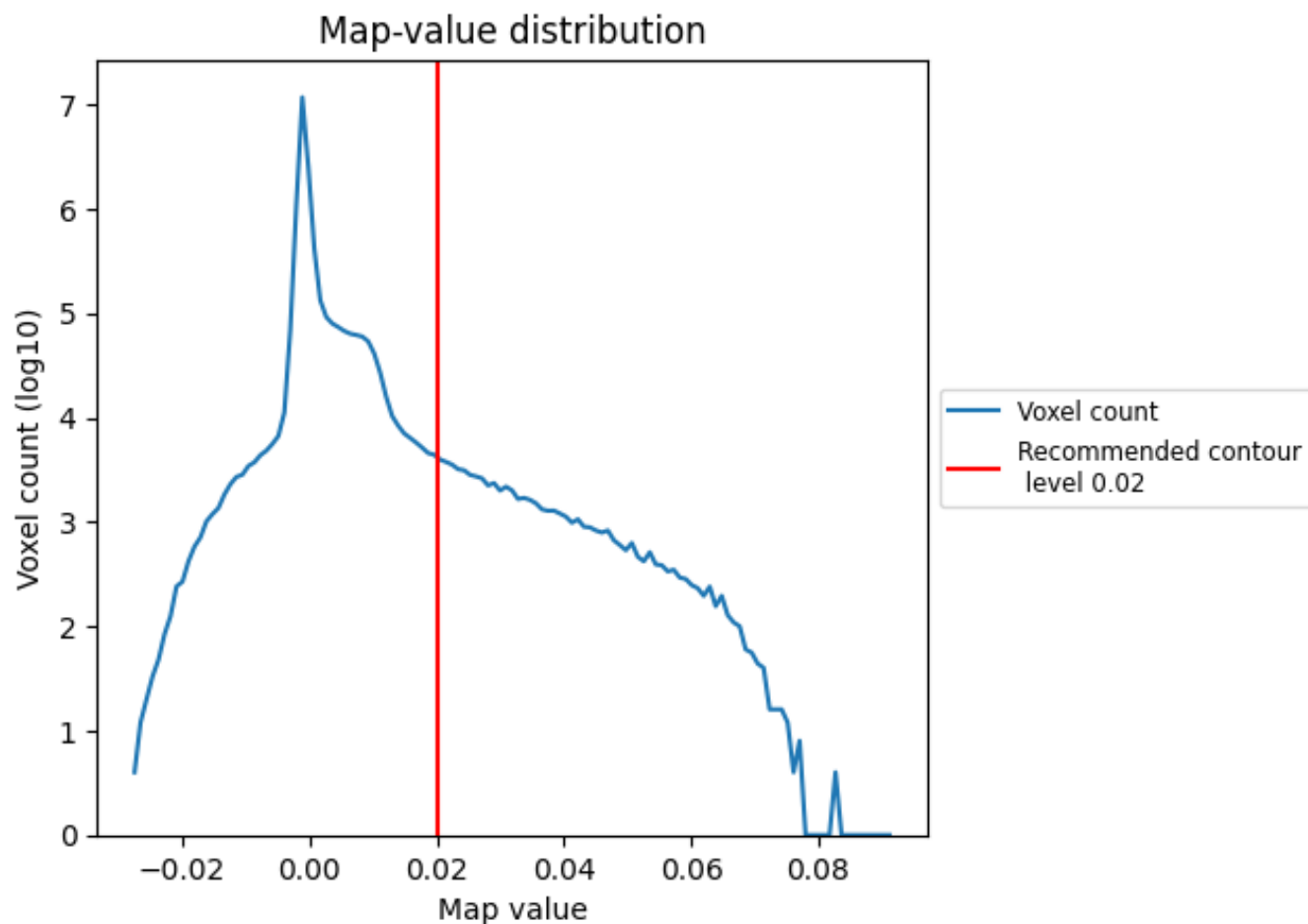
6.5 Mask visualisation [i](#)

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

7 Map analysis [i](#)

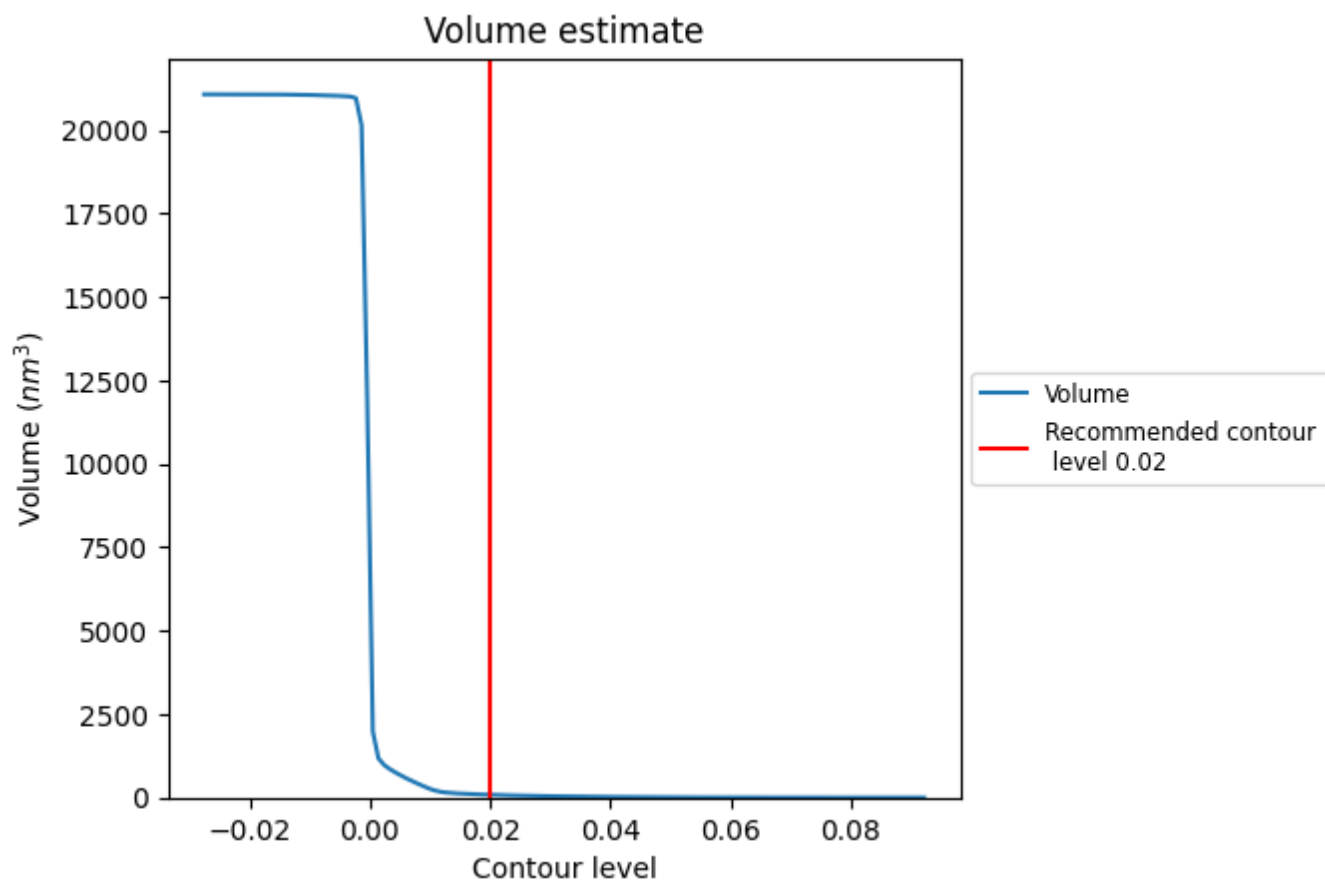
This section contains the results of statistical analysis of the map.

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.

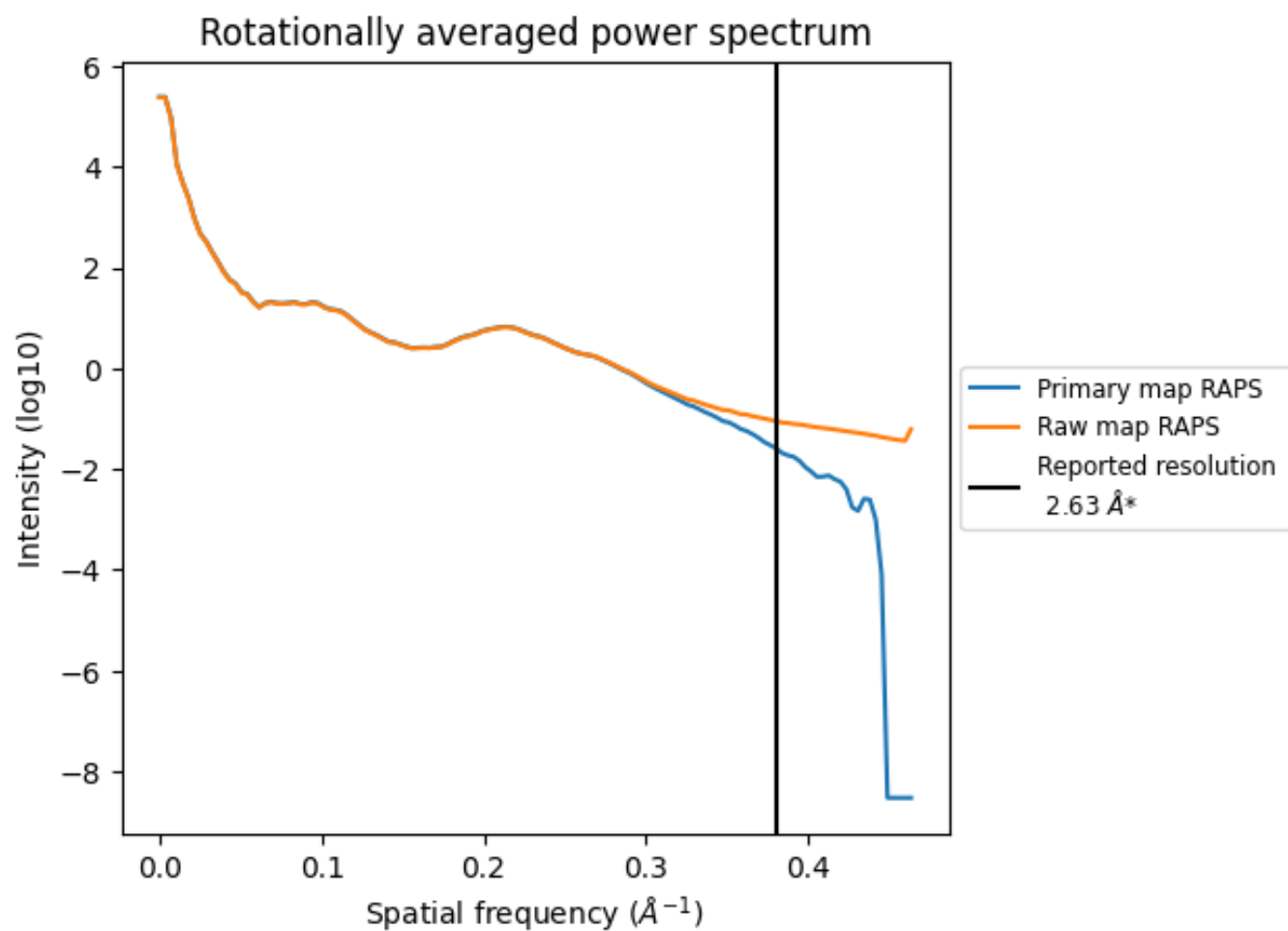
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 82 nm³; this corresponds to an approximate mass of 74 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 ⓘ

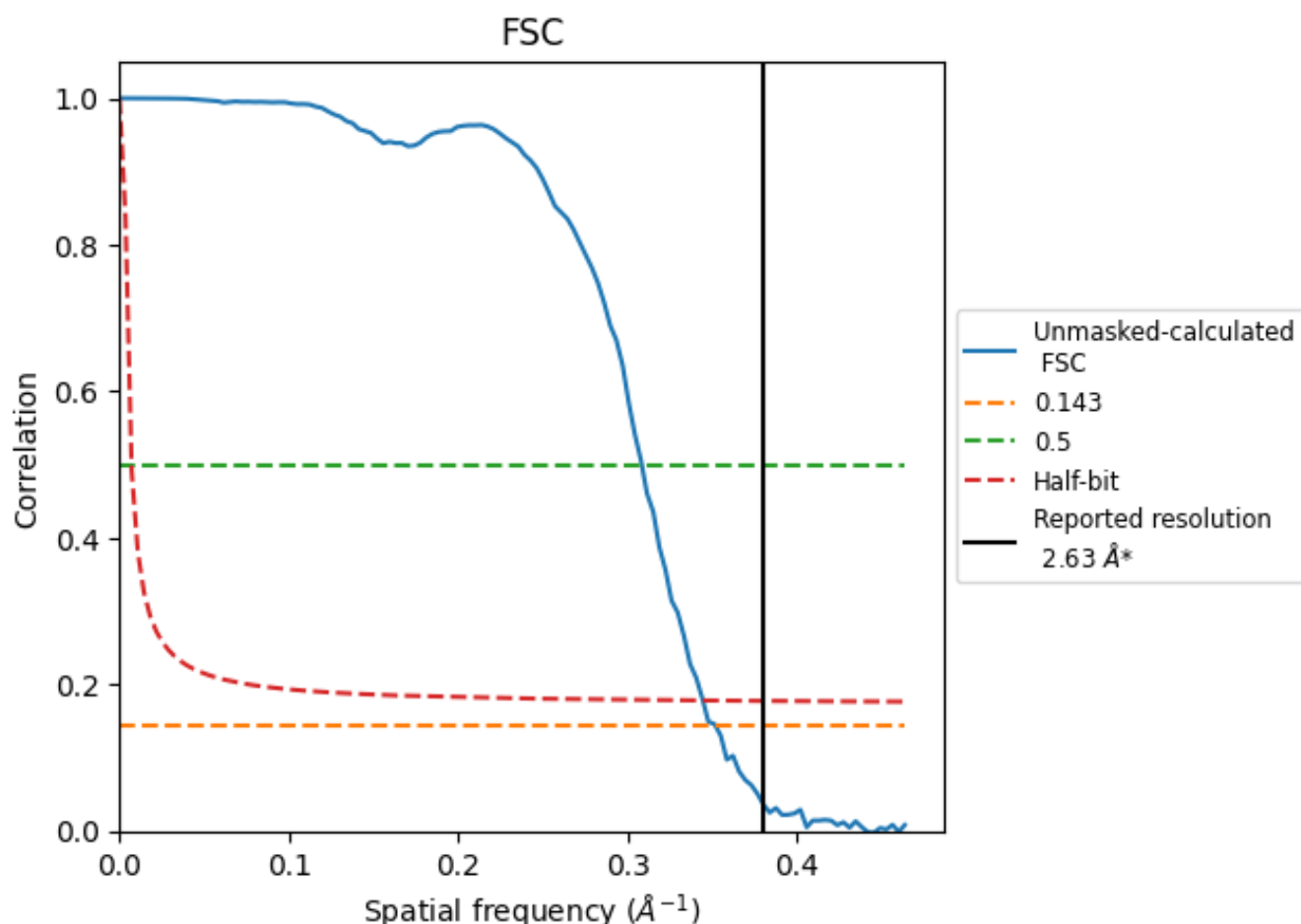


*Reported resolution corresponds to spatial frequency of 0.380 \AA^{-1}

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 0.380 \AA^{-1}

8.2 Resolution estimates [i](#)

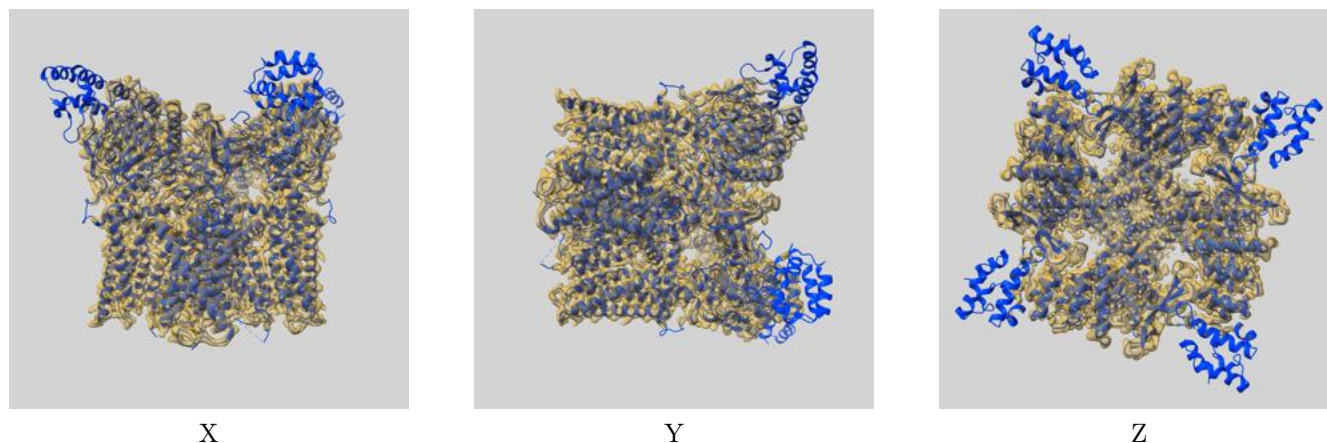
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	2.63	-	-
Author-provided FSC curve	-	-	-
Unmasked-calculated*	2.84	3.24	2.90

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

9 Map-model fit [i](#)

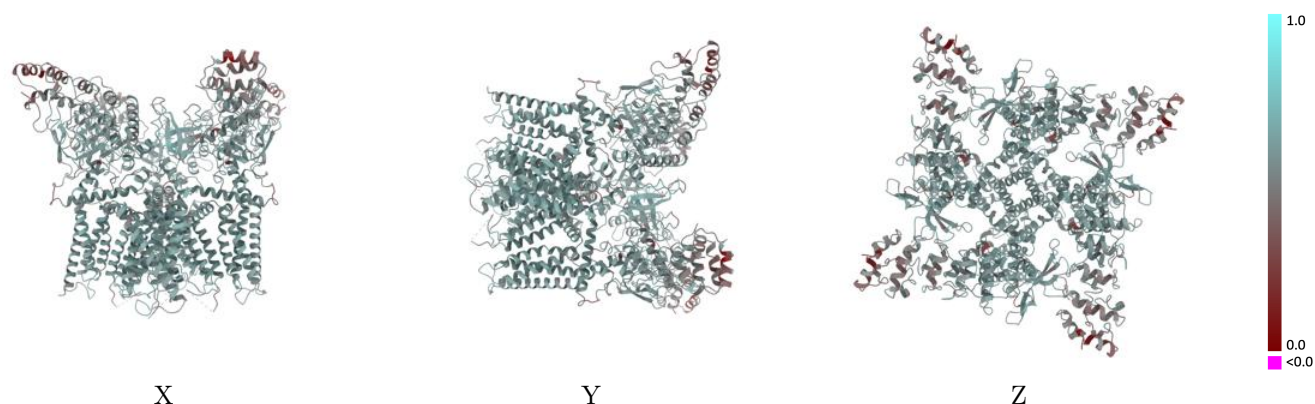
This section contains information regarding the fit between EMDB map EMD-23473 and PDB model 7LP9. Per-residue inclusion information can be found in section 3 on page 11.

9.1 Map-model overlay [i](#)



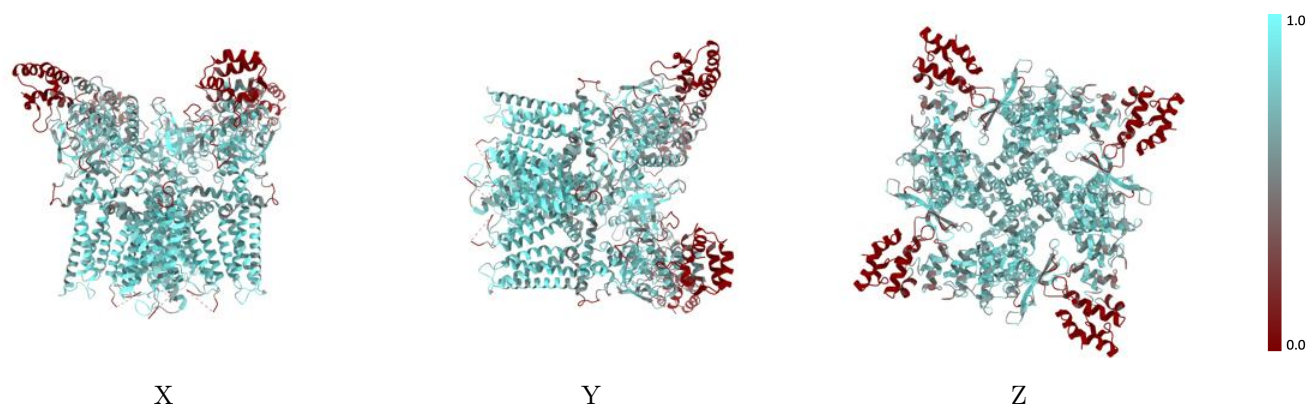
The images above show the 3D surface view of the map at the recommended contour level 0.02 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



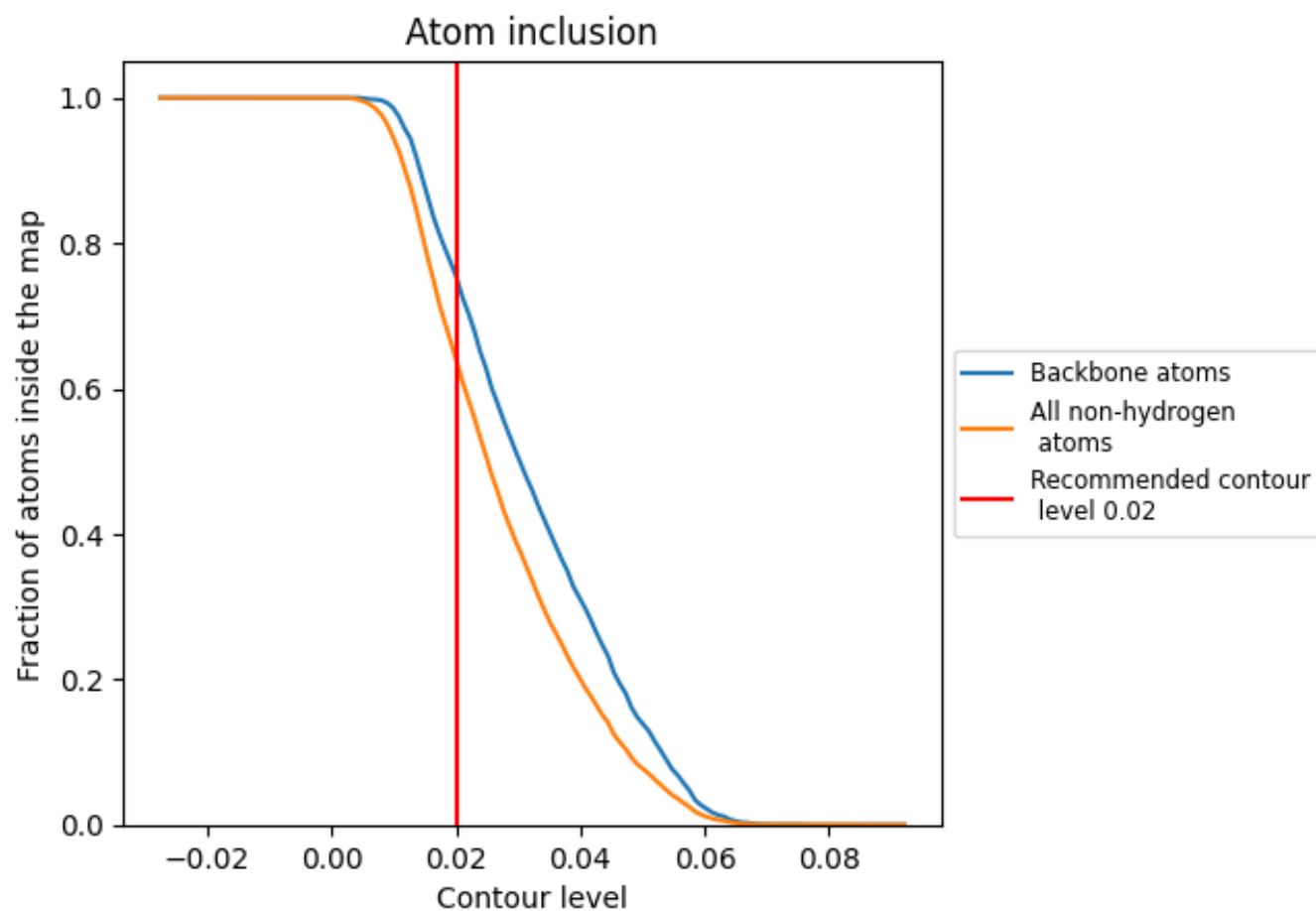
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.02).

9.4 Atom inclusion [i](#)



At the recommended contour level, 75% 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 (0.02) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	<div></div> 0.6407	<div></div> 0.5610
A	<div></div> 0.6432	<div></div> 0.5610
B	<div></div> 0.6416	<div></div> 0.5600
C	<div></div> 0.6375	<div></div> 0.5610
D	<div></div> 0.6405	<div></div> 0.5620

