Full wwPDB EM Validation Report ⓘ

Nov 19, 2022 – 02:18 PM EST

PDB ID	:	7LPC
EMDB ID	:	EMD-23476
Title	:	Cryo-EM structure of full-length TRPV1 at 48 degrees Celsius
Authors	:	Kwon, D.H.; Zhang, F.; Suo, Y.; Lee, S.-Y.
Deposited on	:	2021-02-11
Resolution	:	3.06 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:

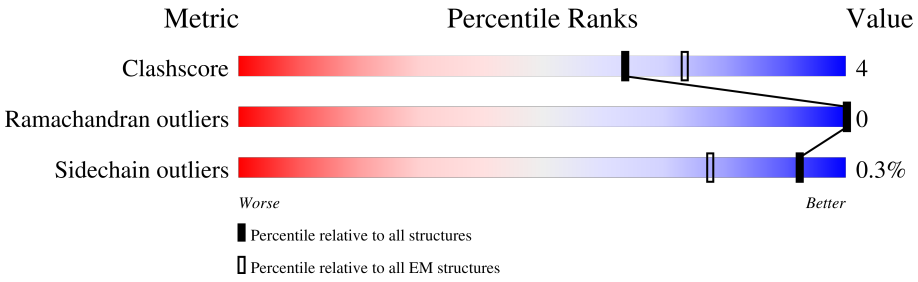
EMDB validation analysis	:	0.0.1.dev43
Mogul	:	1.8.5 (274361), CSD as541be (2020)
MolProbity	:	4.02b-467
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ	:	1.9.9
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.31.2

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
ELECTRON MICROSCOPY

The reported resolution of this entry is 3.06 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 <=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	17% 47% 5% 48%
1	B	868	17% 47% 5% 48%
1	C	868	17% 47% 6% 48%
1	D	868	17% 47% 5% 48%

2 Entry composition (i)

There are 5 unique types of molecules in this entry. The entry contains 15256 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	C	454	Total	C	N	O	S	0	0
			3526	2324	572	609	21		
1	A	454	Total	C	N	O	S	0	0
			3526	2324	572	609	21		
1	B	454	Total	C	N	O	S	0	0
			3526	2324	572	609	21		
1	D	454	Total	C	N	O	S	0	0
			3526	2324	572	609	21		

There are 120 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
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

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Chain	Residue	Modelled	Actual	Comment	Reference
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
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
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

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Chain	Residue	Modelled	Actual	Comment	Reference
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
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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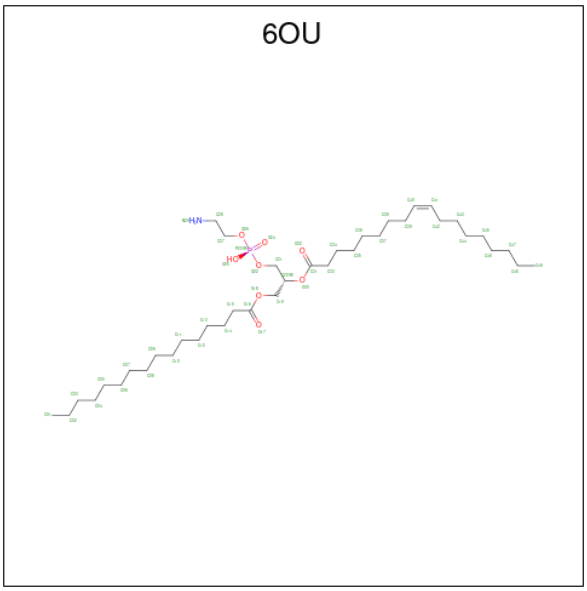
Chain	Residue	Modelled	Actual	Comment	Reference
D	854	ASP	-	expression tag	UNP O35433
D	855	ASP	-	expression tag	UNP O35433
D	856	ASP	-	expression tag	UNP O35433
D	857	LYS	-	expression tag	UNP O35433
D	858	ALA	-	expression tag	UNP O35433
D	859	HIS	-	expression tag	UNP O35433
D	860	HIS	-	expression tag	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 [(2 {R})-1-[2-azanylethoxy(oxidanyl)phosphoryl]oxy-3-hexadecanoyloxy-propan-2-yl] ({Z})-octadec-9-enoate (three-letter code: 6OU) (formula: $C_{39}H_{76}NO_8P$).



Mol	Chain	Residues	Atoms				AltConf
2	C	1	Total	C	O	P	0
			148	110	34	4	
2	C	1	Total	C	O	P	0
			148	110	34	4	
2	C	1	Total	C	O	P	0
			148	110	34	4	

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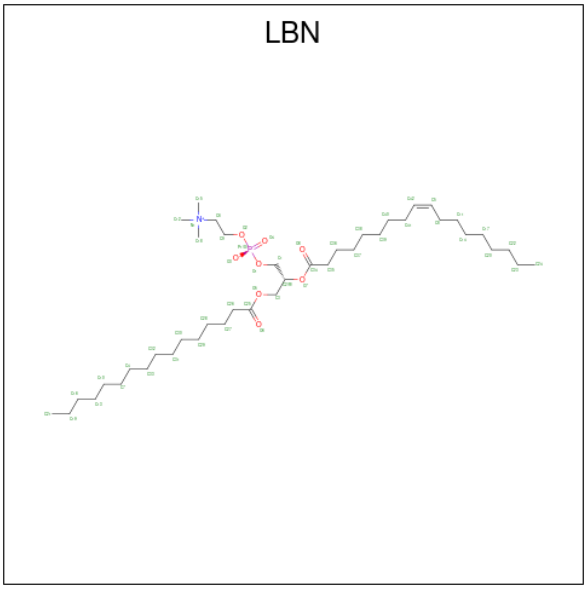
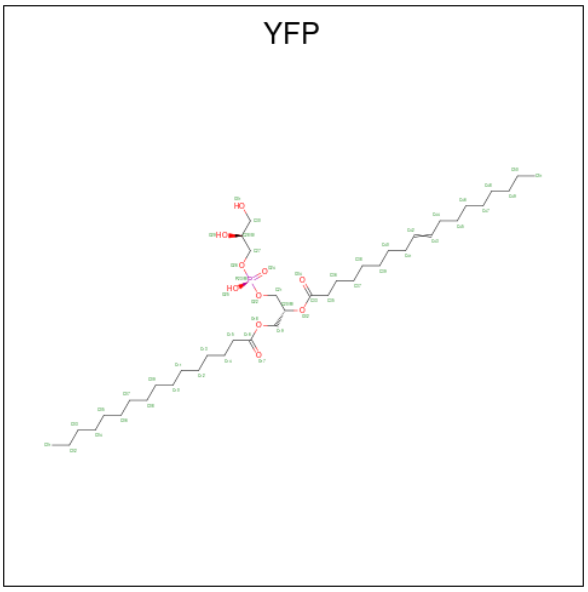
Mol	Chain	Residues	Atoms				AltConf
2	C	1	Total	C	O	P	0
			148	110	34	4	
2	C	1	Total	C	O	P	0
			148	110	34	4	
2	C	1	Total	C	O	P	0
			148	110	34	4	
2	A	1	Total	C	O	P	0
			148	110	34	4	
2	A	1	Total	C	O	P	0
			148	110	34	4	
2	A	1	Total	C	O	P	0
			148	110	34	4	
2	A	1	Total	C	O	P	0
			148	110	34	4	
2	A	1	Total	C	O	P	0
			148	110	34	4	
2	A	1	Total	C	O	P	0
			148	110	34	4	
2	B	1	Total	C	O	P	0
			148	110	34	4	
2	B	1	Total	C	O	P	0
			148	110	34	4	
2	B	1	Total	C	O	P	0
			148	110	34	4	
2	B	1	Total	C	O	P	0
			148	110	34	4	
2	B	1	Total	C	O	P	0
			148	110	34	4	
2	B	1	Total	C	O	P	0
			148	110	34	4	
2	D	1	Total	C	O	P	0
			148	110	34	4	
2	D	1	Total	C	O	P	0
			148	110	34	4	
2	D	1	Total	C	O	P	0
			148	110	34	4	
2	D	1	Total	C	O	P	0
			148	110	34	4	
2	D	1	Total	C	O	P	0
			148	110	34	4	
2	D	1	Total	C	O	P	0
			148	110	34	4	

- Molecule 3 is 1-palmitoyl-2-oleoyl-sn-glycero-3-phosphocholine (three-letter code: LBN) (formula: $C_{42}H_{82}NO_8P$).



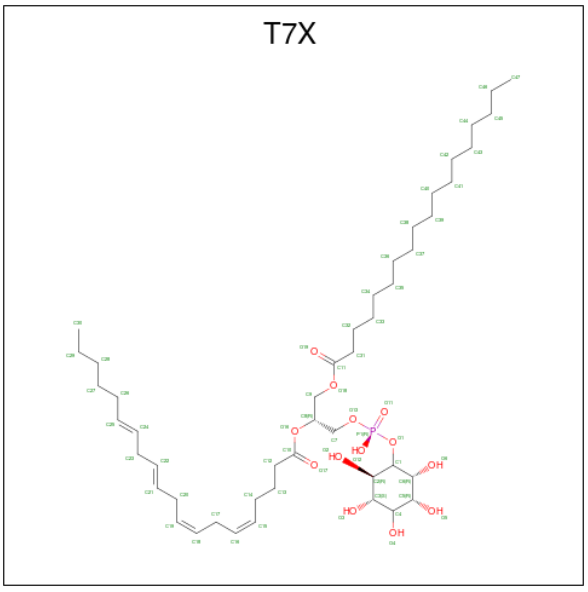
Mol	Chain	Residues	Atoms					AltConf
3	C	1	Total	C	N	O	P	0
			65	50	1	13	1	
3	C	1	Total	C	N	O	P	0
			65	50	1	13	1	
3	A	1	Total	C	N	O	P	0
			65	50	1	13	1	
3	A	1	Total	C	N	O	P	0
			65	50	1	13	1	
3	B	1	Total	C	N	O	P	0
			65	50	1	13	1	
3	B	1	Total	C	N	O	P	0
			65	50	1	13	1	
3	D	1	Total	C	N	O	P	0
			65	50	1	13	1	
3	D	1	Total	C	N	O	P	0
			65	50	1	13	1	

- Molecule 4 is 1-palmitoyl-2-oleoyl-sn-glycero-3-phosphoglycerol (three-letter code: YFP) (formula: $C_{40}H_{77}O_{10}P$).



Mol	Chain	Residues	Atoms				AltConf
4	C	1	Total	C	O	P	0
			32	23	8	1	
4	A	1	Total	C	O	P	0
			32	23	8	1	
4	B	1	Total	C	O	P	0
			32	23	8	1	
4	D	1	Total	C	O	P	0
			32	23	8	1	

- Molecule 5 is Phosphatidylinositol (three-letter code: T7X) (formula: $C_{47}H_{83}O_{13}P$).

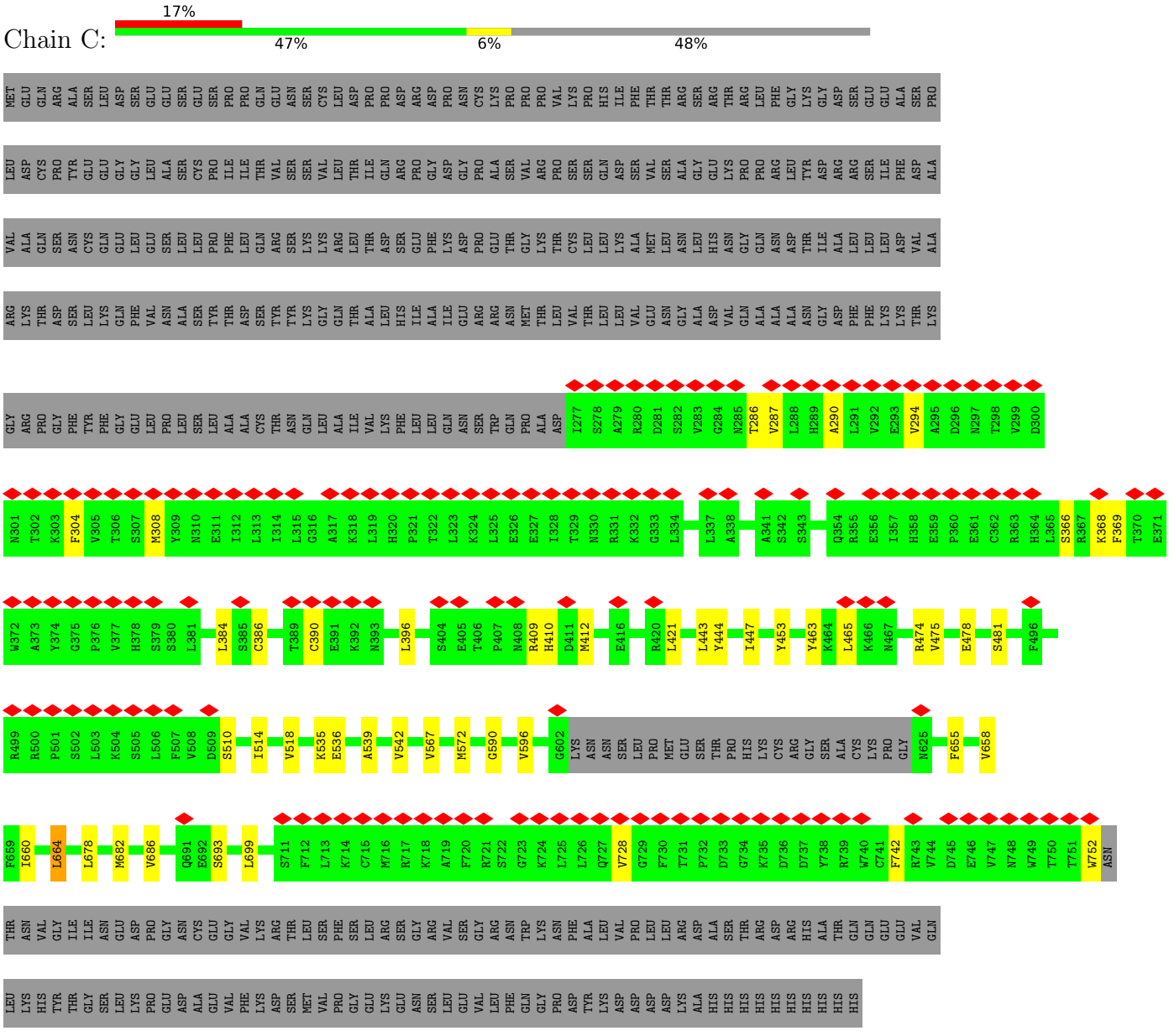


Mol	Chain	Residues	Atoms				AltConf
5	C	1	Total	C	O	P	0
			43	29	13	1	
5	A	1	Total	C	O	P	0
			43	29	13	1	
5	B	1	Total	C	O	P	0
			43	29	13	1	
5	D	1	Total	C	O	P	0
			43	29	13	1	

3 Residue-property plots (i)

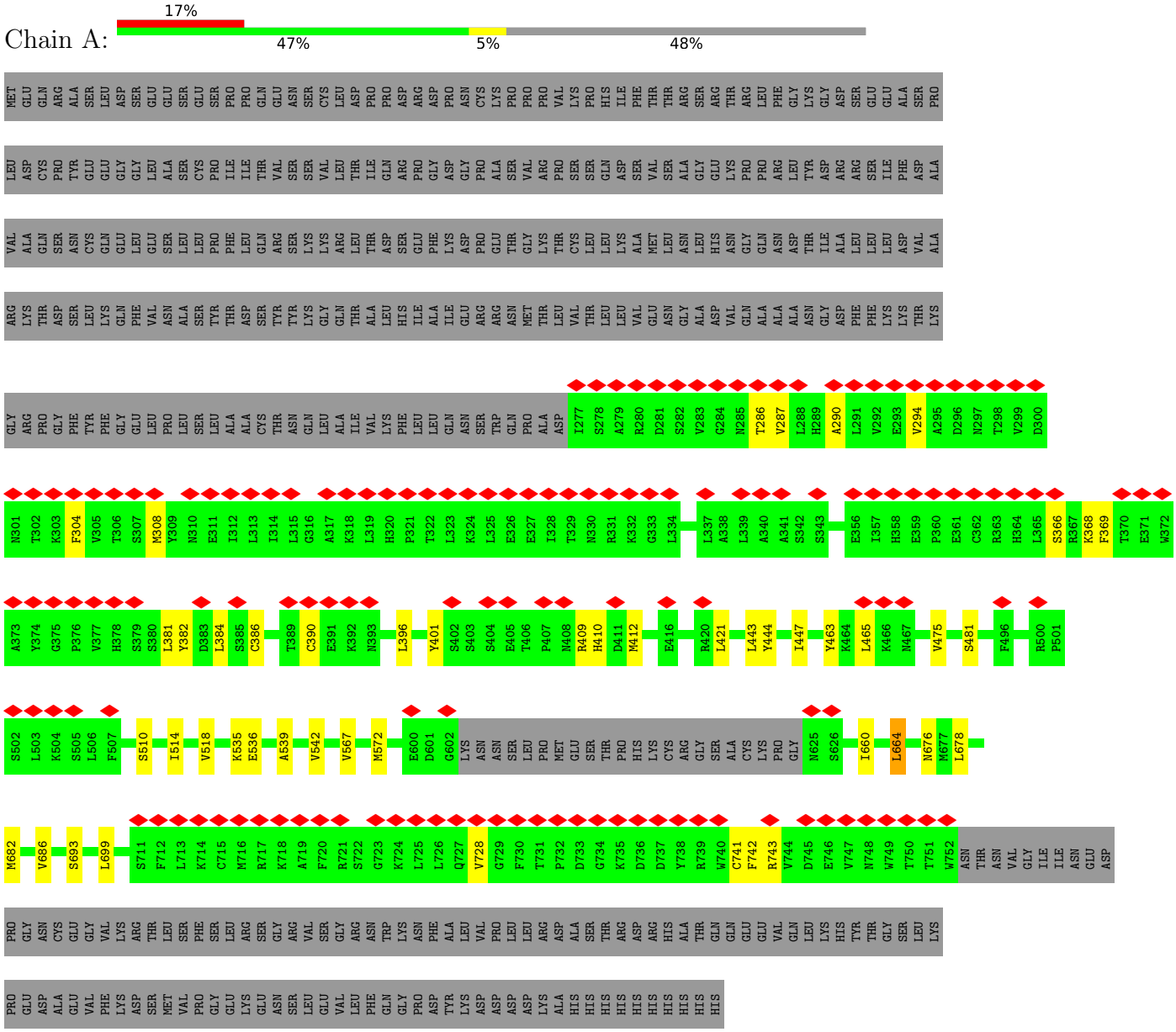
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion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



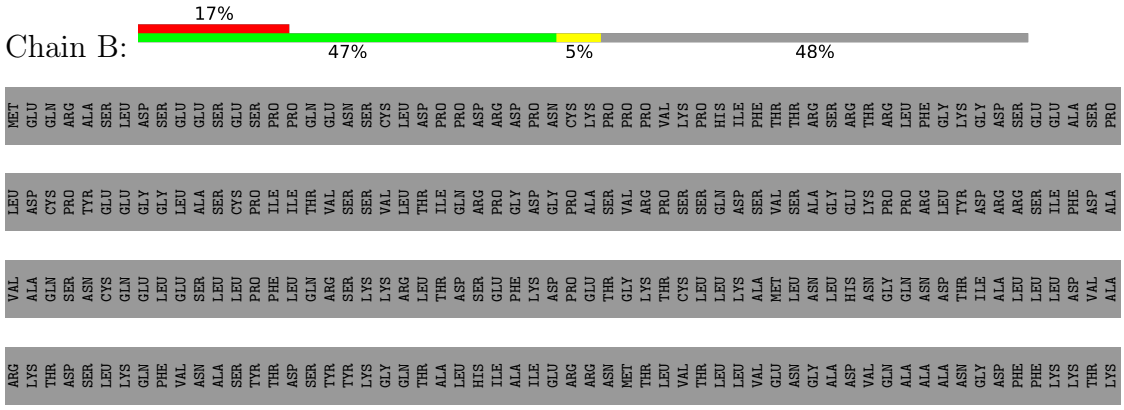
• Molecule 1: Transient receptor potential cation channel subfamily V member 1

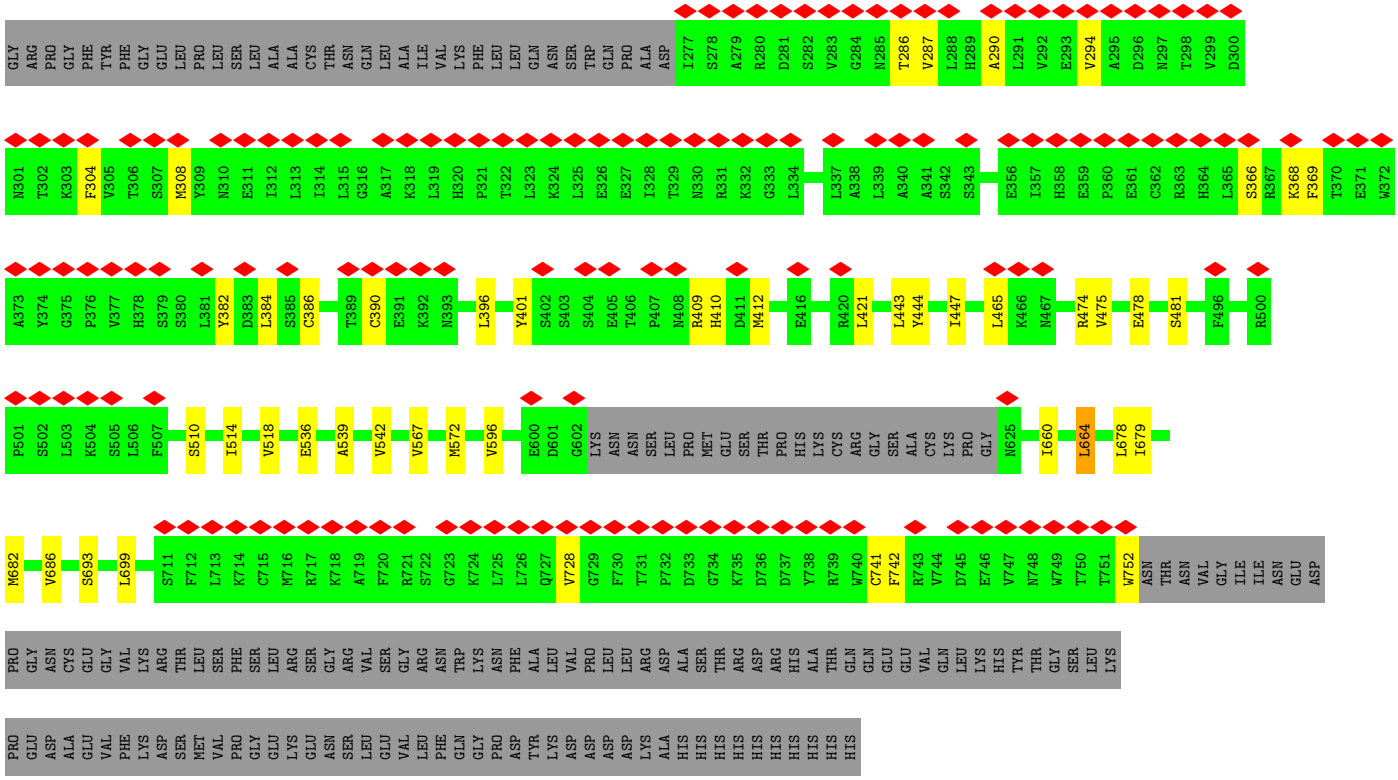
Chain A:



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

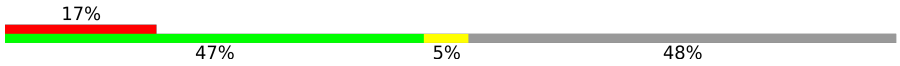
Chain B:

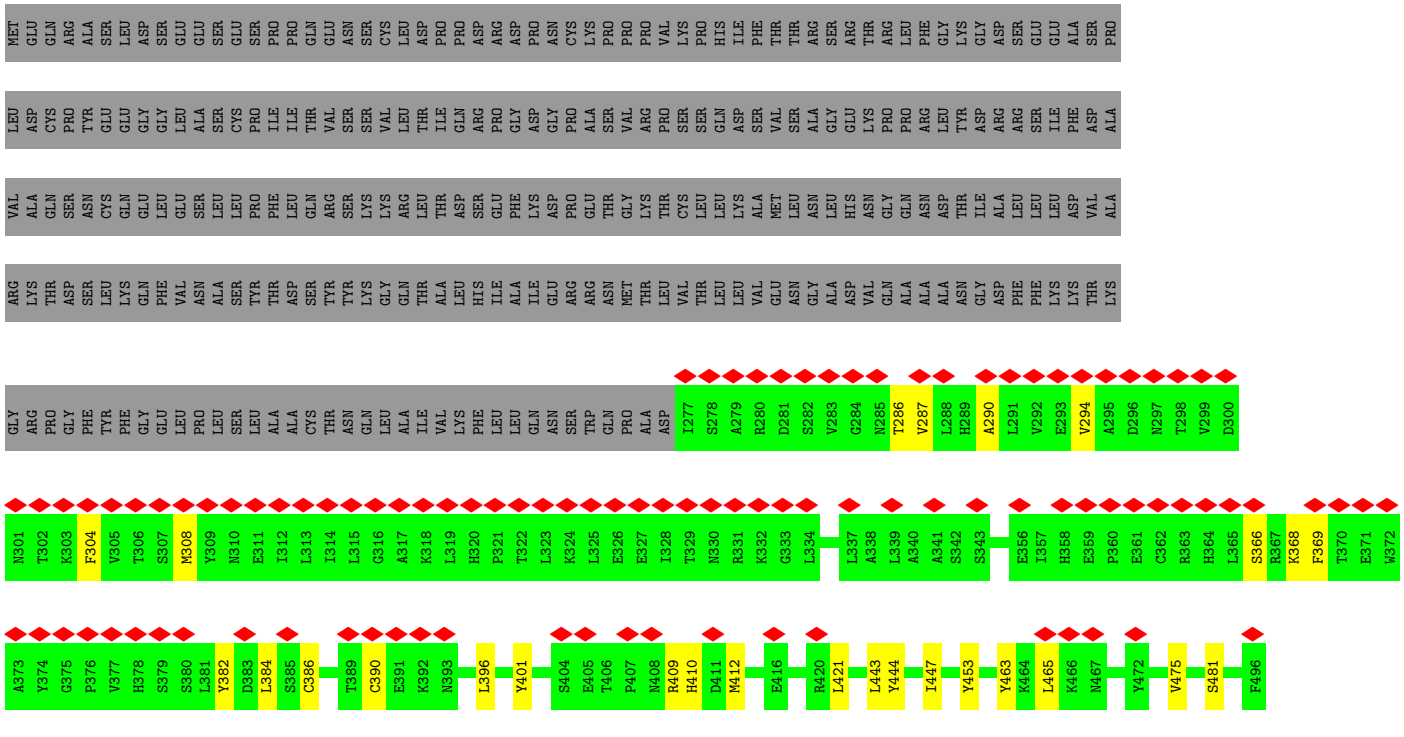


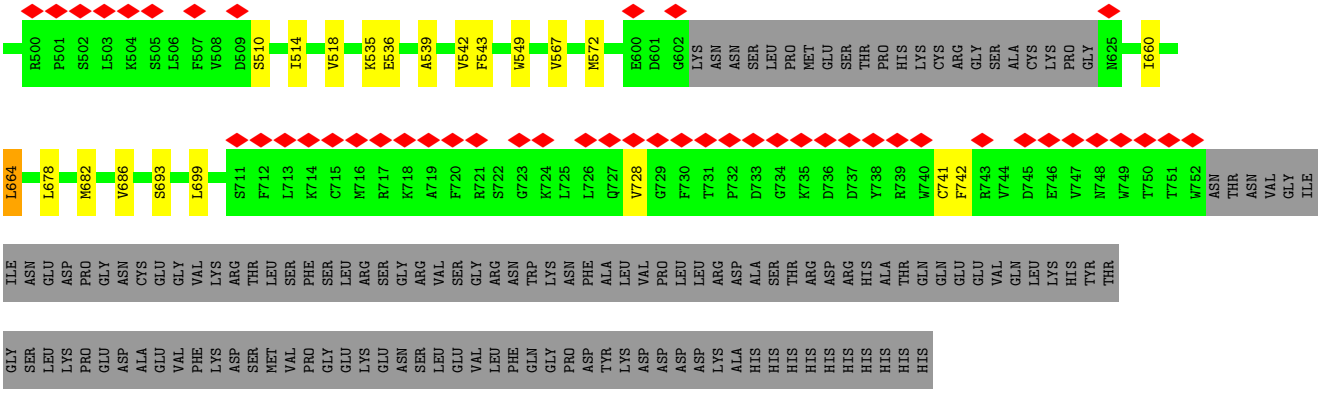


• Molecule 1: Transient receptor potential cation channel subfamily V member 1

Chain D:






R500 P501 S502 L503 K504 S505 L506 F507 V508 D509 S510 I514 V518 K535 E536 A539 V542 F543 W549 V567 M572 E600 D601 G602 LYS ASN ASN SER LEU PRO MET GLU SER THR PRO HIS LYS CYS ARG GLY SER ALA CYS LYS PRO GLY N625 I660
L664 L678 M682 V686 S693 L699 S711 F712 L713 K714 C715 M716 R717 K718 A719 F720 R721 S722 G723 K724 L725 L726 Q727 V728 G729 F730 T731 P732 D733 G734 K735 D736 D737 Y738 R739 W740 C741 F742 R743 V744 D745 E746 V747 N748 W749 T750 T751 W752 ASN THR ASN VAL GLY ILE
ILE ASN GLU ASP PRO GLY ASN CYS GLU GLY VAL LYS ARG THR LEU SER PHE SER LEU ARG SER GLY ARG VAL SER GLY ARG ASN TRP LYS ASN PHE ALA LEU VAL PRO LEU LEU ARG ASP ALA SER THR ARG ASP ARG HIS ALA THR GLN GLN GLU GLU VAL GLN LEU LYS HIS TYR THR
GLY SER LEU LYS PRO GLU ASP ALA GLU VAL PHE LYS ASP SER MET VAL PRO GLY GLU LYS GLU ASN SER LEU GLU VAL LEU PHE GLN GLY PRO ASP TYR LYS ASP ASP ASP ASP LYS ALA HIS HIS HIS HIS HIS HIS HIS HIS HIS HIS

4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	29611	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 ($e^-/Å^2$)	50	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	0.266	Depositor
Minimum map value	-0.145	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.007	Depositor
Recommended contour level	0.04	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, 6OU, LBN, YFP

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	0.45	0/3615	0.48	0/4914
1	B	0.45	0/3615	0.48	0/4914
1	C	0.45	0/3615	0.48	0/4914
1	D	0.45	0/3615	0.48	0/4914
All	All	0.45	0/14460	0.48	0/19656

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

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	3526	0	3396	31	0
1	B	3526	0	3396	34	0
1	C	3526	0	3396	36	0
1	D	3526	0	3396	32	0
2	A	148	0	0	1	0
2	B	148	0	0	2	0
2	C	148	0	0	2	0
2	D	148	0	0	1	0
3	A	65	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	B	65	0	0	0	0
3	C	65	0	0	0	0
3	D	65	0	0	0	0
4	A	32	0	0	0	0
4	B	32	0	0	0	0
4	C	32	0	0	0	0
4	D	32	0	0	0	0
5	A	43	0	0	0	0
5	B	43	0	0	0	0
5	C	43	0	0	0	0
5	D	43	0	0	0	0
All	All	15256	0	13584	125	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 (125) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:536:GLU:N	1:A:536:GLU:OE1	2.19	0.76
1:B:536:GLU:N	1:B:536:GLU:OE1	2.19	0.75
1:D:536:GLU:N	1:D:536:GLU:OE1	2.19	0.75
1:C:536:GLU:N	1:C:536:GLU:OE1	2.19	0.74
1:C:660:ILE:O	1:C:664:LEU:HD12	1.94	0.68
1:B:660:ILE:O	1:B:664:LEU:HD12	1.94	0.67
1:A:660:ILE:O	1:A:664:LEU:HD12	1.94	0.66
1:D:660:ILE:O	1:D:664:LEU:HD12	1.94	0.66
1:C:369:PHE:CE2	1:C:728:VAL:HG11	2.31	0.66
1:B:369:PHE:CE2	1:B:728:VAL:HG11	2.31	0.65
1:D:369:PHE:CE2	1:D:728:VAL:HG11	2.31	0.65
1:A:369:PHE:CE2	1:A:728:VAL:HG11	2.31	0.64
1:A:384:LEU:HD11	1:A:742:PHE:HB2	1.79	0.64
1:C:384:LEU:HD11	1:C:742:PHE:HB2	1.79	0.64
1:D:384:LEU:HD11	1:D:742:PHE:HB2	1.79	0.63
1:B:384:LEU:HD11	1:B:742:PHE:HB2	1.79	0.62
1:C:596:VAL:HG11	1:D:453:TYR:HE1	1.68	0.58
1:C:369:PHE:CD2	1:C:728:VAL:HG11	2.39	0.57
1:B:369:PHE:CD2	1:B:728:VAL:HG11	2.39	0.57
1:D:369:PHE:CD2	1:D:728:VAL:HG11	2.39	0.57
1:A:369:PHE:CD2	1:A:728:VAL:HG11	2.39	0.57
1:A:676:ASN:HB3	1:B:679:ILE:HG12	1.88	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:752:TRP:HZ2	1:B:304:PHE:CE2	2.25	0.55
1:D:290:ALA:O	1:D:294:VAL:HG23	2.08	0.54
1:C:290:ALA:O	1:C:294:VAL:HG23	2.08	0.54
1:A:304:PHE:CE2	1:A:308:MET:SD	3.02	0.54
1:B:304:PHE:CE2	1:B:308:MET:SD	3.02	0.53
1:A:290:ALA:O	1:A:294:VAL:HG23	2.08	0.53
1:D:304:PHE:CE2	1:D:308:MET:SD	3.02	0.53
1:C:304:PHE:CE2	1:C:308:MET:SD	3.02	0.53
1:A:409:ARG:HA	1:A:412:MET:HG3	1.91	0.53
1:B:290:ALA:O	1:B:294:VAL:HG23	2.08	0.53
1:A:539:ALA:O	1:A:542:VAL:HG22	2.09	0.53
1:B:409:ARG:HA	1:B:412:MET:HG3	1.91	0.53
1:B:539:ALA:O	1:B:542:VAL:HG22	2.09	0.52
1:D:409:ARG:HA	1:D:412:MET:HG3	1.91	0.52
2:C:901:6OU:O17	2:B:906:6OU:C33	2.58	0.52
1:C:409:ARG:HA	1:C:412:MET:HG3	1.91	0.51
1:C:539:ALA:O	1:C:542:VAL:HG22	2.09	0.51
1:D:539:ALA:O	1:D:542:VAL:HG22	2.09	0.51
1:C:596:VAL:HG11	1:D:453:TYR:CE1	2.45	0.51
2:C:906:6OU:C33	2:D:901:6OU:O17	2.60	0.50
1:B:572:MET:HE1	1:B:686:VAL:HG23	1.94	0.49
1:C:514:ILE:O	1:C:518:VAL:HG23	2.13	0.49
1:D:514:ILE:O	1:D:518:VAL:HG23	2.13	0.49
1:B:514:ILE:O	1:B:518:VAL:HG23	2.13	0.49
1:D:366:SER:OG	1:D:369:PHE:HE1	1.96	0.49
1:A:366:SER:OG	1:A:369:PHE:HE1	1.96	0.48
1:A:514:ILE:O	1:A:518:VAL:HG23	2.13	0.48
1:C:368:LYS:C	1:C:369:PHE:CD1	2.87	0.48
1:A:510:SER:O	1:A:514:ILE:HD12	2.14	0.48
1:C:465:LEU:HD13	1:C:475:VAL:HG21	1.95	0.48
1:C:510:SER:O	1:C:514:ILE:HD12	2.14	0.48
1:D:465:LEU:HD13	1:D:475:VAL:HG21	1.95	0.48
1:C:366:SER:OG	1:C:369:PHE:HE1	1.96	0.48
1:B:465:LEU:HD13	1:B:475:VAL:HG21	1.95	0.48
1:B:366:SER:OG	1:B:369:PHE:HE1	1.96	0.48
1:B:368:LYS:C	1:B:369:PHE:CD1	2.87	0.47
1:A:368:LYS:C	1:A:369:PHE:CD1	2.87	0.47
1:B:510:SER:O	1:B:514:ILE:HD12	2.14	0.47
1:D:368:LYS:C	1:D:369:PHE:CD1	2.87	0.47
1:A:678:LEU:O	1:A:682:MET:HG3	2.15	0.47
1:D:510:SER:O	1:D:514:ILE:HD12	2.14	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:906:6OU:C33	2:B:901:6OU:O17	2.63	0.47
1:B:678:LEU:O	1:B:682:MET:HG3	2.15	0.47
1:D:678:LEU:O	1:D:682:MET:HG3	2.15	0.47
1:A:465:LEU:HD13	1:A:475:VAL:HG21	1.95	0.47
1:C:453:TYR:HE1	1:B:596:VAL:HG11	1.80	0.46
1:C:678:LEU:O	1:C:682:MET:HG3	2.15	0.46
1:A:304:PHE:CE2	1:B:752:TRP:HZ2	2.33	0.46
1:A:572:MET:HE1	1:A:686:VAL:HG23	1.97	0.46
1:D:572:MET:HE1	1:D:686:VAL:HG23	1.98	0.46
1:C:590:GLY:HA2	1:D:549:TRP:CD1	2.52	0.45
1:A:396:LEU:HD11	1:A:421:LEU:HD22	1.98	0.45
1:C:655:PHE:CZ	1:D:536:GLU:HA	2.51	0.45
1:D:396:LEU:HD11	1:D:421:LEU:HD22	1.98	0.45
1:D:567:VAL:HG11	1:D:693:SER:HA	1.98	0.45
1:C:658:VAL:HG13	1:D:543:PHE:CZ	2.52	0.45
1:B:567:VAL:HG11	1:B:693:SER:HA	1.99	0.45
1:A:567:VAL:HG11	1:A:693:SER:HA	1.98	0.44
1:C:396:LEU:HD11	1:C:421:LEU:HD22	1.98	0.44
1:B:396:LEU:HD11	1:B:421:LEU:HD22	1.98	0.44
1:D:443:LEU:O	1:D:447:ILE:HG12	2.18	0.44
1:B:443:LEU:O	1:B:447:ILE:HG12	2.18	0.44
1:C:567:VAL:HG11	1:C:693:SER:HA	1.99	0.44
1:C:443:LEU:O	1:C:447:ILE:HG12	2.18	0.43
1:A:443:LEU:O	1:A:447:ILE:HG12	2.18	0.43
1:A:286:THR:HG22	1:A:287:VAL:N	2.34	0.43
1:B:286:THR:HG22	1:B:287:VAL:N	2.34	0.43
1:A:286:THR:HG22	1:A:287:VAL:H	1.83	0.43
1:D:286:THR:HG22	1:D:287:VAL:H	1.83	0.42
1:D:286:THR:HG22	1:D:287:VAL:N	2.34	0.42
1:C:286:THR:HG22	1:C:287:VAL:N	2.34	0.42
1:C:286:THR:HG22	1:C:287:VAL:H	1.83	0.42
1:C:386:CYS:HA	1:C:390:CYS:HB2	2.02	0.42
1:B:286:THR:HG22	1:B:287:VAL:H	1.83	0.42
1:C:444:TYR:HE1	1:C:481:SER:HA	1.85	0.42
1:C:752:TRP:CZ2	1:B:304:PHE:CE2	3.08	0.42
1:D:386:CYS:HA	1:D:390:CYS:HB2	2.02	0.42
1:C:453:TYR:CE1	1:B:596:VAL:HG11	2.55	0.41
1:B:369:PHE:CD2	1:B:728:VAL:CG1	3.04	0.41
1:B:410:HIS:ND1	1:B:699:LEU:HD12	2.36	0.41
1:C:572:MET:HE1	1:C:686:VAL:HG23	2.03	0.41
1:A:386:CYS:HA	1:A:390:CYS:HB2	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:463:TYR:OH	1:A:535:LYS:NZ	2.54	0.41
1:D:382:TYR:O	1:D:741:CYS:HA	2.21	0.41
1:C:369:PHE:CD2	1:C:728:VAL:CG1	3.04	0.41
1:D:410:HIS:ND1	1:D:699:LEU:HD12	2.36	0.41
1:D:444:TYR:HE1	1:D:481:SER:HA	1.85	0.41
1:C:463:TYR:OH	1:C:535:LYS:NZ	2.54	0.41
1:C:410:HIS:ND1	1:C:699:LEU:HD12	2.35	0.41
1:A:410:HIS:ND1	1:A:699:LEU:HD12	2.35	0.41
1:A:444:TYR:HE1	1:A:481:SER:HA	1.85	0.41
1:B:386:CYS:HA	1:B:390:CYS:HB2	2.02	0.41
1:B:444:TYR:HE1	1:B:481:SER:HA	1.85	0.41
1:A:369:PHE:CD2	1:A:728:VAL:CG1	3.04	0.40
1:C:474:ARG:NH2	1:C:478:GLU:OE1	2.54	0.40
1:A:382:TYR:O	1:A:741:CYS:HA	2.21	0.40
1:A:381:LEU:HD23	1:A:743:ARG:HA	2.04	0.40
1:B:382:TYR:O	1:B:741:CYS:HA	2.21	0.40
1:B:401:TYR:N	1:B:401:TYR:CD1	2.90	0.40
1:B:474:ARG:NH2	1:B:478:GLU:OE1	2.54	0.40
1:D:463:TYR:OH	1:D:535:LYS:NZ	2.54	0.40
1:A:401:TYR:N	1:A:401:TYR:CD1	2.90	0.40
1:D:401:TYR:N	1:D:401:TYR:CD1	2.90	0.40

There are no symmetry-related clashes.

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	450/868 (52%)	441 (98%)	9 (2%)	0	100	100
1	B	450/868 (52%)	441 (98%)	9 (2%)	0	100	100
1	C	450/868 (52%)	441 (98%)	9 (2%)	0	100	100
1	D	450/868 (52%)	441 (98%)	9 (2%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
All	All	1800/3472 (52%)	1764 (98%)	36 (2%)	0	100 100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains (i)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	A	355/770 (46%)	354 (100%)	1 (0%)	92 96
1	B	355/770 (46%)	354 (100%)	1 (0%)	92 96
1	C	355/770 (46%)	354 (100%)	1 (0%)	92 96
1	D	355/770 (46%)	354 (100%)	1 (0%)	92 96
All	All	1420/3080 (46%)	1416 (100%)	4 (0%)	92 96

All (4) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	C	664	LEU
1	A	664	LEU
1	B	664	LEU
1	D	664	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (4) such sidechains are listed below:

Mol	Chain	Res	Type
1	C	700	GLN
1	A	700	GLN
1	B	700	GLN
1	D	700	GLN

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

40 ligands are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
2	6OU	A	907	-	24,24,48	1.91	3 (12%)	28,29,53	1.00	2 (7%)
5	T7X	A	904	-	43,43,61	1.00	4 (9%)	53,55,73	1.11	4 (7%)
4	YFP	B	903	-	31,31,50	1.55	4 (12%)	35,36,56	1.43	4 (11%)
3	LBN	B	905	-	32,32,51	1.42	4 (12%)	38,40,59	0.96	2 (5%)
3	LBN	D	902	-	31,31,51	0.92	1 (3%)	33,33,59	0.74	0
4	YFP	C	903	-	31,31,50	1.55	4 (12%)	35,36,56	1.44	4 (11%)
2	6OU	C	906	-	34,34,48	1.68	4 (11%)	37,39,53	0.91	2 (5%)
2	6OU	B	901	-	32,32,48	1.53	4 (12%)	34,37,53	0.82	2 (5%)
2	6OU	C	908	-	13,13,48	1.19	2 (15%)	12,13,53	0.71	0
2	6OU	D	907	-	24,24,48	1.90	3 (12%)	28,29,53	1.01	2 (7%)
2	6OU	B	908	-	13,13,48	1.20	2 (15%)	12,13,53	0.72	0
3	LBN	A	905	-	32,32,51	1.42	4 (12%)	38,40,59	0.96	2 (5%)
2	6OU	A	909	-	9,9,48	0.47	0	8,8,53	0.39	0
3	LBN	D	905	-	32,32,51	1.42	4 (12%)	38,40,59	0.96	2 (5%)
5	T7X	D	904	-	43,43,61	1.00	4 (9%)	53,55,73	1.12	4 (7%)
3	LBN	B	902	-	31,31,51	0.92	1 (3%)	33,33,59	0.74	0
2	6OU	C	907	-	24,24,48	1.91	3 (12%)	28,29,53	1.00	2 (7%)
2	6OU	C	910	-	30,30,48	1.83	5 (16%)	34,35,53	0.93	2 (5%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
2	6OU	B	909	-	9,9,48	0.47	0	8,8,53	0.39	0
2	6OU	B	910	-	30,30,48	1.82	5 (16%)	34,35,53	0.93	2 (5%)
5	T7X	B	904	-	43,43,61	1.00	4 (9%)	53,55,73	1.12	4 (7%)
2	6OU	B	906	-	34,34,48	1.68	4 (11%)	37,39,53	0.91	2 (5%)
2	6OU	C	909	-	9,9,48	0.47	0	8,8,53	0.39	0
4	YFP	A	903	-	31,31,50	1.55	4 (12%)	35,36,56	1.44	4 (11%)
2	6OU	A	906	-	34,34,48	1.68	4 (11%)	37,39,53	0.91	2 (5%)
3	LBN	C	902	-	31,31,51	0.92	1 (3%)	33,33,59	0.74	0
2	6OU	A	908	-	13,13,48	1.20	2 (15%)	12,13,53	0.72	0
5	T7X	C	904	-	43,43,61	1.00	4 (9%)	53,55,73	1.11	4 (7%)
2	6OU	D	910	-	30,30,48	1.83	5 (16%)	34,35,53	0.94	2 (5%)
2	6OU	D	909	-	9,9,48	0.47	0	8,8,53	0.39	0
2	6OU	A	901	-	32,32,48	1.53	4 (12%)	34,37,53	0.83	2 (5%)
2	6OU	B	907	-	24,24,48	1.90	3 (12%)	28,29,53	1.00	2 (7%)
3	LBN	C	905	-	32,32,51	1.42	4 (12%)	38,40,59	0.96	2 (5%)
4	YFP	D	903	-	31,31,50	1.55	4 (12%)	35,36,56	1.43	4 (11%)
2	6OU	D	901	-	32,32,48	1.53	4 (12%)	34,37,53	0.82	2 (5%)
2	6OU	A	910	-	30,30,48	1.83	5 (16%)	34,35,53	0.93	2 (5%)
2	6OU	D	906	-	34,34,48	1.67	4 (11%)	37,39,53	0.91	2 (5%)
3	LBN	A	902	-	31,31,51	0.92	1 (3%)	33,33,59	0.74	0
2	6OU	C	901	-	32,32,48	1.53	4 (12%)	34,37,53	0.83	2 (5%)
2	6OU	D	908	-	13,13,48	1.19	2 (15%)	12,13,53	0.72	0

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	6OU	A	907	-	-	16/26/26/52	-
5	T7X	A	904	-	-	16/38/62/80	0/1/1/1
4	YFP	B	903	-	-	16/33/33/55	-
3	LBN	B	905	-	-	22/36/36/55	-
3	LBN	D	902	-	-	17/33/33/55	-
4	YFP	C	903	-	-	16/33/33/55	-
2	6OU	C	906	-	-	16/36/36/52	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	6OU	B	901	-	-	21/36/36/52	-
2	6OU	C	908	-	-	8/11/11/52	-
2	6OU	D	907	-	-	16/26/26/52	-
2	6OU	B	908	-	-	8/11/11/52	-
3	LBN	A	905	-	-	22/36/36/55	-
2	6OU	A	909	-	-	5/7/7/52	-
3	LBN	D	905	-	-	22/36/36/55	-
5	T7X	D	904	-	-	16/38/62/80	0/1/1/1
3	LBN	B	902	-	-	17/33/33/55	-
2	6OU	C	907	-	-	16/26/26/52	-
2	6OU	C	910	-	-	17/32/32/52	-
2	6OU	B	909	-	-	5/7/7/52	-
2	6OU	B	910	-	-	17/32/32/52	-
5	T7X	B	904	-	-	16/38/62/80	0/1/1/1
2	6OU	B	906	-	-	16/36/36/52	-
2	6OU	C	909	-	-	5/7/7/52	-
4	YFP	A	903	-	-	16/33/33/55	-
2	6OU	A	906	-	-	16/36/36/52	-
3	LBN	C	902	-	-	17/33/33/55	-
2	6OU	A	908	-	-	8/11/11/52	-
5	T7X	C	904	-	-	16/38/62/80	0/1/1/1
2	6OU	D	910	-	-	17/32/32/52	-
2	6OU	D	909	-	-	5/7/7/52	-
2	6OU	A	901	-	-	21/36/36/52	-
2	6OU	B	907	-	-	16/26/26/52	-
3	LBN	C	905	-	-	22/36/36/55	-
4	YFP	D	903	-	-	16/33/33/55	-
2	6OU	D	901	-	-	21/36/36/52	-
2	6OU	A	910	-	-	17/32/32/52	-
2	6OU	D	906	-	-	16/36/36/52	-
3	LBN	A	902	-	-	17/33/33/55	-
2	6OU	C	901	-	-	21/36/36/52	-
2	6OU	D	908	-	-	8/11/11/52	-

All (124) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	910	6OU	P23-O22	5.64	1.78	1.60
2	A	910	6OU	P23-O22	5.63	1.78	1.60
2	C	910	6OU	P23-O22	5.63	1.78	1.60
2	B	910	6OU	P23-O22	5.62	1.78	1.60
2	A	907	6OU	P23-O22	5.45	1.77	1.60
2	B	907	6OU	P23-O22	5.44	1.77	1.60
2	C	907	6OU	P23-O22	5.44	1.77	1.60
2	D	907	6OU	P23-O22	5.43	1.77	1.60
2	D	906	6OU	P23-O22	5.24	1.77	1.60
2	C	906	6OU	P23-O22	5.24	1.77	1.60
2	B	906	6OU	P23-O22	5.24	1.77	1.60
2	A	906	6OU	P23-O22	5.22	1.77	1.60
2	D	906	6OU	P23-O26	4.82	1.73	1.54
3	B	905	LBN	P1-O2	4.82	1.78	1.59
2	A	906	6OU	P23-O26	4.82	1.73	1.54
3	D	905	LBN	P1-O2	4.81	1.78	1.59
3	A	905	LBN	P1-O2	4.81	1.78	1.59
3	C	905	LBN	P1-O2	4.81	1.78	1.59
2	C	906	6OU	P23-O26	4.81	1.73	1.54
2	B	906	6OU	P23-O26	4.81	1.73	1.54
2	A	910	6OU	P23-O26	4.72	1.73	1.54
2	D	910	6OU	P23-O26	4.71	1.73	1.54
2	C	910	6OU	P23-O26	4.70	1.73	1.54
2	B	910	6OU	P23-O26	4.69	1.72	1.54
2	D	907	6OU	P23-O26	4.68	1.72	1.54
2	A	907	6OU	P23-O26	4.67	1.72	1.54
2	C	907	6OU	P23-O26	4.67	1.72	1.54
2	B	907	6OU	P23-O26	4.66	1.72	1.54
2	B	901	6OU	P23-O22	4.40	1.77	1.59
2	D	901	6OU	P23-O22	4.39	1.77	1.59
2	C	901	6OU	P23-O22	4.39	1.77	1.59
2	A	901	6OU	P23-O22	4.37	1.77	1.59
4	B	903	YFP	P23-O26	4.27	1.71	1.54
4	D	903	YFP	P23-O26	4.27	1.71	1.54
4	C	903	YFP	P23-O26	4.26	1.71	1.54
4	A	903	YFP	P23-O26	4.25	1.71	1.54
2	A	901	6OU	P23-O26	3.48	1.73	1.59
2	D	901	6OU	P23-O26	3.48	1.73	1.59
2	B	901	6OU	P23-O26	3.48	1.73	1.59
2	C	901	6OU	P23-O26	3.47	1.73	1.59
4	B	903	YFP	C19-C20	3.39	1.61	1.50
4	A	903	YFP	C19-C20	3.36	1.61	1.50
4	D	903	YFP	C19-C20	3.36	1.61	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	C	903	YFP	C19-C20	3.35	1.61	1.50
3	C	905	LBN	C1-C2	2.85	1.59	1.50
3	A	905	LBN	C1-C2	2.84	1.59	1.50
3	B	905	LBN	C1-C2	2.83	1.59	1.50
3	D	905	LBN	C1-C2	2.83	1.59	1.50
5	D	904	T7X	O16-C8	-2.68	1.39	1.46
5	C	904	T7X	O16-C8	-2.66	1.39	1.46
5	B	904	T7X	O16-C8	-2.65	1.40	1.46
2	B	908	6OU	O30-C31	2.65	1.39	1.30
2	D	910	6OU	C21-C20	2.65	1.58	1.50
4	A	903	YFP	P23-O22	2.65	1.68	1.60
2	C	910	6OU	C21-C20	2.65	1.58	1.50
2	D	908	6OU	O30-C31	2.64	1.39	1.30
2	B	910	6OU	C21-C20	2.64	1.58	1.50
5	A	904	T7X	O16-C8	-2.64	1.40	1.46
4	C	903	YFP	P23-O22	2.64	1.68	1.60
2	A	910	6OU	C21-C20	2.64	1.58	1.50
4	B	903	YFP	P23-O22	2.64	1.68	1.60
2	A	908	6OU	O30-C31	2.64	1.39	1.30
2	C	908	6OU	O30-C31	2.63	1.39	1.30
4	D	903	YFP	P23-O22	2.63	1.68	1.60
2	B	910	6OU	C19-C20	2.62	1.58	1.50
2	C	910	6OU	C19-C20	2.60	1.58	1.50
2	A	910	6OU	C19-C20	2.59	1.58	1.50
2	D	910	6OU	C19-C20	2.59	1.58	1.50
3	A	902	LBN	C1-C2	2.57	1.57	1.51
3	B	902	LBN	C1-C2	2.56	1.57	1.51
3	C	902	LBN	C1-C2	2.54	1.57	1.51
2	D	901	6OU	C21-C20	2.53	1.58	1.50
3	D	902	LBN	C1-C2	2.53	1.57	1.51
2	C	901	6OU	C21-C20	2.51	1.58	1.50
2	B	901	6OU	C21-C20	2.51	1.58	1.50
2	C	907	6OU	C21-C20	2.51	1.58	1.50
2	A	901	6OU	C21-C20	2.50	1.58	1.50
2	D	906	6OU	C21-C20	2.50	1.58	1.50
2	C	906	6OU	C21-C20	2.50	1.58	1.50
2	A	906	6OU	C21-C20	2.50	1.58	1.50
2	B	907	6OU	C21-C20	2.50	1.58	1.50
2	A	907	6OU	C21-C20	2.49	1.58	1.50
2	B	906	6OU	C21-C20	2.49	1.58	1.50
2	D	907	6OU	C21-C20	2.49	1.58	1.50
5	D	904	T7X	O18-C9	-2.39	1.39	1.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	B	904	T7X	O18-C9	-2.37	1.39	1.45
5	C	904	T7X	O18-C9	-2.36	1.39	1.45
5	A	904	T7X	O18-C9	-2.35	1.39	1.45
4	D	903	YFP	C21-C20	2.35	1.57	1.50
4	A	903	YFP	C21-C20	2.33	1.57	1.50
5	A	904	T7X	O18-C11	2.31	1.40	1.33
5	C	904	T7X	O18-C11	2.31	1.40	1.33
5	D	904	T7X	O18-C11	2.31	1.40	1.33
4	C	903	YFP	C21-C20	2.31	1.57	1.50
5	B	904	T7X	O18-C11	2.30	1.40	1.33
4	B	903	YFP	C21-C20	2.29	1.57	1.50
2	A	908	6OU	C33-C31	2.27	1.55	1.50
2	C	908	6OU	C33-C31	2.25	1.55	1.50
2	D	910	6OU	O18-C16	2.25	1.39	1.33
2	B	908	6OU	C33-C31	2.25	1.55	1.50
5	B	904	T7X	O16-C10	2.25	1.40	1.34
2	A	910	6OU	O18-C16	2.24	1.39	1.33
5	A	904	T7X	O16-C10	2.24	1.40	1.34
5	C	904	T7X	O16-C10	2.23	1.40	1.34
5	D	904	T7X	O16-C10	2.21	1.40	1.34
2	D	908	6OU	C33-C31	2.21	1.55	1.50
2	C	910	6OU	O18-C16	2.21	1.39	1.33
2	B	910	6OU	O18-C16	2.18	1.39	1.33
3	B	905	LBN	O2-C9	-2.16	1.35	1.44
3	D	905	LBN	O2-C9	-2.16	1.35	1.44
3	C	905	LBN	O2-C9	-2.16	1.35	1.44
2	B	906	6OU	C19-C20	2.15	1.57	1.50
2	A	906	6OU	C19-C20	2.15	1.57	1.50
2	C	906	6OU	C19-C20	2.15	1.57	1.50
3	A	905	LBN	O2-C9	-2.15	1.35	1.44
2	D	906	6OU	C19-C20	2.13	1.57	1.50
3	A	905	LBN	P1-O1	2.11	1.67	1.59
2	D	901	6OU	C19-C20	2.10	1.57	1.50
2	C	901	6OU	C19-C20	2.10	1.57	1.50
2	B	901	6OU	C19-C20	2.10	1.57	1.50
3	C	905	LBN	P1-O1	2.10	1.67	1.59
3	B	905	LBN	P1-O1	2.09	1.67	1.59
3	D	905	LBN	P1-O1	2.09	1.67	1.59
2	A	901	6OU	C19-C20	2.08	1.57	1.50

All (72) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	A	903	YFP	O32-C33-C35	5.51	123.37	111.50
4	C	903	YFP	O32-C33-C35	5.51	123.37	111.50
4	D	903	YFP	O32-C33-C35	5.49	123.34	111.50
4	B	903	YFP	O32-C33-C35	5.49	123.34	111.50
5	D	904	T7X	O16-C10-C12	3.51	119.06	111.50
5	C	904	T7X	O16-C10-C12	3.51	119.06	111.50
5	A	904	T7X	O16-C10-C12	3.51	119.06	111.50
5	B	904	T7X	O16-C10-C12	3.49	119.02	111.50
2	B	907	6OU	O25-P23-O24	3.48	124.29	110.68
2	D	907	6OU	O25-P23-O24	3.48	124.29	110.68
2	C	907	6OU	O25-P23-O24	3.47	124.27	110.68
2	A	907	6OU	O25-P23-O24	3.47	124.26	110.68
2	D	906	6OU	O25-P23-O24	3.44	124.14	110.68
2	A	906	6OU	O25-P23-O24	3.43	124.11	110.68
2	C	906	6OU	O25-P23-O24	3.43	124.11	110.68
2	B	906	6OU	O25-P23-O24	3.42	124.09	110.68
2	A	910	6OU	O25-P23-O24	3.36	123.84	110.68
2	D	910	6OU	O25-P23-O24	3.36	123.82	110.68
2	C	910	6OU	O25-P23-O24	3.35	123.81	110.68
2	B	910	6OU	O25-P23-O24	3.35	123.81	110.68
3	A	905	LBN	O3-P1-O4	3.31	128.60	112.24
3	B	905	LBN	O3-P1-O4	3.31	128.59	112.24
3	C	905	LBN	O3-P1-O4	3.31	128.59	112.24
3	D	905	LBN	O3-P1-O4	3.31	128.59	112.24
4	A	903	YFP	O18-C16-C15	3.27	122.18	111.91
4	C	903	YFP	O18-C16-C15	3.27	122.16	111.91
4	B	903	YFP	O18-C16-C15	3.27	122.16	111.91
4	D	903	YFP	O18-C16-C15	3.26	122.12	111.91
4	B	903	YFP	O18-C16-O17	-2.95	116.16	123.59
4	C	903	YFP	O18-C16-O17	-2.94	116.18	123.59
4	A	903	YFP	O18-C16-O17	-2.93	116.19	123.59
4	D	903	YFP	O18-C16-O17	-2.93	116.19	123.59
5	B	904	T7X	C12-C13-C14	-2.77	108.29	113.23
4	A	903	YFP	O32-C33-O34	-2.77	117.00	123.70
4	C	903	YFP	O32-C33-O34	-2.76	117.04	123.70
4	D	903	YFP	O32-C33-O34	-2.75	117.06	123.70
4	B	903	YFP	O32-C33-O34	-2.74	117.08	123.70
5	C	904	T7X	C12-C13-C14	-2.74	108.35	113.23
5	D	904	T7X	C12-C13-C14	-2.72	108.38	113.23
5	A	904	T7X	C12-C13-C14	-2.71	108.39	113.23
5	D	904	T7X	O18-C11-C31	2.60	120.08	111.91
5	C	904	T7X	O18-C11-C31	2.60	120.06	111.91
5	B	904	T7X	O18-C11-C31	2.60	120.06	111.91

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
5	A	904	T7X	O18-C11-C31	2.58	120.01	111.91
2	D	910	6OU	O30-C31-C33	2.53	116.96	111.50
2	C	910	6OU	O30-C31-C33	2.52	116.93	111.50
2	A	910	6OU	O30-C31-C33	2.52	116.92	111.50
2	B	910	6OU	O30-C31-C33	2.50	116.89	111.50
2	A	901	6OU	O30-C31-C33	2.47	116.81	111.50
2	C	901	6OU	O30-C31-C33	2.46	116.80	111.50
2	C	906	6OU	O30-C31-C33	2.45	116.78	111.50
2	D	901	6OU	O30-C31-C33	2.45	116.78	111.50
2	A	906	6OU	O30-C31-C33	2.44	116.77	111.50
2	D	906	6OU	O30-C31-C33	2.44	116.76	111.50
2	B	906	6OU	O30-C31-C33	2.44	116.76	111.50
2	B	901	6OU	O30-C31-C33	2.44	116.75	111.50
2	B	901	6OU	O25-P23-O24	2.42	124.22	112.24
2	C	901	6OU	O25-P23-O24	2.41	124.16	112.24
2	A	901	6OU	O25-P23-O24	2.41	124.16	112.24
2	D	901	6OU	O25-P23-O24	2.41	124.15	112.24
2	C	907	6OU	O30-C31-C33	2.38	116.64	111.50
2	D	907	6OU	O30-C31-C33	2.38	116.63	111.50
2	B	907	6OU	O30-C31-C33	2.38	116.62	111.50
2	A	907	6OU	O30-C31-C33	2.38	116.62	111.50
5	B	904	T7X	C6-C1-C2	2.34	114.23	110.85
5	A	904	T7X	C6-C1-C2	2.34	114.22	110.85
5	D	904	T7X	C6-C1-C2	2.34	114.22	110.85
5	C	904	T7X	C6-C1-C2	2.33	114.21	110.85
3	B	905	LBN	O2-P1-O4	-2.04	101.11	109.07
3	D	905	LBN	O2-P1-O4	-2.03	101.12	109.07
3	A	905	LBN	O2-P1-O4	-2.03	101.13	109.07
3	C	905	LBN	O2-P1-O4	-2.03	101.14	109.07

There are no chirality outliers.

All (616) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	C	901	6OU	C21-O22-P23-O24
2	C	901	6OU	C21-O22-P23-O25
2	C	906	6OU	C15-C16-O18-C19
2	C	906	6OU	O17-C16-O18-C19
2	C	906	6OU	C40-C41-C42-C43
2	C	907	6OU	C21-O22-P23-O24
2	C	907	6OU	C21-O22-P23-O25
2	C	907	6OU	C21-O22-P23-O26

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Mol	Chain	Res	Type	Atoms
2	C	910	6OU	C21-O22-P23-O25
2	C	910	6OU	O32-C31-O30-C20
2	A	901	6OU	C21-O22-P23-O24
2	A	901	6OU	C21-O22-P23-O25
2	A	906	6OU	C15-C16-O18-C19
2	A	906	6OU	O17-C16-O18-C19
2	A	906	6OU	C40-C41-C42-C43
2	A	907	6OU	C21-O22-P23-O24
2	A	907	6OU	C21-O22-P23-O25
2	A	907	6OU	C21-O22-P23-O26
2	A	910	6OU	C21-O22-P23-O25
2	A	910	6OU	O32-C31-O30-C20
2	B	901	6OU	C21-O22-P23-O24
2	B	901	6OU	C21-O22-P23-O25
2	B	906	6OU	C15-C16-O18-C19
2	B	906	6OU	O17-C16-O18-C19
2	B	906	6OU	C40-C41-C42-C43
2	B	907	6OU	C21-O22-P23-O24
2	B	907	6OU	C21-O22-P23-O25
2	B	907	6OU	C21-O22-P23-O26
2	B	910	6OU	C21-O22-P23-O25
2	B	910	6OU	O32-C31-O30-C20
2	D	901	6OU	C21-O22-P23-O24
2	D	901	6OU	C21-O22-P23-O25
2	D	906	6OU	C15-C16-O18-C19
2	D	906	6OU	O17-C16-O18-C19
2	D	906	6OU	C40-C41-C42-C43
2	D	907	6OU	C21-O22-P23-O24
2	D	907	6OU	C21-O22-P23-O25
2	D	907	6OU	C21-O22-P23-O26
2	D	910	6OU	C21-O22-P23-O25
2	D	910	6OU	O32-C31-O30-C20
3	C	902	LBN	C35-C34-O7-C2
3	C	902	LBN	O8-C34-O7-C2
3	C	905	LBN	O1-C1-C2-O7
3	C	905	LBN	C1-O1-P1-O4
3	C	905	LBN	C9-O2-P1-O4
3	C	905	LBN	N1-C6-C9-O2
3	C	905	LBN	C35-C34-O7-C2
3	A	902	LBN	C35-C34-O7-C2
3	A	902	LBN	O8-C34-O7-C2
3	A	905	LBN	C1-O1-P1-O4

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Mol	Chain	Res	Type	Atoms
3	A	905	LBN	C9-O2-P1-O4
3	A	905	LBN	N1-C6-C9-O2
3	A	905	LBN	C35-C34-O7-C2
3	B	902	LBN	C35-C34-O7-C2
3	B	902	LBN	O8-C34-O7-C2
3	B	905	LBN	C1-O1-P1-O4
3	B	905	LBN	C9-O2-P1-O4
3	B	905	LBN	N1-C6-C9-O2
3	B	905	LBN	C35-C34-O7-C2
3	D	902	LBN	C35-C34-O7-C2
3	D	902	LBN	O8-C34-O7-C2
3	D	905	LBN	O1-C1-C2-O7
3	D	905	LBN	C1-O1-P1-O4
3	D	905	LBN	C9-O2-P1-O4
3	D	905	LBN	N1-C6-C9-O2
3	D	905	LBN	C35-C34-O7-C2
4	C	903	YFP	C21-O22-P23-O25
4	C	903	YFP	C21-O22-P23-O26
4	A	903	YFP	C21-O22-P23-O25
4	A	903	YFP	C21-O22-P23-O26
4	B	903	YFP	C21-O22-P23-O25
4	B	903	YFP	C21-O22-P23-O26
4	D	903	YFP	C21-O22-P23-O25
4	D	903	YFP	C21-O22-P23-O26
5	C	904	T7X	O13-C7-C8-O16
5	A	904	T7X	O13-C7-C8-O16
5	B	904	T7X	O13-C7-C8-O16
5	D	904	T7X	O13-C7-C8-O16
5	C	904	T7X	O19-C11-O18-C9
5	A	904	T7X	O19-C11-O18-C9
5	B	904	T7X	O19-C11-O18-C9
5	D	904	T7X	O19-C11-O18-C9
3	C	905	LBN	O8-C34-O7-C2
3	A	905	LBN	O8-C34-O7-C2
3	B	905	LBN	O8-C34-O7-C2
3	D	905	LBN	O8-C34-O7-C2
2	C	901	6OU	C15-C16-O18-C19
2	A	901	6OU	C15-C16-O18-C19
2	B	901	6OU	C15-C16-O18-C19
2	D	901	6OU	C15-C16-O18-C19
3	C	905	LBN	C26-C25-O5-C3
3	A	905	LBN	C26-C25-O5-C3

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Mol	Chain	Res	Type	Atoms
3	B	905	LBN	C26-C25-O5-C3
3	D	905	LBN	C26-C25-O5-C3
2	C	910	6OU	C33-C31-O30-C20
2	A	910	6OU	C33-C31-O30-C20
2	B	910	6OU	C33-C31-O30-C20
2	D	910	6OU	C33-C31-O30-C20
5	C	904	T7X	C31-C11-O18-C9
5	A	904	T7X	C31-C11-O18-C9
5	B	904	T7X	C31-C11-O18-C9
5	D	904	T7X	C31-C11-O18-C9
2	C	901	6OU	C12-C13-C14-C15
2	A	901	6OU	C12-C13-C14-C15
2	B	901	6OU	C12-C13-C14-C15
2	D	901	6OU	C12-C13-C14-C15
2	C	901	6OU	O17-C16-O18-C19
2	A	901	6OU	O17-C16-O18-C19
2	B	901	6OU	O17-C16-O18-C19
2	D	901	6OU	O17-C16-O18-C19
3	C	905	LBN	O6-C25-O5-C3
3	A	905	LBN	O6-C25-O5-C3
3	B	905	LBN	O6-C25-O5-C3
3	D	905	LBN	O6-C25-O5-C3
4	C	903	YFP	C15-C16-O18-C19
4	A	903	YFP	C15-C16-O18-C19
4	B	903	YFP	C15-C16-O18-C19
4	D	903	YFP	C15-C16-O18-C19
3	A	905	LBN	O1-C1-C2-O7
3	B	905	LBN	O1-C1-C2-O7
5	C	904	T7X	C11-C31-C32-C33
5	A	904	T7X	C11-C31-C32-C33
5	B	904	T7X	C11-C31-C32-C33
5	D	904	T7X	C11-C31-C32-C33
2	C	910	6OU	C13-C14-C15-C16
2	A	910	6OU	C13-C14-C15-C16
2	B	910	6OU	C13-C14-C15-C16
2	D	910	6OU	C13-C14-C15-C16
4	C	903	YFP	O17-C16-O18-C19
4	A	903	YFP	O17-C16-O18-C19
4	B	903	YFP	O17-C16-O18-C19
4	D	903	YFP	O17-C16-O18-C19
2	C	901	6OU	C31-C33-C34-C35
2	A	901	6OU	C31-C33-C34-C35

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Mol	Chain	Res	Type	Atoms
2	B	901	6OU	C31-C33-C34-C35
2	D	901	6OU	C31-C33-C34-C35
2	C	901	6OU	C13-C14-C15-C16
2	A	901	6OU	C13-C14-C15-C16
2	B	901	6OU	C13-C14-C15-C16
2	D	901	6OU	C13-C14-C15-C16
2	C	901	6OU	C21-O22-P23-O26
2	A	901	6OU	C21-O22-P23-O26
2	B	901	6OU	C21-O22-P23-O26
2	D	901	6OU	C21-O22-P23-O26
5	C	904	T7X	C7-O13-P1-O1
5	A	904	T7X	C7-O13-P1-O1
5	B	904	T7X	C7-O13-P1-O1
5	D	904	T7X	C7-O13-P1-O1
2	C	906	6OU	C34-C35-C36-C37
2	C	910	6OU	C34-C35-C36-C37
2	A	906	6OU	C34-C35-C36-C37
2	A	910	6OU	C34-C35-C36-C37
2	B	906	6OU	C34-C35-C36-C37
2	B	910	6OU	C34-C35-C36-C37
2	D	906	6OU	C34-C35-C36-C37
3	C	905	LBN	C27-C28-C29-C30
3	A	905	LBN	C27-C28-C29-C30
3	B	905	LBN	C27-C28-C29-C30
3	D	905	LBN	C27-C28-C29-C30
2	D	910	6OU	C34-C35-C36-C37
2	B	901	6OU	C34-C35-C36-C37
2	C	901	6OU	C34-C35-C36-C37
2	C	908	6OU	C34-C35-C36-C37
2	A	901	6OU	C34-C35-C36-C37
2	A	908	6OU	C34-C35-C36-C37
2	B	908	6OU	C34-C35-C36-C37
2	D	901	6OU	C34-C35-C36-C37
2	D	908	6OU	C34-C35-C36-C37
3	C	905	LBN	C29-C30-C31-C32
3	A	905	LBN	C29-C30-C31-C32
3	B	905	LBN	C29-C30-C31-C32
3	D	905	LBN	C29-C30-C31-C32
5	C	904	T7X	C34-C35-C36-C37
5	A	904	T7X	C34-C35-C36-C37
5	B	904	T7X	C34-C35-C36-C37
5	D	904	T7X	C34-C35-C36-C37

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Mol	Chain	Res	Type	Atoms
2	C	907	6OU	C31-C33-C34-C35
2	A	907	6OU	C31-C33-C34-C35
2	B	907	6OU	C31-C33-C34-C35
2	D	907	6OU	C31-C33-C34-C35
2	C	909	6OU	C44-C45-C46-C47
2	A	909	6OU	C44-C45-C46-C47
2	B	909	6OU	C44-C45-C46-C47
2	D	909	6OU	C44-C45-C46-C47
3	C	902	LBN	C34-C35-C36-C37
3	A	902	LBN	C34-C35-C36-C37
3	B	902	LBN	C34-C35-C36-C37
3	D	902	LBN	C34-C35-C36-C37
2	C	907	6OU	C33-C31-O30-C20
2	A	907	6OU	C33-C31-O30-C20
2	B	907	6OU	C33-C31-O30-C20
2	D	907	6OU	C33-C31-O30-C20
2	D	910	6OU	C12-C13-C14-C15
4	C	903	YFP	C13-C14-C15-C16
4	A	903	YFP	C13-C14-C15-C16
4	B	903	YFP	C13-C14-C15-C16
4	D	903	YFP	C13-C14-C15-C16
2	C	910	6OU	C12-C13-C14-C15
2	A	909	6OU	C45-C46-C47-C48
2	A	910	6OU	C12-C13-C14-C15
2	B	910	6OU	C12-C13-C14-C15
2	C	909	6OU	C45-C46-C47-C48
2	A	907	6OU	C12-C13-C14-C15
2	B	907	6OU	C12-C13-C14-C15
2	B	909	6OU	C45-C46-C47-C48
2	D	907	6OU	C12-C13-C14-C15
2	D	909	6OU	C45-C46-C47-C48
2	C	907	6OU	C12-C13-C14-C15
2	C	910	6OU	C36-C37-C38-C39
2	A	910	6OU	C36-C37-C38-C39
2	B	910	6OU	C36-C37-C38-C39
2	D	910	6OU	C36-C37-C38-C39
2	C	910	6OU	C15-C16-O18-C19
2	A	910	6OU	C15-C16-O18-C19
2	B	910	6OU	C15-C16-O18-C19
2	D	910	6OU	C15-C16-O18-C19
4	C	903	YFP	C06-C07-C08-C09
4	A	903	YFP	C06-C07-C08-C09

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Mol	Chain	Res	Type	Atoms
4	B	903	YFP	C06-C07-C08-C09
4	D	903	YFP	C06-C07-C08-C09
2	C	907	6OU	O32-C31-O30-C20
2	A	907	6OU	O32-C31-O30-C20
2	B	907	6OU	O32-C31-O30-C20
2	D	907	6OU	O32-C31-O30-C20
2	A	907	6OU	C33-C34-C35-C36
2	A	910	6OU	O17-C16-O18-C19
2	B	910	6OU	O17-C16-O18-C19
2	C	907	6OU	C33-C34-C35-C36
2	B	907	6OU	C33-C34-C35-C36
2	D	907	6OU	C33-C34-C35-C36
4	C	903	YFP	C12-C13-C14-C15
4	A	903	YFP	C12-C13-C14-C15
4	B	903	YFP	C12-C13-C14-C15
4	D	903	YFP	C12-C13-C14-C15
3	C	902	LBN	C28-C29-C30-C31
3	A	902	LBN	C28-C29-C30-C31
3	D	902	LBN	C28-C29-C30-C31
2	C	910	6OU	O17-C16-O18-C19
2	D	910	6OU	O17-C16-O18-C19
3	B	902	LBN	C28-C29-C30-C31
2	C	901	6OU	C37-C38-C39-C40
2	A	901	6OU	C37-C38-C39-C40
2	B	901	6OU	C37-C38-C39-C40
2	D	901	6OU	C37-C38-C39-C40
5	C	904	T7X	C10-C12-C13-C14
5	B	904	T7X	C10-C12-C13-C14
2	C	907	6OU	C15-C16-O18-C19
2	A	907	6OU	C15-C16-O18-C19
2	B	907	6OU	C15-C16-O18-C19
2	D	907	6OU	C15-C16-O18-C19
2	B	908	6OU	C35-C36-C37-C38
3	A	905	LBN	C36-C37-C38-C39
2	C	908	6OU	C35-C36-C37-C38
2	A	908	6OU	C35-C36-C37-C38
2	D	908	6OU	C35-C36-C37-C38
3	C	905	LBN	C36-C37-C38-C39
3	B	905	LBN	C36-C37-C38-C39
3	D	905	LBN	C36-C37-C38-C39
5	A	904	T7X	C10-C12-C13-C14
5	D	904	T7X	C10-C12-C13-C14

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Mol	Chain	Res	Type	Atoms
2	B	901	6OU	C33-C34-C35-C36
2	C	901	6OU	C33-C34-C35-C36
2	A	901	6OU	C33-C34-C35-C36
2	D	901	6OU	C33-C34-C35-C36
2	C	910	6OU	C35-C36-C37-C38
2	A	910	6OU	C35-C36-C37-C38
2	B	910	6OU	C35-C36-C37-C38
2	D	910	6OU	C35-C36-C37-C38
3	A	902	LBN	C37-C38-C39-C40
3	D	902	LBN	C37-C38-C39-C40
3	C	902	LBN	C37-C38-C39-C40
3	B	902	LBN	C37-C38-C39-C40
3	C	905	LBN	C1-O1-P1-O2
3	A	905	LBN	C1-O1-P1-O2
3	B	905	LBN	C1-O1-P1-O2
3	D	905	LBN	C1-O1-P1-O2
2	C	909	6OU	C42-C43-C44-C45
2	A	909	6OU	C42-C43-C44-C45
2	B	909	6OU	C42-C43-C44-C45
2	D	909	6OU	C42-C43-C44-C45
2	B	906	6OU	C10-C11-C12-C13
2	D	906	6OU	C10-C11-C12-C13
2	C	906	6OU	C10-C11-C12-C13
2	A	906	6OU	C10-C11-C12-C13
2	C	906	6OU	C38-C39-C40-C41
2	A	906	6OU	C38-C39-C40-C41
2	B	906	6OU	C38-C39-C40-C41
2	D	906	6OU	C38-C39-C40-C41
2	A	907	6OU	O17-C16-O18-C19
2	D	907	6OU	O17-C16-O18-C19
2	C	907	6OU	O18-C19-C20-C21
2	A	907	6OU	O18-C19-C20-C21
2	B	907	6OU	O18-C19-C20-C21
2	D	907	6OU	O18-C19-C20-C21
3	C	902	LBN	C1-C2-C3-O5
3	A	902	LBN	C1-C2-C3-O5
3	B	902	LBN	C1-C2-C3-O5
3	D	902	LBN	C1-C2-C3-O5
2	C	907	6OU	O17-C16-O18-C19
4	C	903	YFP	C07-C08-C09-C10
4	A	903	YFP	C07-C08-C09-C10
4	B	903	YFP	C07-C08-C09-C10

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Mol	Chain	Res	Type	Atoms
4	D	903	YFP	C07-C08-C09-C10
2	B	907	6OU	O17-C16-O18-C19
4	A	903	YFP	C35-C36-C37-C38
4	B	903	YFP	C35-C36-C37-C38
4	D	903	YFP	C35-C36-C37-C38
4	C	903	YFP	C35-C36-C37-C38
2	C	901	6OU	C10-C11-C12-C13
2	A	901	6OU	C10-C11-C12-C13
2	B	901	6OU	C10-C11-C12-C13
2	D	901	6OU	C10-C11-C12-C13
2	A	908	6OU	C36-C37-C38-C39
2	C	908	6OU	C36-C37-C38-C39
2	C	910	6OU	C10-C11-C12-C13
2	A	910	6OU	C10-C11-C12-C13
2	B	908	6OU	C36-C37-C38-C39
2	B	910	6OU	C10-C11-C12-C13
2	D	908	6OU	C36-C37-C38-C39
2	D	910	6OU	C10-C11-C12-C13
3	C	902	LBN	C29-C30-C31-C32
3	A	902	LBN	C29-C30-C31-C32
3	B	902	LBN	C29-C30-C31-C32
3	D	902	LBN	C29-C30-C31-C32
4	C	903	YFP	C21-O22-P23-O24
4	A	903	YFP	C21-O22-P23-O24
4	B	903	YFP	C21-O22-P23-O24
4	D	903	YFP	C21-O22-P23-O24
5	C	904	T7X	C40-C41-C42-C43
5	A	904	T7X	C40-C41-C42-C43
5	B	904	T7X	C40-C41-C42-C43
5	D	904	T7X	C40-C41-C42-C43
3	A	905	LBN	O7-C2-C3-O5
3	B	905	LBN	O7-C2-C3-O5
3	D	905	LBN	O7-C2-C3-O5
2	C	901	6OU	C35-C36-C37-C38
2	A	901	6OU	C35-C36-C37-C38
2	B	901	6OU	C35-C36-C37-C38
2	D	901	6OU	C35-C36-C37-C38
3	C	905	LBN	O1-C1-C2-C3
3	A	905	LBN	O1-C1-C2-C3
3	B	905	LBN	O1-C1-C2-C3
3	D	905	LBN	O1-C1-C2-C3
3	C	902	LBN	C38-C39-C40-C41

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Mol	Chain	Res	Type	Atoms
3	A	902	LBN	C38-C39-C40-C41
3	B	902	LBN	C38-C39-C40-C41
3	D	902	LBN	C38-C39-C40-C41
2	D	906	6OU	C08-C09-C10-C11
2	C	906	6OU	C08-C09-C10-C11
2	A	906	6OU	C08-C09-C10-C11
2	B	906	6OU	C08-C09-C10-C11
4	B	903	YFP	O18-C19-C20-C21
2	C	906	6OU	C35-C36-C37-C38
2	A	906	6OU	C35-C36-C37-C38
2	B	906	6OU	C35-C36-C37-C38
2	D	906	6OU	C35-C36-C37-C38
2	C	910	6OU	O30-C20-C21-O22
2	A	910	6OU	O30-C20-C21-O22
2	B	910	6OU	O30-C20-C21-O22
2	D	910	6OU	O30-C20-C21-O22
3	C	905	LBN	O7-C2-C3-O5
2	C	907	6OU	C10-C11-C12-C13
2	A	907	6OU	C10-C11-C12-C13
2	D	907	6OU	C10-C11-C12-C13
2	B	907	6OU	C10-C11-C12-C13
3	B	905	LBN	C26-C27-C28-C29
3	D	905	LBN	C26-C27-C28-C29
3	C	905	LBN	C26-C27-C28-C29
3	A	905	LBN	C26-C27-C28-C29
2	C	901	6OU	C40-C41-C42-C43
2	C	908	6OU	C40-C41-C42-C43
2	A	901	6OU	C40-C41-C42-C43
2	A	908	6OU	C40-C41-C42-C43
2	B	901	6OU	C40-C41-C42-C43
2	B	908	6OU	C40-C41-C42-C43
2	D	901	6OU	C40-C41-C42-C43
2	D	908	6OU	C40-C41-C42-C43
2	C	906	6OU	C19-C20-C21-O22
2	A	906	6OU	C19-C20-C21-O22
2	B	906	6OU	C19-C20-C21-O22
2	D	906	6OU	C19-C20-C21-O22
4	C	903	YFP	C19-C20-C21-O22
4	A	903	YFP	C19-C20-C21-O22
4	B	903	YFP	C19-C20-C21-O22
4	D	903	YFP	C19-C20-C21-O22
5	C	904	T7X	O13-C7-C8-C9

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Mol	Chain	Res	Type	Atoms
5	A	904	T7X	O13-C7-C8-C9
5	B	904	T7X	O13-C7-C8-C9
5	D	904	T7X	O13-C7-C8-C9
2	C	908	6OU	C37-C38-C39-C40
2	A	908	6OU	C37-C38-C39-C40
2	B	908	6OU	C37-C38-C39-C40
2	D	908	6OU	C37-C38-C39-C40
2	C	901	6OU	C19-C20-O30-C31
2	A	901	6OU	C19-C20-O30-C31
2	B	901	6OU	C19-C20-O30-C31
2	D	901	6OU	C19-C20-O30-C31
2	C	901	6OU	O18-C19-C20-C21
2	A	901	6OU	O18-C19-C20-C21
2	B	901	6OU	O18-C19-C20-C21
2	D	901	6OU	O18-C19-C20-C21
4	C	903	YFP	O18-C19-C20-C21
4	A	903	YFP	O18-C19-C20-C21
4	D	903	YFP	O18-C19-C20-C21
4	C	903	YFP	O32-C20-C21-O22
4	A	903	YFP	O32-C20-C21-O22
4	B	903	YFP	O32-C20-C21-O22
4	D	903	YFP	O32-C20-C21-O22
2	C	907	6OU	O18-C19-C20-O30
2	A	907	6OU	O18-C19-C20-O30
2	B	907	6OU	O18-C19-C20-O30
2	D	907	6OU	O18-C19-C20-O30
3	C	902	LBN	O7-C2-C3-O5
3	A	902	LBN	O7-C2-C3-O5
3	B	902	LBN	O7-C2-C3-O5
3	D	902	LBN	O7-C2-C3-O5
4	C	903	YFP	O18-C19-C20-O32
4	A	903	YFP	O18-C19-C20-O32
4	B	903	YFP	O18-C19-C20-O32
4	D	903	YFP	O18-C19-C20-O32
2	A	908	6OU	C33-C34-C35-C36
2	B	908	6OU	C33-C34-C35-C36
2	C	908	6OU	C33-C34-C35-C36
2	D	908	6OU	C33-C34-C35-C36
3	C	902	LBN	C36-C37-C38-C39
3	D	902	LBN	C36-C37-C38-C39
3	A	902	LBN	C36-C37-C38-C39
3	B	902	LBN	C36-C37-C38-C39

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Mol	Chain	Res	Type	Atoms
3	C	905	LBN	C9-O2-P1-O1
3	A	905	LBN	C9-O2-P1-O1
3	B	905	LBN	C9-O2-P1-O1
3	D	905	LBN	C9-O2-P1-O1
3	C	905	LBN	C35-C36-C37-C38
3	A	905	LBN	C35-C36-C37-C38
3	B	905	LBN	C35-C36-C37-C38
3	D	905	LBN	C35-C36-C37-C38
5	C	904	T7X	C7-O13-P1-O12
5	A	904	T7X	C7-O13-P1-O12
5	B	904	T7X	C7-O13-P1-O12
5	D	904	T7X	C7-O13-P1-O12
2	C	910	6OU	C19-C20-C21-O22
2	A	910	6OU	C19-C20-C21-O22
2	B	910	6OU	C19-C20-C21-O22
2	D	910	6OU	C19-C20-C21-O22
2	C	906	6OU	O30-C20-C21-O22
2	A	906	6OU	O30-C20-C21-O22
2	B	906	6OU	O30-C20-C21-O22
2	D	906	6OU	O30-C20-C21-O22
3	A	902	LBN	C35-C36-C37-C38
3	C	902	LBN	C35-C36-C37-C38
3	B	902	LBN	C35-C36-C37-C38
5	C	904	T7X	C36-C37-C38-C39
5	B	904	T7X	C36-C37-C38-C39
5	D	904	T7X	C36-C37-C38-C39
5	A	904	T7X	C36-C37-C38-C39
2	C	901	6OU	O18-C19-C20-O30
2	A	901	6OU	O18-C19-C20-O30
2	B	901	6OU	O18-C19-C20-O30
2	D	901	6OU	O18-C19-C20-O30
3	D	902	LBN	C35-C36-C37-C38
4	C	903	YFP	C19-C20-O32-C33
4	A	903	YFP	C19-C20-O32-C33
4	B	903	YFP	C19-C20-O32-C33
4	D	903	YFP	C19-C20-O32-C33
3	C	905	LBN	C1-C2-C3-O5
3	A	905	LBN	C1-C2-C3-O5
3	B	905	LBN	C1-C2-C3-O5
3	D	905	LBN	C1-C2-C3-O5
5	C	904	T7X	C12-C13-C14-C15
5	A	904	T7X	C12-C13-C14-C15

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Mol	Chain	Res	Type	Atoms
5	B	904	T7X	C12-C13-C14-C15
5	D	904	T7X	C12-C13-C14-C15
2	D	910	6OU	C08-C09-C10-C11
2	B	910	6OU	C08-C09-C10-C11
2	C	910	6OU	C08-C09-C10-C11
2	A	910	6OU	C08-C09-C10-C11
2	C	910	6OU	C37-C38-C39-C40
2	A	910	6OU	C37-C38-C39-C40
2	B	910	6OU	C37-C38-C39-C40
2	D	910	6OU	C37-C38-C39-C40
2	C	906	6OU	C36-C37-C38-C39
2	A	906	6OU	C36-C37-C38-C39
2	D	906	6OU	C36-C37-C38-C39
2	B	906	6OU	C36-C37-C38-C39
5	C	904	T7X	C7-C8-O16-C10
5	A	904	T7X	C7-C8-O16-C10
5	B	904	T7X	C7-C8-O16-C10
5	D	904	T7X	C7-C8-O16-C10
3	C	905	LBN	C2-C1-O1-P1
3	A	905	LBN	C2-C1-O1-P1
3	B	905	LBN	C2-C1-O1-P1
3	D	905	LBN	C2-C1-O1-P1
2	A	909	6OU	C46-C47-C48-C49
2	D	909	6OU	C46-C47-C48-C49
2	C	909	6OU	C46-C47-C48-C49
2	B	909	6OU	C46-C47-C48-C49
4	A	903	YFP	C08-C09-C10-C11
4	C	903	YFP	C08-C09-C10-C11
4	B	903	YFP	C08-C09-C10-C11
4	D	903	YFP	C08-C09-C10-C11
3	C	902	LBN	C27-C28-C29-C30
3	B	902	LBN	C27-C28-C29-C30
3	D	902	LBN	C27-C28-C29-C30
3	A	902	LBN	C27-C28-C29-C30
3	C	902	LBN	O1-C1-C2-O7
3	A	902	LBN	O1-C1-C2-O7
3	B	902	LBN	O1-C1-C2-O7
3	D	902	LBN	O1-C1-C2-O7
2	D	906	6OU	C07-C08-C09-C10
2	C	906	6OU	C07-C08-C09-C10
2	A	906	6OU	C07-C08-C09-C10
2	B	906	6OU	C07-C08-C09-C10

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Mol	Chain	Res	Type	Atoms
2	C	909	6OU	C40-C41-C42-C43
2	A	909	6OU	C40-C41-C42-C43
2	B	909	6OU	C40-C41-C42-C43
2	D	909	6OU	C40-C41-C42-C43
2	C	907	6OU	O30-C31-C33-C34
2	A	907	6OU	O30-C31-C33-C34
2	B	907	6OU	O30-C31-C33-C34
2	D	907	6OU	O30-C31-C33-C34
5	C	904	T7X	O18-C11-C31-C32
5	A	904	T7X	O18-C11-C31-C32
5	B	904	T7X	O18-C11-C31-C32
5	D	904	T7X	O18-C11-C31-C32
2	C	906	6OU	C12-C13-C14-C15
2	A	906	6OU	C12-C13-C14-C15
2	D	906	6OU	C12-C13-C14-C15
2	B	906	6OU	C12-C13-C14-C15
5	C	904	T7X	C9-C8-O16-C10
5	A	904	T7X	C9-C8-O16-C10
5	B	904	T7X	C9-C8-O16-C10
5	D	904	T7X	C9-C8-O16-C10
2	C	906	6OU	C11-C12-C13-C14
2	A	906	6OU	C11-C12-C13-C14
2	B	906	6OU	C11-C12-C13-C14
2	D	906	6OU	C11-C12-C13-C14
2	C	908	6OU	O30-C31-C33-C34
2	A	908	6OU	O30-C31-C33-C34
2	B	908	6OU	O30-C31-C33-C34
2	D	908	6OU	O30-C31-C33-C34
2	C	906	6OU	C14-C15-C16-O18
2	A	906	6OU	C14-C15-C16-O18
2	B	906	6OU	C14-C15-C16-O18
2	D	906	6OU	C14-C15-C16-O18
3	C	902	LBN	O7-C34-C35-C36
3	A	902	LBN	O7-C34-C35-C36
3	B	902	LBN	O7-C34-C35-C36
3	D	902	LBN	O7-C34-C35-C36
3	D	905	LBN	C30-C31-C32-C33
3	C	905	LBN	C30-C31-C32-C33
3	A	905	LBN	C30-C31-C32-C33
2	C	910	6OU	C38-C39-C40-C41
2	A	910	6OU	C38-C39-C40-C41
2	B	910	6OU	C38-C39-C40-C41

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Mol	Chain	Res	Type	Atoms
2	D	910	6OU	C38-C39-C40-C41
3	B	905	LBN	C30-C31-C32-C33
2	C	908	6OU	O32-C31-C33-C34
2	A	908	6OU	O32-C31-C33-C34
2	B	908	6OU	O32-C31-C33-C34
2	D	908	6OU	O32-C31-C33-C34
2	C	901	6OU	C14-C15-C16-O18
2	A	901	6OU	C14-C15-C16-O18
2	B	901	6OU	C14-C15-C16-O18
2	D	901	6OU	C14-C15-C16-O18
2	C	901	6OU	C38-C39-C40-C41
2	A	901	6OU	C38-C39-C40-C41
2	B	901	6OU	C38-C39-C40-C41
2	D	901	6OU	C38-C39-C40-C41
3	C	905	LBN	O5-C25-C26-C27
3	A	905	LBN	O5-C25-C26-C27
3	B	905	LBN	O5-C25-C26-C27
3	D	905	LBN	O5-C25-C26-C27
2	C	907	6OU	O32-C31-C33-C34
2	A	907	6OU	O32-C31-C33-C34
2	B	907	6OU	O32-C31-C33-C34
2	D	907	6OU	O32-C31-C33-C34
2	A	907	6OU	C34-C35-C36-C37
2	B	907	6OU	C34-C35-C36-C37
2	C	907	6OU	C34-C35-C36-C37
2	D	907	6OU	C34-C35-C36-C37
2	C	906	6OU	C14-C15-C16-O17
2	B	906	6OU	C14-C15-C16-O17
2	A	906	6OU	C14-C15-C16-O17
2	D	906	6OU	C14-C15-C16-O17
2	C	901	6OU	C20-C21-O22-P23
2	A	901	6OU	C20-C21-O22-P23
2	B	901	6OU	C20-C21-O22-P23
2	D	901	6OU	C20-C21-O22-P23
2	A	910	6OU	C09-C10-C11-C12
2	B	910	6OU	C09-C10-C11-C12
2	D	910	6OU	C09-C10-C11-C12
2	C	910	6OU	C09-C10-C11-C12
3	C	902	LBN	O8-C34-C35-C36
3	A	902	LBN	O8-C34-C35-C36
3	B	902	LBN	O8-C34-C35-C36
3	D	902	LBN	O8-C34-C35-C36

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Mol	Chain	Res	Type	Atoms
3	A	902	LBN	C25-C26-C27-C28
3	D	902	LBN	C25-C26-C27-C28
5	C	904	T7X	O19-C11-C31-C32
5	A	904	T7X	O19-C11-C31-C32
5	B	904	T7X	O19-C11-C31-C32
5	D	904	T7X	O19-C11-C31-C32
3	C	902	LBN	C25-C26-C27-C28
3	B	902	LBN	C25-C26-C27-C28
3	B	905	LBN	O6-C25-C26-C27
3	C	902	LBN	C42-C5-C8-C11
3	A	902	LBN	C42-C5-C8-C11
3	B	902	LBN	C42-C5-C8-C11
3	D	902	LBN	C42-C5-C8-C11
3	D	905	LBN	O6-C25-C26-C27
2	B	901	6OU	C14-C15-C16-O17
3	C	905	LBN	O6-C25-C26-C27
3	A	905	LBN	O6-C25-C26-C27
2	C	901	6OU	C14-C15-C16-O17
2	D	901	6OU	C14-C15-C16-O17
2	A	901	6OU	C14-C15-C16-O17

There are no ring outliers.

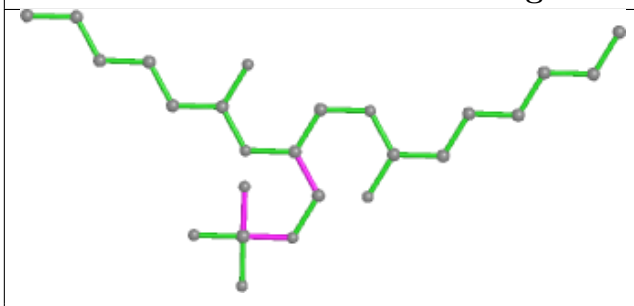
6 monomers are involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	C	906	6OU	1	0
2	B	901	6OU	1	0
2	B	906	6OU	1	0
2	A	906	6OU	1	0
2	D	901	6OU	1	0
2	C	901	6OU	1	0

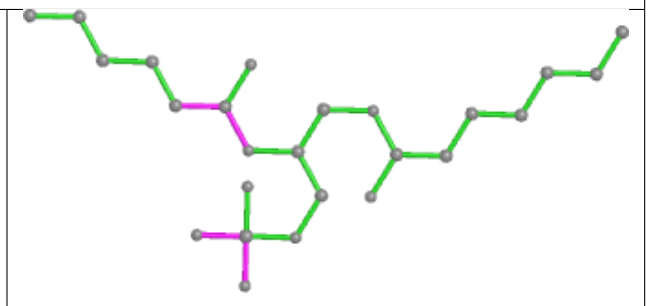
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

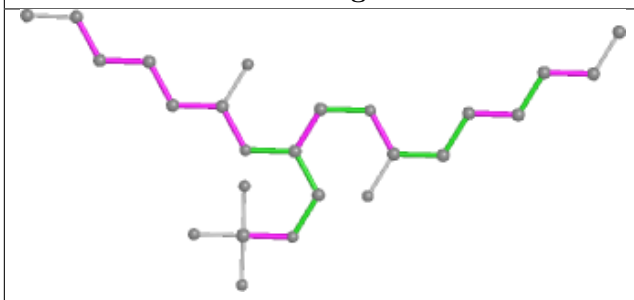
Ligand 6OU A 907



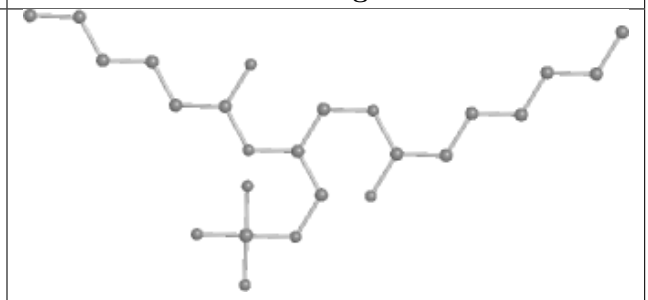
Bond lengths



Bond angles

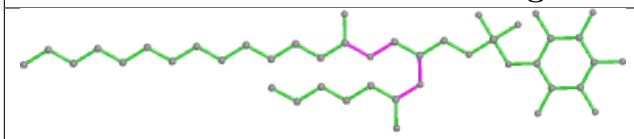


Torsions

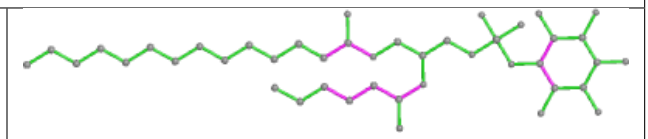


Rings

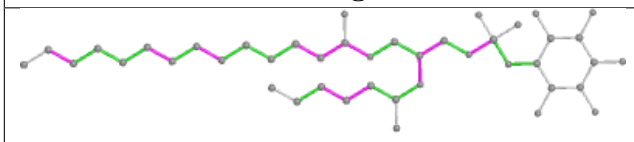
Ligand T7X A 904



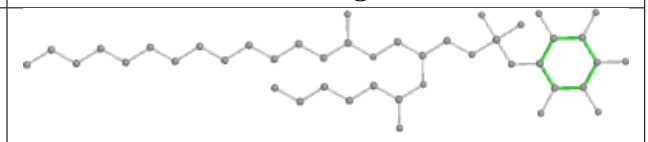
Bond lengths



Bond angles

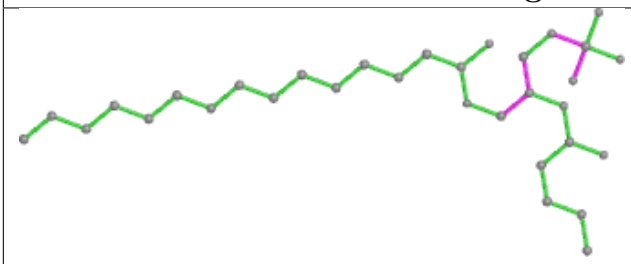


Torsions

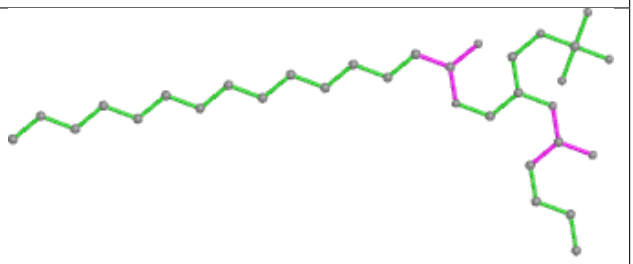


Rings

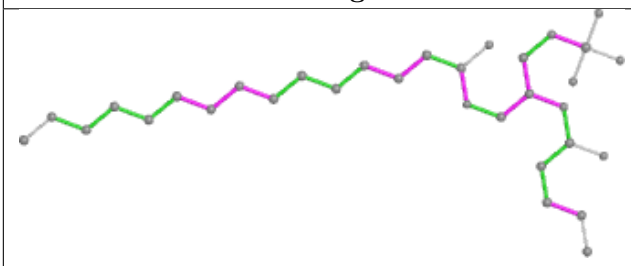
Ligand YFP B 903



Bond lengths



Bond angles



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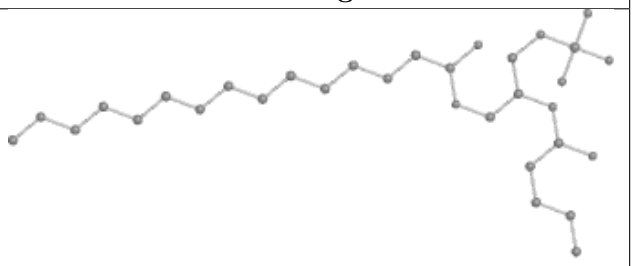
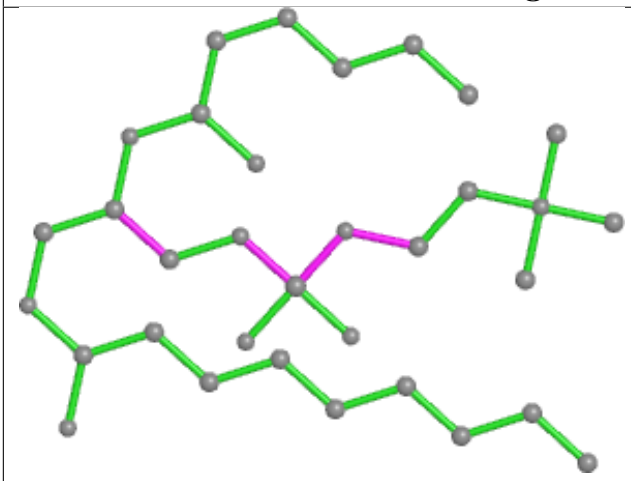
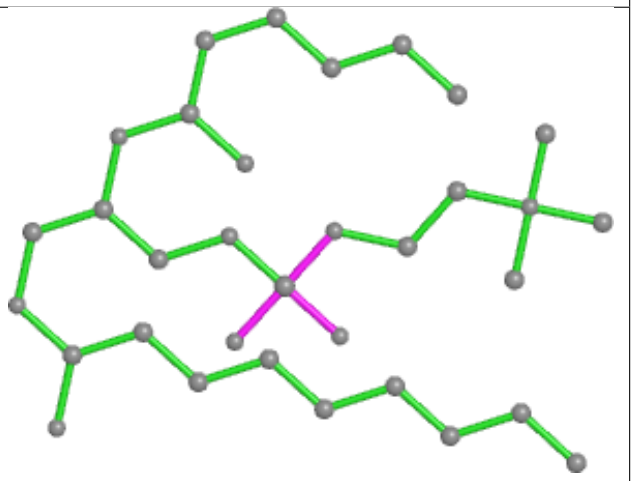


Rings

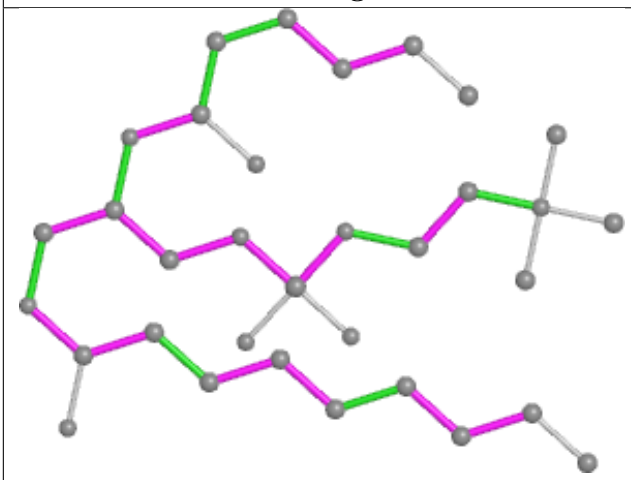
Ligand LBN B 905



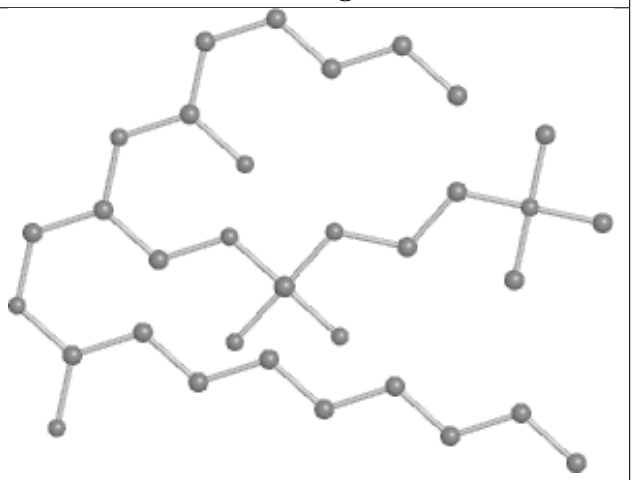
Bond lengths



Bond angles

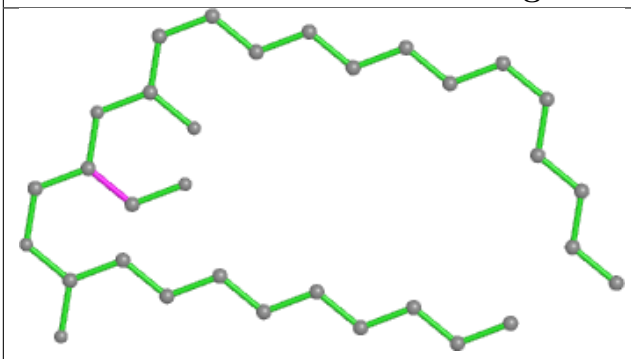


Torsions



Rings

Ligand LBN D 902



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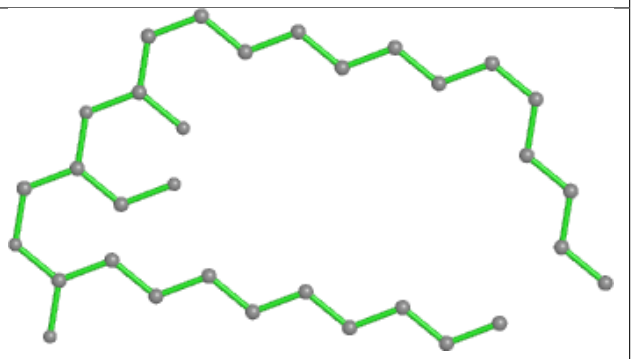
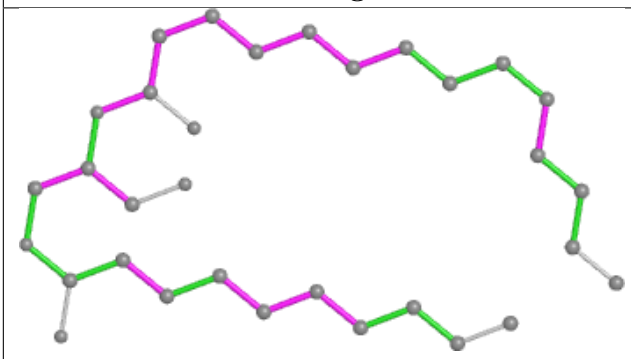
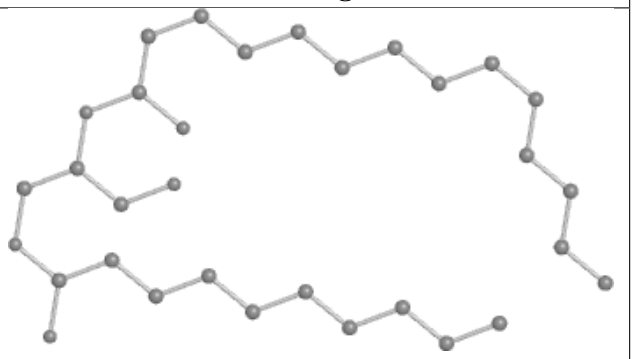


Bond angles

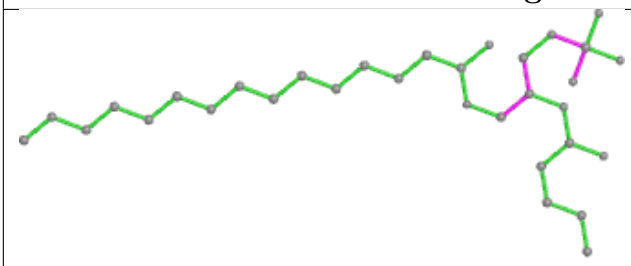


Torsions

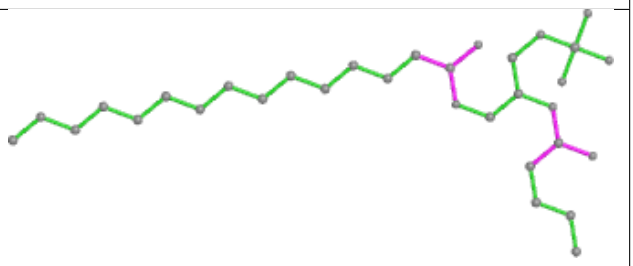


Rings

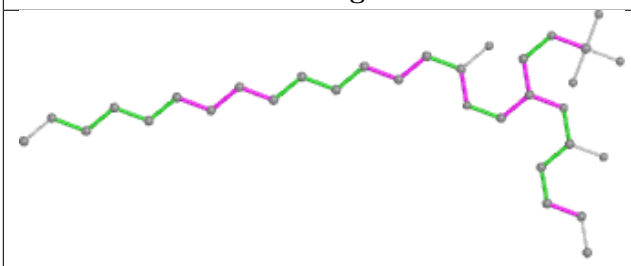
Ligand YFP C 903



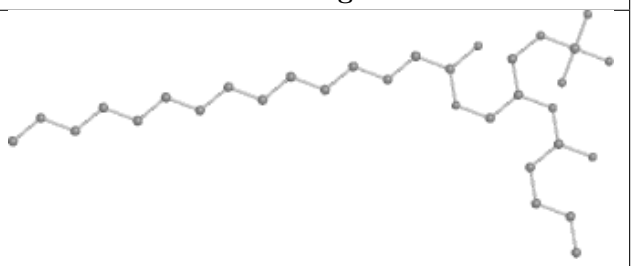
Bond lengths



Bond angles

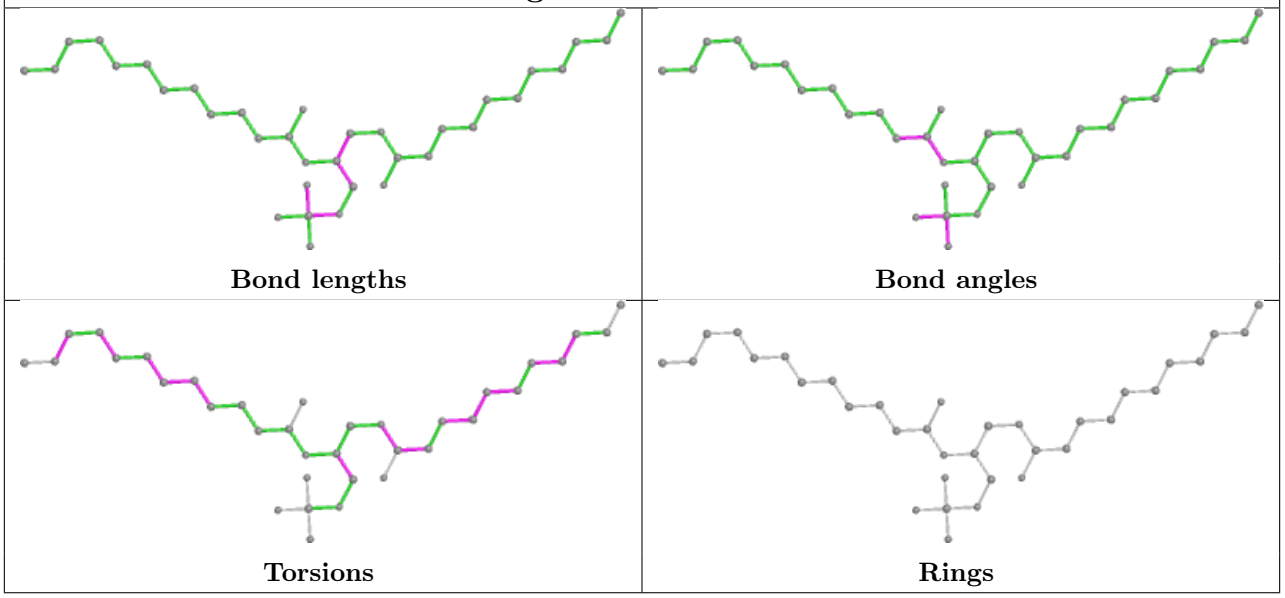


Torsions

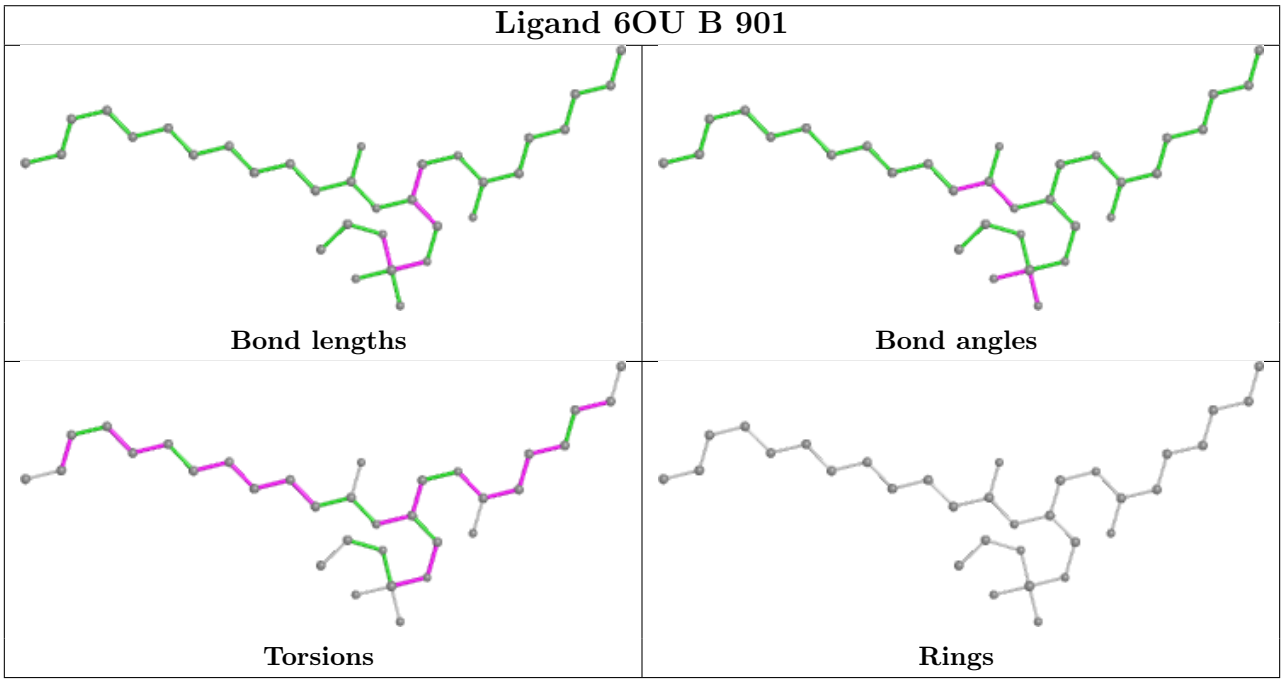


Rings

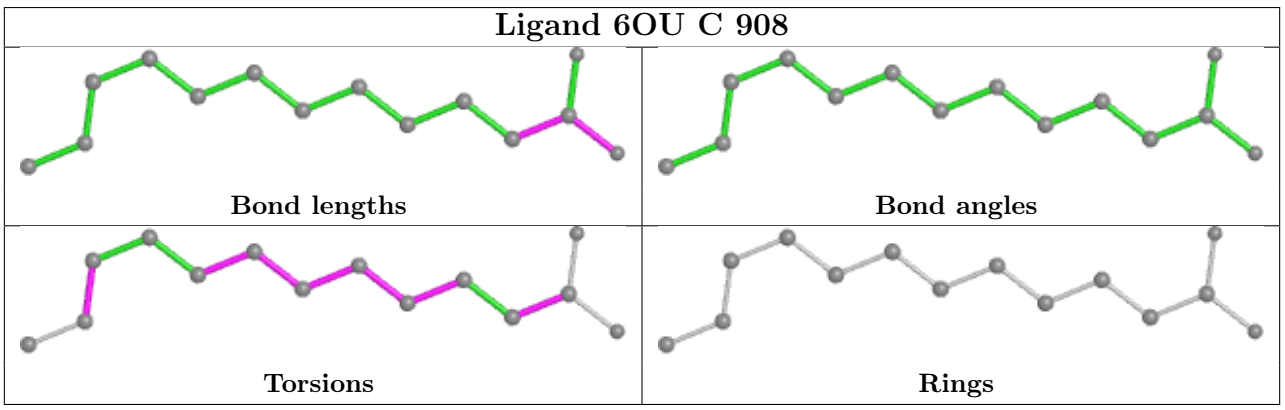
Ligand 6OU C 906



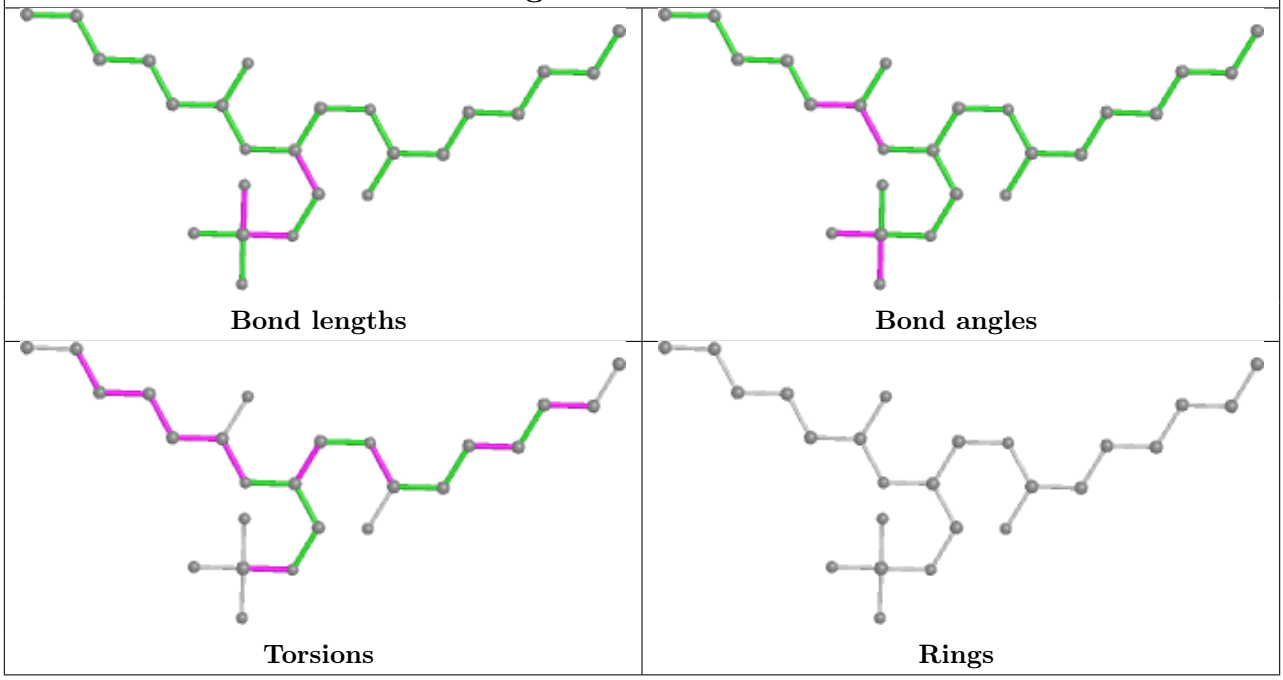
Ligand 6OU B 901



Ligand 6OU C 908



Ligand 6OU D 907



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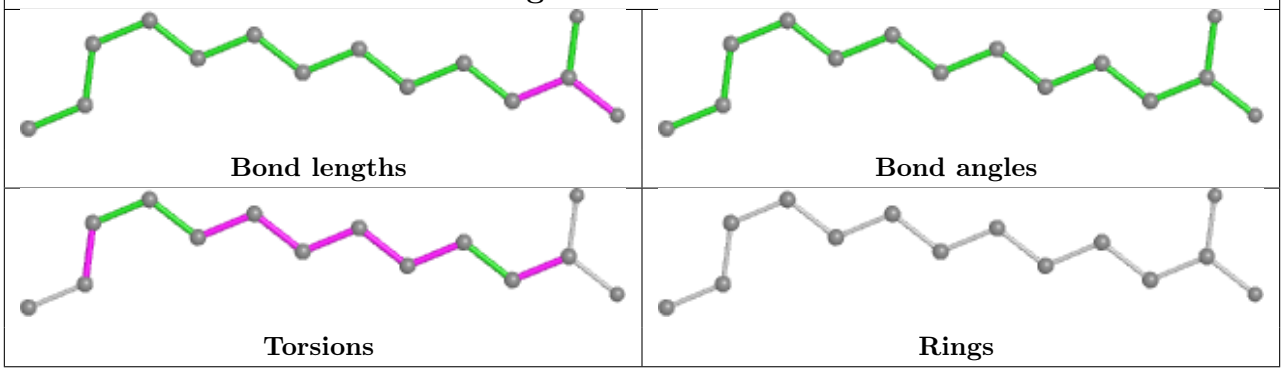
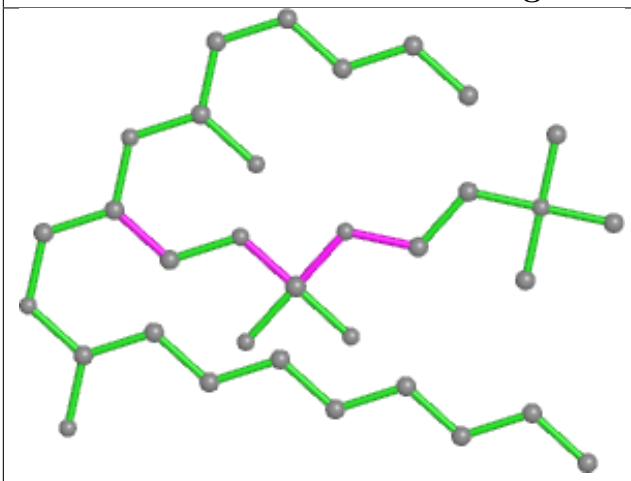
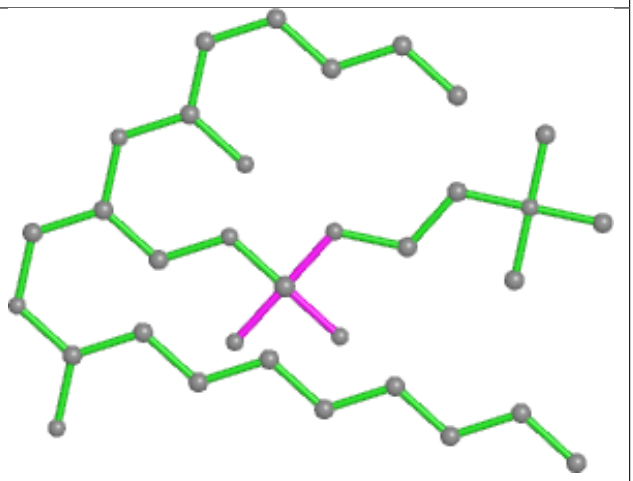


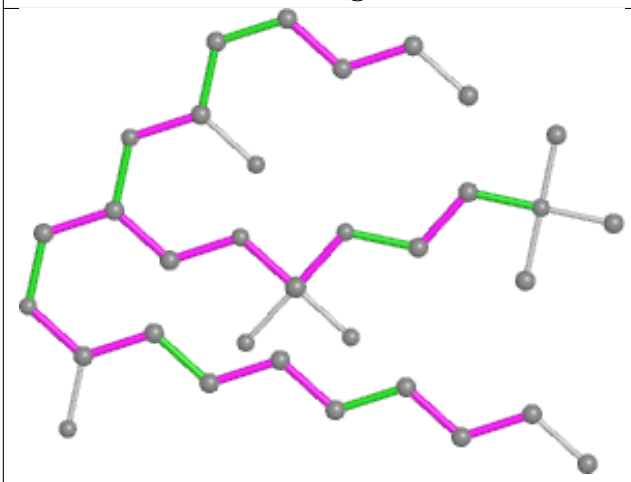
Ligand LBN A 905



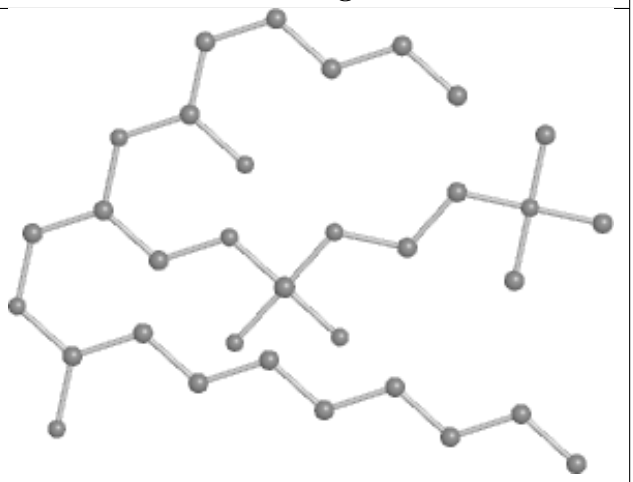
Bond lengths



Bond angles

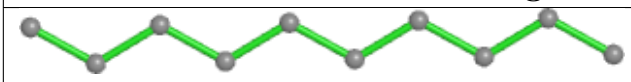


Torsions

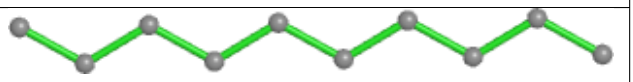


Rings

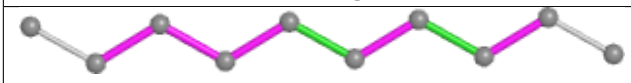
Ligand 6OU A 909



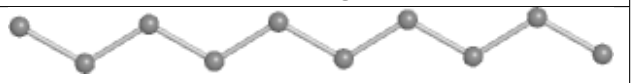
Bond lengths



Bond angles

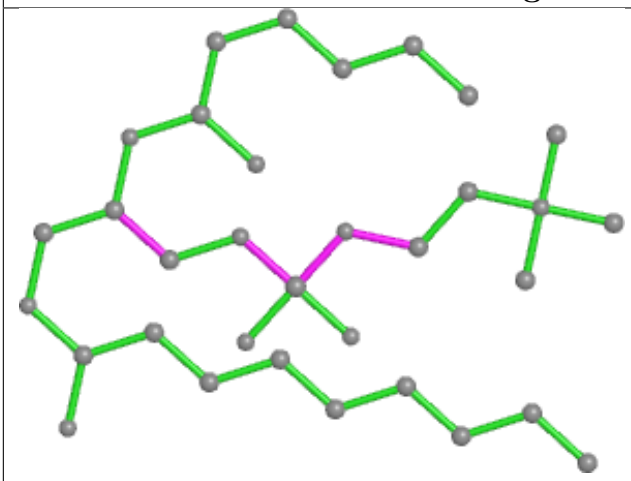


Torsions

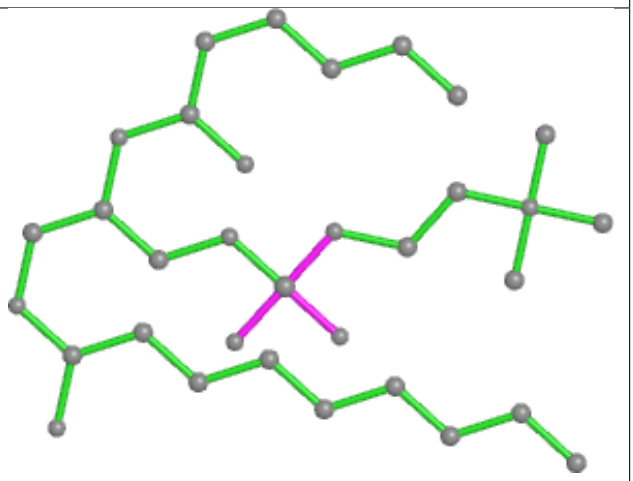


Rings

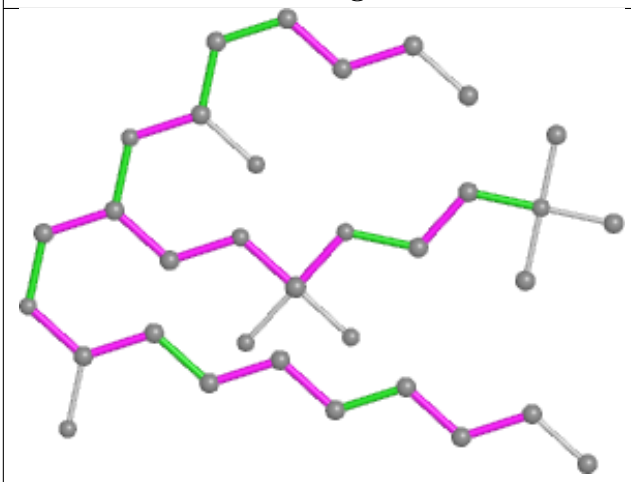
Ligand LBN D 905



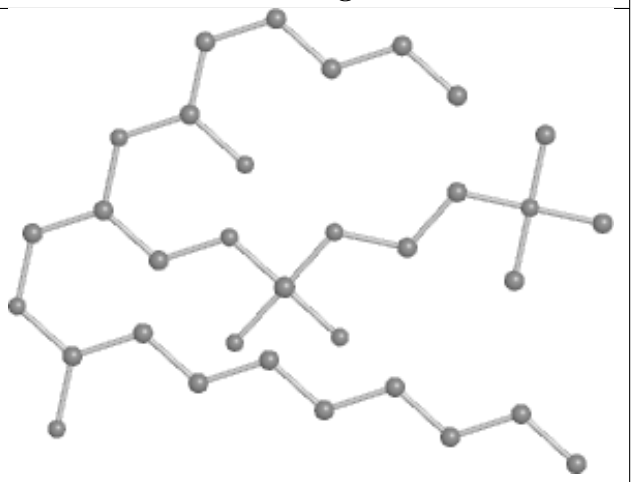
Bond lengths



Bond angles

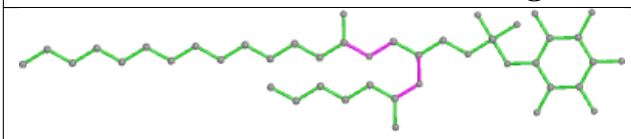


Torsions

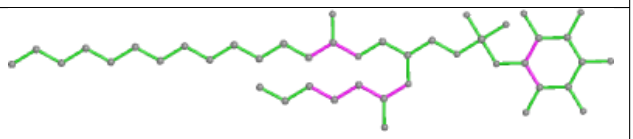


Rings

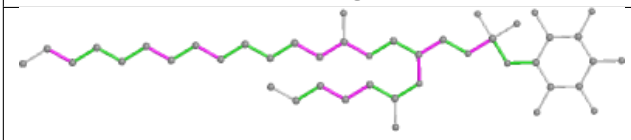
Ligand T7X D 904



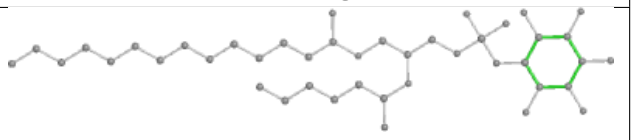
Bond lengths



Bond angles

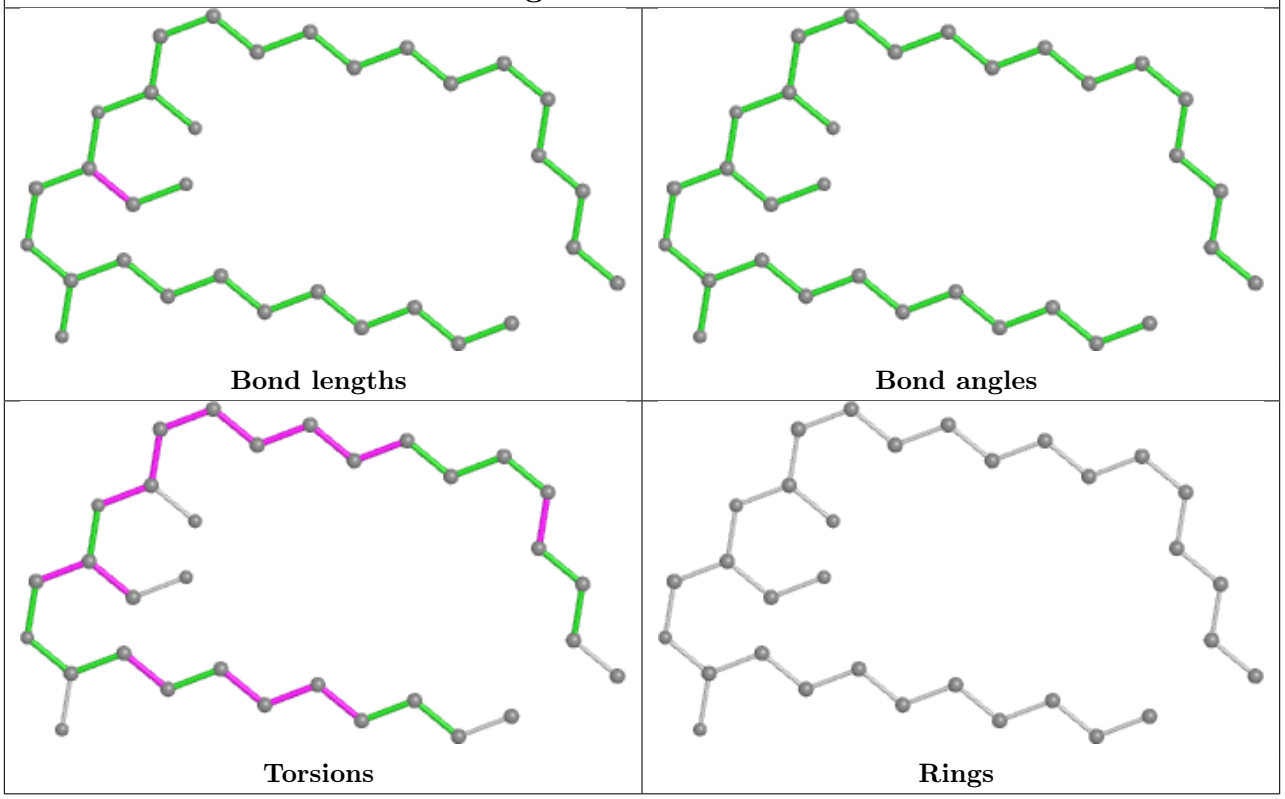


Torsions

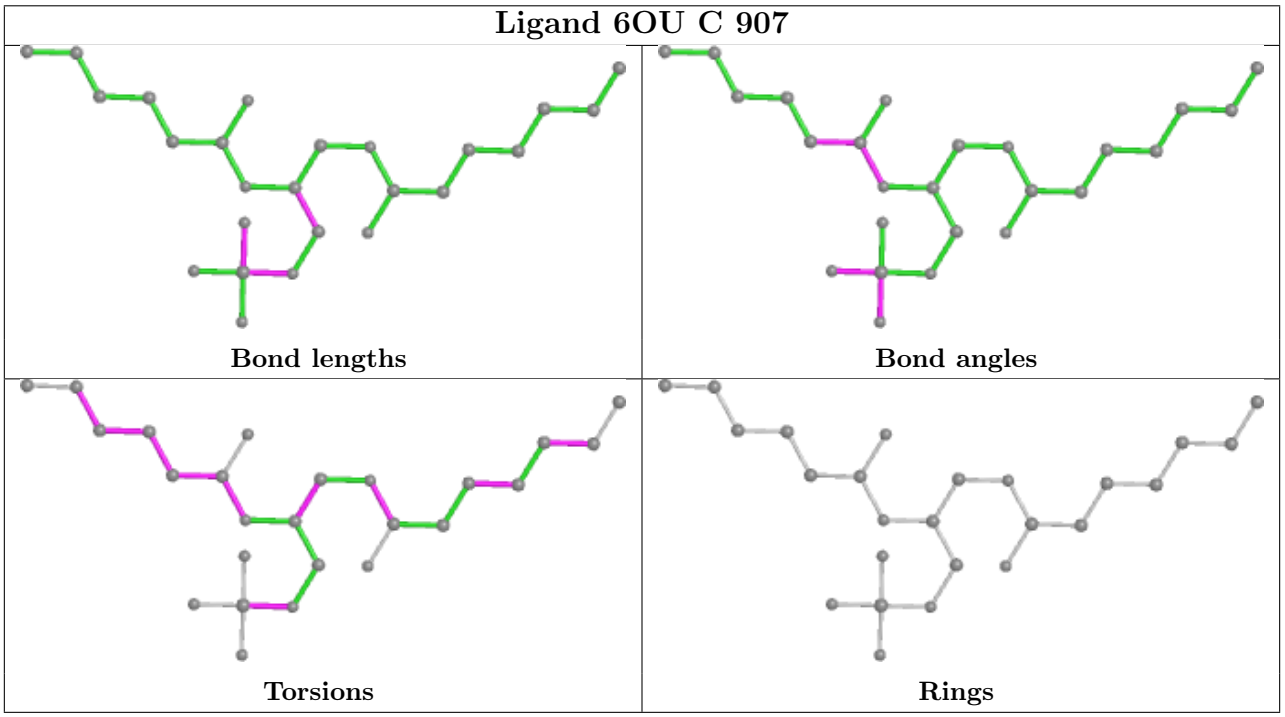


Rings

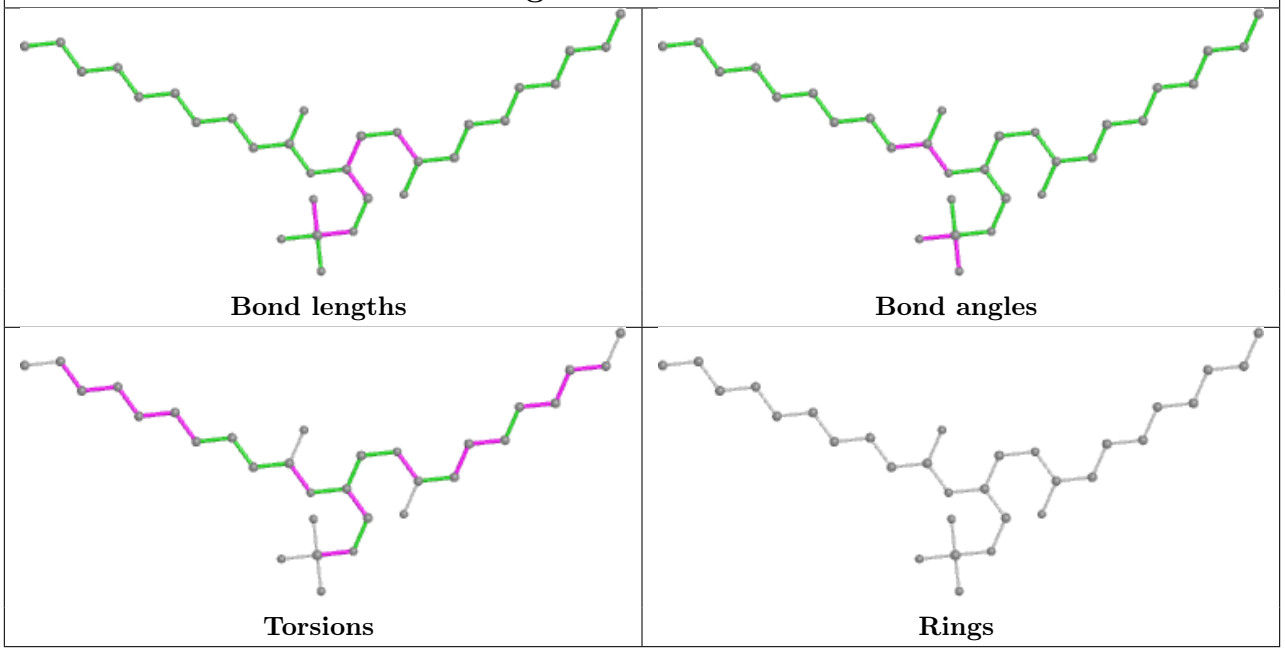
Ligand LBN B 902



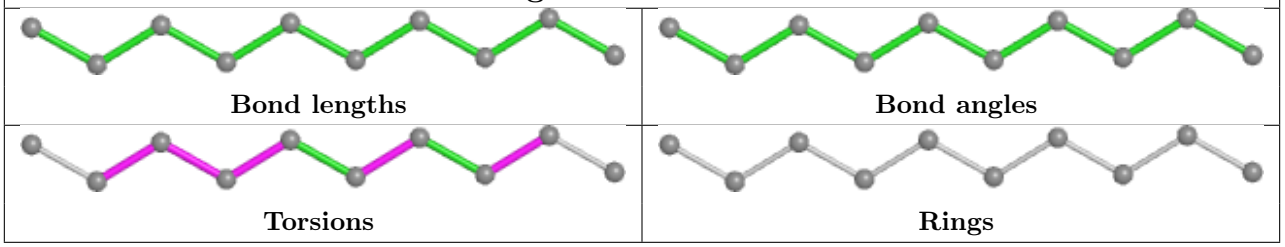
Ligand 6OU C 907



Ligand 6OU C 910



Ligand 6OU B 909



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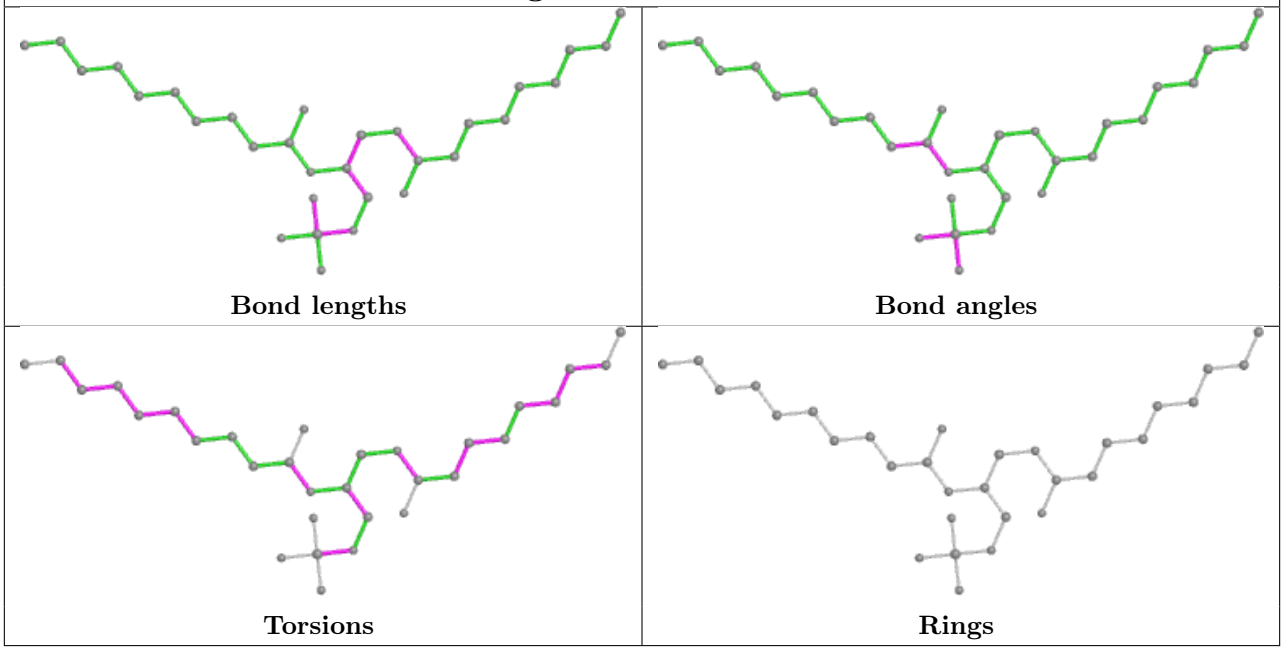
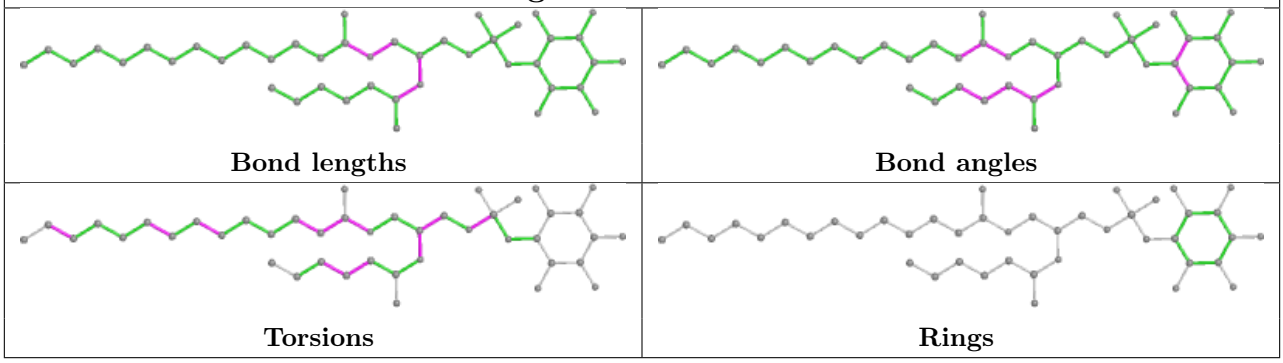
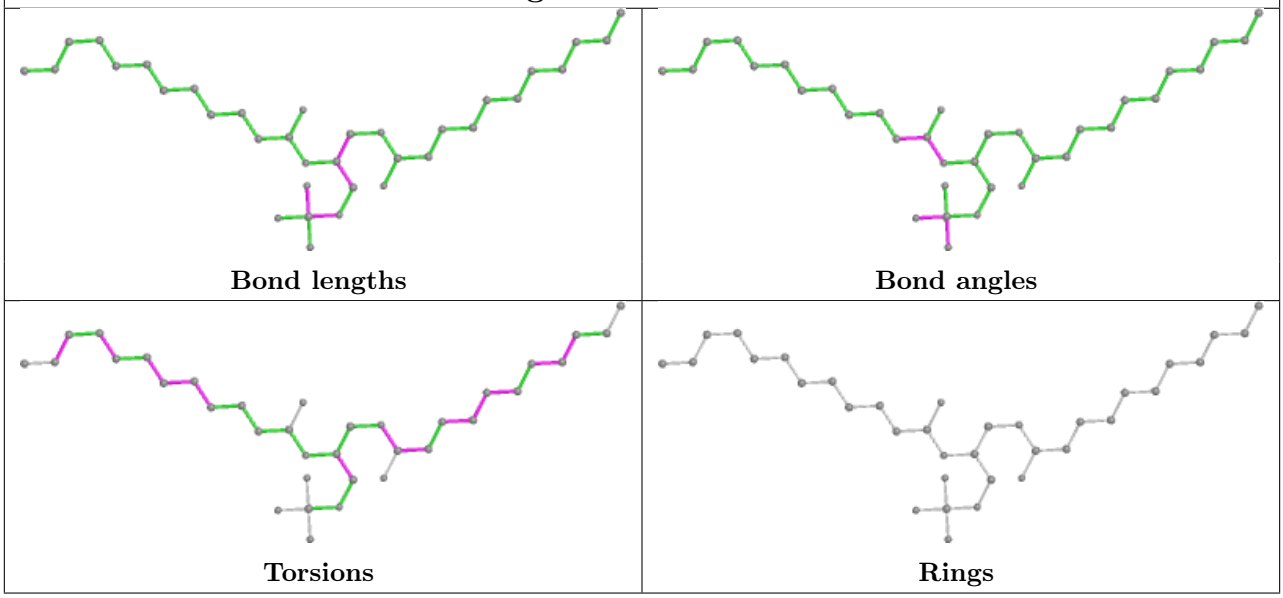


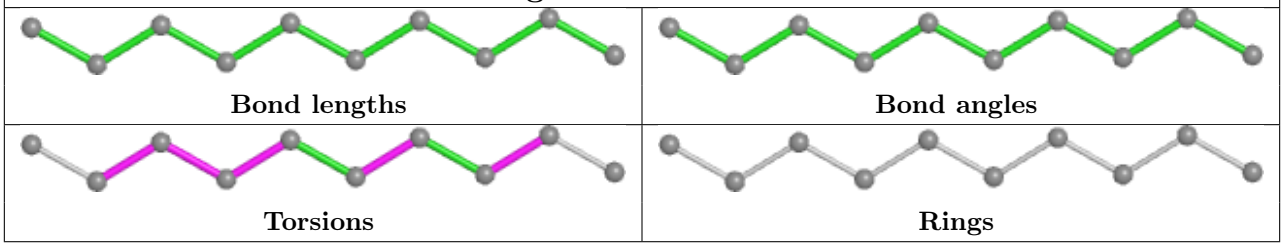
Ligand T7X B 904



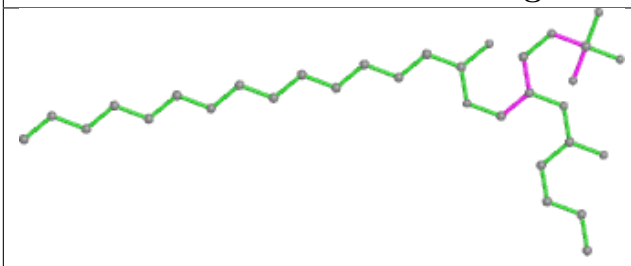
Ligand 6OU B 906



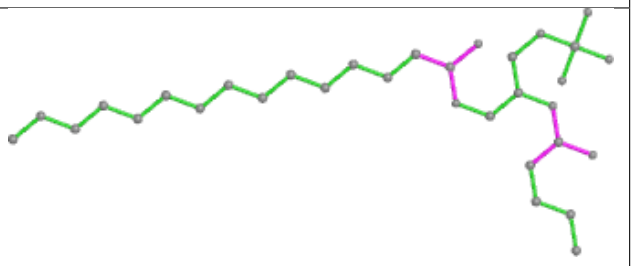
Ligand 6OU C 909



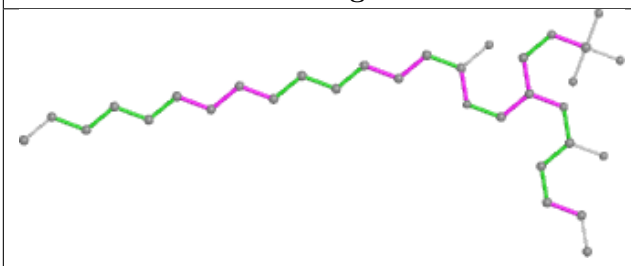
Ligand YFP A 903



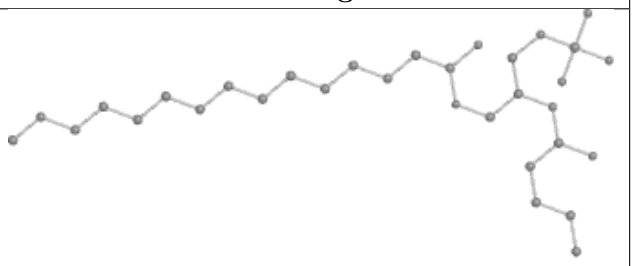
Bond lengths



Bond angles

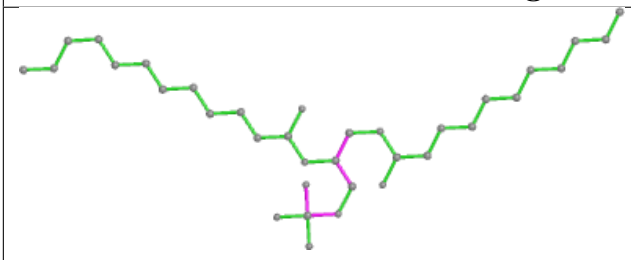


Torsions

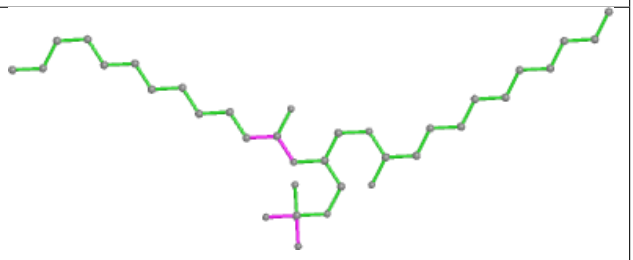


Rings

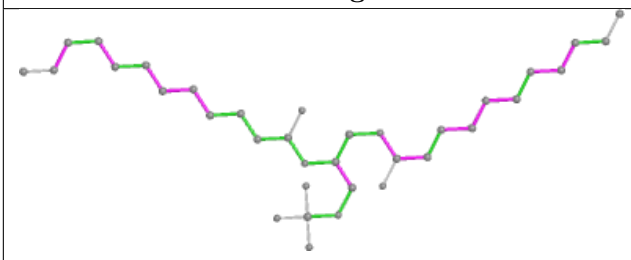
Ligand 6OU A 906



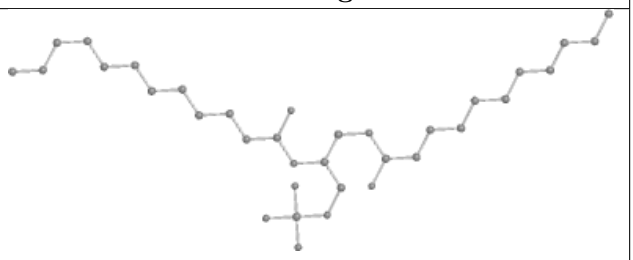
Bond lengths



Bond angles

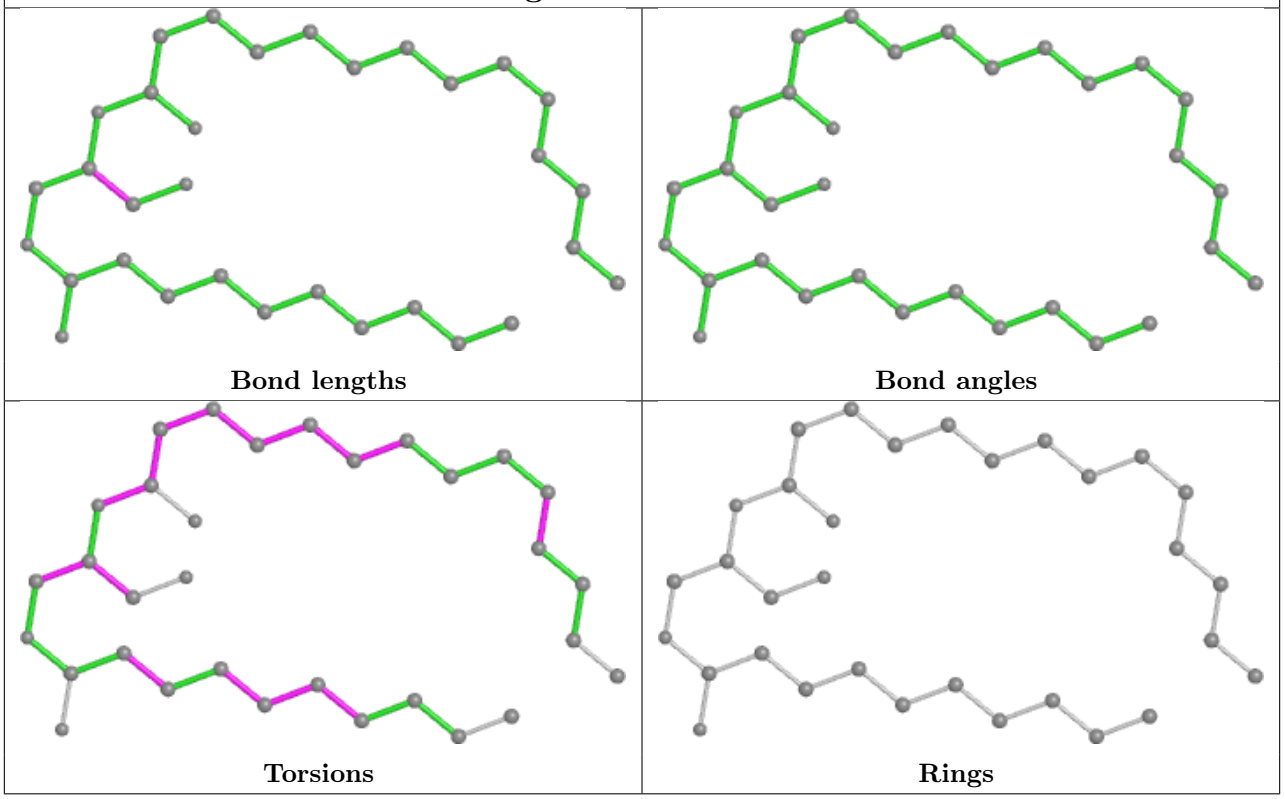


Torsions

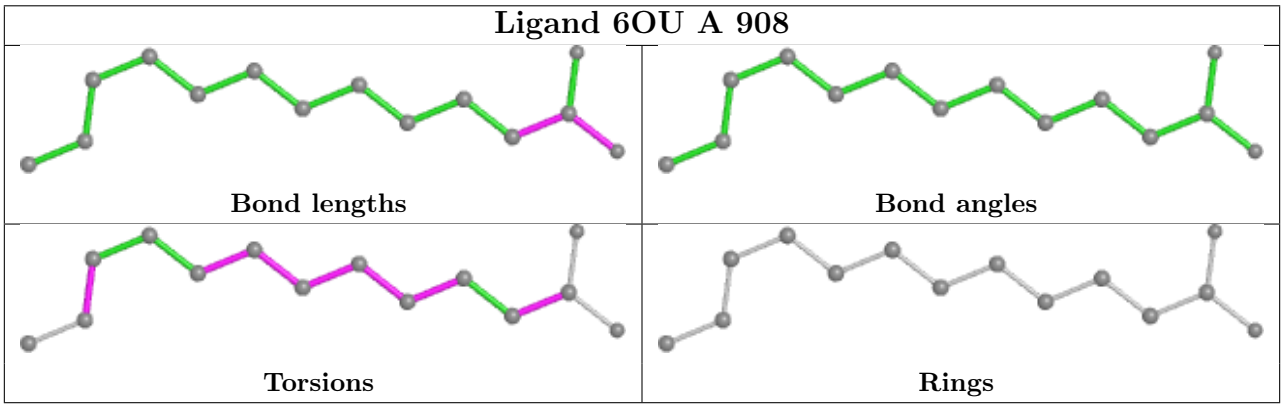


Rings

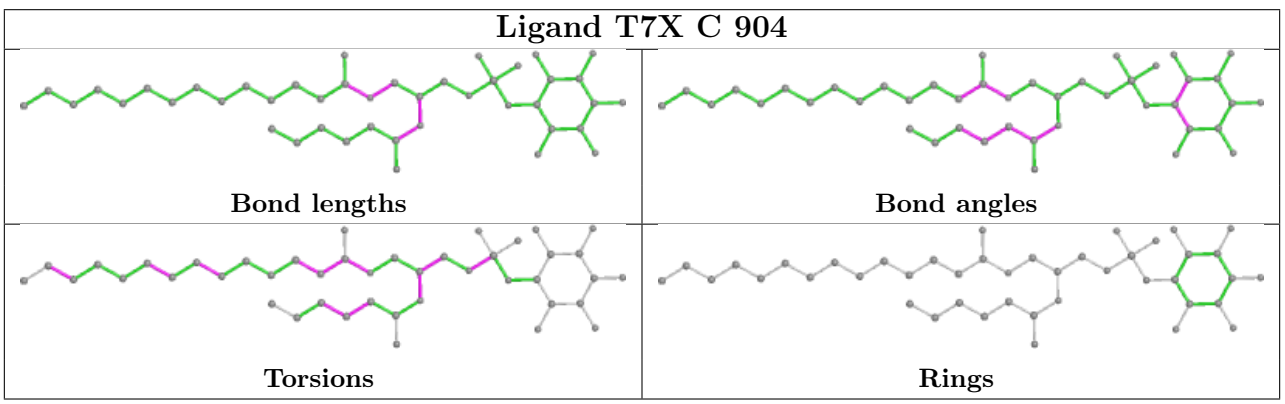
Ligand LBN C 902



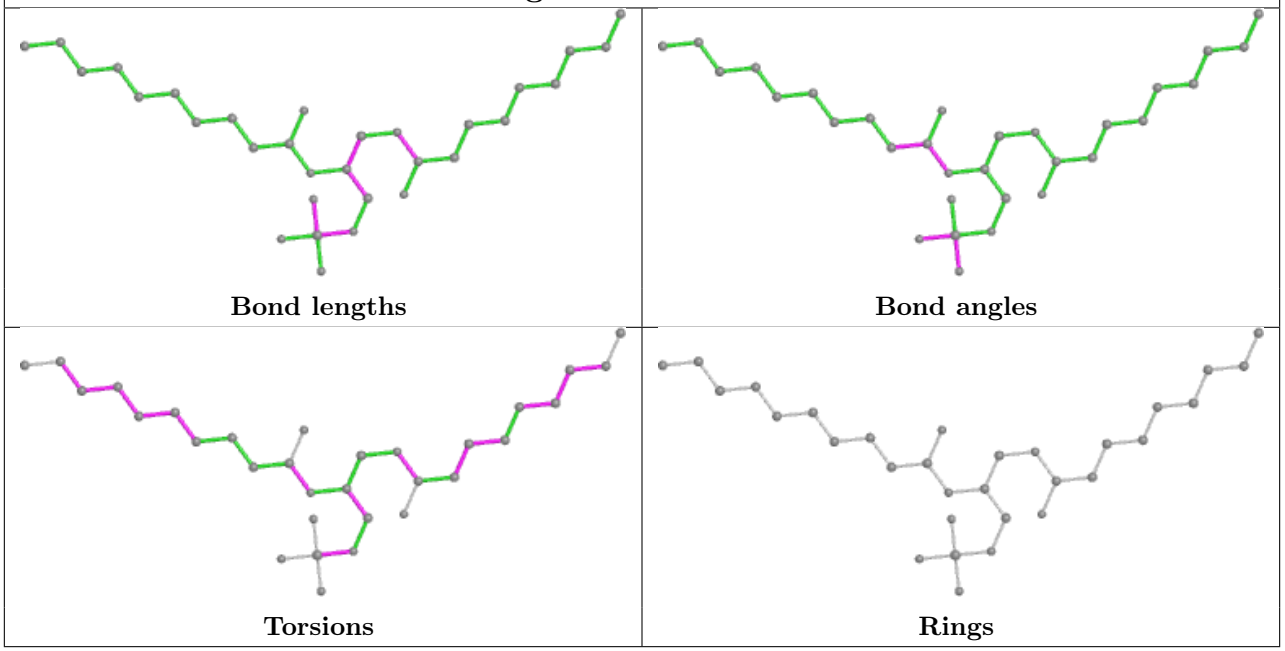
Ligand 6OU A 908



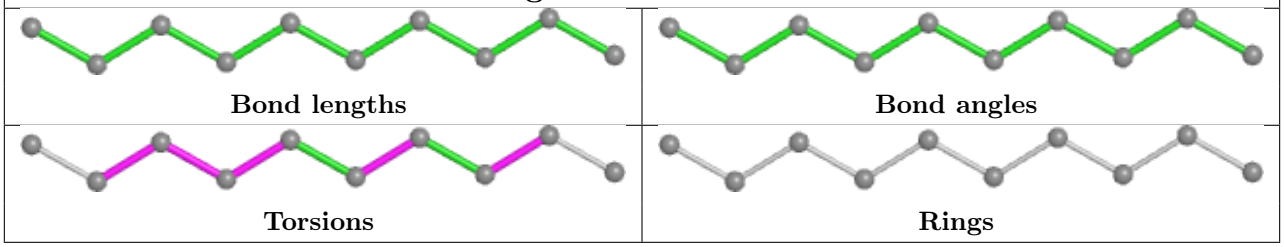
Ligand T7X C 904



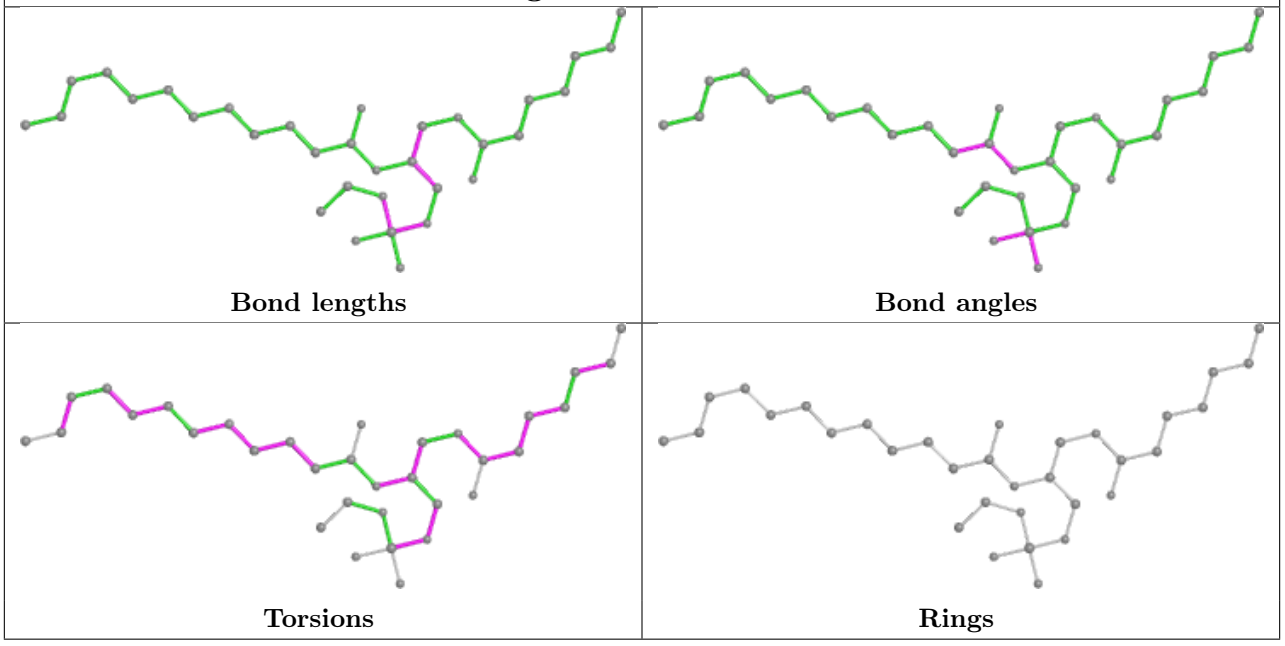
Ligand 6OU D 910



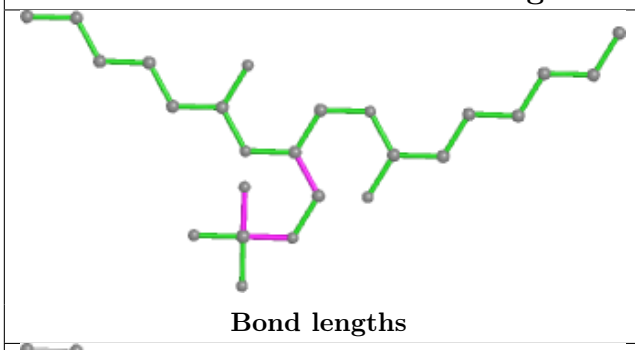
Ligand 6OU D 909



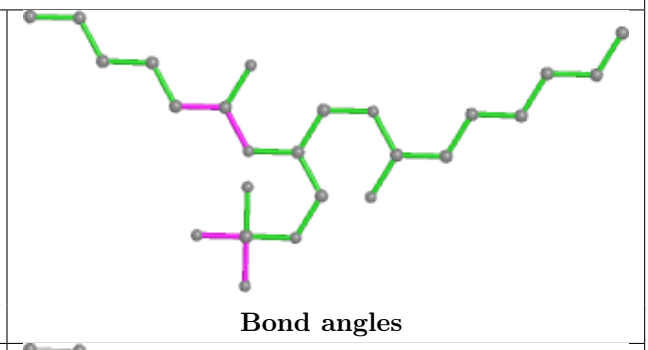
Ligand 6OU A 901



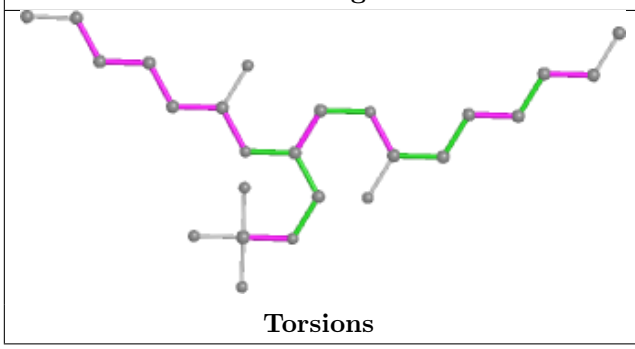
Ligand 6OU B 907



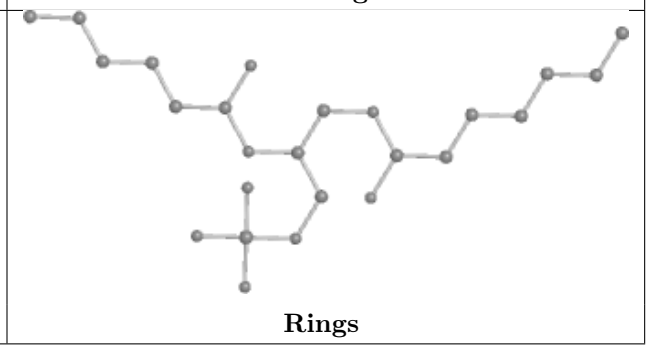
Bond lengths



Bond angles

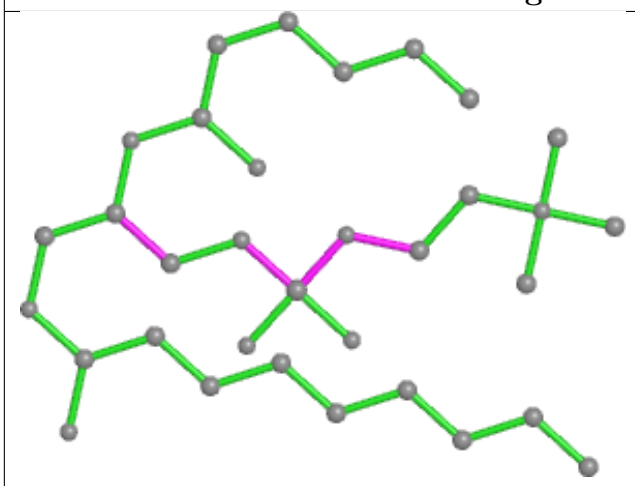


Torsions

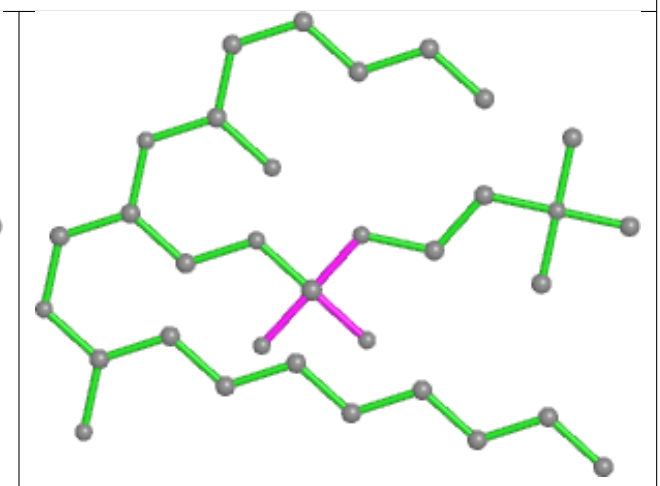


Rings

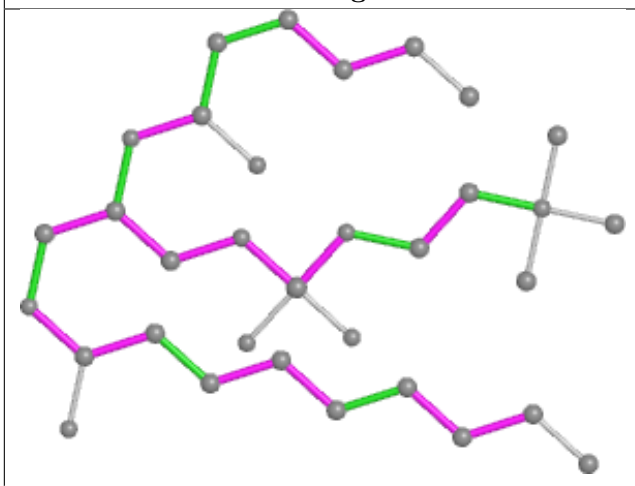
Ligand LBN C 905



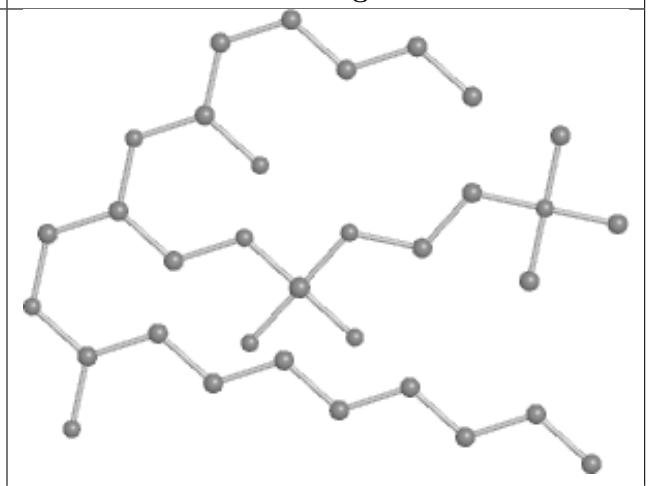
Bond lengths



Bond angles

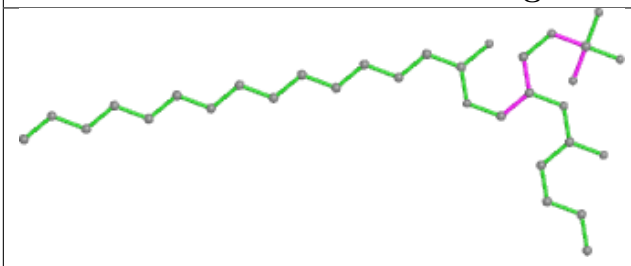


Torsions

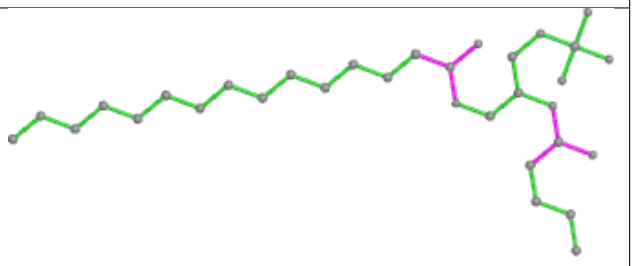


Rings

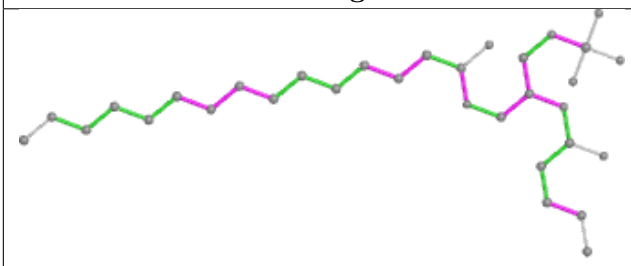
Ligand YFP D 903



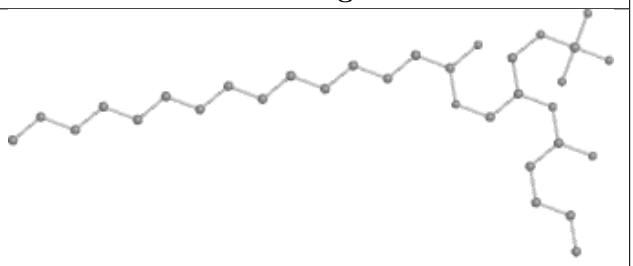
Bond lengths



Bond angles

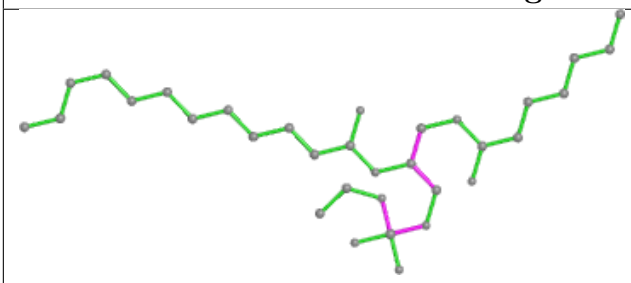


Torsions

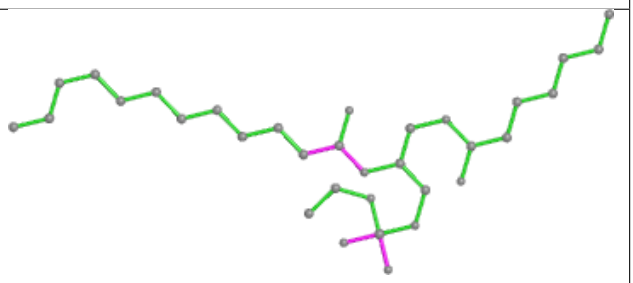


Rings

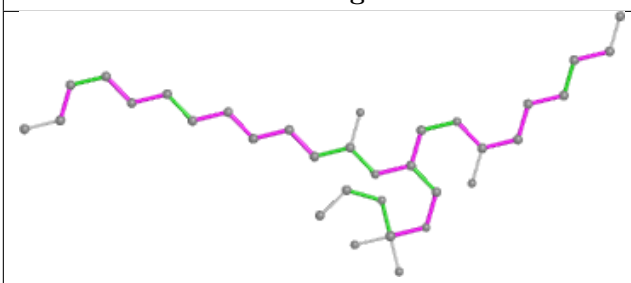
Ligand 6OU D 901



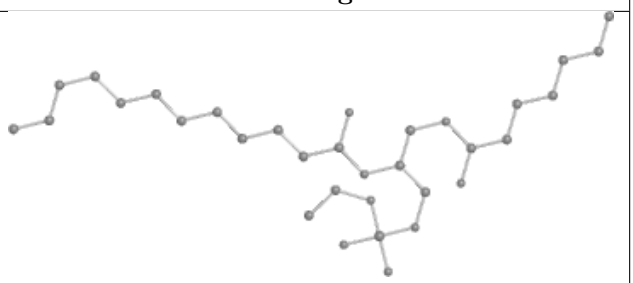
Bond lengths



Bond angles

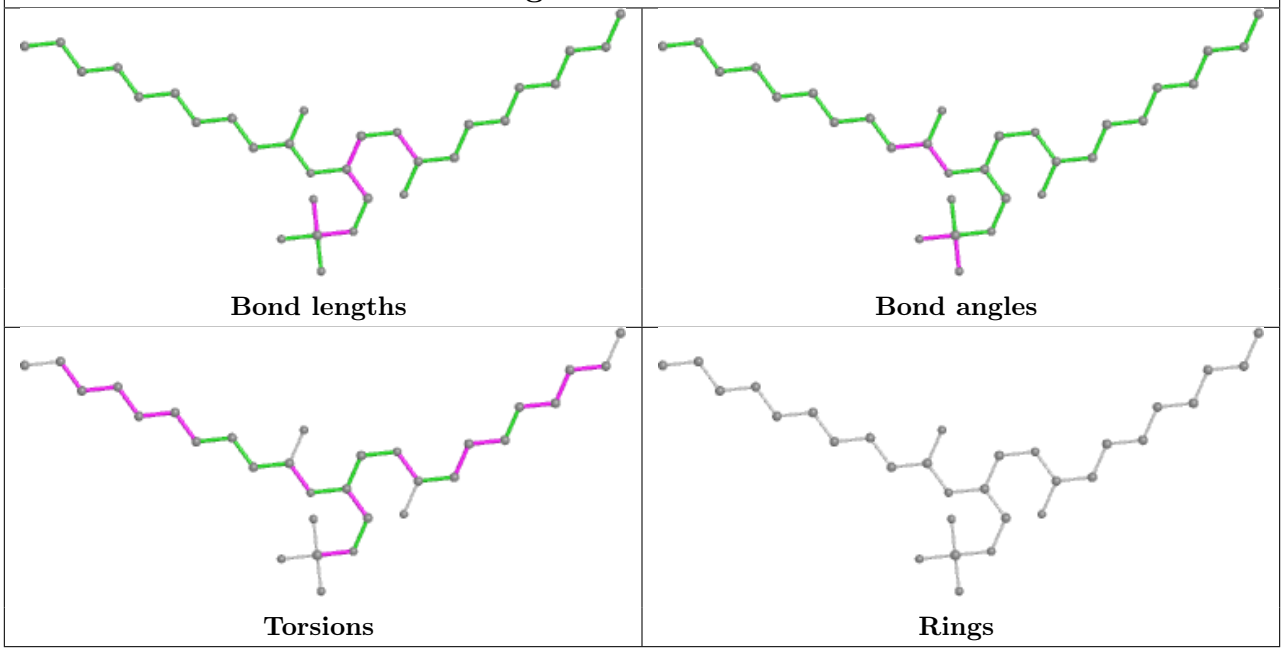


Torsions

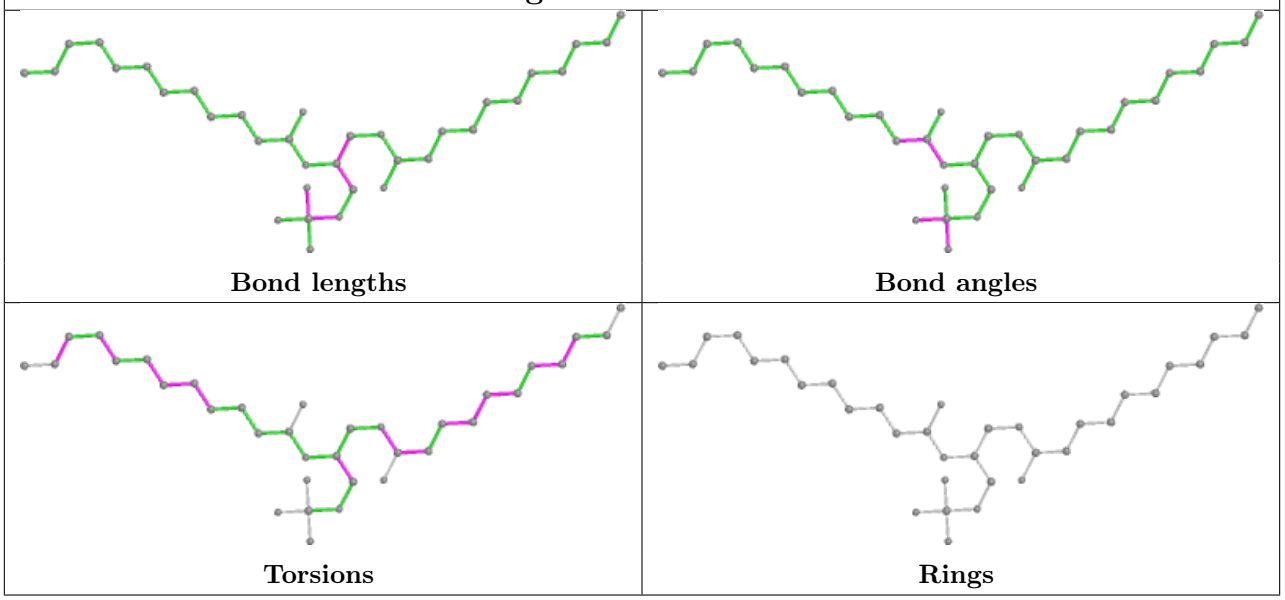


Rings

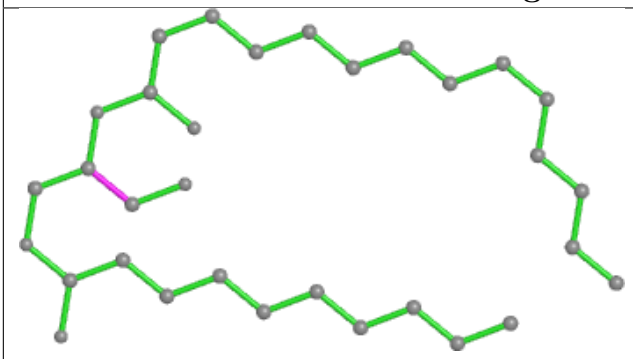
Ligand 6OU A 910



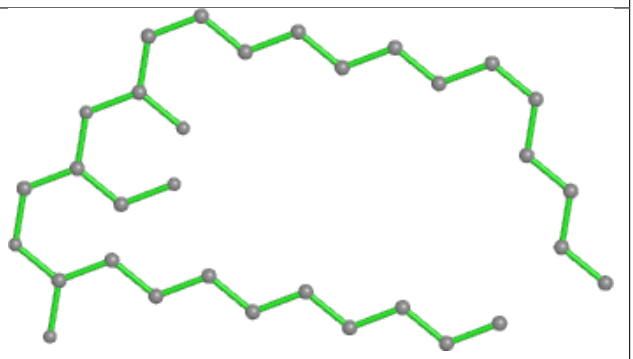
Ligand 6OU D 906



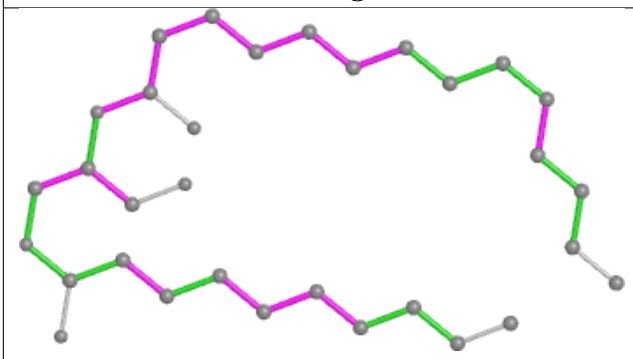
Ligand LBN A 902



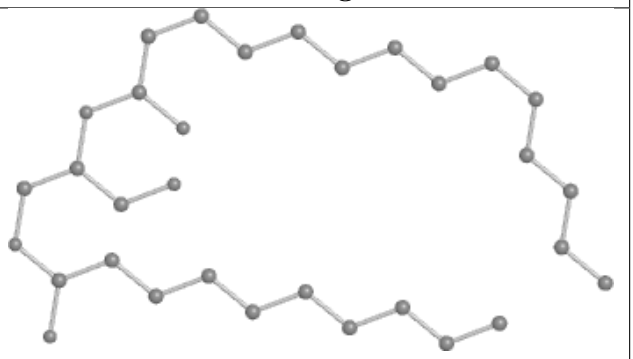
Bond lengths



Bond angles

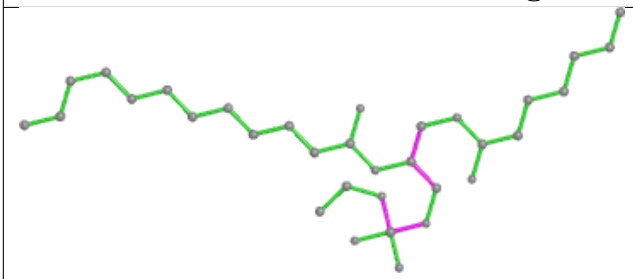


Torsions

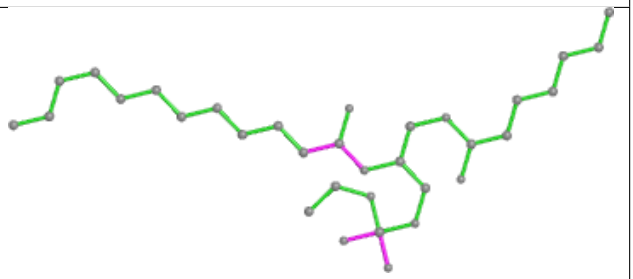


Rings

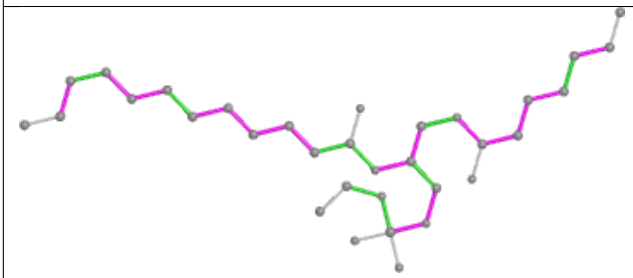
Ligand 6OU C 901



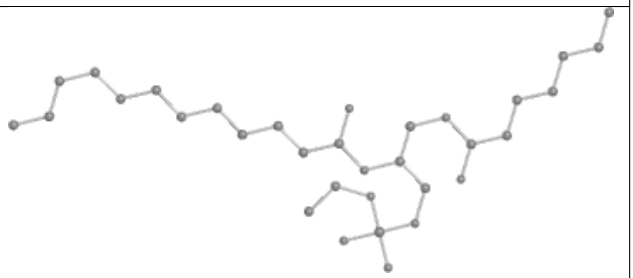
Bond lengths



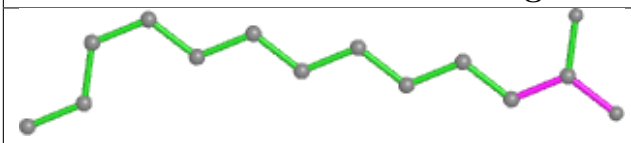
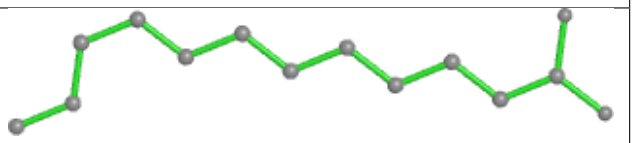
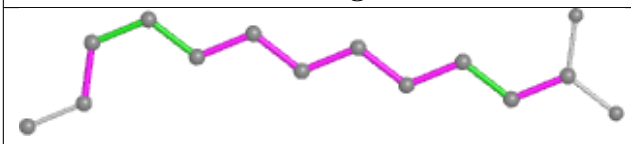
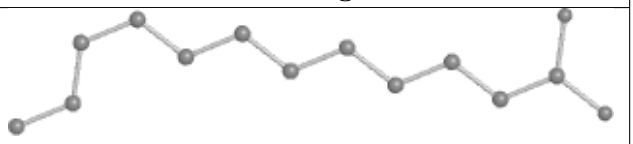
Bond angles



Torsions



Rings

Ligand 6OU D 908	
 Bond lengths	 Bond angles
 Torsions	 Rings

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

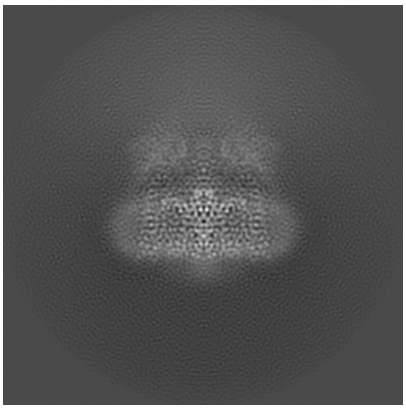
6 Map visualisation

This section contains visualisations of the EMDB entry EMD-23476. These allow visual inspection of the internal detail of the map and identification of artifacts.

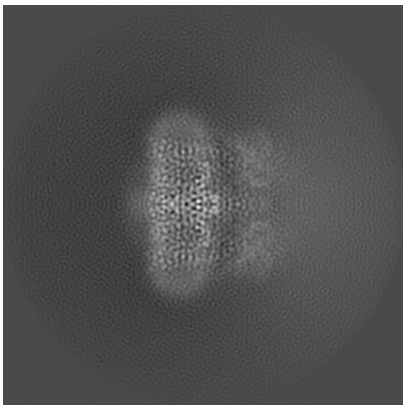
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections

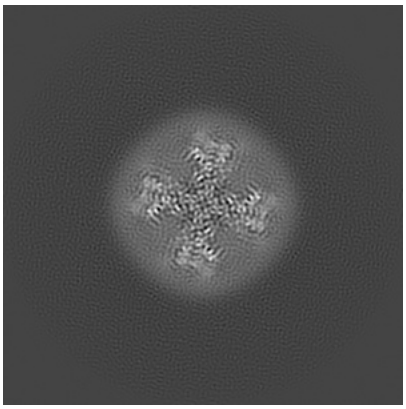
6.1.1 Primary map



X

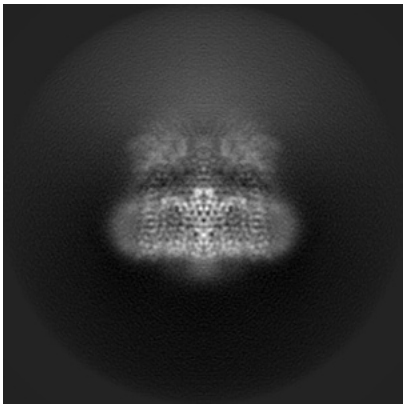


Y

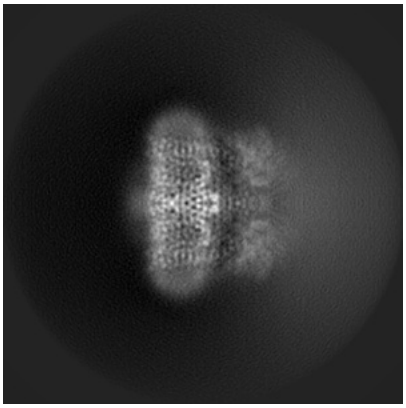


Z

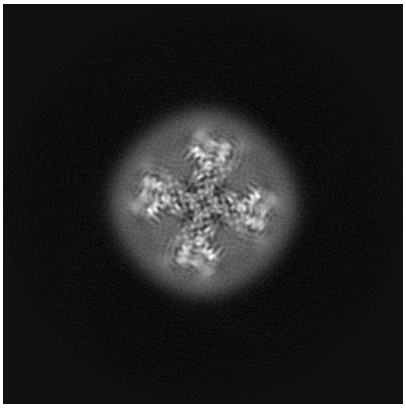
6.1.2 Raw map



X



Y

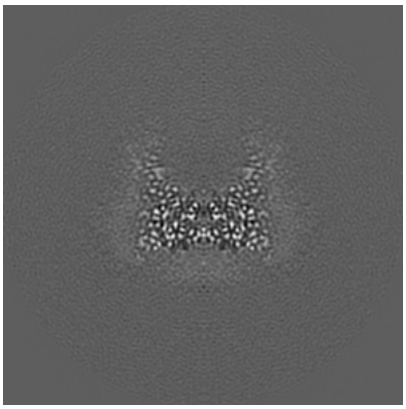


Z

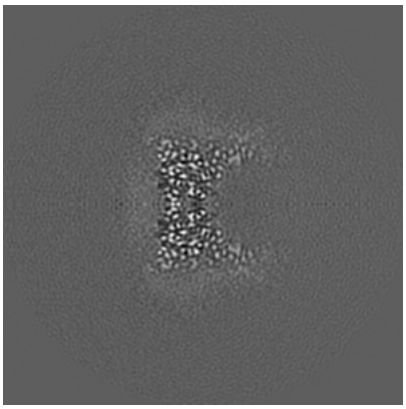
The images above show the map projected in three orthogonal directions.

6.2 Central slices (i)

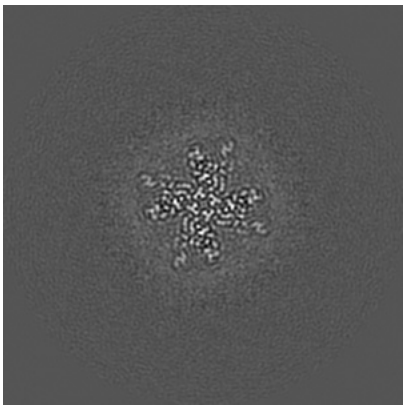
6.2.1 Primary map



X Index: 128

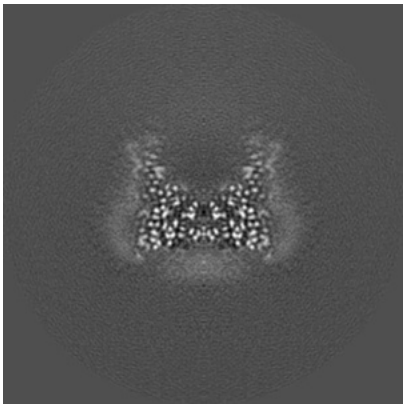


Y Index: 128

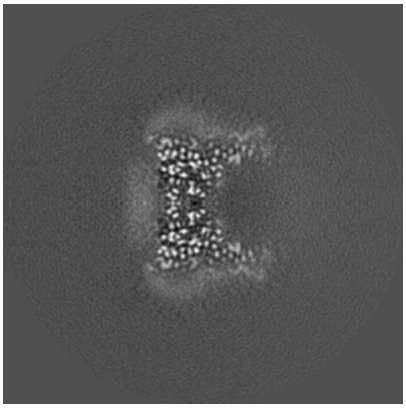


Z Index: 128

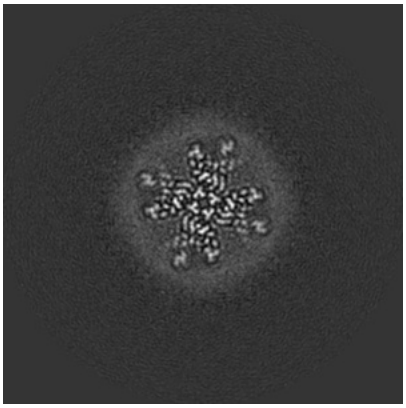
6.2.2 Raw map



X Index: 128



Y Index: 128

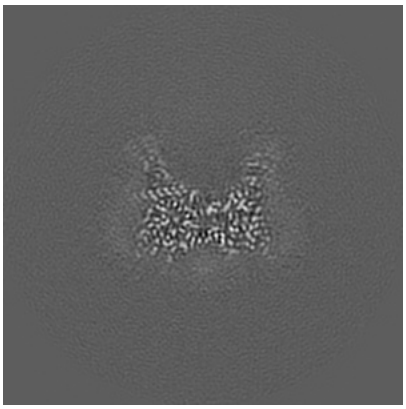


Z Index: 128

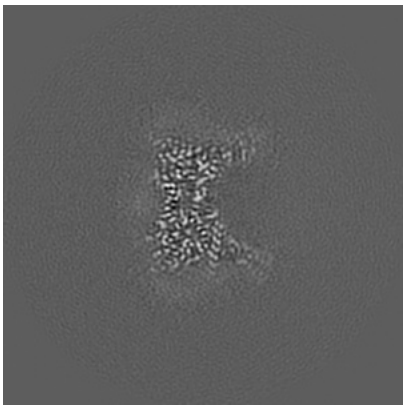
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

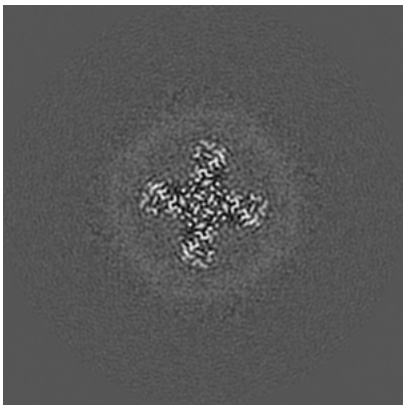
6.3.1 Primary map



X Index: 126

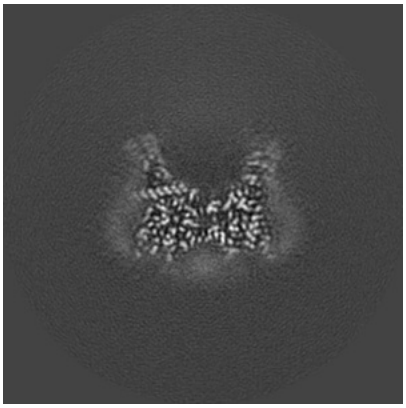


Y Index: 130

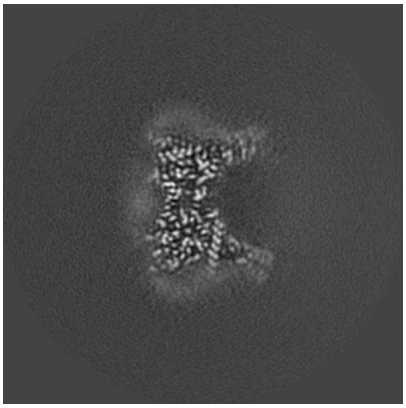


Z Index: 111

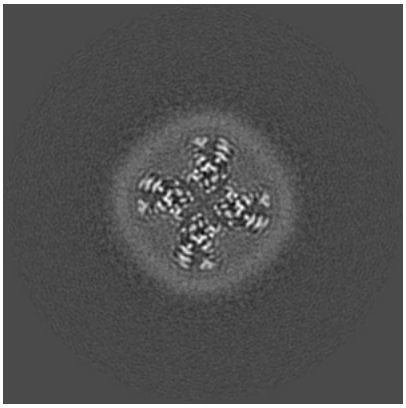
6.3.2 Raw map



X Index: 126



Y Index: 130

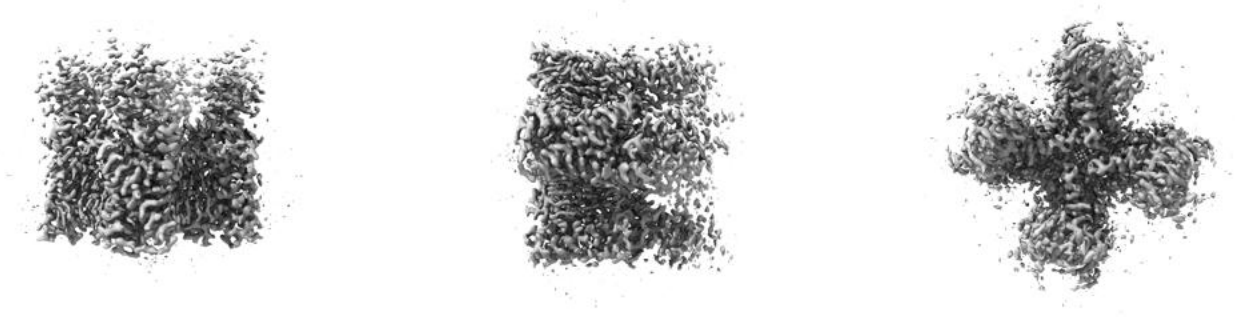


Z Index: 102

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

6.4 Orthogonal surface views (i)

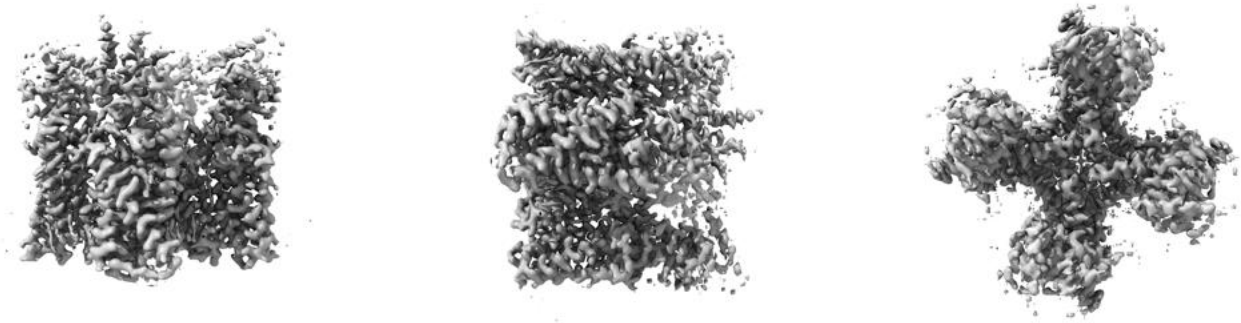
6.4.1 Primary map



X Y Z

The images above show the 3D surface view of the map at the recommended contour level 0.04. 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



X Y Z

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.

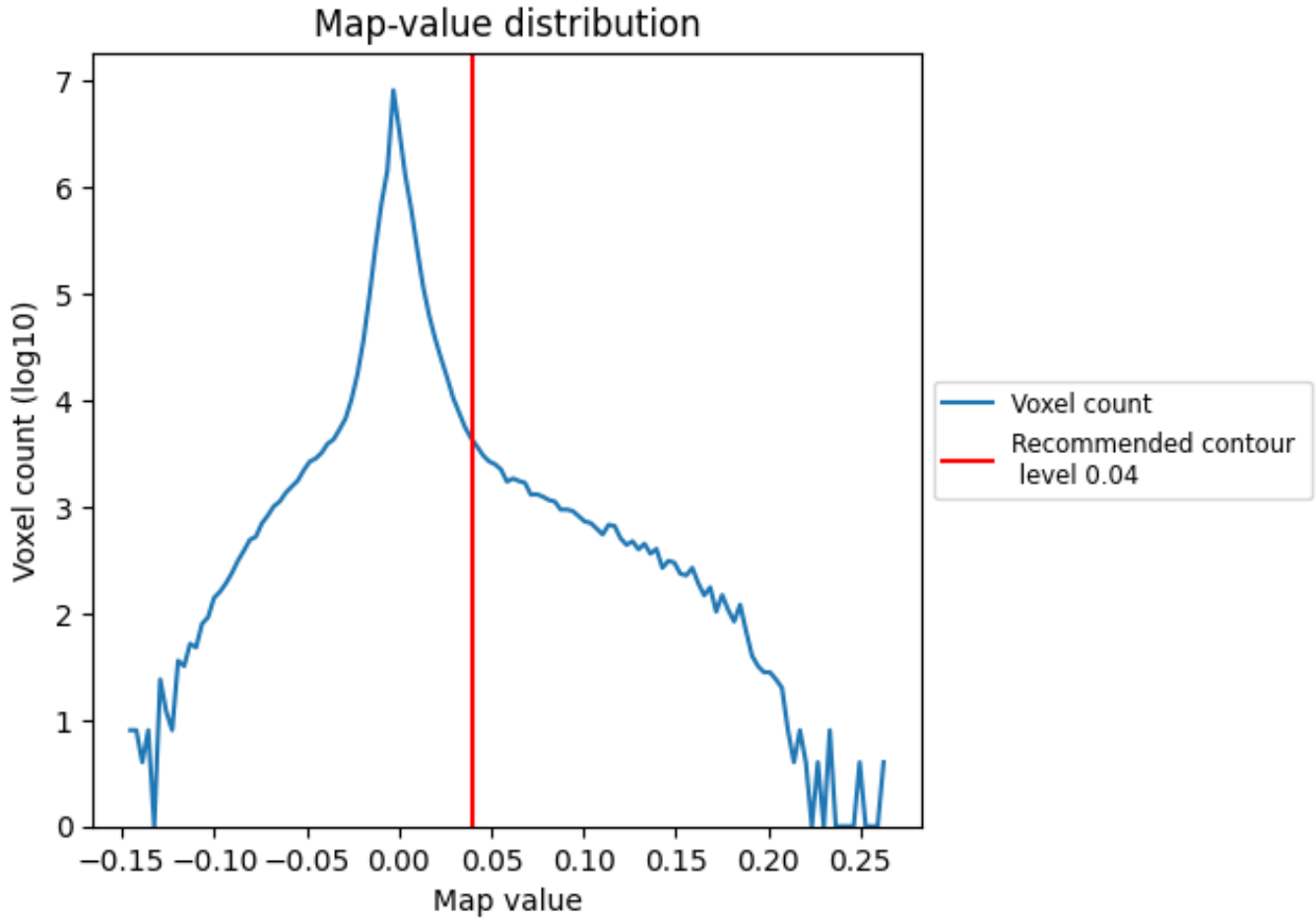
6.5 Mask visualisation (i)

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

7 Map analysis

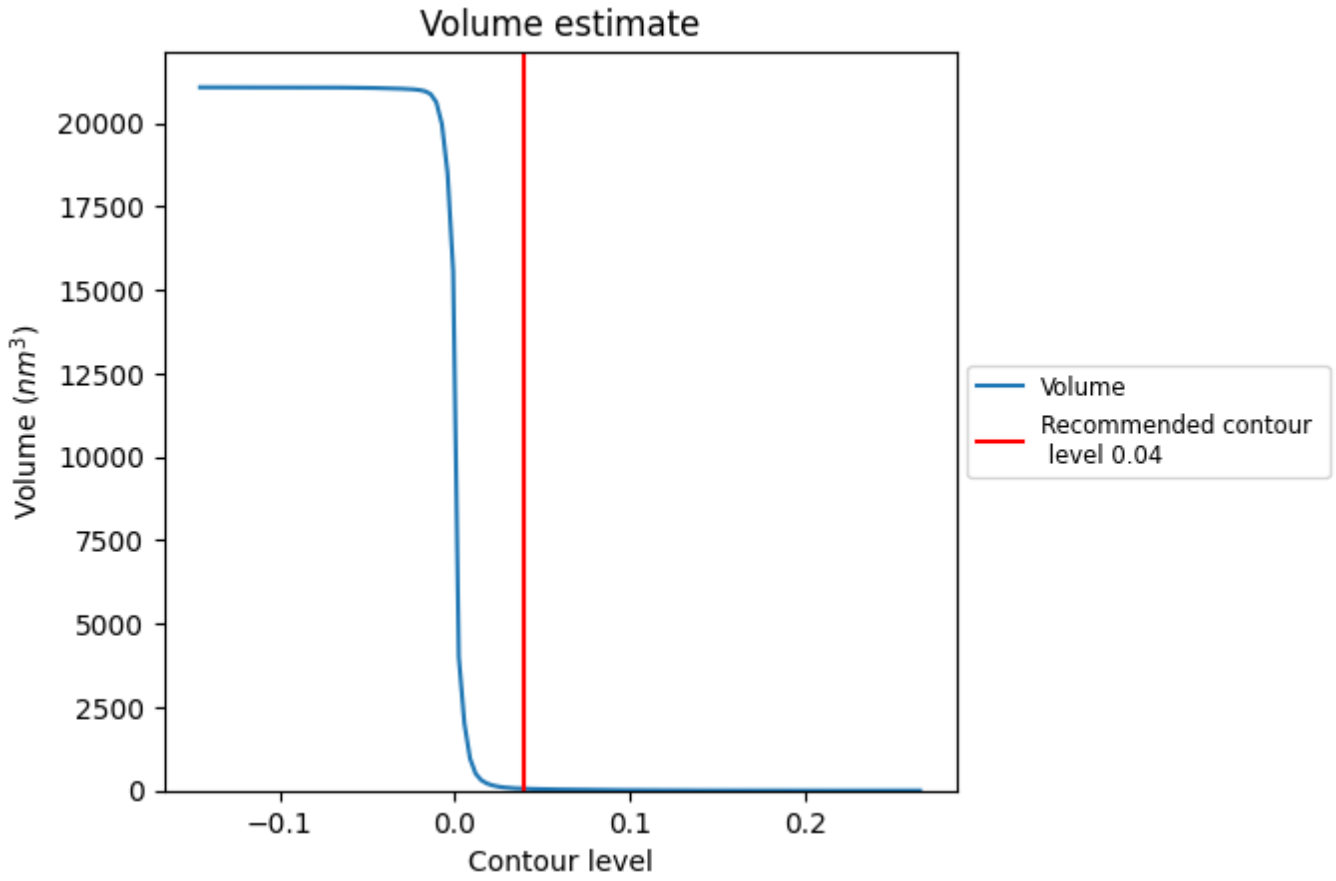
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution



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.

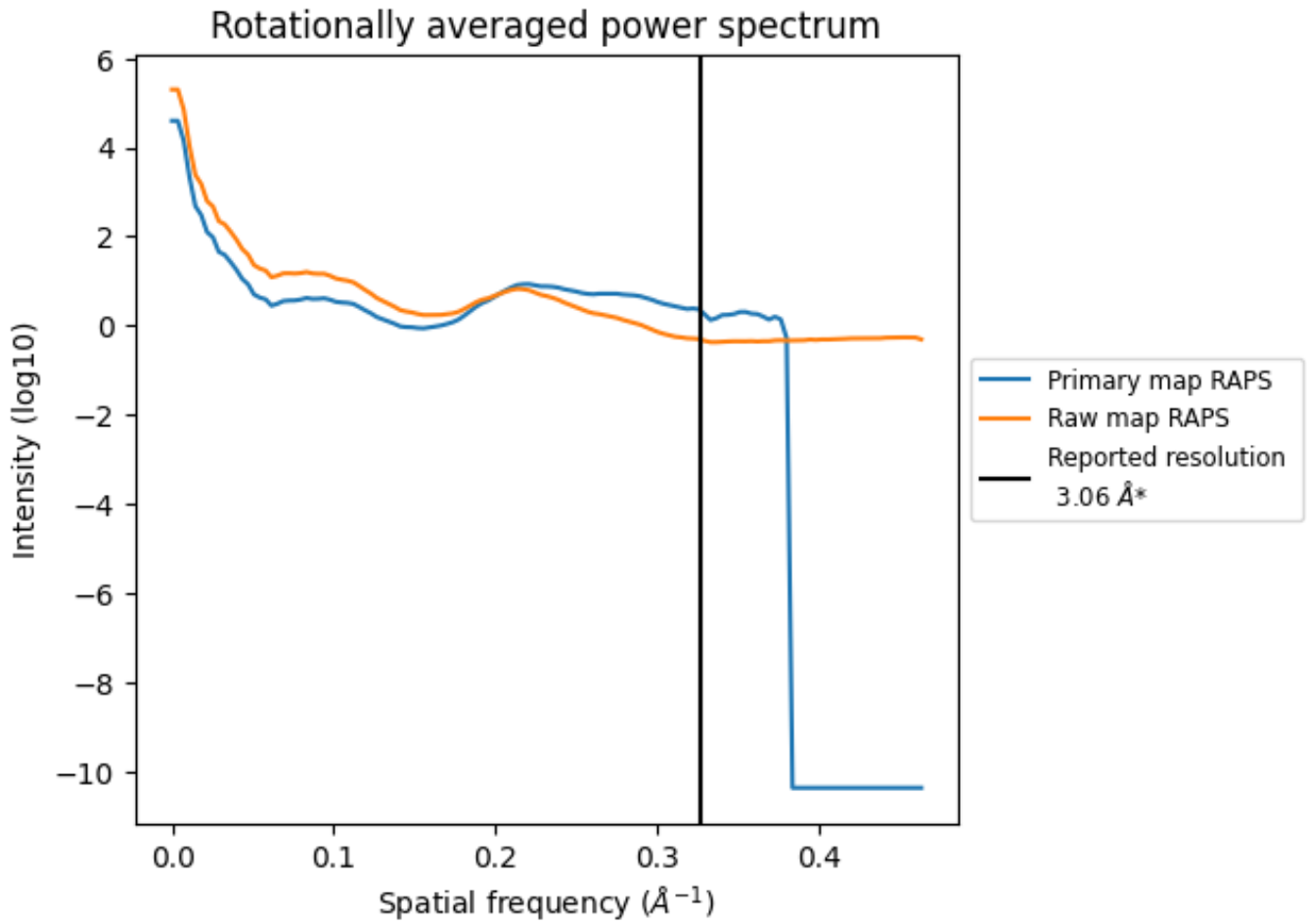
7.2 Volume estimate



The volume at the recommended contour level is 56 nm^3; this corresponds to an approximate mass of 50 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 (i)

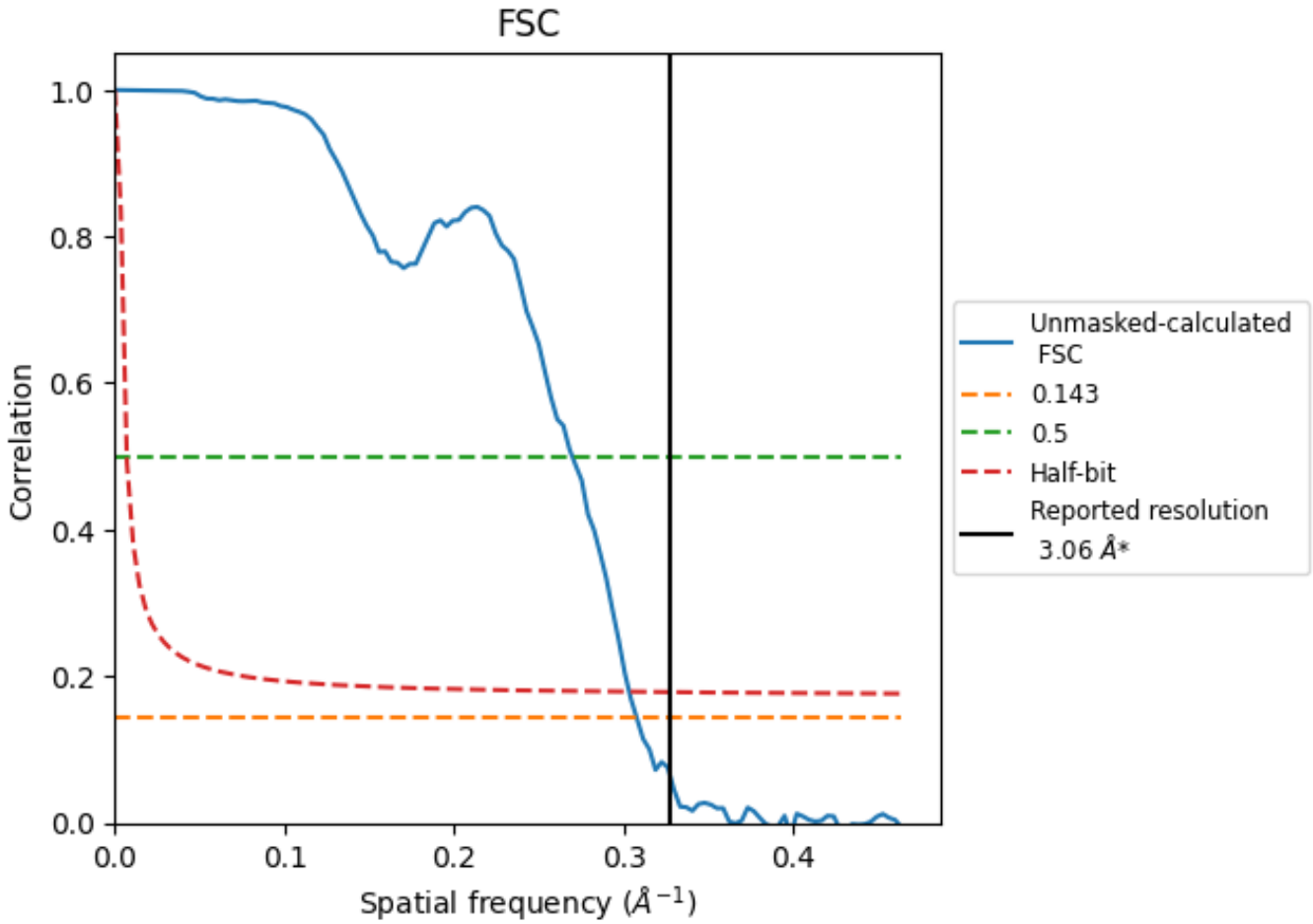


*Reported resolution corresponds to spatial frequency of 0.327 Å^{-1}

8 Fourier-Shell correlation

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



*Reported resolution corresponds to spatial frequency of 0.327 Å^{-1}

8.2 Resolution estimates (i)

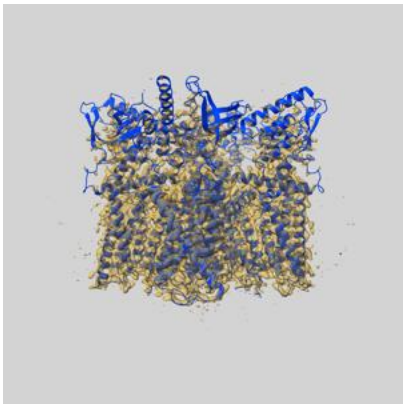
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.06	-	-
Author-provided FSC curve	-	-	-
Unmasked-calculated*	3.25	3.71	3.30

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

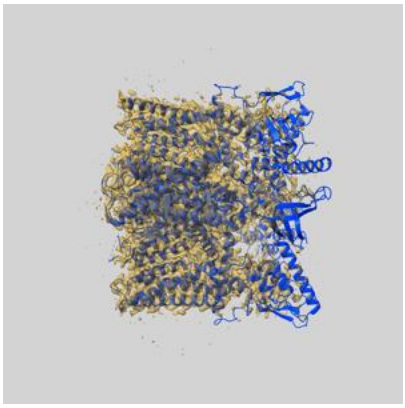
9 Map-model fit

This section contains information regarding the fit between EMDB map EMD-23476 and PDB model 7LPC. Per-residue inclusion information can be found in section 3 on page 11.

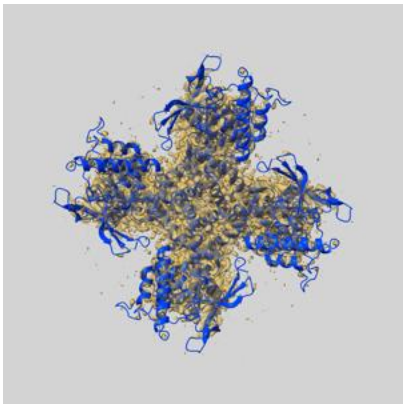
9.1 Map-model overlay



X



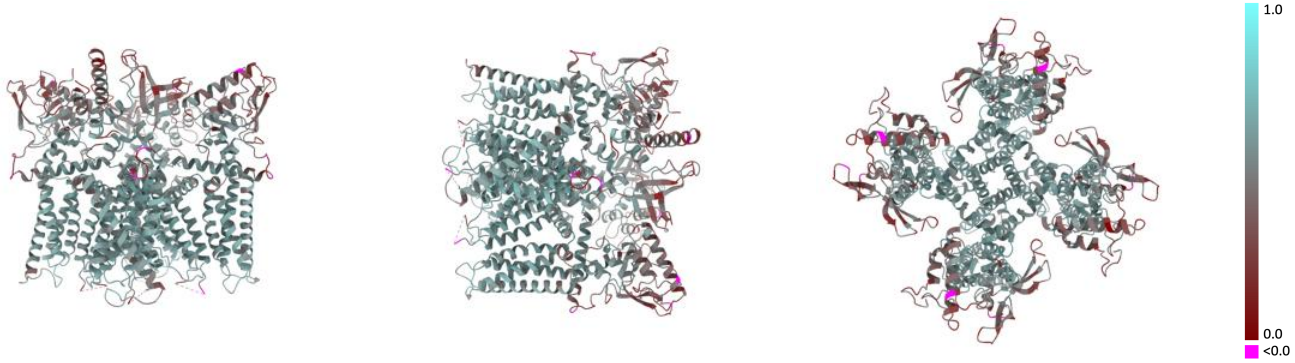
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.04 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.

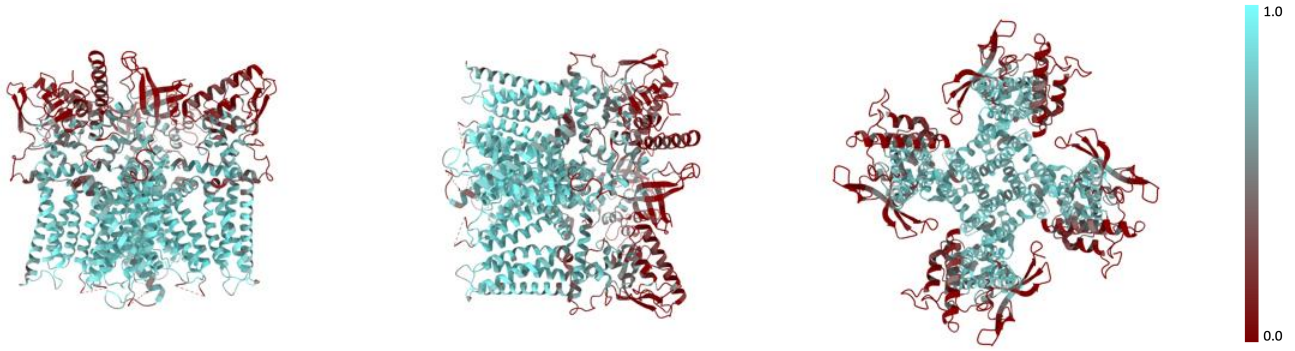
9.2 Q-score mapped to coordinate model (i)



X Y Z

The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions at which atoms can be resolved. Low Q-score values may therefore be expected for many entries.

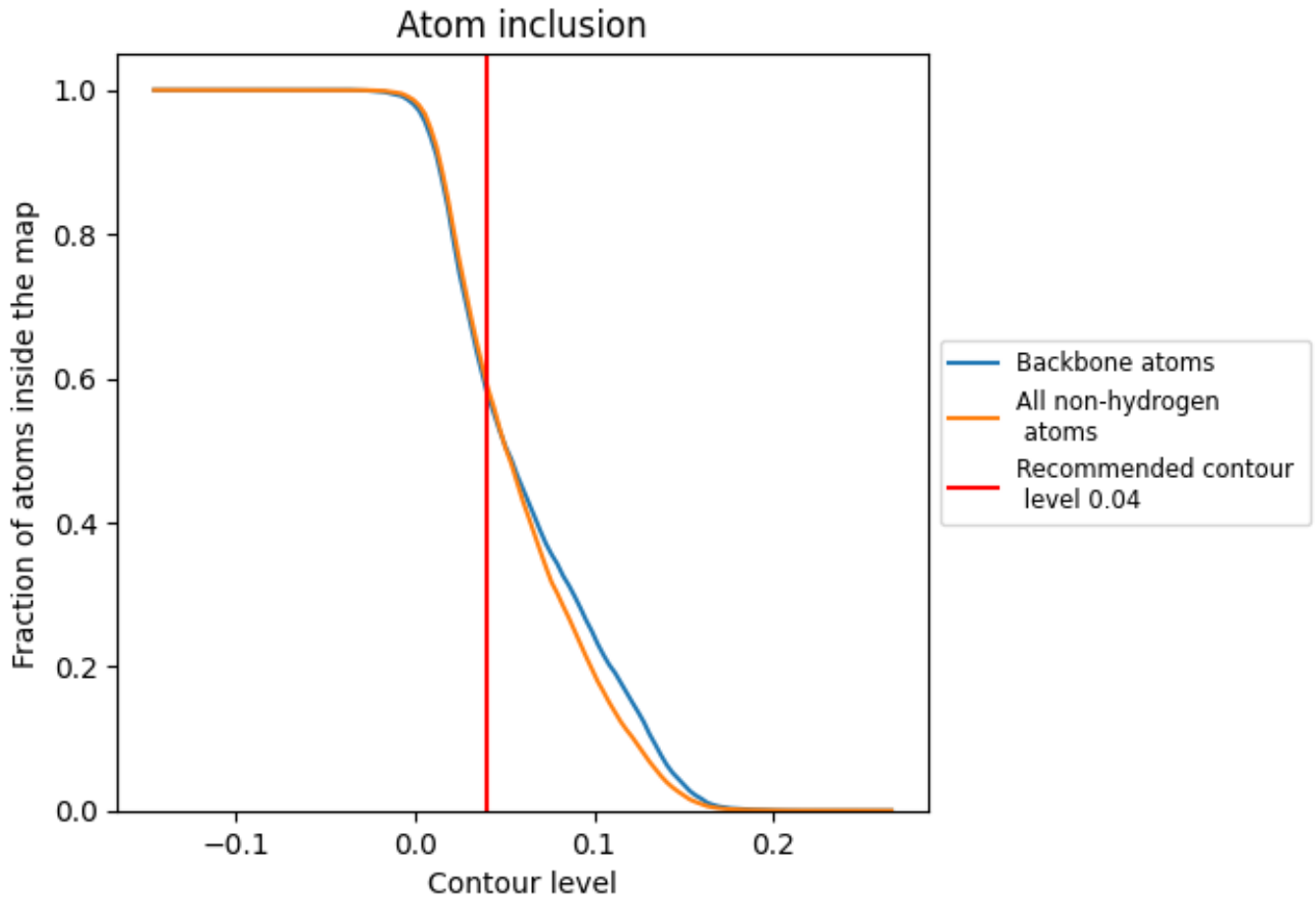
9.3 Atom inclusion mapped to coordinate model (i)



X Y Z

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 (0.04).

9.4 Atom inclusion (i)



At the recommended contour level, 58% of all backbone atoms, 59% 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 (0.04) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.5925	0.5290
A	0.5904	0.5260
B	0.5960	0.5340
C	0.5891	0.5220
D	0.5947	0.5330