Full wwPDB EM Validation Report ⓘ

Nov 12, 2022 – 01:23 PM EST

PDB ID	:	6PQO
EMDB ID	:	EMD-20449
Title	:	Cryo-EM structure of the human TRPA1 ion channel in complex with the covalent agonist JT010
Authors	:	Suo, Y.; Wang, Z.; Zubcevic, L.; Hsu, A.L.; He, Q.; Borgnia, M.J.; Ji, R.-R.; Lee, S.-Y.
Deposited on	:	2019-07-09
Resolution	:	2.88 Å(reported)
Based on initial model	:	3J9P

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

We welcome your comments at *validation@mail.wwpdb.org*
A user guide is available at
https://www.wwpdb.org/validation/2017/EMValidationReportHelp
with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at
http://www.wwpdb.org/validation/2017/FAQs#types.

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

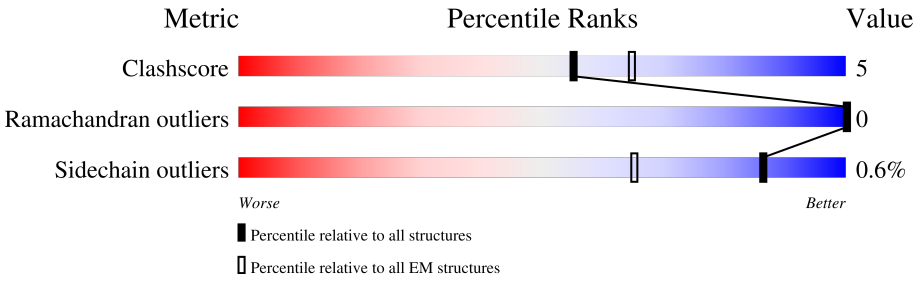
EMDB validation analysis	:	0.0.1.dev43
Mogul	:	1.8.5 (274361), CSD as541be (2020)
MolProbity	:	4.02b-467
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ	:	1.9.9
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry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

1 Overall quality at a glance

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

The reported resolution of this entry is 2.88 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	1152	49% · 47%
1	B	1152	50% · 47%
1	C	1152	49% · 47%
1	D	1152	49% · 47%
2	E	2	100%
2	F	2	100%
2	G	2	100%
2	H	2	100%

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	NAG	E	1	-	-	X	-
2	NAG	F	1	-	-	X	-
2	NAG	G	1	-	-	X	-
2	NAG	H	1	-	-	X	-

2 Entry composition (i)

There are 5 unique types of molecules in this entry. The entry contains 20312 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 A member 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	D	612	Total	C	N	O	S	0	0
			4813	3151	794	833	35		
1	A	612	Total	C	N	O	S	0	0
			4813	3151	794	833	35		
1	B	612	Total	C	N	O	S	0	0
			4813	3151	794	833	35		
1	C	612	Total	C	N	O	S	0	0
			4813	3151	794	833	35		

There are 136 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
D	0	MET	-	expression tag	UNP O75762
D	1	ALA	-	expression tag	UNP O75762
D	1120	SER	-	expression tag	UNP O75762
D	1121	ASN	-	expression tag	UNP O75762
D	1122	SER	-	expression tag	UNP O75762
D	1123	LEU	-	expression tag	UNP O75762
D	1124	GLU	-	expression tag	UNP O75762
D	1125	VAL	-	expression tag	UNP O75762
D	1126	LEU	-	expression tag	UNP O75762
D	1127	PHE	-	expression tag	UNP O75762
D	1128	GLN	-	expression tag	UNP O75762
D	1129	GLY	-	expression tag	UNP O75762
D	1130	PRO	-	expression tag	UNP O75762
D	1131	ALA	-	expression tag	UNP O75762
D	1132	ALA	-	expression tag	UNP O75762
D	1133	ASP	-	expression tag	UNP O75762
D	1134	TYR	-	expression tag	UNP O75762
D	1135	LYS	-	expression tag	UNP O75762
D	1136	ASP	-	expression tag	UNP O75762
D	1137	ASP	-	expression tag	UNP O75762
D	1138	ASP	-	expression tag	UNP O75762

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Chain	Residue	Modelled	Actual	Comment	Reference
D	1139	ASP	-	expression tag	UNP O75762
D	1140	LYS	-	expression tag	UNP O75762
D	1141	ALA	-	expression tag	UNP O75762
D	1142	HIS	-	expression tag	UNP O75762
D	1143	HIS	-	expression tag	UNP O75762
D	1144	HIS	-	expression tag	UNP O75762
D	1145	HIS	-	expression tag	UNP O75762
D	1146	HIS	-	expression tag	UNP O75762
D	1147	HIS	-	expression tag	UNP O75762
D	1148	HIS	-	expression tag	UNP O75762
D	1149	HIS	-	expression tag	UNP O75762
D	1150	HIS	-	expression tag	UNP O75762
D	1151	HIS	-	expression tag	UNP O75762
A	0	MET	-	expression tag	UNP O75762
A	1	ALA	-	expression tag	UNP O75762
A	1120	SER	-	expression tag	UNP O75762
A	1121	ASN	-	expression tag	UNP O75762
A	1122	SER	-	expression tag	UNP O75762
A	1123	LEU	-	expression tag	UNP O75762
A	1124	GLU	-	expression tag	UNP O75762
A	1125	VAL	-	expression tag	UNP O75762
A	1126	LEU	-	expression tag	UNP O75762
A	1127	PHE	-	expression tag	UNP O75762
A	1128	GLN	-	expression tag	UNP O75762
A	1129	GLY	-	expression tag	UNP O75762
A	1130	PRO	-	expression tag	UNP O75762
A	1131	ALA	-	expression tag	UNP O75762
A	1132	ALA	-	expression tag	UNP O75762
A	1133	ASP	-	expression tag	UNP O75762
A	1134	TYR	-	expression tag	UNP O75762
A	1135	LYS	-	expression tag	UNP O75762
A	1136	ASP	-	expression tag	UNP O75762
A	1137	ASP	-	expression tag	UNP O75762
A	1138	ASP	-	expression tag	UNP O75762
A	1139	ASP	-	expression tag	UNP O75762
A	1140	LYS	-	expression tag	UNP O75762
A	1141	ALA	-	expression tag	UNP O75762
A	1142	HIS	-	expression tag	UNP O75762
A	1143	HIS	-	expression tag	UNP O75762
A	1144	HIS	-	expression tag	UNP O75762
A	1145	HIS	-	expression tag	UNP O75762
A	1146	HIS	-	expression tag	UNP O75762

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Chain	Residue	Modelled	Actual	Comment	Reference
A	1147	HIS	-	expression tag	UNP O75762
A	1148	HIS	-	expression tag	UNP O75762
A	1149	HIS	-	expression tag	UNP O75762
A	1150	HIS	-	expression tag	UNP O75762
A	1151	HIS	-	expression tag	UNP O75762
B	0	MET	-	expression tag	UNP O75762
B	1	ALA	-	expression tag	UNP O75762
B	1120	SER	-	expression tag	UNP O75762
B	1121	ASN	-	expression tag	UNP O75762
B	1122	SER	-	expression tag	UNP O75762
B	1123	LEU	-	expression tag	UNP O75762
B	1124	GLU	-	expression tag	UNP O75762
B	1125	VAL	-	expression tag	UNP O75762
B	1126	LEU	-	expression tag	UNP O75762
B	1127	PHE	-	expression tag	UNP O75762
B	1128	GLN	-	expression tag	UNP O75762
B	1129	GLY	-	expression tag	UNP O75762
B	1130	PRO	-	expression tag	UNP O75762
B	1131	ALA	-	expression tag	UNP O75762
B	1132	ALA	-	expression tag	UNP O75762
B	1133	ASP	-	expression tag	UNP O75762
B	1134	TYR	-	expression tag	UNP O75762
B	1135	LYS	-	expression tag	UNP O75762
B	1136	ASP	-	expression tag	UNP O75762
B	1137	ASP	-	expression tag	UNP O75762
B	1138	ASP	-	expression tag	UNP O75762
B	1139	ASP	-	expression tag	UNP O75762
B	1140	LYS	-	expression tag	UNP O75762
B	1141	ALA	-	expression tag	UNP O75762
B	1142	HIS	-	expression tag	UNP O75762
B	1143	HIS	-	expression tag	UNP O75762
B	1144	HIS	-	expression tag	UNP O75762
B	1145	HIS	-	expression tag	UNP O75762
B	1146	HIS	-	expression tag	UNP O75762
B	1147	HIS	-	expression tag	UNP O75762
B	1148	HIS	-	expression tag	UNP O75762
B	1149	HIS	-	expression tag	UNP O75762
B	1150	HIS	-	expression tag	UNP O75762
B	1151	HIS	-	expression tag	UNP O75762
C	0	MET	-	expression tag	UNP O75762
C	1	ALA	-	expression tag	UNP O75762
C	1120	SER	-	expression tag	UNP O75762

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Chain	Residue	Modelled	Actual	Comment	Reference
C	1121	ASN	-	expression tag	UNP O75762
C	1122	SER	-	expression tag	UNP O75762
C	1123	LEU	-	expression tag	UNP O75762
C	1124	GLU	-	expression tag	UNP O75762
C	1125	VAL	-	expression tag	UNP O75762
C	1126	LEU	-	expression tag	UNP O75762
C	1127	PHE	-	expression tag	UNP O75762
C	1128	GLN	-	expression tag	UNP O75762
C	1129	GLY	-	expression tag	UNP O75762
C	1130	PRO	-	expression tag	UNP O75762
C	1131	ALA	-	expression tag	UNP O75762
C	1132	ALA	-	expression tag	UNP O75762
C	1133	ASP	-	expression tag	UNP O75762
C	1134	TYR	-	expression tag	UNP O75762
C	1135	LYS	-	expression tag	UNP O75762
C	1136	ASP	-	expression tag	UNP O75762
C	1137	ASP	-	expression tag	UNP O75762
C	1138	ASP	-	expression tag	UNP O75762
C	1139	ASP	-	expression tag	UNP O75762
C	1140	LYS	-	expression tag	UNP O75762
C	1141	ALA	-	expression tag	UNP O75762
C	1142	HIS	-	expression tag	UNP O75762
C	1143	HIS	-	expression tag	UNP O75762
C	1144	HIS	-	expression tag	UNP O75762
C	1145	HIS	-	expression tag	UNP O75762
C	1146	HIS	-	expression tag	UNP O75762
C	1147	HIS	-	expression tag	UNP O75762
C	1148	HIS	-	expression tag	UNP O75762
C	1149	HIS	-	expression tag	UNP O75762
C	1150	HIS	-	expression tag	UNP O75762
C	1151	HIS	-	expression tag	UNP O75762

- Molecule 2 is an oligosaccharide called 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose.

Mol	Chain	Residues	Atoms				AltConf	Trace
2	E	2	Total	C	N	O	0	0
			28	16	2	10		

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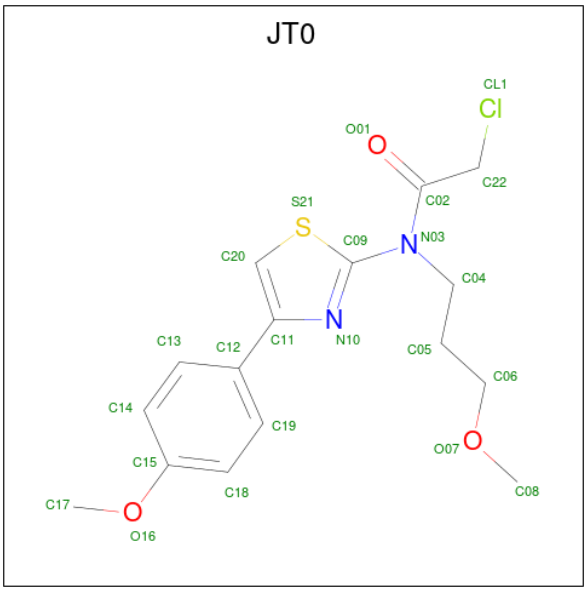
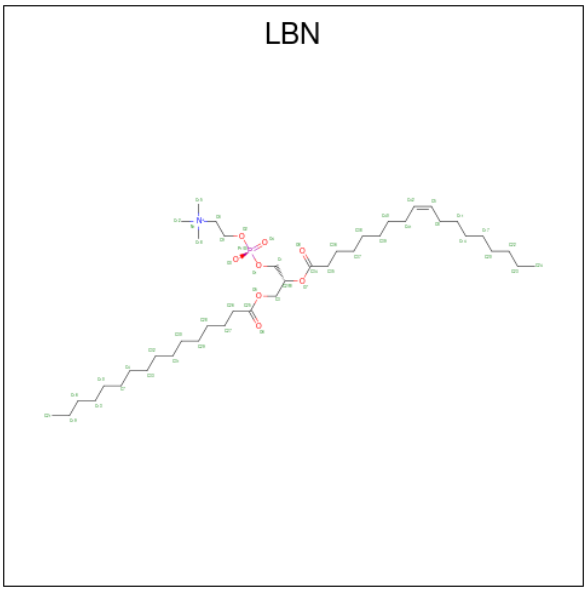
Mol	Chain	Residues	Atoms				AltConf	Trace
2	F	2	Total	C	N	O	0	0
			28	16	2	10		
2	G	2	Total	C	N	O	0	0
			28	16	2	10		
2	H	2	Total	C	N	O	0	0
			28	16	2	10		

- Molecule 3 is 2-chloro-N-[4-(4-methoxyphenyl)-1,3-thiazol-2-yl]-N-(3-methoxypropyl)acetamide (three-letter code: JT0) (formula: $C_{16}H_{19}ClN_2O_3S$) (labeled as "Ligand of Interest" by depositor).



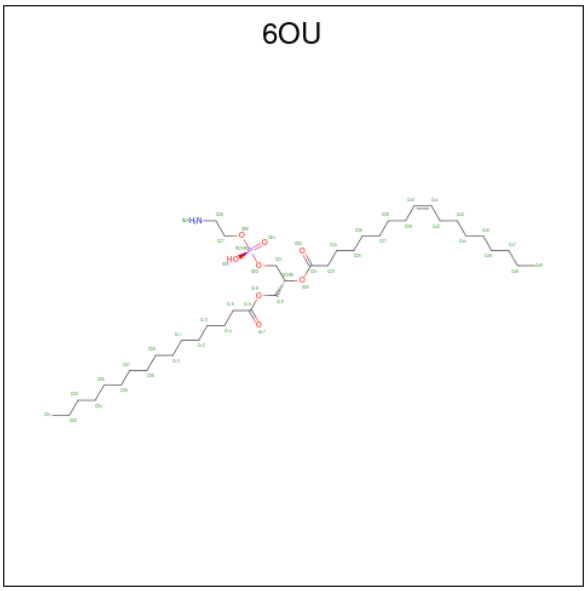
Mol	Chain	Residues	Atoms					AltConf
3	D	1	Total	C	N	O	S	0
			22	16	2	3	1	
3	A	1	Total	C	N	O	S	0
			22	16	2	3	1	
3	B	1	Total	C	N	O	S	0
			22	16	2	3	1	
3	C	1	Total	C	N	O	S	0
			22	16	2	3	1	

- Molecule 4 is 1-palmitoyl-2-oleoyl-sn-glycero-3-phosphocholine (three-letter code: LBN) (formula: $C_{42}H_{82}NO_8P$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms					AltConf
4	D	1	Total	C	N	O	P	0
			84	64	2	16	2	
4	D	1	Total	C	N	O	P	0
			84	64	2	16	2	
4	A	1	Total	C	N	O	P	0
			84	64	2	16	2	
4	A	1	Total	C	N	O	P	0
			84	64	2	16	2	
4	B	1	Total	C	N	O	P	0
			84	64	2	16	2	
4	B	1	Total	C	N	O	P	0
			84	64	2	16	2	
4	C	1	Total	C	N	O	P	0
			84	64	2	16	2	
4	C	1	Total	C	N	O	P	0
			84	64	2	16	2	

- Molecule 5 is [(2 {R})-1-[2-azanylethoxy(oxidanyl)phosphoryl]oxy-3-hexadecanoyloxy-propan-2-yl] ({Z})-octadec-9-enoate (three-letter code: 6OU) (formula: $C_{39}H_{76}NO_8P$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms					AltConf
5	D	1	Total	C	N	O	P	0
			172	124	3	40	5	
5	D	1	Total	C	N	O	P	0
			172	124	3	40	5	
5	D	1	Total	C	N	O	P	0
			172	124	3	40	5	
5	D	1	Total	C	N	O	P	0
			172	124	3	40	5	
5	D	1	Total	C	N	O	P	0
			172	124	3	40	5	
5	A	1	Total	C	N	O	P	0
			90	62	1	24	3	
5	A	1	Total	C	N	O	P	0
			90	62	1	24	3	
5	A	1	Total	C	N	O	P	0
			90	62	1	24	3	
5	B	1	Total	C	N	O	P	0
			131	93	2	32	4	
5	B	1	Total	C	N	O	P	0
			131	93	2	32	4	
5	B	1	Total	C	N	O	P	0
			131	93	2	32	4	
5	B	1	Total	C	N	O	P	0
			131	93	2	32	4	
5	C	1	Total	C	N	O	P	0
			131	93	2	32	4	
5	C	1	Total	C	N	O	P	0
			131	93	2	32	4	

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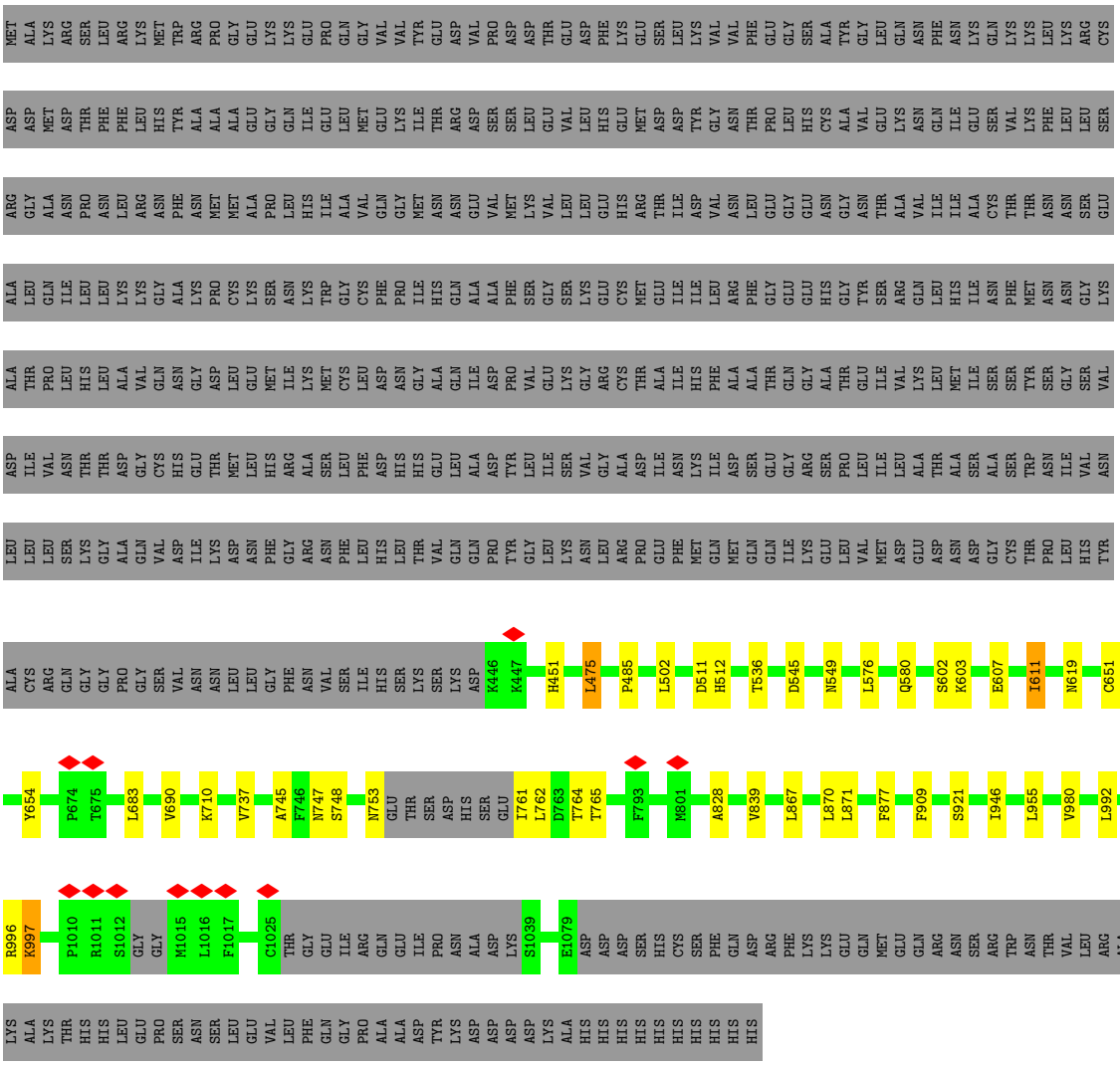
Mol	Chain	Residues	Atoms					AltConf
5	C	1	Total	C	N	O	P	0
			131	93	2	32	4	
5	C	1	Total	C	N	O	P	0
			131	93	2	32	4	

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.

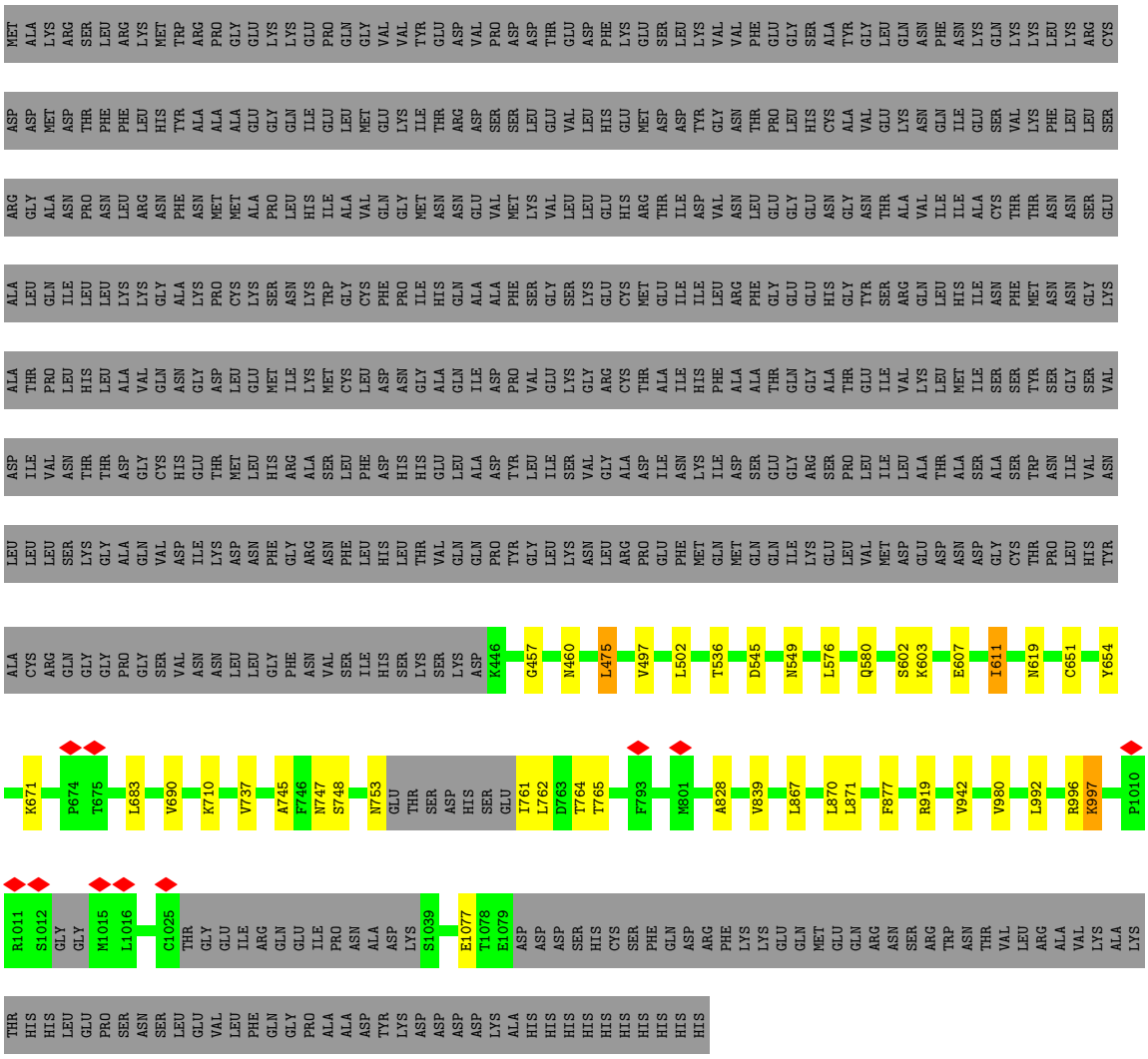
• Molecule 1: Transient receptor potential cation channel subfamily A member 1

Chain D:



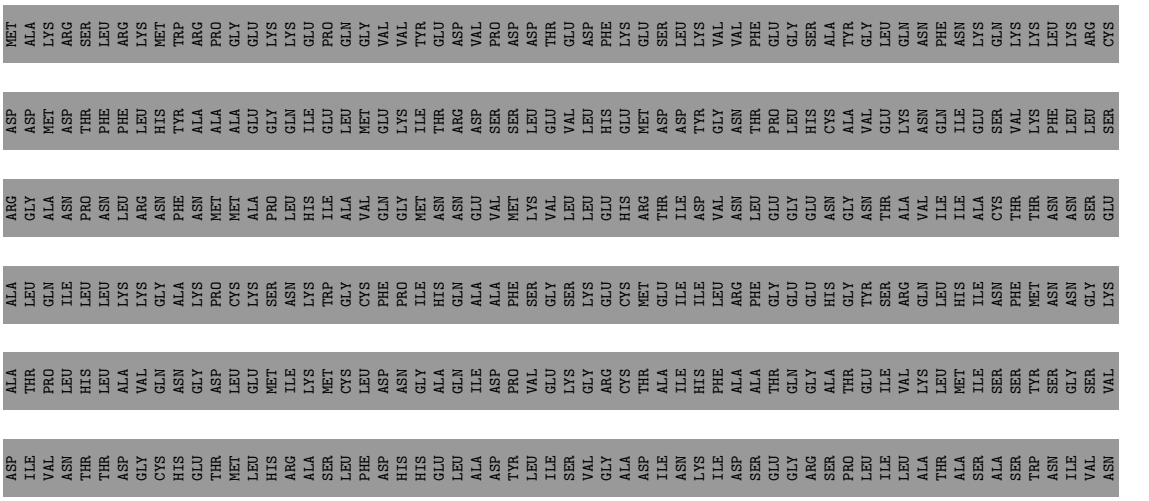
• Molecule 1: Transient receptor potential cation channel subfamily A member 1

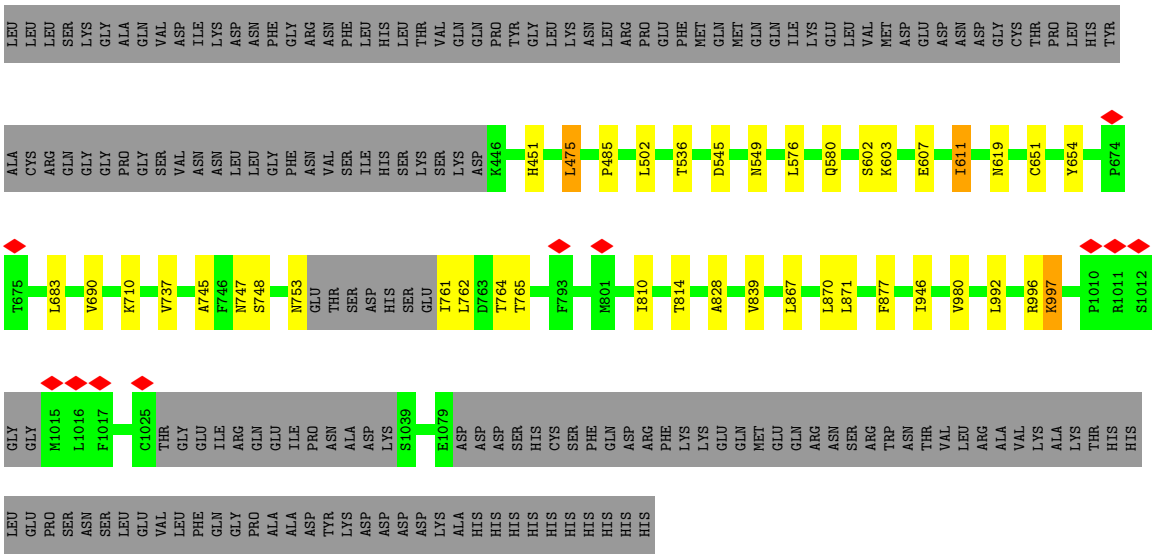
Chain A:



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

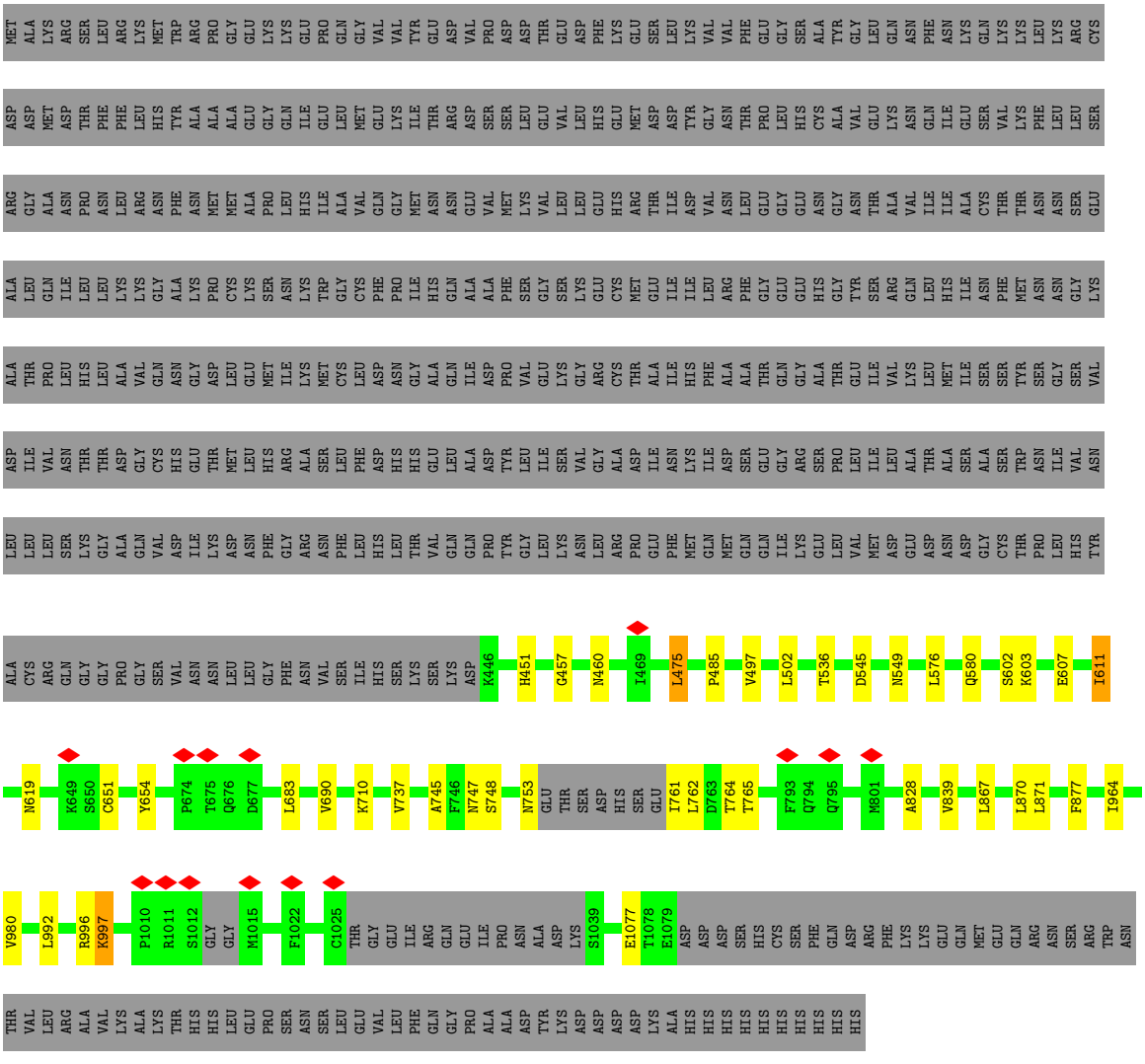
Chain B:





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

Chain C:



• Molecule 2: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain E: 100%

• Molecule 2: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain F: 100%

• Molecule 2: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain G: 100%

• Molecule 2: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain H: 100%

4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C4	Depositor
Number of particles used	189927	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 ($e^-/Å^2$)	42	Depositor
Minimum defocus (nm)	1250	Depositor
Maximum defocus (nm)	3000	Depositor
Magnification	75000	Depositor
Image detector	FEI FALCON III (4k x 4k)	Depositor
Maximum map value	0.273	Depositor
Minimum map value	-0.143	Depositor
Average map value	-0.000	Depositor
Map value standard deviation	0.008	Depositor
Recommended contour level	0.025	Depositor
Map size (Å)	276.48, 276.48, 276.48	wwPDB
Map dimensions	256, 256, 256	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.08, 1.08, 1.08	Depositor

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: 6OU, NAG, LBN, JT0

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	0.36	0/4920	0.58	0/6673
1	B	0.36	0/4920	0.58	0/6673
1	C	0.36	0/4920	0.58	0/6673
1	D	0.36	0/4920	0.58	0/6673
All	All	0.36	0/19680	0.58	0/26692

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	4813	0	4839	54	0
1	B	4813	0	4839	48	0
1	C	4813	0	4839	52	0
1	D	4813	0	4839	51	0
2	E	28	0	25	15	0
2	F	28	0	25	16	0
2	G	28	0	25	15	0
2	H	28	0	25	16	0
3	A	22	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	B	22	0	0	0	0
3	C	22	0	0	0	0
3	D	22	0	0	0	0
4	A	84	0	0	7	0
4	B	84	0	0	7	0
4	C	84	0	0	7	0
4	D	84	0	0	7	0
5	A	90	0	0	3	0
5	B	131	0	0	3	0
5	C	131	0	0	3	0
5	D	172	0	0	4	0
All	All	20312	0	19456	211	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 5.

All (211) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:747:ASN:ND2	2:G:1:NAG:C1	1.78	1.46
1:D:747:ASN:ND2	2:E:1:NAG:C1	1.78	1.46
1:C:747:ASN:ND2	2:H:1:NAG:C1	1.78	1.46
1:A:747:ASN:ND2	2:F:1:NAG:C1	1.78	1.44
1:D:871:LEU:CD1	4:D:1305:LBN:C41	2.39	1.01
1:A:871:LEU:CD1	4:A:1206:LBN:C41	2.39	0.99
1:B:871:LEU:CD1	4:B:1206:LBN:C41	2.39	0.99
1:C:871:LEU:CD1	4:C:1207:LBN:C41	2.39	0.99
1:C:747:ASN:HD22	2:H:1:NAG:C1	1.57	0.95
1:B:747:ASN:HD22	2:G:1:NAG:C1	1.57	0.94
1:D:747:ASN:HD22	2:E:1:NAG:C1	1.57	0.92
1:A:747:ASN:HD22	2:F:1:NAG:C1	1.57	0.90
1:C:871:LEU:HG	4:C:1207:LBN:C41	2.05	0.87
1:D:871:LEU:HG	4:D:1305:LBN:C41	2.05	0.87
1:A:871:LEU:HG	4:A:1206:LBN:C41	2.05	0.87
1:B:871:LEU:HG	4:B:1206:LBN:C41	2.05	0.86
1:A:762:LEU:HD11	2:F:1:NAG:H61	1.57	0.85
1:D:762:LEU:HD11	2:E:1:NAG:H61	1.57	0.85
1:C:762:LEU:HD11	2:H:1:NAG:H61	1.57	0.84
1:B:762:LEU:HD11	2:G:1:NAG:H61	1.57	0.84
1:D:871:LEU:CG	4:D:1305:LBN:C41	2.59	0.81
1:C:871:LEU:CG	4:C:1207:LBN:C41	2.59	0.80

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:871:LEU:CG	4:A:1206:LBN:C41	2.59	0.80
1:B:871:LEU:CG	4:B:1206:LBN:C41	2.59	0.79
1:D:762:LEU:HD21	2:E:1:NAG:C6	2.15	0.77
1:C:762:LEU:HD21	2:H:1:NAG:C6	2.15	0.77
1:B:762:LEU:HD21	2:G:1:NAG:C6	2.15	0.77
1:D:762:LEU:HD21	2:E:1:NAG:H5	1.68	0.76
1:A:762:LEU:HD21	2:F:1:NAG:C6	2.15	0.76
1:C:762:LEU:HD21	2:H:1:NAG:H5	1.68	0.76
1:A:762:LEU:HD21	2:F:1:NAG:H5	1.68	0.76
1:B:762:LEU:HD21	2:G:1:NAG:H5	1.68	0.75
1:A:747:ASN:HD21	2:F:1:NAG:C1	1.98	0.74
1:A:747:ASN:ND2	2:F:1:NAG:C2	2.51	0.74
1:A:871:LEU:HD12	4:A:1206:LBN:C41	2.18	0.73
1:C:871:LEU:HD12	4:C:1207:LBN:C41	2.18	0.73
1:D:871:LEU:HD12	4:D:1305:LBN:C41	2.18	0.73
1:D:747:ASN:ND2	2:E:1:NAG:C2	2.51	0.73
1:B:747:ASN:OD1	1:B:748:SER:N	2.22	0.73
1:B:747:ASN:ND2	2:G:1:NAG:C2	2.51	0.72
1:B:747:ASN:HD21	2:G:1:NAG:C1	1.98	0.72
1:C:747:ASN:OD1	1:C:748:SER:N	2.22	0.72
1:B:871:LEU:HD12	4:B:1206:LBN:C41	2.18	0.72
1:C:747:ASN:ND2	2:H:1:NAG:C2	2.51	0.72
1:B:871:LEU:HD11	4:B:1206:LBN:C41	2.19	0.72
1:A:747:ASN:OD1	1:A:748:SER:N	2.22	0.72
1:D:747:ASN:OD1	1:D:748:SER:N	2.22	0.71
1:C:747:ASN:HD21	2:H:1:NAG:C1	1.98	0.70
1:C:871:LEU:HD11	4:C:1207:LBN:C41	2.19	0.70
1:D:871:LEU:HD11	4:D:1305:LBN:C39	2.22	0.70
1:A:871:LEU:HD11	4:A:1206:LBN:C41	2.19	0.70
1:B:871:LEU:HD11	4:B:1206:LBN:C39	2.22	0.69
1:C:871:LEU:HD11	4:C:1207:LBN:C39	2.22	0.69
1:A:871:LEU:HD11	4:A:1206:LBN:C39	2.22	0.69
1:D:871:LEU:HD11	4:D:1305:LBN:C41	2.19	0.69
1:D:747:ASN:HD21	2:E:1:NAG:C1	1.98	0.68
1:C:762:LEU:HD11	2:H:1:NAG:C6	2.25	0.67
1:D:762:LEU:HD11	2:E:1:NAG:C6	2.25	0.66
1:D:867:LEU:O	1:D:871:LEU:HD13	1.95	0.66
1:A:762:LEU:HD11	2:F:1:NAG:C6	2.25	0.66
1:B:747:ASN:HD21	2:G:1:NAG:C7	2.09	0.66
1:C:867:LEU:O	1:C:871:LEU:HD13	1.95	0.66
1:A:747:ASN:HD21	2:F:1:NAG:C7	2.09	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:867:LEU:O	1:A:871:LEU:HD13	1.95	0.66
1:D:747:ASN:HD21	2:E:1:NAG:C7	2.09	0.66
1:C:762:LEU:HD21	2:H:1:NAG:C5	2.25	0.66
1:D:762:LEU:HD21	2:E:1:NAG:C5	2.25	0.66
1:A:762:LEU:HD21	2:F:1:NAG:C5	2.25	0.66
1:C:747:ASN:HD21	2:H:1:NAG:C7	2.09	0.65
1:B:762:LEU:HD21	2:G:1:NAG:C5	2.25	0.65
1:B:867:LEU:O	1:B:871:LEU:HD13	1.95	0.64
1:B:762:LEU:HD11	2:G:1:NAG:C6	2.25	0.63
1:B:747:ASN:CG	2:G:1:NAG:C1	2.66	0.61
1:D:747:ASN:CG	2:E:1:NAG:C1	2.66	0.60
1:C:747:ASN:CG	2:H:1:NAG:C1	2.66	0.59
1:D:737:VAL:HG21	1:D:839:VAL:HG21	1.86	0.58
1:C:737:VAL:HG21	1:C:839:VAL:HG21	1.86	0.58
1:A:737:VAL:HG21	1:A:839:VAL:HG21	1.86	0.58
1:B:737:VAL:HG21	1:B:839:VAL:HG21	1.86	0.58
1:D:611:ILE:HD12	1:D:611:ILE:H	1.69	0.58
1:B:611:ILE:HD12	1:B:611:ILE:H	1.69	0.58
1:C:611:ILE:HD12	1:C:611:ILE:H	1.69	0.57
1:A:611:ILE:HD12	1:A:611:ILE:H	1.69	0.57
1:B:992:LEU:CD2	1:B:996:ARG:HE	2.18	0.57
1:A:992:LEU:CD2	1:A:996:ARG:HE	2.18	0.57
1:C:992:LEU:CD2	1:C:996:ARG:HE	2.18	0.57
1:D:992:LEU:CD2	1:D:996:ARG:HE	2.18	0.56
1:A:747:ASN:CG	2:F:1:NAG:C1	2.66	0.56
1:D:871:LEU:HD11	4:D:1305:LBN:C40	2.36	0.56
1:A:871:LEU:HD11	4:A:1206:LBN:C40	2.36	0.56
1:C:753:ASN:HB3	1:C:761:ILE:HD11	1.88	0.56
1:C:871:LEU:HD11	4:C:1207:LBN:C40	2.36	0.55
1:D:580:GLN:O	1:D:619:ASN:ND2	2.39	0.55
1:B:753:ASN:HB3	1:B:761:ILE:HD11	1.88	0.55
1:B:871:LEU:HD11	4:B:1206:LBN:C40	2.36	0.55
1:C:762:LEU:HD21	2:H:1:NAG:H62	1.89	0.55
1:C:580:GLN:O	1:C:619:ASN:ND2	2.39	0.55
5:A:1201:6OU:C19	5:A:1201:6OU:C14	2.86	0.54
1:A:580:GLN:O	1:A:619:ASN:ND2	2.39	0.54
1:B:870:LEU:HD12	1:B:877:PHE:HE2	1.73	0.54
1:D:762:LEU:HD21	2:E:1:NAG:H62	1.89	0.54
1:A:753:ASN:HB3	1:A:761:ILE:HD11	1.88	0.54
1:B:580:GLN:O	1:B:619:ASN:ND2	2.39	0.54
1:D:753:ASN:HB3	1:D:761:ILE:HD11	1.88	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:D:1310:6OU:C19	5:D:1310:6OU:C14	2.86	0.54
5:C:1202:6OU:C19	5:C:1202:6OU:C14	2.86	0.54
1:D:870:LEU:HD12	1:D:877:PHE:HE2	1.73	0.54
1:B:747:ASN:HD21	2:G:1:NAG:C2	2.20	0.53
1:D:921:SER:OG	1:A:919:ARG:NH2	2.41	0.53
5:B:1201:6OU:C14	5:B:1201:6OU:C19	2.86	0.53
1:C:762:LEU:CD1	2:H:2:NAG:H82	2.39	0.53
1:A:762:LEU:HD21	2:F:1:NAG:H62	1.89	0.53
1:D:762:LEU:CD1	2:E:2:NAG:H82	2.39	0.53
1:B:762:LEU:CD1	2:G:2:NAG:H82	2.39	0.53
1:C:870:LEU:HD12	1:C:877:PHE:HE2	1.73	0.53
1:C:747:ASN:HD21	2:H:1:NAG:C2	2.20	0.52
1:C:992:LEU:HD21	1:C:996:ARG:HE	1.74	0.52
1:A:870:LEU:HD12	1:A:877:PHE:HE2	1.73	0.52
1:B:992:LEU:HD21	1:B:996:ARG:HE	1.74	0.52
1:A:762:LEU:CD1	2:F:2:NAG:H82	2.39	0.52
1:B:762:LEU:HD21	2:G:1:NAG:H62	1.89	0.52
1:A:870:LEU:CD1	1:A:877:PHE:HE2	2.23	0.51
1:B:870:LEU:CD1	1:B:877:PHE:HE2	2.23	0.51
1:D:870:LEU:CD1	1:D:877:PHE:HE2	2.23	0.51
1:C:870:LEU:CD1	1:C:877:PHE:HE2	2.23	0.51
1:D:683:LEU:HD21	1:D:710:LYS:HE3	1.93	0.51
1:B:683:LEU:HD21	1:B:710:LYS:HE3	1.93	0.51
1:C:683:LEU:HD21	1:C:710:LYS:HE3	1.93	0.51
1:A:683:LEU:HD21	1:A:710:LYS:HE3	1.93	0.51
1:C:745:ALA:HB2	1:C:828:ALA:HB2	1.93	0.51
1:A:992:LEU:HD21	1:A:996:ARG:HE	1.74	0.50
1:B:745:ALA:HB2	1:B:828:ALA:HB2	1.93	0.50
1:D:745:ALA:HB2	1:D:828:ALA:HB2	1.93	0.50
1:D:992:LEU:HD21	1:D:996:ARG:HE	1.74	0.50
5:D:1307:6OU:C15	5:A:1201:6OU:O32	2.60	0.50
1:D:909:PHE:CE2	1:A:942:VAL:HG23	2.45	0.50
5:D:1310:6OU:O32	5:C:1209:6OU:C15	2.60	0.50
5:A:1207:6OU:C15	5:B:1201:6OU:O32	2.60	0.50
1:A:745:ALA:HB2	1:A:828:ALA:HB2	1.93	0.49
1:A:747:ASN:HD21	2:F:1:NAG:C2	2.20	0.49
1:D:997:LYS:HD2	1:D:997:LYS:O	2.13	0.49
1:A:997:LYS:HD2	1:A:997:LYS:O	2.13	0.49
1:B:997:LYS:HD2	1:B:997:LYS:O	2.13	0.49
5:B:1208:6OU:C15	5:C:1202:6OU:O32	2.60	0.49
1:D:690:VAL:HG21	1:D:980:VAL:HG11	1.95	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:690:VAL:HG21	1:B:980:VAL:HG11	1.95	0.49
1:C:997:LYS:HD2	1:C:997:LYS:O	2.13	0.48
1:D:747:ASN:HD21	2:E:1:NAG:C2	2.20	0.48
1:D:955:LEU:HA	1:C:964:ILE:HD11	1.96	0.48
1:A:690:VAL:HG21	1:A:980:VAL:HG11	1.95	0.48
1:C:690:VAL:HG21	1:C:980:VAL:HG11	1.95	0.48
1:A:607:GLU:O	1:A:611:ILE:HD11	2.15	0.47
1:C:607:GLU:O	1:C:611:ILE:HD11	2.15	0.47
1:B:607:GLU:O	1:B:611:ILE:HD11	2.15	0.47
1:C:545:ASP:OD1	1:C:549:ASN:N	2.47	0.46
1:C:602:SER:OG	1:C:603:LYS:N	2.49	0.46
1:B:602:SER:OG	1:B:603:LYS:N	2.49	0.46
1:D:545:ASP:OD1	1:D:549:ASN:N	2.47	0.46
1:D:651:CYS:HB2	1:D:654:TYR:HB2	1.98	0.46
2:E:1:NAG:H61	2:E:2:NAG:HN2	1.81	0.46
1:A:602:SER:OG	1:A:603:LYS:N	2.49	0.45
1:D:607:GLU:O	1:D:611:ILE:HD11	2.15	0.45
1:D:602:SER:OG	1:D:603:LYS:N	2.49	0.45
2:F:1:NAG:H61	2:F:2:NAG:HN2	1.81	0.45
1:A:651:CYS:HB2	1:A:654:TYR:HB2	1.98	0.45
1:A:1077:GLU:HA	1:C:460:ASN:HD22	1.81	0.45
1:A:607:GLU:O	1:A:611:ILE:CD1	2.65	0.45
2:H:1:NAG:H61	2:H:2:NAG:HN2	1.81	0.45
1:A:545:ASP:OD1	1:A:549:ASN:N	2.47	0.45
1:B:545:ASP:OD1	1:B:549:ASN:N	2.47	0.45
1:D:607:GLU:O	1:D:611:ILE:CD1	2.64	0.45
1:B:651:CYS:HB2	1:B:654:TYR:HB2	1.98	0.45
1:B:607:GLU:O	1:B:611:ILE:CD1	2.64	0.44
1:C:607:GLU:O	1:C:611:ILE:CD1	2.64	0.44
1:C:651:CYS:HB2	1:C:654:TYR:HB2	1.98	0.44
2:G:1:NAG:H61	2:G:2:NAG:HN2	1.81	0.44
5:D:1308:6OU:C38	5:D:1310:6OU:C13	2.95	0.44
1:D:576:LEU:HB3	1:D:580:GLN:HA	2.00	0.44
1:C:867:LEU:O	1:C:871:LEU:CD1	2.65	0.44
1:A:576:LEU:HB3	1:A:580:GLN:HA	2.00	0.44
1:A:870:LEU:HD21	1:B:946:ILE:HG23	2.01	0.43
1:D:867:LEU:O	1:D:871:LEU:CD1	2.65	0.43
1:A:460:ASN:HD22	1:C:1077:GLU:HA	1.84	0.43
1:B:576:LEU:HB3	1:B:580:GLN:HA	2.00	0.43
1:B:475:LEU:HD22	1:B:475:LEU:O	2.19	0.42
1:A:867:LEU:O	1:A:871:LEU:CD1	2.65	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:475:LEU:O	1:C:475:LEU:HD22	2.19	0.42
1:C:576:LEU:HB3	1:C:580:GLN:HA	2.00	0.42
1:B:867:LEU:O	1:B:871:LEU:CD1	2.65	0.42
1:D:946:ILE:HG23	1:C:870:LEU:HD21	2.01	0.42
1:D:475:LEU:O	1:D:475:LEU:HD22	2.19	0.42
1:A:475:LEU:O	1:A:475:LEU:HD22	2.19	0.42
1:D:764:THR:HG22	1:D:765:THR:H	1.85	0.41
1:D:502:LEU:HD13	1:D:536:THR:HG21	2.02	0.41
1:C:764:THR:HG22	1:C:765:THR:H	1.85	0.41
1:A:502:LEU:HD13	1:A:536:THR:HG21	2.02	0.41
1:B:451:HIS:HD2	1:B:485:PRO:HG3	1.86	0.41
1:C:451:HIS:HD2	1:C:485:PRO:HG3	1.86	0.41
1:D:451:HIS:HD2	1:D:485:PRO:HG3	1.86	0.41
1:B:810:ILE:O	1:B:814:THR:OG1	2.30	0.41
1:A:457:GLY:HA2	1:A:497:VAL:HG21	2.03	0.41
1:A:764:THR:HG22	1:A:765:THR:H	1.85	0.41
1:B:502:LEU:HD13	1:B:536:THR:HG21	2.02	0.41
1:C:502:LEU:HD13	1:C:536:THR:HG21	2.02	0.41
1:A:870:LEU:HD12	1:A:877:PHE:CE2	2.56	0.41
1:C:457:GLY:HA2	1:C:497:VAL:HG21	2.03	0.40
1:B:764:THR:HG22	1:B:765:THR:H	1.85	0.40
1:A:762:LEU:HD12	2:F:2:NAG:H82	2.03	0.40
1:C:762:LEU:HD12	2:H:2:NAG:H82	2.04	0.40
1:D:511:ASP:OD1	1:D:512:HIS:N	2.54	0.40
1:A:671:LYS:HG3	1:A:992:LEU:HD12	2.04	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	604/1152 (52%)	583 (96%)	21 (4%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	B	604/1152 (52%)	583 (96%)	21 (4%)	0	100	100
1	C	604/1152 (52%)	583 (96%)	21 (4%)	0	100	100
1	D	604/1152 (52%)	583 (96%)	21 (4%)	0	100	100
All	All	2416/4608 (52%)	2332 (96%)	84 (4%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains (i)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	514/1023 (50%)	511 (99%)	3 (1%)	86	95
1	B	514/1023 (50%)	511 (99%)	3 (1%)	86	95
1	C	514/1023 (50%)	511 (99%)	3 (1%)	86	95
1	D	514/1023 (50%)	511 (99%)	3 (1%)	86	95
All	All	2056/4092 (50%)	2044 (99%)	12 (1%)	86	95

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

Mol	Chain	Res	Type
1	D	475	LEU
1	D	611	ILE
1	D	997	LYS
1	A	475	LEU
1	A	611	ILE
1	A	997	LYS
1	B	475	LEU
1	B	611	ILE
1	B	997	LYS
1	C	475	LEU
1	C	611	ILE
1	C	997	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (22) such sidechains are listed below:

Mol	Chain	Res	Type
1	D	451	HIS
1	D	512	HIS
1	D	519	HIS
1	D	570	HIS
1	D	805	ASN
1	A	451	HIS
1	A	460	ASN
1	A	512	HIS
1	A	519	HIS
1	A	570	HIS
1	A	805	ASN
1	B	451	HIS
1	B	512	HIS
1	B	519	HIS
1	B	570	HIS
1	B	805	ASN
1	B	1061	GLN
1	C	451	HIS
1	C	460	ASN
1	C	512	HIS
1	C	519	HIS
1	C	805	ASN

5.3.3 RNA

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates

8 monosaccharides 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	NAG	E	1	2	14,14,15	0.28	0	17,19,21	0.62	0
2	NAG	E	2	2	14,14,15	0.28	0	17,19,21	0.58	0
2	NAG	F	1	2	14,14,15	0.28	0	17,19,21	0.63	0
2	NAG	F	2	2	14,14,15	0.27	0	17,19,21	0.57	0
2	NAG	G	1	2	14,14,15	0.28	0	17,19,21	0.63	0
2	NAG	G	2	2	14,14,15	0.28	0	17,19,21	0.58	0
2	NAG	H	1	2	14,14,15	0.28	0	17,19,21	0.63	0
2	NAG	H	2	2	14,14,15	0.29	0	17,19,21	0.58	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	NAG	E	1	2	-	2/6/23/26	0/1/1/1
2	NAG	E	2	2	-	4/6/23/26	0/1/1/1
2	NAG	F	1	2	-	2/6/23/26	0/1/1/1
2	NAG	F	2	2	-	4/6/23/26	0/1/1/1
2	NAG	G	1	2	-	2/6/23/26	0/1/1/1
2	NAG	G	2	2	-	4/6/23/26	0/1/1/1
2	NAG	H	1	2	-	2/6/23/26	0/1/1/1
2	NAG	H	2	2	-	4/6/23/26	0/1/1/1

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (24) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	E	2	NAG	C3-C2-N2-C7
2	E	2	NAG	C8-C7-N2-C2
2	E	2	NAG	O7-C7-N2-C2
2	F	2	NAG	C3-C2-N2-C7
2	F	2	NAG	C8-C7-N2-C2
2	F	2	NAG	O7-C7-N2-C2

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Mol	Chain	Res	Type	Atoms
2	G	2	NAG	C3-C2-N2-C7
2	G	2	NAG	C8-C7-N2-C2
2	G	2	NAG	O7-C7-N2-C2
2	H	2	NAG	C3-C2-N2-C7
2	H	2	NAG	C8-C7-N2-C2
2	H	2	NAG	O7-C7-N2-C2
2	E	1	NAG	C8-C7-N2-C2
2	F	1	NAG	C8-C7-N2-C2
2	G	1	NAG	C8-C7-N2-C2
2	H	1	NAG	C8-C7-N2-C2
2	E	1	NAG	O7-C7-N2-C2
2	F	1	NAG	O7-C7-N2-C2
2	G	1	NAG	O7-C7-N2-C2
2	H	1	NAG	O7-C7-N2-C2
2	E	2	NAG	C1-C2-N2-C7
2	F	2	NAG	C1-C2-N2-C7
2	G	2	NAG	C1-C2-N2-C7
2	H	2	NAG	C1-C2-N2-C7

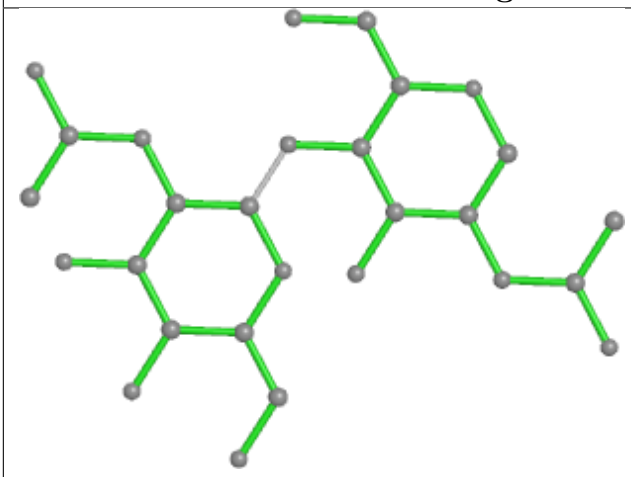
There are no ring outliers.

8 monomers are involved in 62 short contacts:

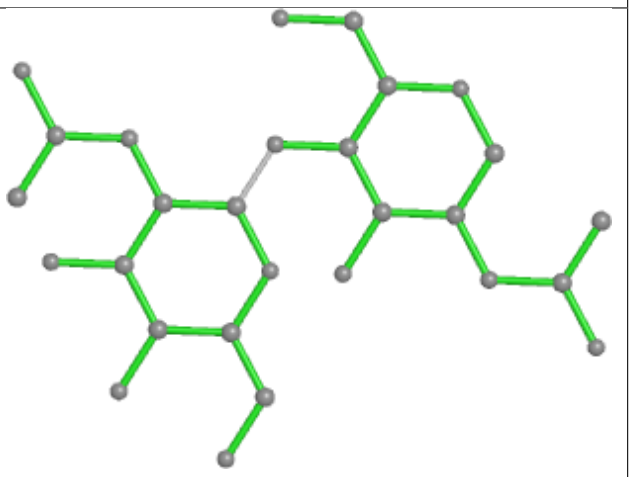
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	G	1	NAG	14	0
2	G	2	NAG	2	0
2	F	1	NAG	14	0
2	F	2	NAG	3	0
2	E	1	NAG	14	0
2	E	2	NAG	2	0
2	H	2	NAG	3	0
2	H	1	NAG	14	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for oligosaccharide.

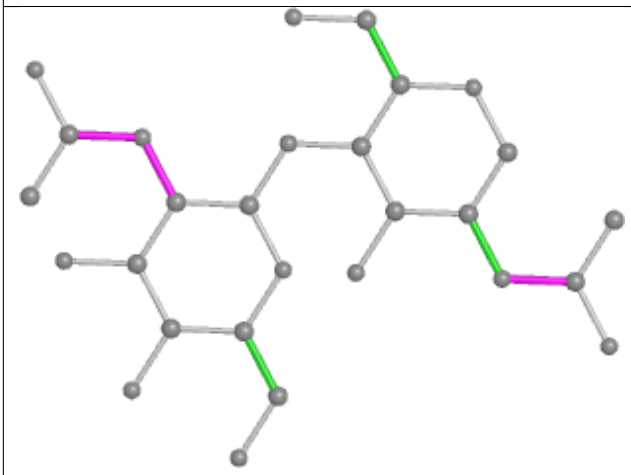
Oligosaccharide Chain E



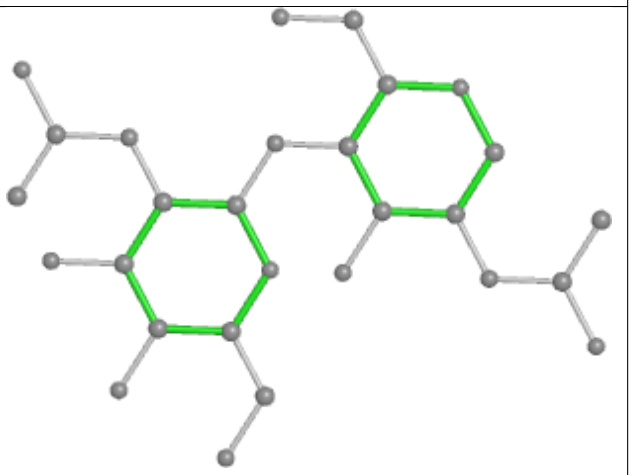
Bond lengths



Bond angles

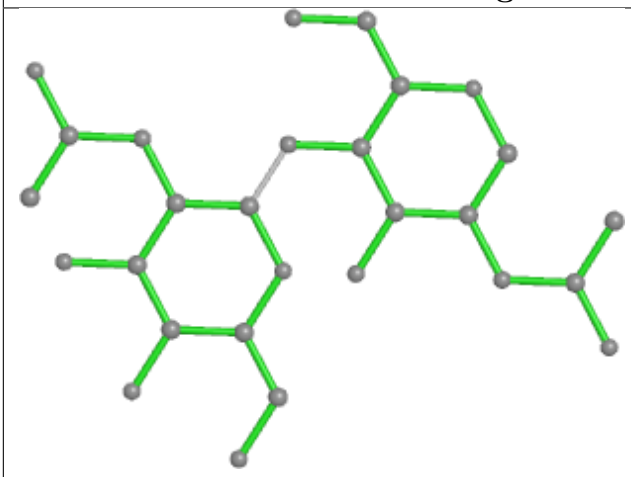


Torsions

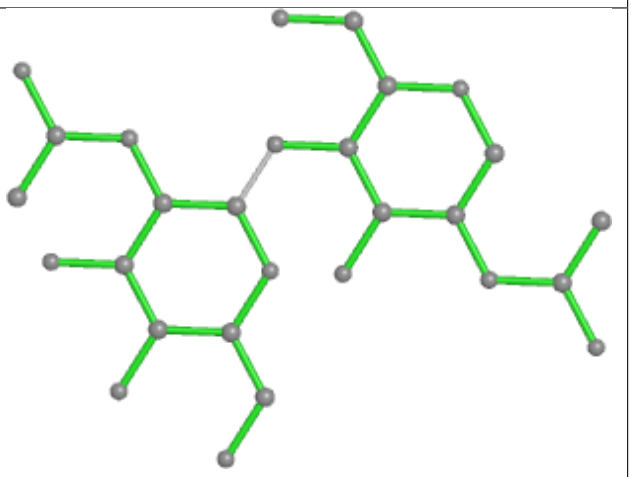


Rings

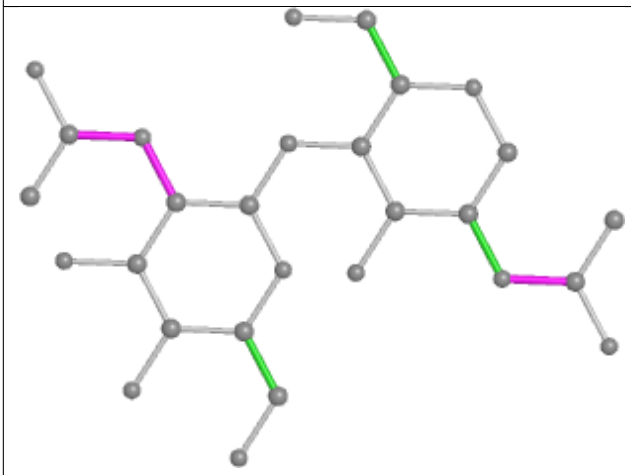
Oligosaccharide Chain F



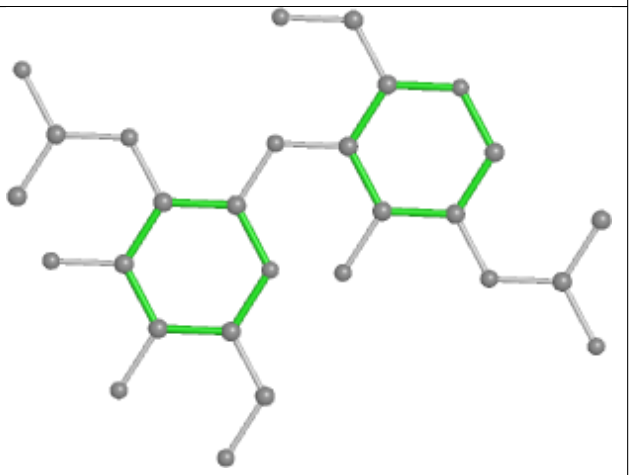
Bond lengths



Bond angles

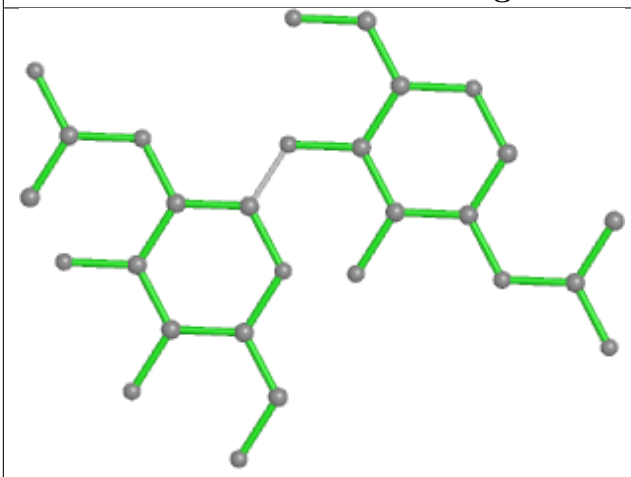


Torsions

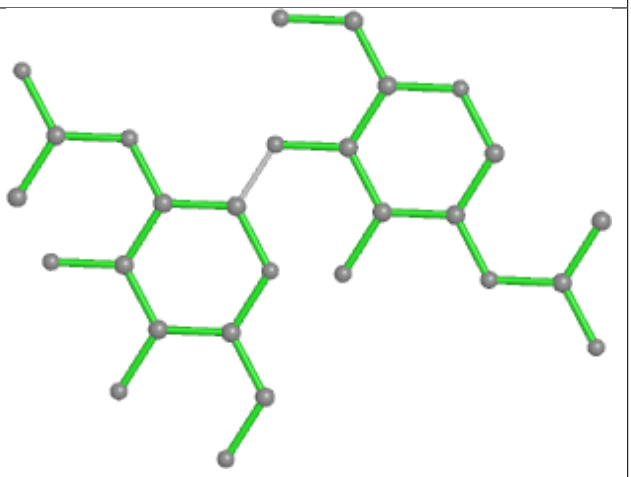


Rings

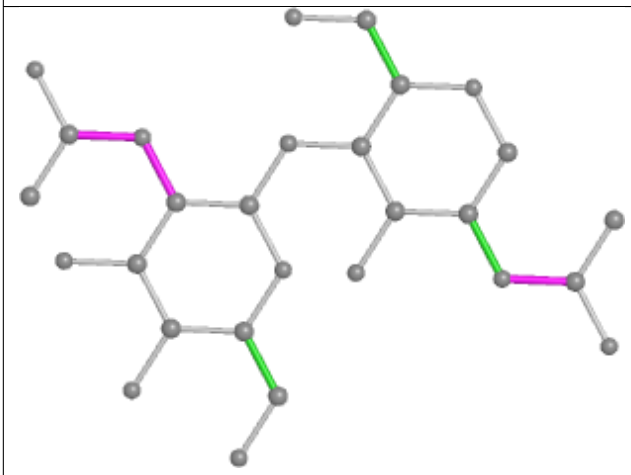
Oligosaccharide Chain G



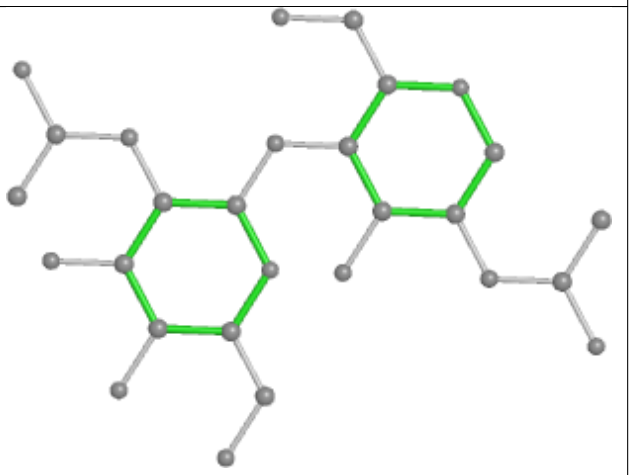
Bond lengths



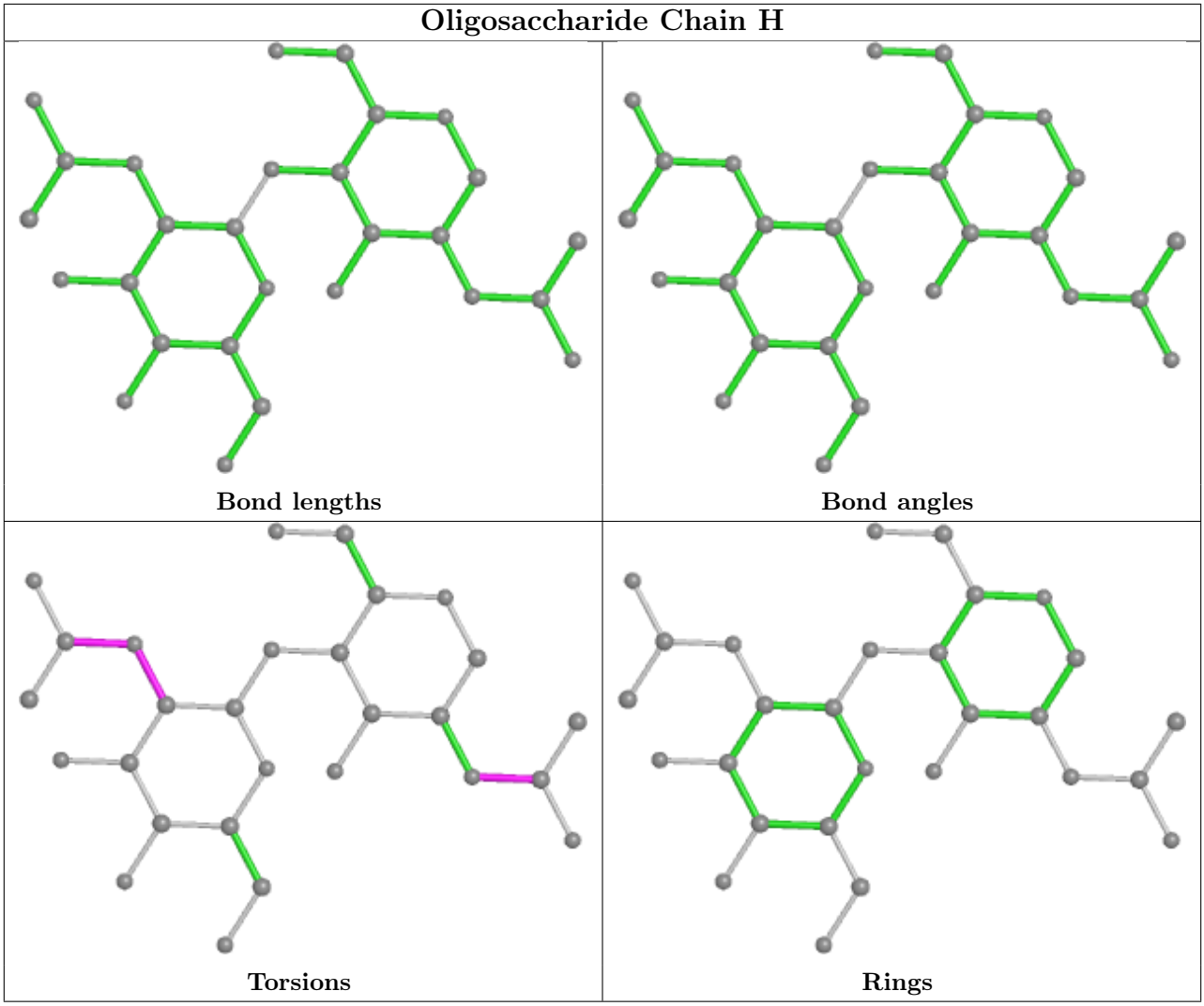
Bond angles



Torsions



Rings



5.6 Ligand geometry (i)

28 ligands are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
5	6OU	C	1201	-	28,28,48	1.92	7 (25%)	32,33,53	1.05	2 (6%)
4	LBN	B	1206	-	51,51,51	1.15	4 (7%)	57,59,59	0.90	3 (5%)
4	LBN	D	1304	-	31,31,51	1.41	3 (9%)	37,39,59	0.96	2 (5%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
3	JT0	D	1303	1	19,23,24	1.59	3 (15%)	23,30,31	1.60	6 (26%)
5	6OU	B	1207	-	40,40,48	1.17	3 (7%)	43,45,53	1.01	3 (6%)
4	LBN	D	1305	-	51,51,51	1.15	4 (7%)	57,59,59	0.90	3 (5%)
5	6OU	A	1207	-	27,27,48	1.94	7 (25%)	31,32,53	1.05	2 (6%)
5	6OU	D	1308	-	40,40,48	1.17	3 (7%)	43,45,53	1.00	3 (6%)
5	6OU	B	1209	-	28,28,48	1.92	7 (25%)	32,33,53	1.05	2 (6%)
5	6OU	C	1202	-	32,32,48	1.68	7 (21%)	35,37,53	0.91	2 (5%)
4	LBN	A	1206	-	51,51,51	1.15	4 (7%)	57,59,59	0.90	3 (5%)
3	JT0	B	1204	1	19,23,24	1.60	3 (15%)	23,30,31	1.60	6 (26%)
4	LBN	C	1207	-	51,51,51	1.15	4 (7%)	57,59,59	0.90	3 (5%)
5	6OU	D	1306	-	40,40,48	1.17	3 (7%)	43,45,53	1.01	3 (6%)
5	6OU	B	1201	-	32,32,48	1.68	7 (21%)	35,37,53	0.91	2 (5%)
4	LBN	B	1205	-	31,31,51	1.41	3 (9%)	37,39,59	0.96	2 (5%)
5	6OU	C	1208	-	40,40,48	1.17	3 (7%)	43,45,53	1.01	3 (6%)
5	6OU	D	1309	-	28,28,48	1.92	7 (25%)	32,33,53	1.05	2 (6%)
5	6OU	D	1310	-	32,32,48	1.68	7 (21%)	35,37,53	0.90	2 (5%)
4	LBN	C	1206	-	31,31,51	1.41	3 (9%)	37,39,59	0.96	2 (5%)
5	6OU	A	1201	-	32,32,48	1.68	7 (21%)	35,37,53	0.91	2 (5%)
3	JT0	A	1204	1	19,23,24	1.59	3 (15%)	23,30,31	1.61	6 (26%)
5	6OU	A	1208	-	28,28,48	1.92	7 (25%)	32,33,53	1.05	2 (6%)
3	JT0	C	1205	1	19,23,24	1.60	3 (15%)	23,30,31	1.60	6 (26%)
5	6OU	B	1208	-	27,27,48	1.94	7 (25%)	31,32,53	1.06	2 (6%)
4	LBN	A	1205	-	31,31,51	1.41	3 (9%)	37,39,59	0.97	2 (5%)
5	6OU	C	1209	-	27,27,48	1.94	7 (25%)	31,32,53	1.05	2 (6%)
5	6OU	D	1307	-	27,27,48	1.94	7 (25%)	31,32,53	1.05	2 (6%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	6OU	C	1201	-	-	16/30/30/52	-
4	LBN	B	1206	-	-	30/55/55/55	-
4	LBN	D	1304	-	-	16/35/35/55	-
3	JT0	D	1303	1	-	9/15/19/21	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	6OU	B	1207	-	-	17/44/44/52	-
4	LBN	D	1305	-	-	30/55/55/55	-
5	6OU	A	1207	-	-	14/29/29/52	-
5	6OU	D	1308	-	-	17/44/44/52	-
5	6OU	B	1209	-	-	16/30/30/52	-
5	6OU	C	1202	-	-	21/36/36/52	-
4	LBN	A	1206	-	-	30/55/55/55	-
3	JT0	B	1204	1	-	9/15/19/21	0/2/2/2
4	LBN	C	1207	-	-	30/55/55/55	-
5	6OU	D	1306	-	-	17/44/44/52	-
5	6OU	B	1201	-	-	21/36/36/52	-
4	LBN	B	1205	-	-	16/35/35/55	-
5	6OU	C	1208	-	-	17/44/44/52	-
5	6OU	D	1309	-	-	16/30/30/52	-
5	6OU	D	1310	-	-	21/36/36/52	-
4	LBN	C	1206	-	-	16/35/35/55	-
5	6OU	A	1201	-	-	21/36/36/52	-
3	JT0	A	1204	1	-	9/15/19/21	0/2/2/2
5	6OU	A	1208	-	-	16/30/30/52	-
3	JT0	C	1205	1	-	9/15/19/21	0/2/2/2
5	6OU	B	1208	-	-	14/29/29/52	-
4	LBN	A	1205	-	-	16/35/35/55	-
5	6OU	C	1209	-	-	14/29/29/52	-
5	6OU	D	1307	-	-	14/29/29/52	-

All (136) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	1204	JT0	C02-N03	4.70	1.42	1.36
3	C	1205	JT0	C02-N03	4.67	1.42	1.36
3	D	1303	JT0	C02-N03	4.67	1.42	1.36
5	D	1309	6OU	P23-O26	4.62	1.72	1.54
3	A	1204	JT0	C02-N03	4.62	1.42	1.36
5	C	1201	6OU	P23-O26	4.61	1.72	1.54
5	B	1209	6OU	P23-O26	4.61	1.72	1.54
5	B	1208	6OU	P23-O26	4.61	1.72	1.54
5	A	1208	6OU	P23-O26	4.60	1.72	1.54

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	D	1307	6OU	P23-O26	4.59	1.72	1.54
5	C	1209	6OU	P23-O26	4.59	1.72	1.54
5	A	1207	6OU	P23-O26	4.57	1.72	1.54
4	B	1205	LBN	P1-O2	4.49	1.77	1.59
4	A	1205	LBN	P1-O2	4.49	1.77	1.59
4	D	1304	LBN	P1-O2	4.48	1.77	1.59
4	C	1206	LBN	P1-O2	4.48	1.77	1.59
4	A	1206	LBN	P1-O2	4.41	1.77	1.59
4	C	1207	LBN	P1-O2	4.40	1.77	1.59
4	D	1305	LBN	P1-O2	4.39	1.77	1.59
4	B	1206	LBN	P1-O2	4.38	1.77	1.59
5	A	1208	6OU	P23-O22	4.33	1.74	1.60
5	A	1207	6OU	P23-O22	4.33	1.74	1.60
5	D	1307	6OU	P23-O22	4.32	1.74	1.60
5	C	1209	6OU	P23-O22	4.32	1.74	1.60
5	B	1208	6OU	P23-O22	4.31	1.74	1.60
5	C	1201	6OU	P23-O22	4.31	1.74	1.60
5	B	1209	6OU	P23-O22	4.31	1.74	1.60
5	D	1309	6OU	P23-O22	4.31	1.74	1.60
5	C	1202	6OU	P23-O22	3.67	1.74	1.59
5	B	1201	6OU	P23-O22	3.66	1.74	1.59
5	D	1310	6OU	P23-O22	3.66	1.74	1.59
5	A	1201	6OU	P23-O22	3.65	1.74	1.59
5	D	1308	6OU	P23-O22	3.49	1.73	1.59
5	C	1208	6OU	P23-O22	3.49	1.73	1.59
5	B	1207	6OU	P23-O22	3.48	1.73	1.59
5	D	1306	6OU	P23-O22	3.47	1.73	1.59
5	B	1201	6OU	P23-O26	3.31	1.72	1.59
5	C	1202	6OU	P23-O26	3.30	1.72	1.59
5	A	1201	6OU	P23-O26	3.30	1.72	1.59
5	D	1310	6OU	P23-O26	3.27	1.72	1.59
5	C	1208	6OU	P23-O26	3.24	1.72	1.59
5	D	1306	6OU	P23-O26	3.23	1.72	1.59
5	B	1207	6OU	P23-O26	3.22	1.72	1.59
5	D	1308	6OU	P23-O26	3.22	1.72	1.59
5	A	1207	6OU	C19-C20	3.02	1.60	1.50
5	D	1307	6OU	C19-C20	3.01	1.59	1.50
5	C	1209	6OU	C19-C20	3.00	1.59	1.50
5	B	1208	6OU	C19-C20	3.00	1.59	1.50
5	A	1208	6OU	C21-C20	2.97	1.59	1.50
5	B	1209	6OU	C21-C20	2.96	1.59	1.50
5	D	1309	6OU	C19-C20	2.96	1.59	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	D	1309	6OU	C21-C20	2.96	1.59	1.50
5	C	1201	6OU	C19-C20	2.96	1.59	1.50
5	D	1310	6OU	C19-C20	2.96	1.59	1.50
5	A	1201	6OU	C19-C20	2.96	1.59	1.50
5	C	1201	6OU	C21-C20	2.95	1.59	1.50
5	C	1202	6OU	C21-C20	2.95	1.59	1.50
5	D	1310	6OU	C21-C20	2.95	1.59	1.50
5	B	1201	6OU	C21-C20	2.95	1.59	1.50
5	B	1209	6OU	C19-C20	2.95	1.59	1.50
5	B	1201	6OU	C19-C20	2.95	1.59	1.50
5	C	1202	6OU	C19-C20	2.94	1.59	1.50
5	A	1208	6OU	C19-C20	2.94	1.59	1.50
5	A	1201	6OU	C21-C20	2.94	1.59	1.50
5	B	1208	6OU	C21-C20	2.94	1.59	1.50
5	A	1207	6OU	C21-C20	2.92	1.59	1.50
5	D	1307	6OU	C21-C20	2.92	1.59	1.50
5	C	1209	6OU	C21-C20	2.91	1.59	1.50
5	A	1207	6OU	O30-C31	2.74	1.42	1.34
5	D	1307	6OU	O30-C31	2.72	1.42	1.34
5	B	1208	6OU	O30-C31	2.72	1.42	1.34
5	C	1201	6OU	O30-C31	2.72	1.42	1.34
5	D	1309	6OU	O30-C31	2.71	1.42	1.34
5	C	1202	6OU	O30-C31	2.71	1.42	1.34
5	B	1209	6OU	O30-C31	2.71	1.42	1.34
5	A	1208	6OU	O30-C31	2.71	1.42	1.34
5	C	1209	6OU	O30-C31	2.71	1.42	1.34
5	A	1201	6OU	O30-C31	2.70	1.41	1.34
5	B	1201	6OU	O30-C31	2.68	1.41	1.34
5	D	1310	6OU	O30-C31	2.68	1.41	1.34
5	B	1208	6OU	O18-C16	2.53	1.40	1.33
5	A	1207	6OU	O18-C16	2.53	1.40	1.33
5	D	1307	6OU	O18-C16	2.53	1.40	1.33
5	C	1209	6OU	O18-C16	2.53	1.40	1.33
5	B	1209	6OU	O18-C16	2.52	1.40	1.33
5	A	1208	6OU	O18-C16	2.52	1.40	1.33
5	C	1201	6OU	O18-C16	2.51	1.40	1.33
5	D	1309	6OU	O18-C16	2.51	1.40	1.33
5	A	1201	6OU	O18-C16	2.51	1.40	1.33
3	C	1205	JT0	C11-N10	2.51	1.45	1.37
5	B	1201	6OU	O18-C16	2.51	1.40	1.33
5	C	1202	6OU	O18-C16	2.51	1.40	1.33
3	D	1303	JT0	C11-N10	2.50	1.45	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	1204	JT0	C11-N10	2.50	1.45	1.37
3	A	1204	JT0	C11-N10	2.50	1.45	1.37
5	D	1310	6OU	O18-C16	2.49	1.40	1.33
5	D	1310	6OU	C33-C31	2.47	1.57	1.50
5	B	1201	6OU	C33-C31	2.46	1.57	1.50
4	B	1206	LBN	P1-O1	2.46	1.69	1.59
5	C	1202	6OU	C33-C31	2.46	1.57	1.50
5	C	1209	6OU	C33-C31	2.46	1.57	1.50
5	A	1201	6OU	C33-C31	2.46	1.57	1.50
4	D	1305	LBN	P1-O1	2.45	1.69	1.59
4	C	1207	LBN	P1-O1	2.45	1.69	1.59
4	A	1206	LBN	P1-O1	2.45	1.69	1.59
5	D	1307	6OU	C33-C31	2.45	1.57	1.50
5	B	1208	6OU	C33-C31	2.44	1.57	1.50
5	A	1208	6OU	C33-C31	2.43	1.57	1.50
5	A	1207	6OU	C33-C31	2.43	1.57	1.50
5	D	1309	6OU	C33-C31	2.43	1.57	1.50
5	B	1209	6OU	C33-C31	2.42	1.57	1.50
4	C	1207	LBN	O2-C9	-2.41	1.34	1.44
5	C	1201	6OU	C33-C31	2.41	1.57	1.50
4	D	1305	LBN	O2-C9	-2.40	1.34	1.44
4	A	1206	LBN	O2-C9	-2.39	1.34	1.44
4	B	1206	LBN	O2-C9	-2.37	1.35	1.44
4	B	1205	LBN	O2-C9	-2.29	1.35	1.44
4	D	1304	LBN	O2-C9	-2.27	1.35	1.44
4	C	1206	LBN	O2-C9	-2.27	1.35	1.44
4	A	1205	LBN	O2-C9	-2.26	1.35	1.44
3	C	1205	JT0	C12-C11	2.25	1.52	1.48
3	A	1204	JT0	C12-C11	2.24	1.52	1.48
3	B	1204	JT0	C12-C11	2.24	1.52	1.48
3	D	1303	JT0	C12-C11	2.22	1.52	1.48
4	C	1207	LBN	C1-C2	2.18	1.57	1.50
4	D	1305	LBN	C1-C2	2.18	1.57	1.50
4	B	1206	LBN	C1-C2	2.18	1.57	1.50
4	A	1206	LBN	C1-C2	2.18	1.57	1.50
5	D	1308	6OU	C21-C20	2.14	1.57	1.50
5	C	1208	6OU	C21-C20	2.14	1.57	1.50
5	D	1306	6OU	C21-C20	2.13	1.57	1.50
5	B	1207	6OU	C21-C20	2.12	1.57	1.50
4	C	1206	LBN	P1-O1	2.09	1.67	1.59
4	D	1304	LBN	P1-O1	2.08	1.67	1.59
4	A	1205	LBN	P1-O1	2.08	1.67	1.59

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	B	1205	LBN	P1-O1	2.06	1.67	1.59

All (80) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	A	1204	JT0	C20-C11-C12	-4.26	123.52	129.44
3	C	1205	JT0	C20-C11-C12	-4.25	123.54	129.44
3	D	1303	JT0	C20-C11-C12	-4.24	123.54	129.44
3	B	1204	JT0	C20-C11-C12	-4.24	123.55	129.44
4	A	1205	LBN	O3-P1-O4	3.34	128.74	112.24
4	D	1304	LBN	O3-P1-O4	3.34	128.73	112.24
4	B	1205	LBN	O3-P1-O4	3.33	128.71	112.24
4	C	1206	LBN	O3-P1-O4	3.33	128.69	112.24
5	C	1208	6OU	O25-P23-O24	3.28	128.45	112.24
5	B	1207	6OU	O25-P23-O24	3.28	128.44	112.24
5	D	1306	6OU	O25-P23-O24	3.27	128.41	112.24
5	D	1308	6OU	O25-P23-O24	3.27	128.41	112.24
4	C	1207	LBN	C2-O7-C34	3.18	125.62	117.79
4	B	1206	LBN	C2-O7-C34	3.17	125.60	117.79
4	D	1305	LBN	C2-O7-C34	3.17	125.59	117.79
4	C	1207	LBN	O3-P1-O4	3.16	127.85	112.24
4	A	1206	LBN	O3-P1-O4	3.15	127.82	112.24
4	D	1305	LBN	O3-P1-O4	3.15	127.80	112.24
4	A	1206	LBN	C2-O7-C34	3.15	125.54	117.79
4	B	1206	LBN	O3-P1-O4	3.14	127.78	112.24
5	C	1209	6OU	O25-P23-O24	2.98	122.34	110.68
5	A	1208	6OU	O25-P23-O24	2.97	122.32	110.68
5	D	1309	6OU	O25-P23-O24	2.97	122.31	110.68
5	C	1201	6OU	O25-P23-O24	2.97	122.31	110.68
5	D	1307	6OU	O25-P23-O24	2.97	122.30	110.68
5	B	1209	6OU	O25-P23-O24	2.97	122.29	110.68
5	B	1208	6OU	O25-P23-O24	2.96	122.28	110.68
5	A	1207	6OU	O25-P23-O24	2.96	122.27	110.68
5	B	1201	6OU	O30-C31-C33	2.64	117.19	111.50
5	C	1202	6OU	O30-C31-C33	2.63	117.17	111.50
5	A	1201	6OU	O30-C31-C33	2.63	117.16	111.50
5	D	1310	6OU	O30-C31-C33	2.62	117.14	111.50
5	A	1208	6OU	O30-C31-C33	2.61	117.13	111.50
5	D	1309	6OU	O30-C31-C33	2.61	117.12	111.50
5	C	1201	6OU	O30-C31-C33	2.61	117.12	111.50
5	B	1209	6OU	O30-C31-C33	2.60	117.11	111.50
5	D	1307	6OU	O30-C31-C33	2.59	117.07	111.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
5	B	1208	6OU	O30-C31-C33	2.58	117.06	111.50
5	A	1207	6OU	O30-C31-C33	2.58	117.06	111.50
5	C	1209	6OU	O30-C31-C33	2.58	117.06	111.50
5	D	1308	6OU	O18-C19-C20	2.50	115.70	108.43
5	C	1208	6OU	O18-C19-C20	2.50	115.70	108.43
5	D	1306	6OU	O18-C19-C20	2.50	115.70	108.43
5	B	1207	6OU	O18-C19-C20	2.49	115.69	108.43
3	B	1204	JT0	C18-C15-C14	-2.45	116.40	120.18
3	A	1204	JT0	C18-C15-C14	-2.45	116.41	120.18
3	C	1205	JT0	C18-C15-C14	-2.44	116.42	120.18
3	D	1303	JT0	C18-C15-C14	-2.44	116.42	120.18
5	B	1207	6OU	O30-C31-C33	2.36	116.59	111.50
5	C	1208	6OU	O30-C31-C33	2.35	116.58	111.50
5	D	1306	6OU	O30-C31-C33	2.35	116.56	111.50
5	D	1308	6OU	O30-C31-C33	2.34	116.54	111.50
3	A	1204	JT0	C14-C13-C12	2.31	124.47	121.13
3	B	1204	JT0	C14-C13-C12	2.31	124.46	121.13
3	A	1204	JT0	C19-C12-C13	-2.31	112.99	117.59
3	D	1303	JT0	C19-C12-C13	-2.30	113.00	117.59
3	B	1204	JT0	C19-C12-C13	-2.30	113.00	117.59
3	D	1303	JT0	C14-C13-C12	2.30	124.44	121.13
3	B	1204	JT0	C11-C20-S21	2.30	114.61	111.79
3	C	1205	JT0	C11-C20-S21	2.29	114.60	111.79
3	D	1303	JT0	C11-C20-S21	2.28	114.59	111.79
3	A	1204	JT0	C11-C20-S21	2.28	114.59	111.79
3	C	1205	JT0	C19-C12-C13	-2.28	113.05	117.59
3	C	1205	JT0	C14-C13-C12	2.28	124.41	121.13
4	B	1206	LBN	O3-P1-O2	-2.27	97.19	107.75
4	A	1206	LBN	O3-P1-O2	-2.27	97.21	107.75
4	D	1305	LBN	O3-P1-O2	-2.27	97.22	107.75
4	C	1207	LBN	O3-P1-O2	-2.26	97.24	107.75
3	A	1204	JT0	C05-C04-N03	2.13	116.99	112.44
3	D	1303	JT0	C05-C04-N03	2.12	116.97	112.44
3	C	1205	JT0	C05-C04-N03	2.12	116.96	112.44
3	B	1204	JT0	C05-C04-N03	2.12	116.95	112.44
5	C	1202	6OU	O25-P23-O24	2.04	122.32	112.24
5	B	1201	6OU	O25-P23-O24	2.04	122.31	112.24
5	A	1201	6OU	O25-P23-O24	2.04	122.30	112.24
4	A	1205	LBN	O2-P1-O4	-2.03	101.13	109.07
4	D	1304	LBN	O2-P1-O4	-2.03	101.14	109.07
4	B	1205	LBN	O2-P1-O4	-2.03	101.14	109.07
5	D	1310	6OU	O25-P23-O24	2.03	122.27	112.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	C	1206	LBN	O2-P1-O4	-2.03	101.15	109.07

There are no chirality outliers.

All (492) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	D	1303	JT0	C22-C02-N03-C04
3	D	1303	JT0	C22-C02-N03-C09
3	D	1303	JT0	O01-C02-N03-C04
3	D	1303	JT0	O01-C02-N03-C09
3	A	1204	JT0	C22-C02-N03-C04
3	A	1204	JT0	C22-C02-N03-C09
3	A	1204	JT0	O01-C02-N03-C04
3	A	1204	JT0	O01-C02-N03-C09
3	B	1204	JT0	C22-C02-N03-C04
3	B	1204	JT0	C22-C02-N03-C09
3	B	1204	JT0	O01-C02-N03-C04
3	B	1204	JT0	O01-C02-N03-C09
3	C	1205	JT0	C22-C02-N03-C04
3	C	1205	JT0	C22-C02-N03-C09
3	C	1205	JT0	O01-C02-N03-C04
3	C	1205	JT0	O01-C02-N03-C09
4	D	1304	LBN	C1-O1-P1-O3
4	D	1305	LBN	C1-O1-P1-O2
4	D	1305	LBN	C1-O1-P1-O3
4	D	1305	LBN	C1-O1-P1-O4
4	A	1205	LBN	C1-O1-P1-O3
4	A	1206	LBN	C1-O1-P1-O2
4	A	1206	LBN	C1-O1-P1-O3
4	A	1206	LBN	C1-O1-P1-O4
4	B	1205	LBN	C1-O1-P1-O3
4	B	1206	LBN	C1-O1-P1-O2
4	B	1206	LBN	C1-O1-P1-O3
4	B	1206	LBN	C1-O1-P1-O4
4	C	1206	LBN	C1-O1-P1-O3
4	C	1207	LBN	C1-O1-P1-O2
4	C	1207	LBN	C1-O1-P1-O3
4	C	1207	LBN	C1-O1-P1-O4
5	D	1306	6OU	O30-C20-C21-O22
5	D	1306	6OU	C21-O22-P23-O24
5	D	1306	6OU	C27-O26-P23-O25
5	D	1306	6OU	O26-C27-C28-N29

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Mol	Chain	Res	Type	Atoms
5	D	1307	6OU	C21-O22-P23-O25
5	D	1307	6OU	C21-O22-P23-O26
5	D	1308	6OU	O30-C20-C21-O22
5	D	1308	6OU	C21-O22-P23-O24
5	D	1308	6OU	C27-O26-P23-O25
5	D	1308	6OU	O26-C27-C28-N29
5	D	1309	6OU	C21-O22-P23-O25
5	D	1309	6OU	C21-O22-P23-O26
5	D	1310	6OU	C21-O22-P23-O25
5	D	1310	6OU	C27-O26-P23-O22
5	A	1201	6OU	C21-O22-P23-O25
5	A	1201	6OU	C27-O26-P23-O22
5	A	1207	6OU	C21-O22-P23-O25
5	A	1207	6OU	C21-O22-P23-O26
5	A	1208	6OU	C21-O22-P23-O25
5	A	1208	6OU	C21-O22-P23-O26
5	B	1201	6OU	C21-O22-P23-O25
5	B	1201	6OU	C27-O26-P23-O22
5	B	1207	6OU	O30-C20-C21-O22
5	B	1207	6OU	C21-O22-P23-O24
5	B	1207	6OU	C27-O26-P23-O25
5	B	1207	6OU	O26-C27-C28-N29
5	B	1208	6OU	C21-O22-P23-O25
5	B	1208	6OU	C21-O22-P23-O26
5	B	1209	6OU	C21-O22-P23-O25
5	B	1209	6OU	C21-O22-P23-O26
5	C	1201	6OU	C21-O22-P23-O25
5	C	1201	6OU	C21-O22-P23-O26
5	C	1202	6OU	C21-O22-P23-O25
5	C	1202	6OU	C27-O26-P23-O22
5	C	1208	6OU	O30-C20-C21-O22
5	C	1208	6OU	C21-O22-P23-O24
5	C	1208	6OU	C27-O26-P23-O25
5	C	1208	6OU	O26-C27-C28-N29
5	C	1209	6OU	C21-O22-P23-O25
5	C	1209	6OU	C21-O22-P23-O26
5	D	1310	6OU	O17-C16-O18-C19
5	A	1201	6OU	O17-C16-O18-C19
5	B	1201	6OU	O17-C16-O18-C19
5	C	1202	6OU	O17-C16-O18-C19
5	D	1310	6OU	C15-C16-O18-C19
5	A	1201	6OU	C15-C16-O18-C19

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Mol	Chain	Res	Type	Atoms
5	B	1201	6OU	C15-C16-O18-C19
5	C	1202	6OU	C15-C16-O18-C19
4	D	1305	LBN	O6-C25-O5-C3
4	A	1206	LBN	O6-C25-O5-C3
4	B	1206	LBN	O6-C25-O5-C3
4	C	1207	LBN	O6-C25-O5-C3
5	D	1309	6OU	O17-C16-O18-C19
5	A	1208	6OU	O17-C16-O18-C19
5	B	1209	6OU	O17-C16-O18-C19
5	C	1201	6OU	O17-C16-O18-C19
4	D	1305	LBN	C26-C25-O5-C3
4	A	1206	LBN	C26-C25-O5-C3
4	B	1206	LBN	C26-C25-O5-C3
4	C	1207	LBN	C26-C25-O5-C3
3	D	1303	JT0	C18-C15-O16-C17
3	A	1204	JT0	C18-C15-O16-C17
3	B	1204	JT0	C18-C15-O16-C17
3	C	1205	JT0	C18-C15-O16-C17
3	D	1303	JT0	C14-C15-O16-C17
3	A	1204	JT0	C14-C15-O16-C17
3	B	1204	JT0	C14-C15-O16-C17
3	C	1205	JT0	C14-C15-O16-C17
5	D	1309	6OU	C15-C16-O18-C19
5	A	1208	6OU	C15-C16-O18-C19
5	B	1209	6OU	C15-C16-O18-C19
5	C	1201	6OU	C15-C16-O18-C19
4	D	1305	LBN	C36-C37-C38-C39
4	A	1206	LBN	C36-C37-C38-C39
4	B	1206	LBN	C36-C37-C38-C39
4	C	1207	LBN	C36-C37-C38-C39
5	D	1306	6OU	C34-C35-C36-C37
5	D	1308	6OU	C34-C35-C36-C37
5	B	1207	6OU	C34-C35-C36-C37
5	C	1208	6OU	C34-C35-C36-C37
3	D	1303	JT0	C04-C05-C06-O07
3	A	1204	JT0	C04-C05-C06-O07
3	B	1204	JT0	C04-C05-C06-O07
3	C	1205	JT0	C04-C05-C06-O07
4	D	1305	LBN	C35-C34-O7-C2
4	A	1206	LBN	C35-C34-O7-C2
4	B	1206	LBN	C35-C34-O7-C2
4	C	1207	LBN	C35-C34-O7-C2

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Mol	Chain	Res	Type	Atoms
5	D	1309	6OU	C31-C33-C34-C35
5	A	1208	6OU	C31-C33-C34-C35
5	B	1209	6OU	C31-C33-C34-C35
5	C	1201	6OU	C31-C33-C34-C35
4	D	1304	LBN	C34-C35-C36-C37
4	A	1205	LBN	C34-C35-C36-C37
4	B	1205	LBN	C34-C35-C36-C37
4	C	1206	LBN	C34-C35-C36-C37
5	D	1307	6OU	C31-C33-C34-C35
5	D	1310	6OU	C31-C33-C34-C35
5	A	1201	6OU	C31-C33-C34-C35
5	A	1207	6OU	C31-C33-C34-C35
5	B	1201	6OU	C31-C33-C34-C35
5	B	1208	6OU	C31-C33-C34-C35
5	C	1202	6OU	C31-C33-C34-C35
5	C	1209	6OU	C31-C33-C34-C35
4	D	1305	LBN	O8-C34-O7-C2
4	A	1206	LBN	O8-C34-O7-C2
4	B	1206	LBN	O8-C34-O7-C2
4	C	1207	LBN	O8-C34-O7-C2
5	D	1307	6OU	C33-C34-C35-C36
5	A	1207	6OU	C33-C34-C35-C36
5	B	1208	6OU	C33-C34-C35-C36
5	C	1209	6OU	C33-C34-C35-C36
4	D	1305	LBN	C14-C11-C8-C5
4	A	1206	LBN	C14-C11-C8-C5
4	C	1207	LBN	C14-C11-C8-C5
5	D	1309	6OU	C33-C34-C35-C36
5	A	1208	6OU	C33-C34-C35-C36
5	C	1201	6OU	C33-C34-C35-C36
4	D	1304	LBN	C1-O1-P1-O2
4	A	1205	LBN	C1-O1-P1-O2
4	B	1205	LBN	C1-O1-P1-O2
4	C	1206	LBN	C1-O1-P1-O2
5	D	1306	6OU	C21-O22-P23-O26
5	D	1306	6OU	C27-O26-P23-O22
5	D	1308	6OU	C21-O22-P23-O26
5	D	1308	6OU	C27-O26-P23-O22
5	D	1310	6OU	C21-O22-P23-O26
5	A	1201	6OU	C21-O22-P23-O26
5	B	1201	6OU	C21-O22-P23-O26
5	B	1207	6OU	C21-O22-P23-O26

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Mol	Chain	Res	Type	Atoms
5	B	1207	6OU	C27-O26-P23-O22
5	C	1202	6OU	C21-O22-P23-O26
5	C	1208	6OU	C21-O22-P23-O26
5	C	1208	6OU	C27-O26-P23-O22
5	B	1209	6OU	C33-C34-C35-C36
3	D	1303	JT0	C20-C11-C12-C13
3	A	1204	JT0	C20-C11-C12-C13
3	B	1204	JT0	C20-C11-C12-C13
3	C	1205	JT0	C20-C11-C12-C13
4	B	1206	LBN	C14-C11-C8-C5
5	D	1310	6OU	C35-C36-C37-C38
5	A	1201	6OU	C35-C36-C37-C38
5	B	1201	6OU	C35-C36-C37-C38
5	C	1202	6OU	C35-C36-C37-C38
5	D	1307	6OU	C35-C36-C37-C38
5	B	1208	6OU	C35-C36-C37-C38
5	C	1209	6OU	C35-C36-C37-C38
5	A	1207	6OU	C35-C36-C37-C38
4	D	1305	LBN	C27-C28-C29-C30
4	A	1206	LBN	C27-C28-C29-C30
4	B	1206	LBN	C27-C28-C29-C30
4	C	1207	LBN	C27-C28-C29-C30
5	D	1309	6OU	C35-C36-C37-C38
5	A	1208	6OU	C35-C36-C37-C38
5	B	1209	6OU	C35-C36-C37-C38
5	C	1201	6OU	C35-C36-C37-C38
4	A	1205	LBN	C29-C30-C31-C32
4	B	1205	LBN	C29-C30-C31-C32
4	C	1206	LBN	C29-C30-C31-C32
5	D	1306	6OU	C09-C10-C11-C12
5	D	1308	6OU	C09-C10-C11-C12
5	B	1207	6OU	C09-C10-C11-C12
5	C	1208	6OU	C09-C10-C11-C12
4	D	1304	LBN	C29-C30-C31-C32
5	D	1310	6OU	C09-C10-C11-C12
5	A	1201	6OU	C09-C10-C11-C12
5	B	1201	6OU	C09-C10-C11-C12
5	C	1202	6OU	C09-C10-C11-C12
5	D	1309	6OU	C37-C38-C39-C40
5	A	1208	6OU	C37-C38-C39-C40
5	B	1209	6OU	C37-C38-C39-C40
5	C	1201	6OU	C37-C38-C39-C40

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Mol	Chain	Res	Type	Atoms
5	D	1306	6OU	C08-C09-C10-C11
5	D	1308	6OU	C08-C09-C10-C11
5	B	1207	6OU	C08-C09-C10-C11
5	C	1208	6OU	C08-C09-C10-C11
4	D	1305	LBN	C7-C10-C13-C16
4	A	1206	LBN	C7-C10-C13-C16
4	B	1206	LBN	C7-C10-C13-C16
4	C	1207	LBN	C7-C10-C13-C16
5	D	1307	6OU	C12-C13-C14-C15
5	A	1207	6OU	C12-C13-C14-C15
5	B	1208	6OU	C12-C13-C14-C15
5	C	1209	6OU	C12-C13-C14-C15
4	D	1304	LBN	C9-C6-N1-C18
4	A	1205	LBN	C9-C6-N1-C18
4	B	1205	LBN	C9-C6-N1-C18
4	C	1206	LBN	C9-C6-N1-C18
4	D	1305	LBN	C34-C35-C36-C37
4	A	1206	LBN	C34-C35-C36-C37
4	B	1206	LBN	C34-C35-C36-C37
4	C	1207	LBN	C34-C35-C36-C37
4	D	1305	LBN	C30-C31-C32-C33
4	A	1206	LBN	C30-C31-C32-C33
4	B	1206	LBN	C30-C31-C32-C33
4	C	1207	LBN	C30-C31-C32-C33
5	B	1207	6OU	C06-C07-C08-C09
5	D	1306	6OU	C06-C07-C08-C09
5	D	1308	6OU	C06-C07-C08-C09
5	C	1208	6OU	C06-C07-C08-C09
4	D	1305	LBN	C32-C33-C4-C7
4	A	1206	LBN	C32-C33-C4-C7
4	B	1206	LBN	C32-C33-C4-C7
4	C	1207	LBN	C32-C33-C4-C7
5	C	1209	6OU	C34-C35-C36-C37
5	D	1307	6OU	C34-C35-C36-C37
5	A	1207	6OU	C34-C35-C36-C37
5	B	1208	6OU	C34-C35-C36-C37
4	D	1305	LBN	C2-C1-O1-P1
4	A	1206	LBN	C2-C1-O1-P1
4	B	1206	LBN	C2-C1-O1-P1
4	C	1207	LBN	C2-C1-O1-P1
5	D	1310	6OU	C37-C38-C39-C40
5	A	1201	6OU	C37-C38-C39-C40

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Mol	Chain	Res	Type	Atoms
5	B	1201	6OU	C37-C38-C39-C40
5	C	1202	6OU	C37-C38-C39-C40
5	C	1202	6OU	C34-C35-C36-C37
5	D	1310	6OU	C34-C35-C36-C37
5	A	1201	6OU	C34-C35-C36-C37
5	B	1201	6OU	C34-C35-C36-C37
5	D	1307	6OU	C37-C38-C39-C40
5	A	1207	6OU	C37-C38-C39-C40
5	B	1208	6OU	C37-C38-C39-C40
5	C	1209	6OU	C37-C38-C39-C40
4	D	1305	LBN	C33-C4-C7-C10
4	A	1206	LBN	C33-C4-C7-C10
4	B	1206	LBN	C33-C4-C7-C10
4	C	1207	LBN	C33-C4-C7-C10
4	D	1305	LBN	C1-C2-O7-C34
4	A	1206	LBN	C1-C2-O7-C34
4	B	1206	LBN	C1-C2-O7-C34
4	C	1207	LBN	C1-C2-O7-C34
5	D	1307	6OU	O30-C20-C21-O22
5	A	1207	6OU	O30-C20-C21-O22
5	B	1208	6OU	O30-C20-C21-O22
5	C	1209	6OU	O30-C20-C21-O22
4	D	1304	LBN	C9-C6-N1-C12
4	A	1205	LBN	C9-C6-N1-C12
4	B	1205	LBN	C9-C6-N1-C12
4	C	1206	LBN	C9-C6-N1-C12
4	C	1207	LBN	C37-C38-C39-C40
4	D	1305	LBN	C37-C38-C39-C40
4	A	1206	LBN	C37-C38-C39-C40
4	B	1206	LBN	C37-C38-C39-C40
5	D	1310	6OU	O18-C19-C20-O30
5	B	1201	6OU	O18-C19-C20-O30
5	C	1202	6OU	O18-C19-C20-O30
5	D	1309	6OU	C34-C35-C36-C37
5	B	1209	6OU	C34-C35-C36-C37
5	A	1208	6OU	C34-C35-C36-C37
5	C	1201	6OU	C34-C35-C36-C37
4	D	1305	LBN	C26-C27-C28-C29
4	B	1206	LBN	C26-C27-C28-C29
4	C	1207	LBN	C26-C27-C28-C29
4	A	1206	LBN	C26-C27-C28-C29
5	D	1306	6OU	C19-C20-C21-O22

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Mol	Chain	Res	Type	Atoms
5	D	1308	6OU	C19-C20-C21-O22
5	B	1207	6OU	C19-C20-C21-O22
5	C	1208	6OU	C19-C20-C21-O22
4	D	1305	LBN	C29-C30-C31-C32
4	A	1206	LBN	C29-C30-C31-C32
4	C	1207	LBN	C29-C30-C31-C32
4	B	1206	LBN	C29-C30-C31-C32
5	D	1306	6OU	C35-C36-C37-C38
5	D	1308	6OU	C35-C36-C37-C38
5	C	1208	6OU	C35-C36-C37-C38
5	B	1207	6OU	C35-C36-C37-C38
5	D	1309	6OU	O18-C19-C20-C21
5	A	1208	6OU	O18-C19-C20-C21
5	B	1209	6OU	O18-C19-C20-C21
5	C	1201	6OU	O18-C19-C20-C21
5	D	1309	6OU	O30-C20-C21-O22
5	D	1310	6OU	O30-C20-C21-O22
5	A	1201	6OU	O30-C20-C21-O22
5	A	1208	6OU	O30-C20-C21-O22
5	B	1201	6OU	O30-C20-C21-O22
5	B	1209	6OU	O30-C20-C21-O22
5	C	1201	6OU	O30-C20-C21-O22
5	C	1202	6OU	O30-C20-C21-O22
5	D	1310	6OU	C33-C34-C35-C36
5	A	1201	6OU	C33-C34-C35-C36
5	B	1201	6OU	C33-C34-C35-C36
5	C	1202	6OU	C33-C34-C35-C36
5	A	1201	6OU	O18-C19-C20-O30
3	D	1303	JT0	C20-C11-C12-C19
3	A	1204	JT0	C20-C11-C12-C19
3	B	1204	JT0	C20-C11-C12-C19
3	C	1205	JT0	C20-C11-C12-C19
4	B	1206	LBN	C31-C32-C33-C4
4	C	1207	LBN	C31-C32-C33-C4
4	D	1305	LBN	C31-C32-C33-C4
4	A	1206	LBN	C31-C32-C33-C4
5	D	1307	6OU	C10-C11-C12-C13
5	A	1207	6OU	C10-C11-C12-C13
5	B	1208	6OU	C10-C11-C12-C13
5	C	1209	6OU	C10-C11-C12-C13
5	B	1207	6OU	C36-C37-C38-C39
5	D	1306	6OU	C36-C37-C38-C39

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Mol	Chain	Res	Type	Atoms
5	D	1308	6OU	C36-C37-C38-C39
5	C	1208	6OU	C36-C37-C38-C39
4	D	1305	LBN	C1-C2-C3-O5
4	A	1206	LBN	C1-C2-C3-O5
4	B	1206	LBN	C1-C2-C3-O5
4	C	1207	LBN	C1-C2-C3-O5
4	D	1305	LBN	O1-C1-C2-O7
4	A	1206	LBN	O1-C1-C2-O7
4	B	1206	LBN	O1-C1-C2-O7
4	C	1207	LBN	O1-C1-C2-O7
5	D	1309	6OU	C12-C13-C14-C15
5	A	1208	6OU	C12-C13-C14-C15
5	B	1209	6OU	C12-C13-C14-C15
5	C	1201	6OU	C12-C13-C14-C15
4	D	1305	LBN	O7-C2-C3-O5
4	A	1206	LBN	O7-C2-C3-O5
4	B	1206	LBN	O7-C2-C3-O5
4	C	1207	LBN	O7-C2-C3-O5
5	D	1309	6OU	O18-C19-C20-O30
5	A	1208	6OU	O18-C19-C20-O30
5	B	1209	6OU	O18-C19-C20-O30
5	C	1201	6OU	O18-C19-C20-O30
4	D	1304	LBN	C9-C6-N1-C15
4	A	1205	LBN	C9-C6-N1-C15
4	B	1205	LBN	C9-C6-N1-C15
4	C	1206	LBN	C9-C6-N1-C15
4	A	1205	LBN	C25-C26-C27-C28
4	D	1304	LBN	C25-C26-C27-C28
4	B	1205	LBN	C25-C26-C27-C28
4	C	1206	LBN	C25-C26-C27-C28
5	D	1310	6OU	C10-C11-C12-C13
5	B	1201	6OU	C10-C11-C12-C13
5	C	1202	6OU	C10-C11-C12-C13
5	A	1201	6OU	C10-C11-C12-C13
5	D	1306	6OU	C21-O22-P23-O25
5	D	1308	6OU	C21-O22-P23-O25
5	D	1310	6OU	C27-O26-P23-O25
5	A	1201	6OU	C27-O26-P23-O25
5	B	1201	6OU	C27-O26-P23-O25
5	B	1207	6OU	C21-O22-P23-O25
5	C	1202	6OU	C27-O26-P23-O25
5	C	1208	6OU	C21-O22-P23-O25

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Mol	Chain	Res	Type	Atoms
4	D	1305	LBN	O1-C1-C2-C3
4	A	1206	LBN	O1-C1-C2-C3
4	B	1206	LBN	O1-C1-C2-C3
4	C	1207	LBN	O1-C1-C2-C3
5	D	1309	6OU	C19-C20-C21-O22
5	D	1310	6OU	C19-C20-C21-O22
5	A	1201	6OU	C19-C20-C21-O22
5	A	1208	6OU	C19-C20-C21-O22
5	B	1201	6OU	C19-C20-C21-O22
5	B	1209	6OU	C19-C20-C21-O22
5	C	1201	6OU	C19-C20-C21-O22
5	C	1202	6OU	C19-C20-C21-O22
5	D	1309	6OU	C10-C11-C12-C13
5	A	1208	6OU	C10-C11-C12-C13
5	B	1209	6OU	C10-C11-C12-C13
5	C	1201	6OU	C10-C11-C12-C13
4	D	1305	LBN	N1-C6-C9-O2
4	A	1206	LBN	N1-C6-C9-O2
4	B	1206	LBN	N1-C6-C9-O2
4	C	1207	LBN	N1-C6-C9-O2
5	D	1310	6OU	O18-C19-C20-C21
5	A	1201	6OU	O18-C19-C20-C21
5	B	1201	6OU	O18-C19-C20-C21
5	C	1202	6OU	O18-C19-C20-C21
5	C	1202	6OU	C12-C13-C14-C15
5	A	1201	6OU	C12-C13-C14-C15
5	D	1310	6OU	C12-C13-C14-C15
5	B	1201	6OU	C12-C13-C14-C15
5	D	1307	6OU	C20-C21-O22-P23
5	A	1207	6OU	C20-C21-O22-P23
5	B	1208	6OU	C20-C21-O22-P23
5	C	1209	6OU	C20-C21-O22-P23
4	D	1305	LBN	C42-C5-C8-C11
4	A	1206	LBN	C42-C5-C8-C11
4	B	1206	LBN	C42-C5-C8-C11
4	C	1207	LBN	C42-C5-C8-C11
5	B	1201	6OU	C36-C37-C38-C39
5	D	1310	6OU	C36-C37-C38-C39
5	A	1201	6OU	C36-C37-C38-C39
5	C	1202	6OU	C36-C37-C38-C39
4	D	1304	LBN	C26-C27-C28-C29
4	B	1205	LBN	C26-C27-C28-C29

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Mol	Chain	Res	Type	Atoms
4	C	1206	LBN	C26-C27-C28-C29
4	A	1205	LBN	C26-C27-C28-C29
4	D	1304	LBN	O8-C34-O7-C2
4	A	1205	LBN	O8-C34-O7-C2
4	B	1205	LBN	O8-C34-O7-C2
4	C	1206	LBN	O8-C34-O7-C2
5	D	1310	6OU	C14-C15-C16-O18
5	A	1201	6OU	C14-C15-C16-O18
5	B	1201	6OU	C14-C15-C16-O18
5	C	1202	6OU	C14-C15-C16-O18
5	A	1207	6OU	C36-C37-C38-C39
5	D	1307	6OU	C36-C37-C38-C39
5	C	1209	6OU	C36-C37-C38-C39
5	B	1208	6OU	C36-C37-C38-C39
4	C	1206	LBN	C35-C34-O7-C2
4	A	1206	LBN	C35-C36-C37-C38
4	B	1206	LBN	C35-C36-C37-C38
4	C	1207	LBN	C35-C36-C37-C38
4	D	1305	LBN	C35-C36-C37-C38
4	D	1304	LBN	C35-C34-O7-C2
4	A	1205	LBN	C35-C34-O7-C2
4	B	1205	LBN	C35-C34-O7-C2
5	D	1307	6OU	O18-C19-C20-O30
5	A	1207	6OU	O18-C19-C20-O30
5	B	1208	6OU	O18-C19-C20-O30
5	C	1209	6OU	O18-C19-C20-O30
5	D	1306	6OU	C40-C41-C42-C43
5	C	1208	6OU	C40-C41-C42-C43
4	D	1304	LBN	O7-C34-C35-C36
4	A	1205	LBN	O7-C34-C35-C36
4	B	1205	LBN	O7-C34-C35-C36
4	C	1206	LBN	O7-C34-C35-C36
5	D	1306	6OU	C38-C39-C40-C41
5	D	1308	6OU	C38-C39-C40-C41
5	D	1308	6OU	C40-C41-C42-C43
5	B	1207	6OU	C38-C39-C40-C41
5	B	1207	6OU	C40-C41-C42-C43
5	C	1208	6OU	C38-C39-C40-C41
5	D	1306	6OU	C37-C38-C39-C40
5	D	1308	6OU	C37-C38-C39-C40
5	B	1207	6OU	C37-C38-C39-C40
5	C	1208	6OU	C37-C38-C39-C40

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Mol	Chain	Res	Type	Atoms
4	D	1305	LBN	O5-C25-C26-C27
4	A	1206	LBN	O5-C25-C26-C27
4	C	1207	LBN	O5-C25-C26-C27
5	D	1307	6OU	C19-C20-C21-O22
5	A	1207	6OU	C19-C20-C21-O22
5	B	1208	6OU	C19-C20-C21-O22
5	C	1209	6OU	C19-C20-C21-O22
4	D	1304	LBN	O5-C25-C26-C27
4	A	1205	LBN	O5-C25-C26-C27
4	B	1205	LBN	O5-C25-C26-C27
4	B	1206	LBN	O5-C25-C26-C27
4	C	1206	LBN	O5-C25-C26-C27
4	B	1205	LBN	C2-C1-O1-P1
4	D	1304	LBN	O8-C34-C35-C36
4	A	1205	LBN	O8-C34-C35-C36
4	B	1205	LBN	O8-C34-C35-C36
4	C	1206	LBN	O8-C34-C35-C36
5	D	1309	6OU	C38-C39-C40-C41
5	A	1208	6OU	C38-C39-C40-C41
5	B	1209	6OU	C38-C39-C40-C41
5	C	1201	6OU	C38-C39-C40-C41
4	D	1304	LBN	C2-C1-O1-P1
4	A	1205	LBN	C2-C1-O1-P1
4	C	1206	LBN	C2-C1-O1-P1
4	D	1305	LBN	O6-C25-C26-C27
4	A	1205	LBN	O6-C25-C26-C27
4	A	1206	LBN	O6-C25-C26-C27
4	B	1205	LBN	O6-C25-C26-C27
4	B	1206	LBN	O6-C25-C26-C27
4	D	1304	LBN	O6-C25-C26-C27
4	C	1206	LBN	O6-C25-C26-C27
4	C	1207	LBN	O6-C25-C26-C27
5	D	1310	6OU	C21-C20-O30-C31
5	A	1201	6OU	C21-C20-O30-C31
5	B	1201	6OU	C21-C20-O30-C31
5	C	1202	6OU	C21-C20-O30-C31

There are no ring outliers.

13 monomers are involved in 37 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	B	1206	LBN	7	0

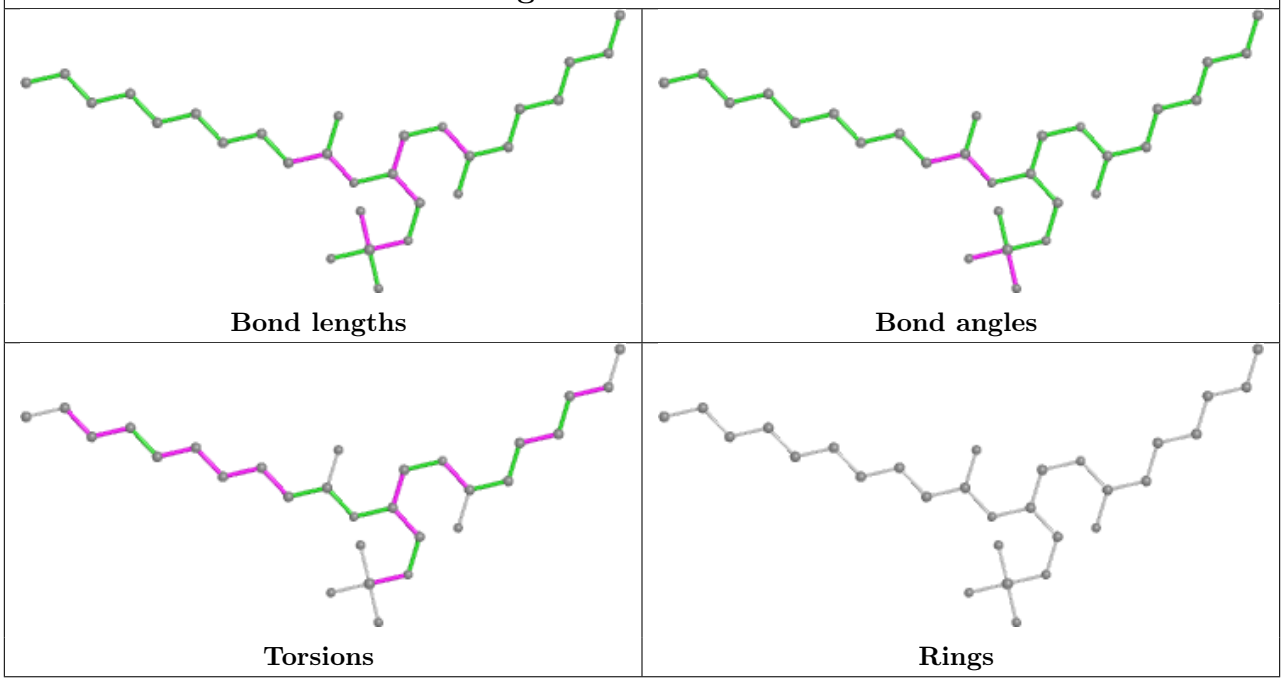
Continued on next page...

Continued from previous page...

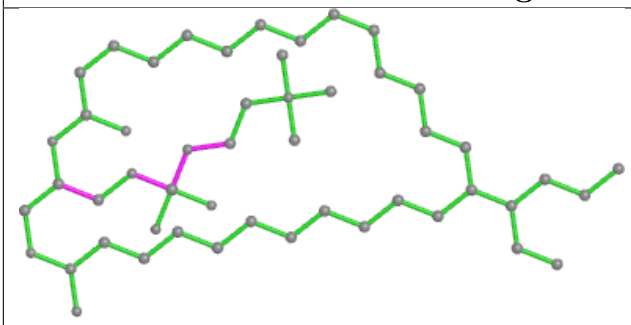
Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	D	1305	LBN	7	0
5	A	1207	6OU	1	0
5	D	1308	6OU	1	0
5	C	1202	6OU	2	0
4	A	1206	LBN	7	0
4	C	1207	LBN	7	0
5	B	1201	6OU	2	0
5	D	1310	6OU	3	0
5	A	1201	6OU	2	0
5	B	1208	6OU	1	0
5	C	1209	6OU	1	0
5	D	1307	6OU	1	0

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.

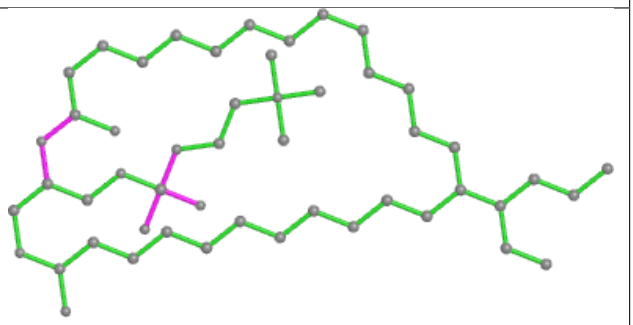
Ligand 6OU C 1201



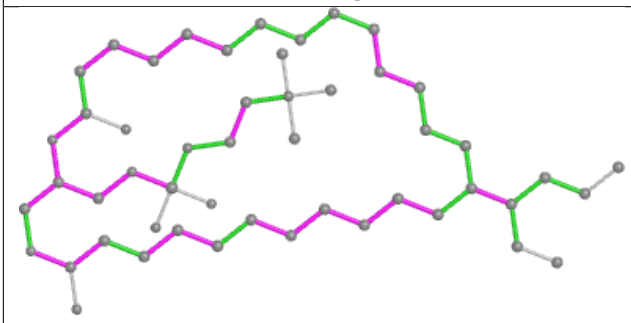
Ligand LBN B 1206



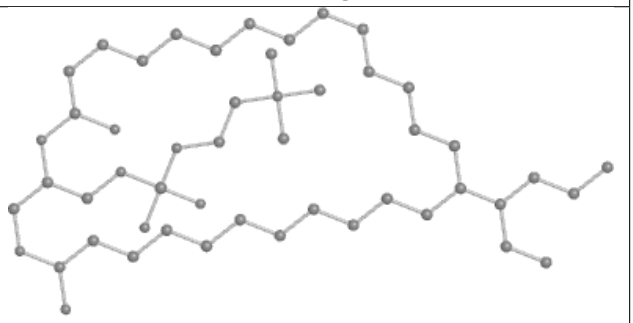
Bond lengths



Bond angles

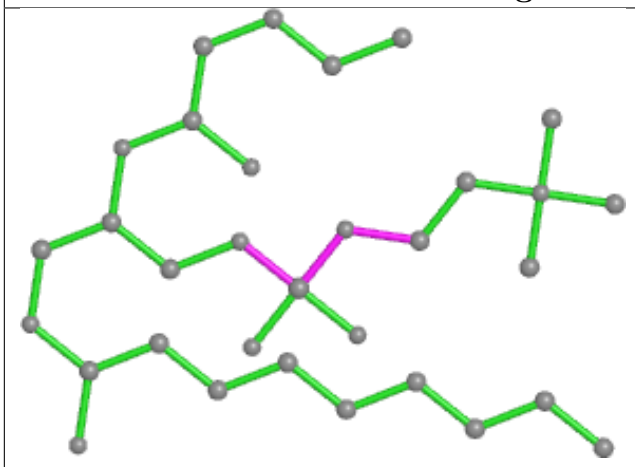


Torsions

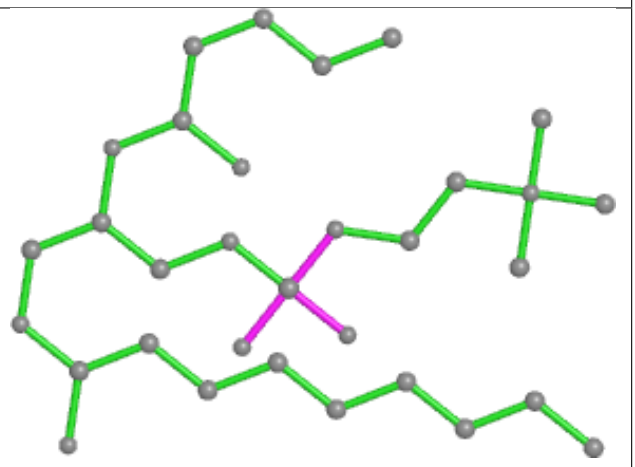


Rings

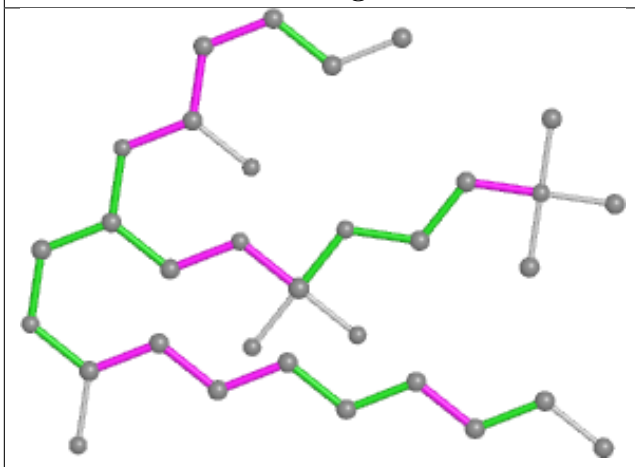
Ligand LBN D 1304



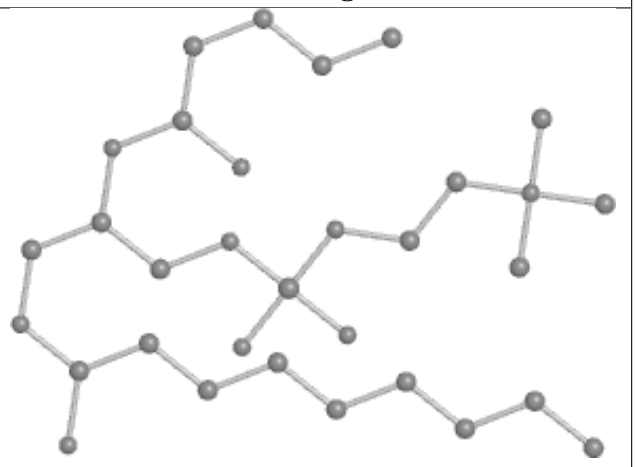
Bond lengths



Bond angles

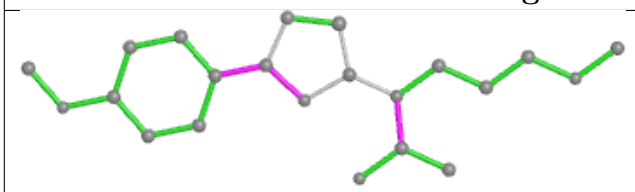


Torsions

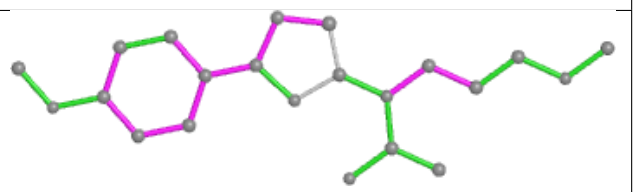


Rings

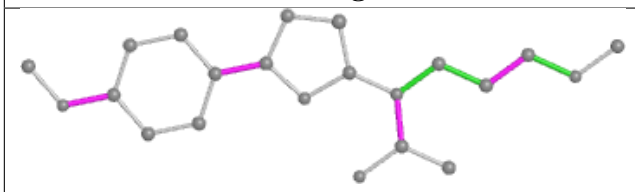
Ligand JT0 D 1303



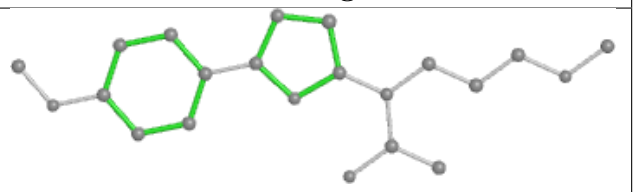
Bond lengths



Bond angles

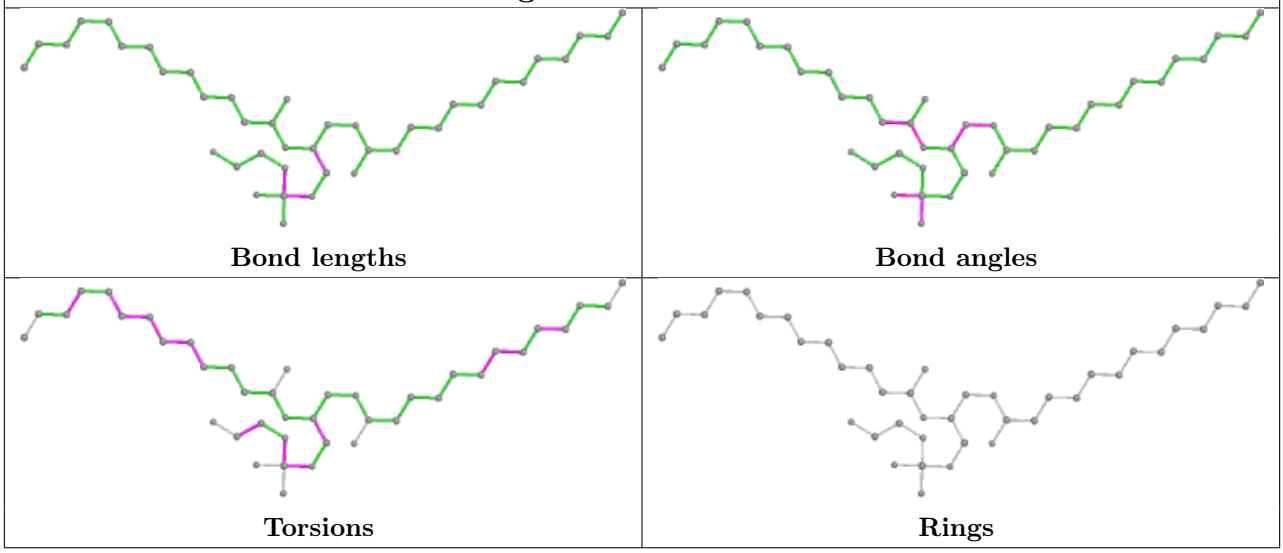


Torsions



Rings

Ligand 6OU B 1207



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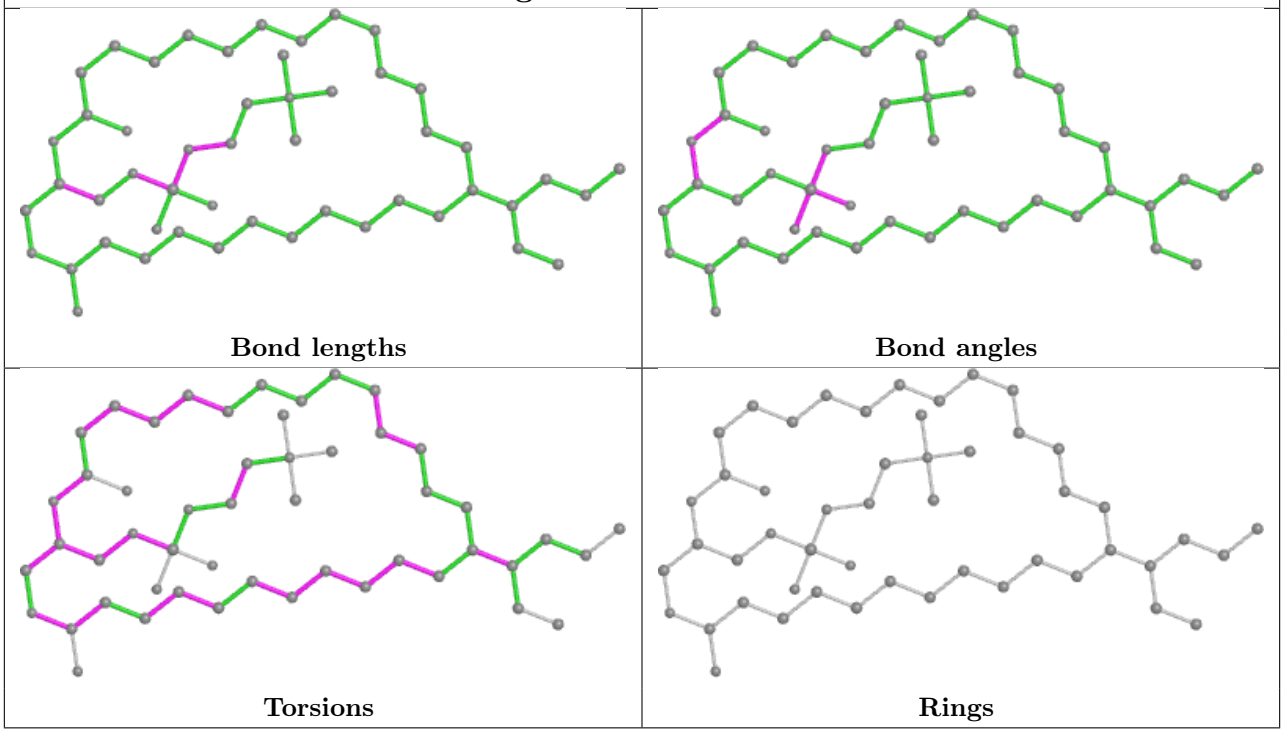
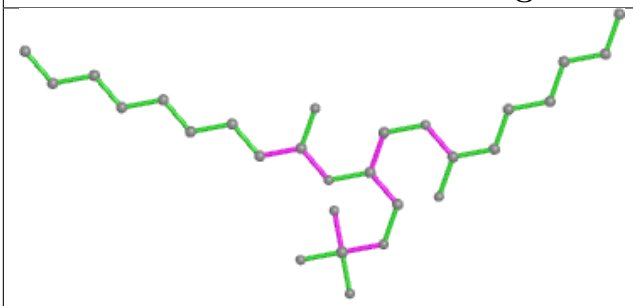


Ligand 6OU A 1207



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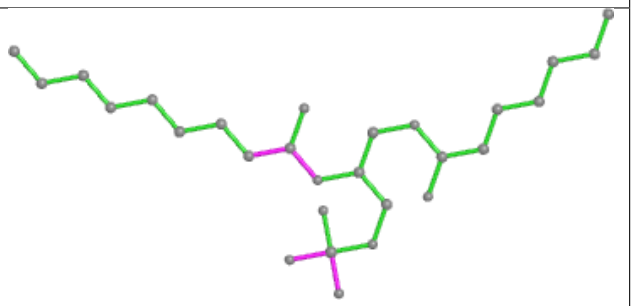

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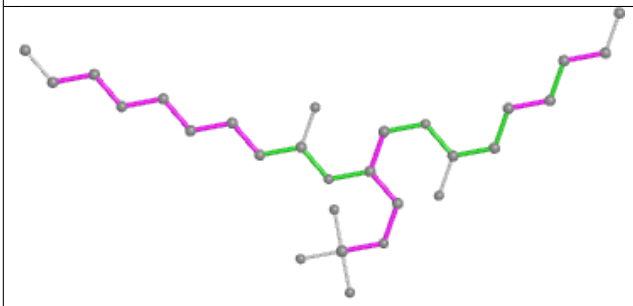

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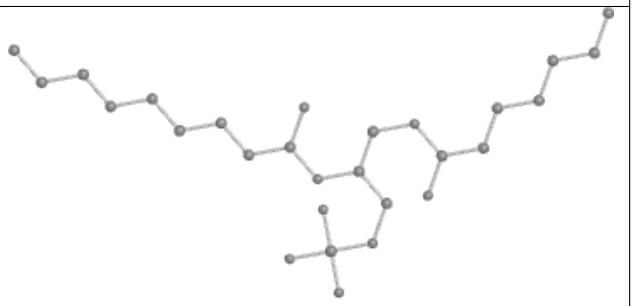
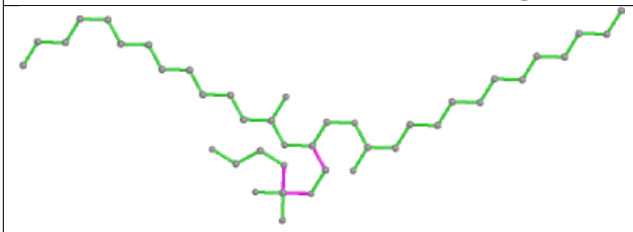


Rings

Ligand 6OU D 1308



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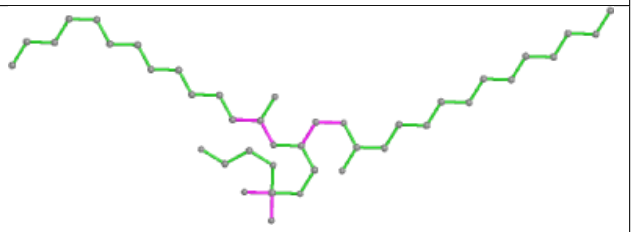

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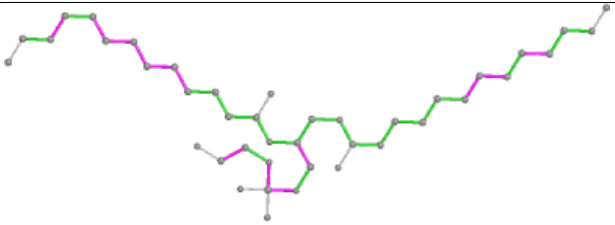

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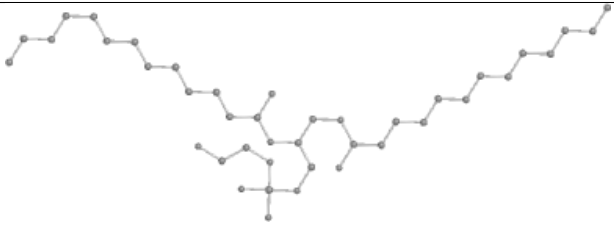
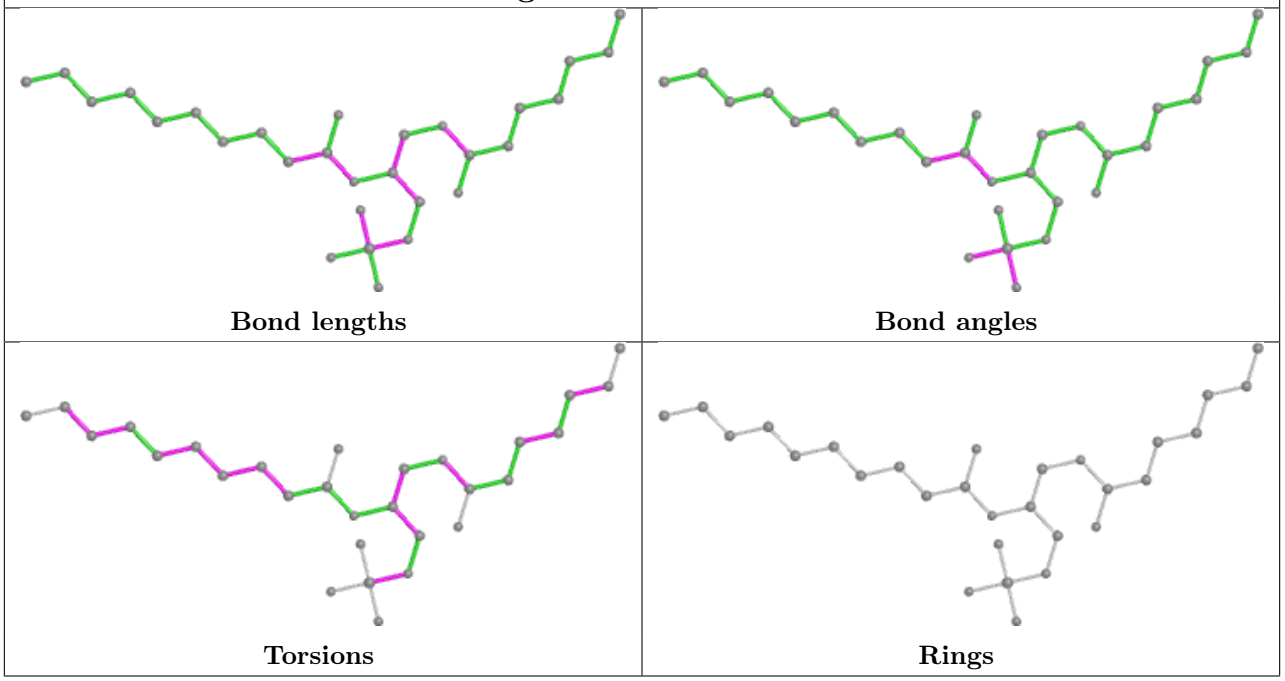
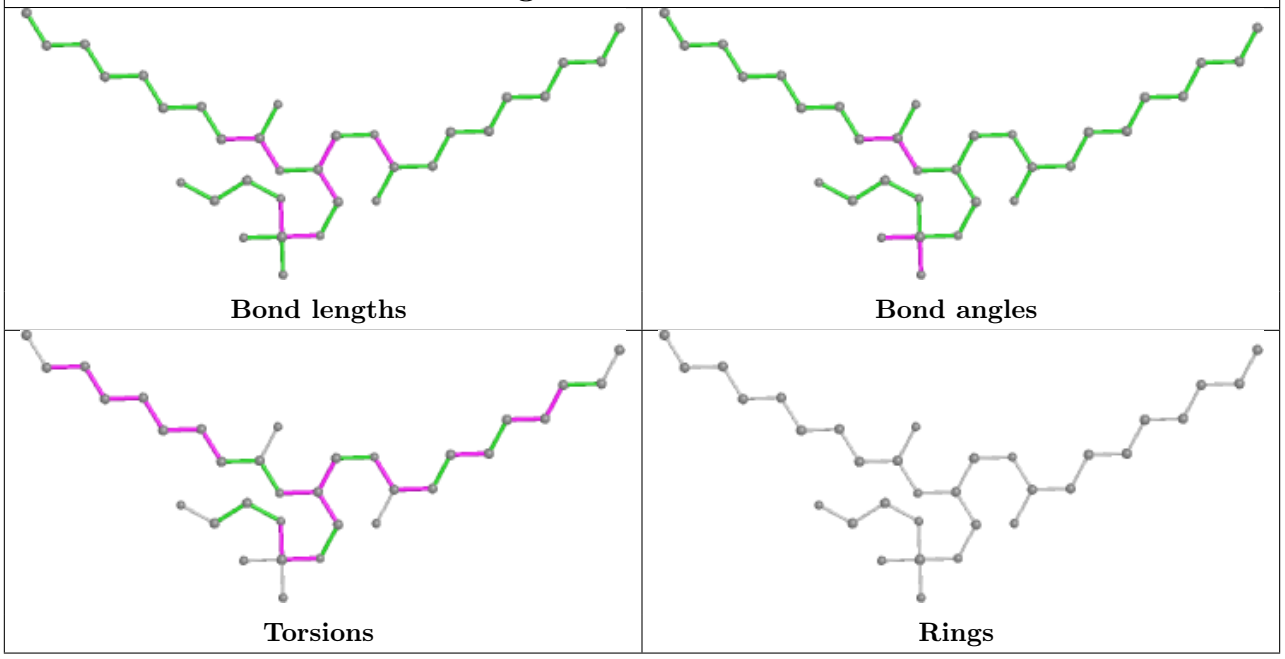


Rings

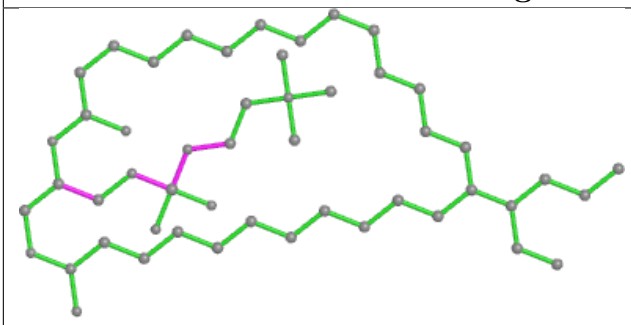
Ligand 6OU B 1209



Ligand 6OU C 1202



Ligand LBN A 1206



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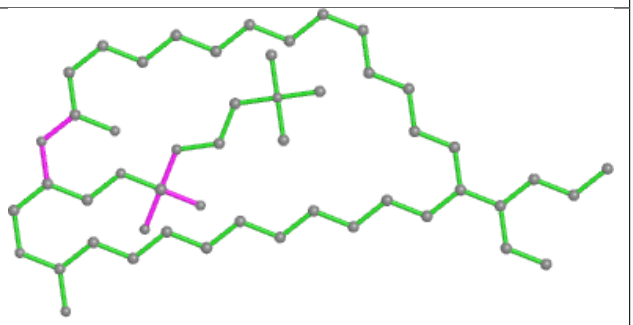
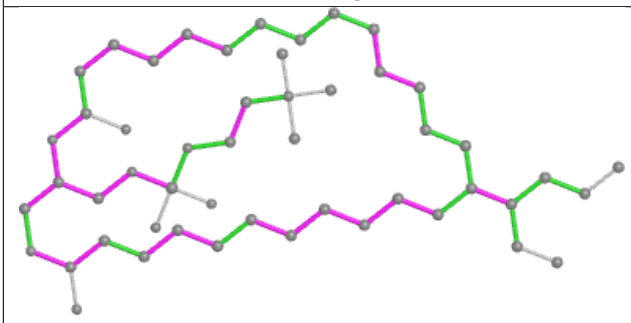


Bond angles



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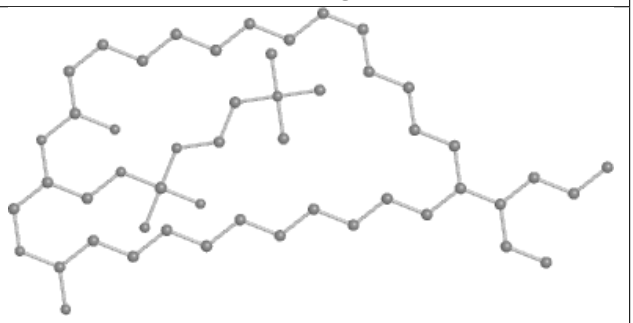
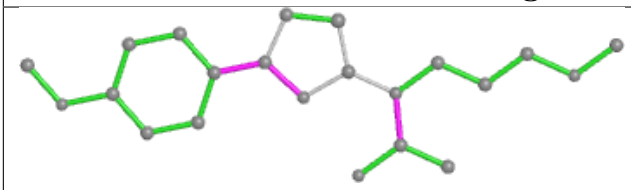


Rings

Ligand JT0 B 1204



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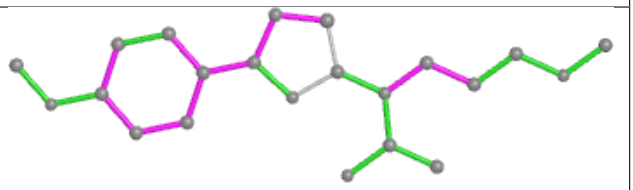

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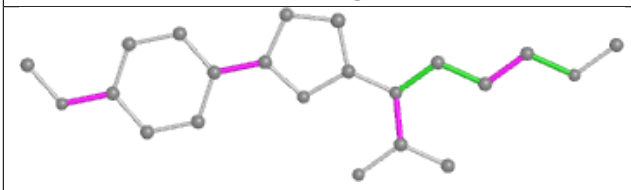

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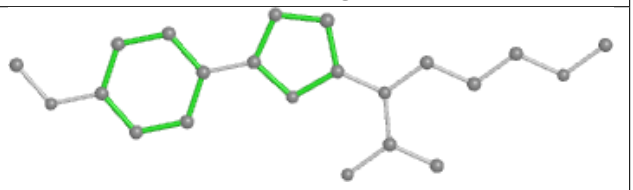
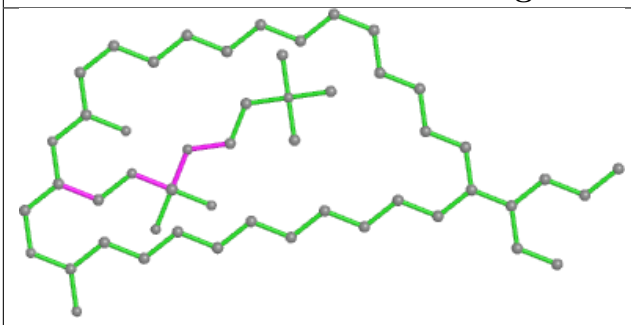
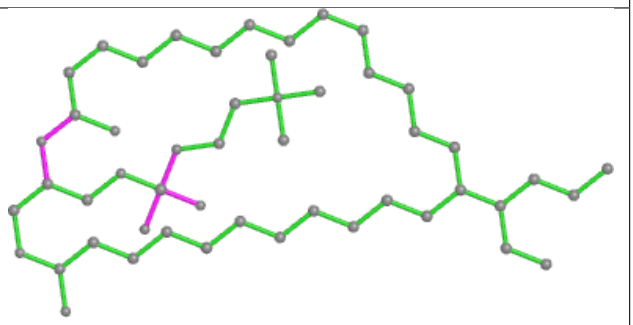


Rings

Ligand LBN C 1207



Bond lengths



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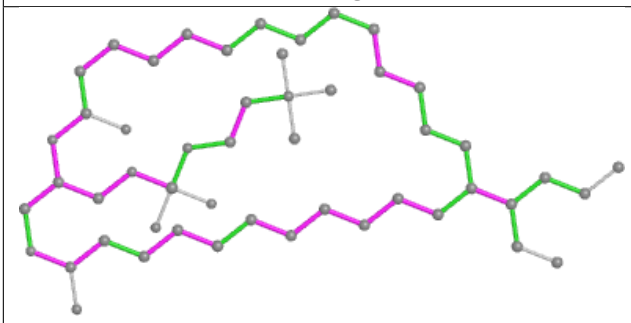

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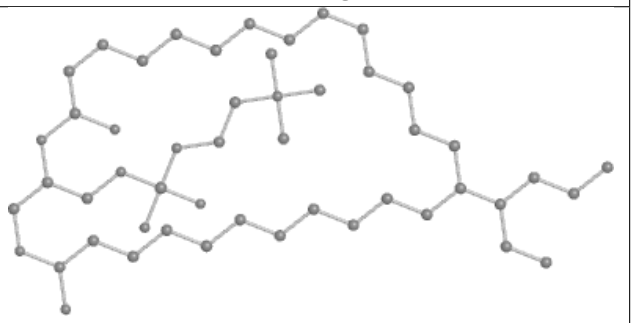
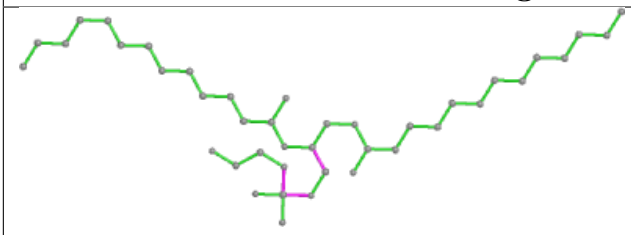


Rings

Ligand 6OU D 1306



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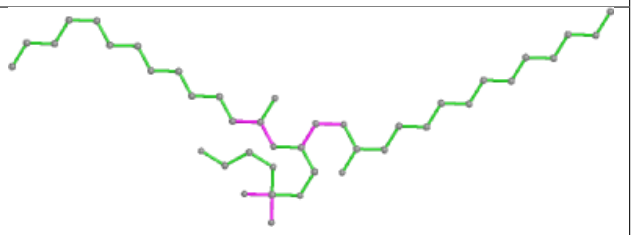
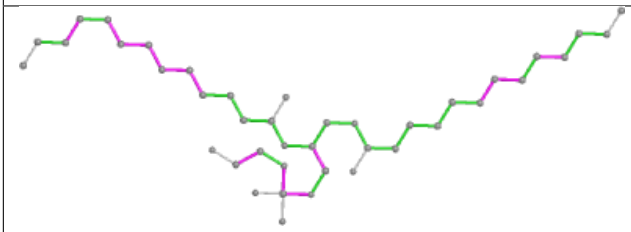
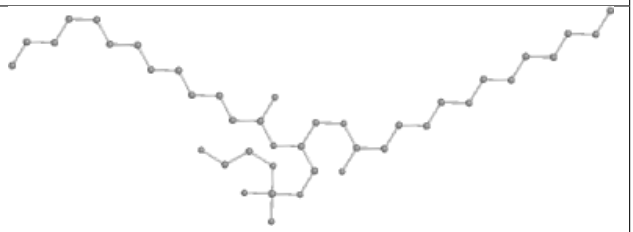


Bond angles

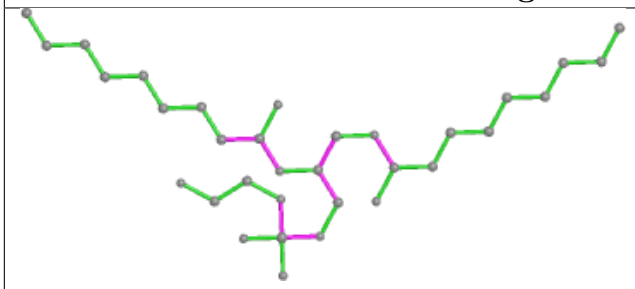


Torsions



Rings

Ligand 6OU B 1201



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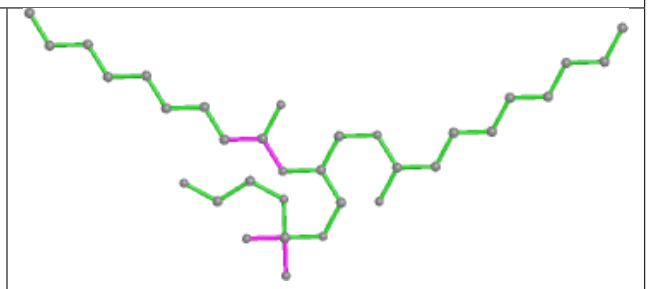
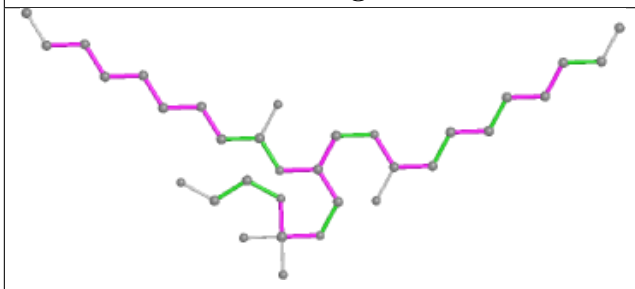
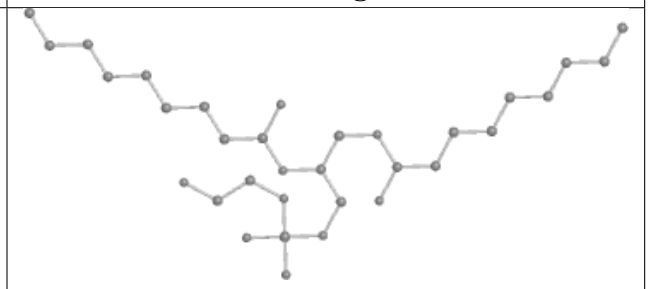


Bond angles

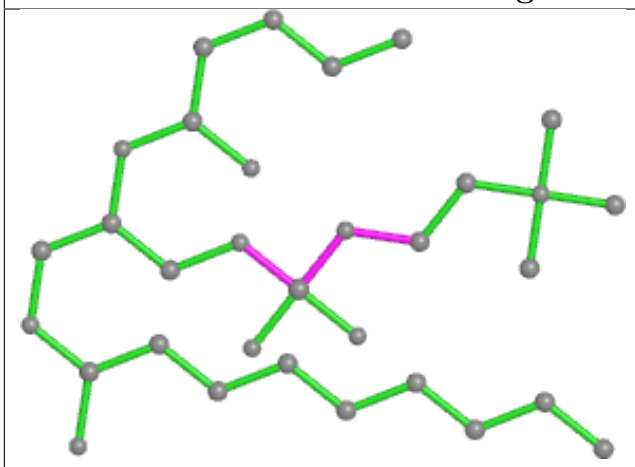


Torsions

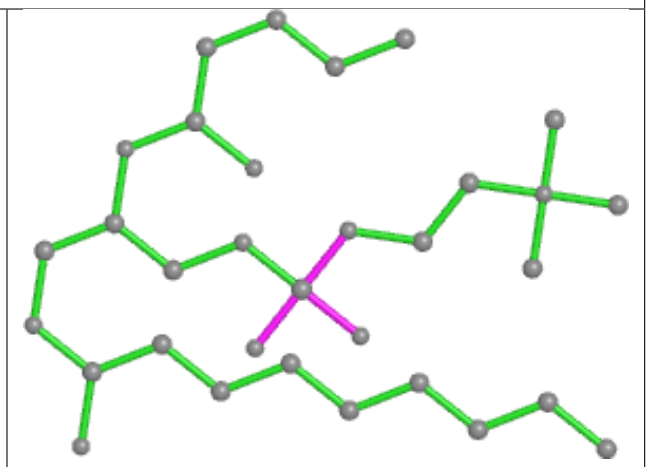


Rings

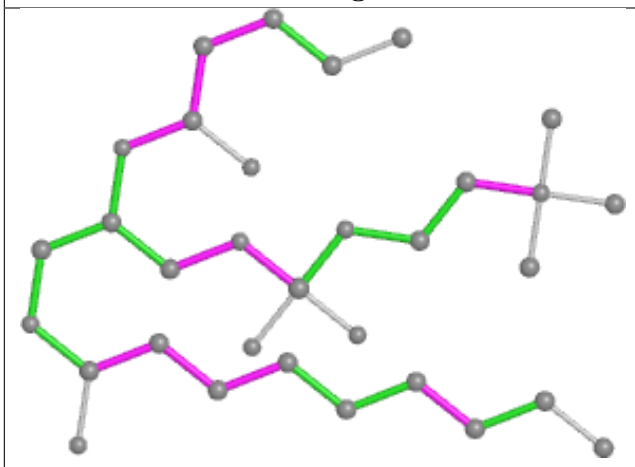
Ligand LBN B 1205



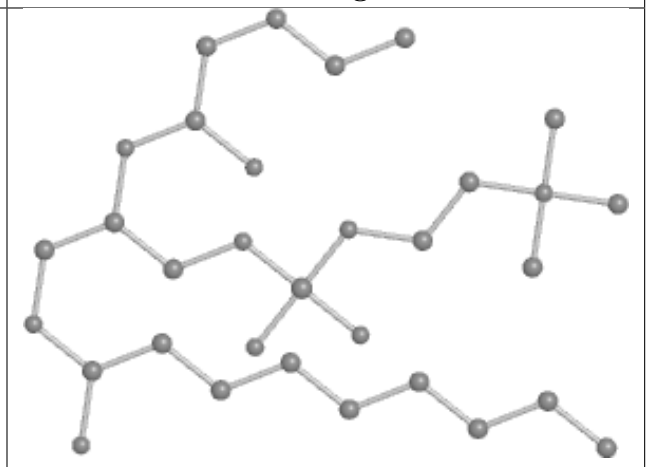
Bond lengths



Bond angles

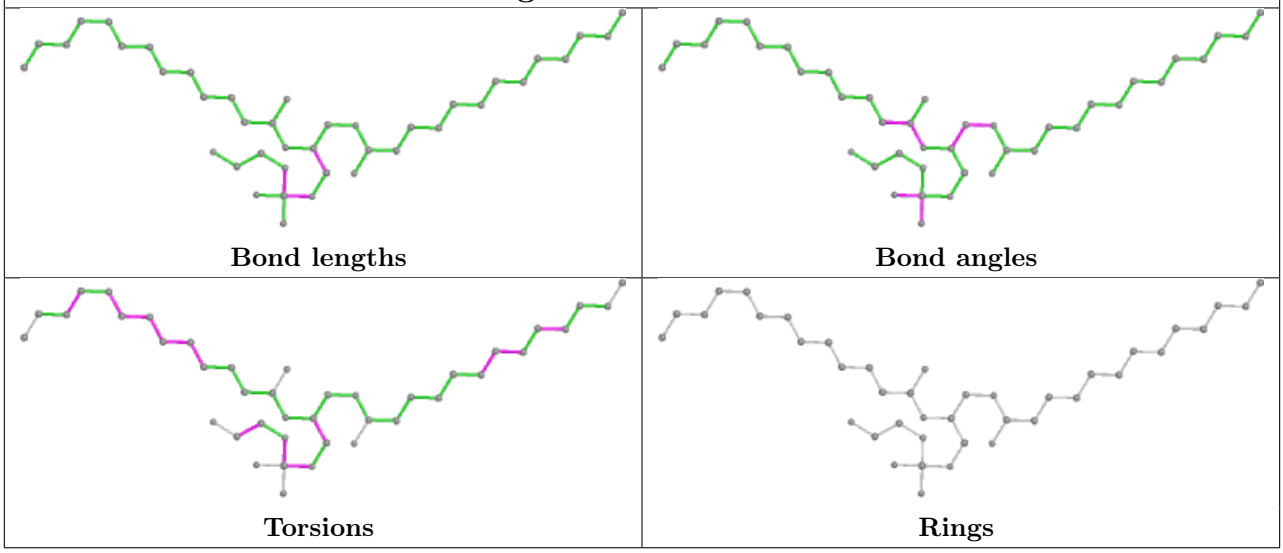


Torsions

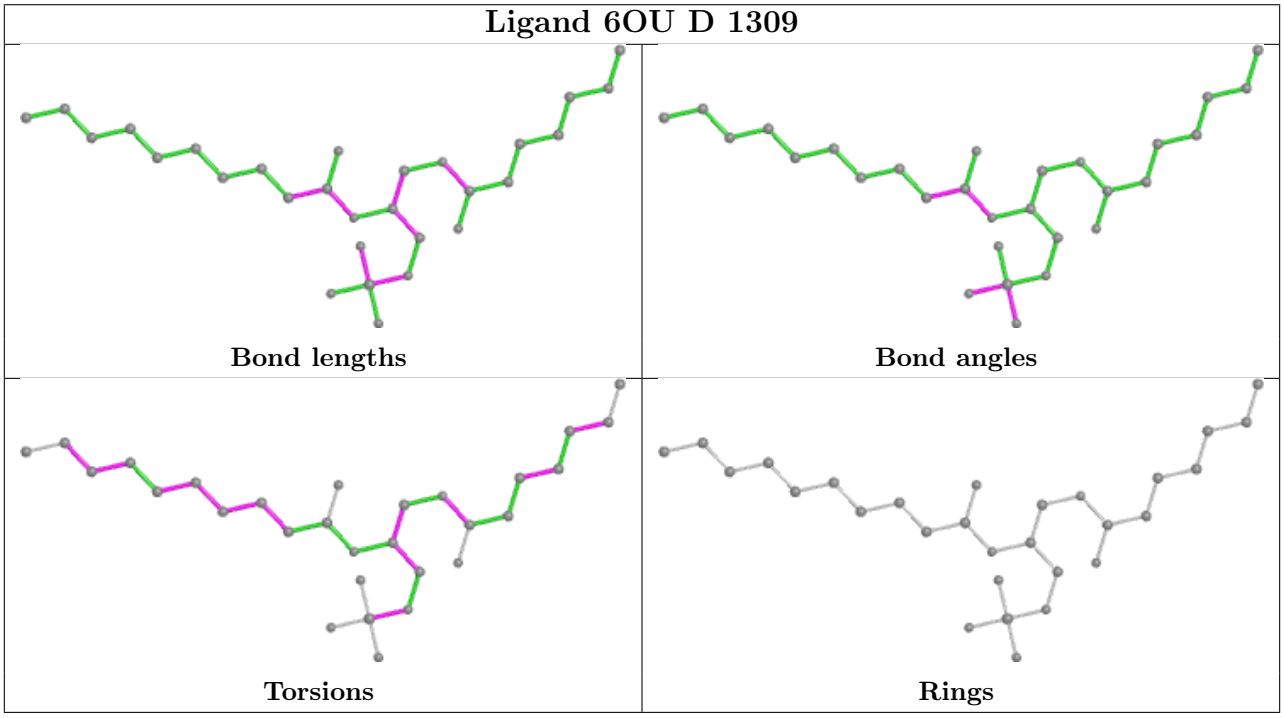


Rings

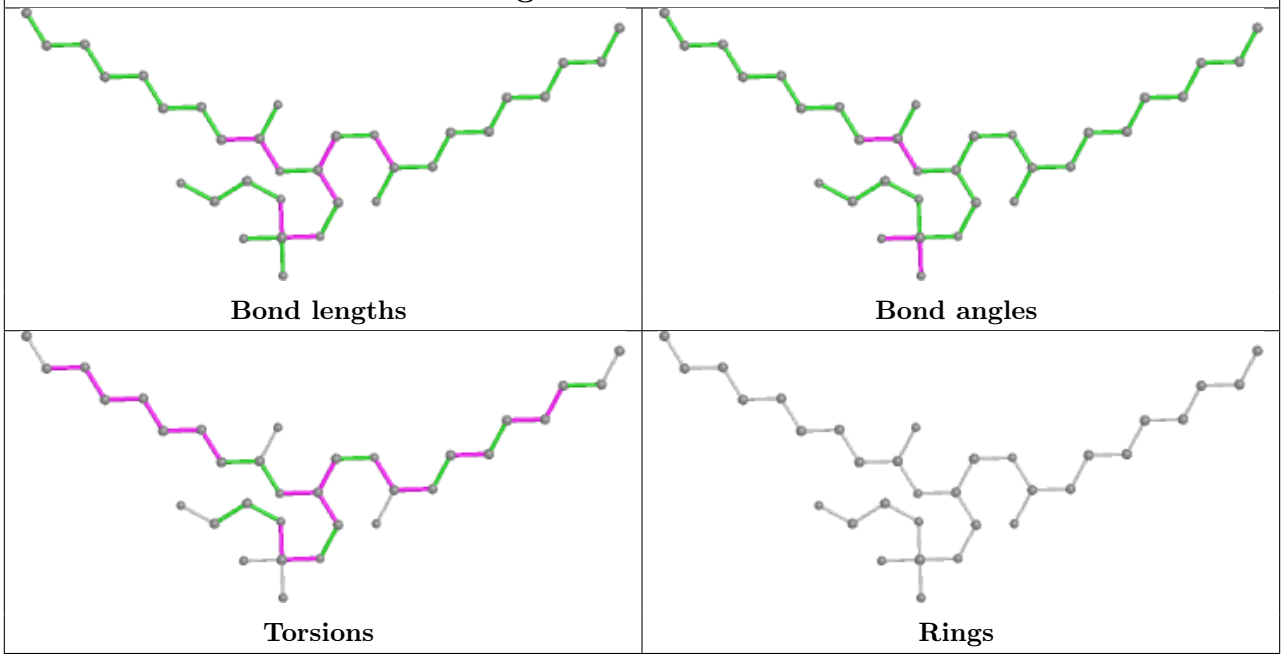
Ligand 6OU C 1208



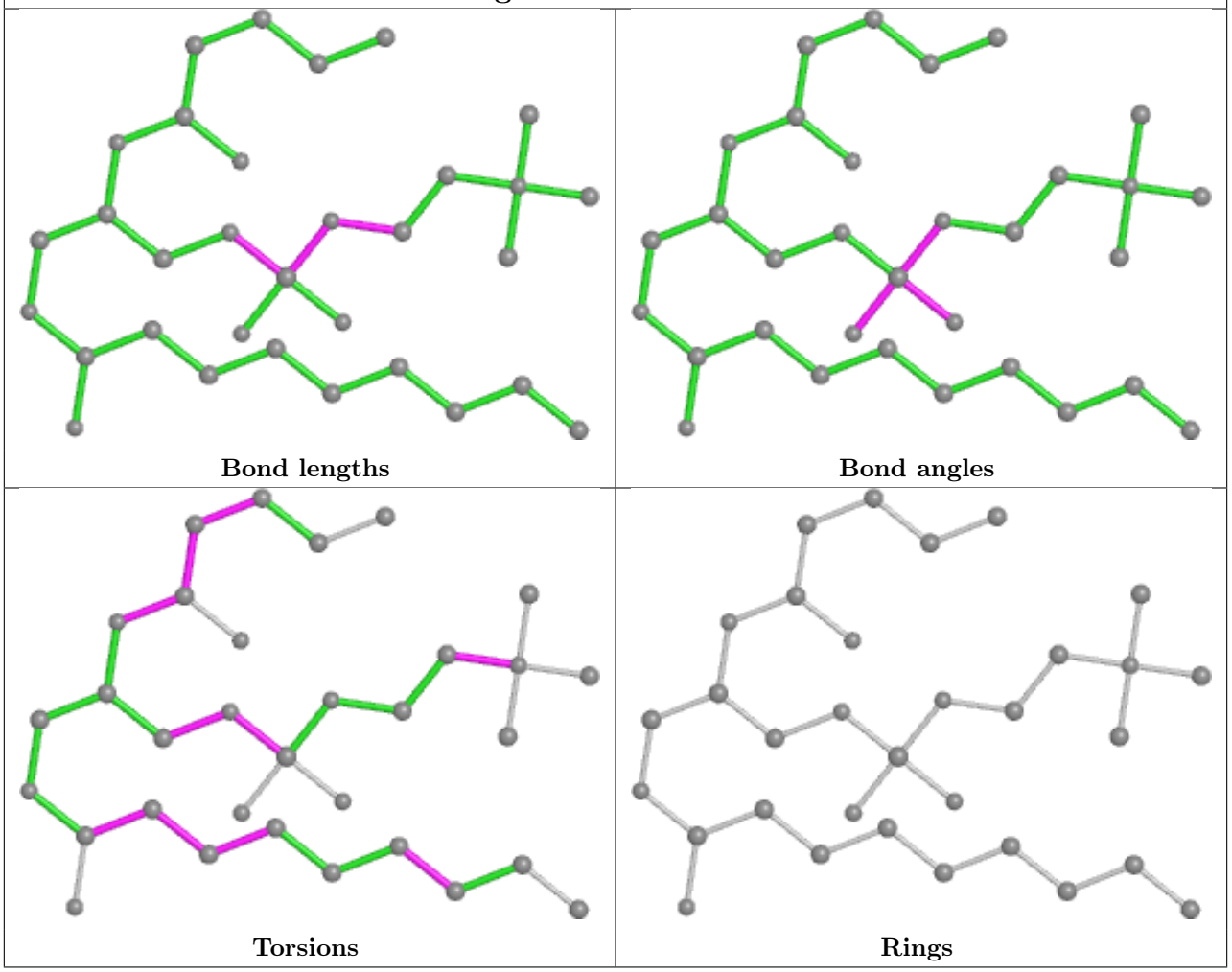
Ligand 6OU D 1309



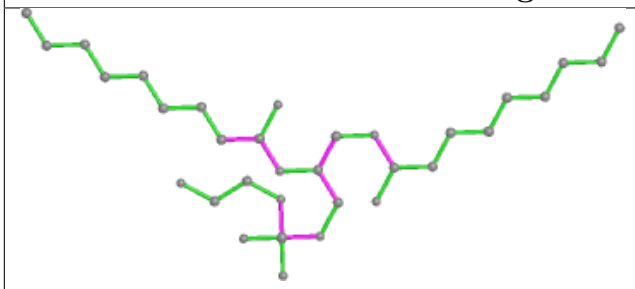
Ligand 6OU D 1310



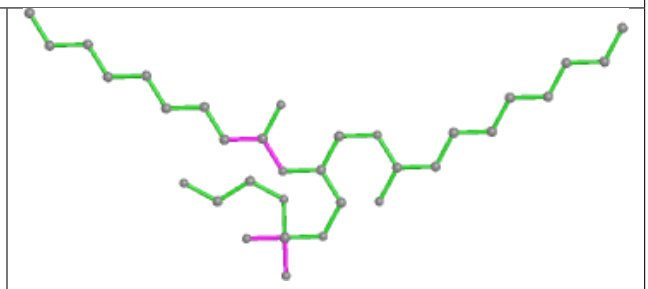
Ligand LBN C 1206



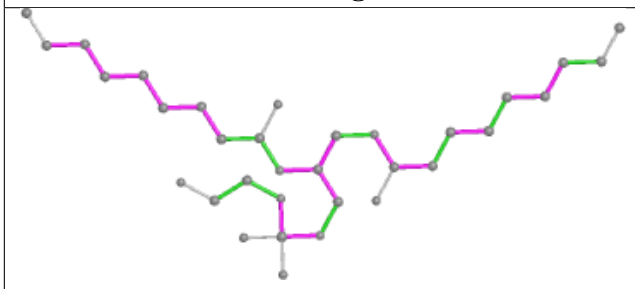
Ligand 6OU A 1201



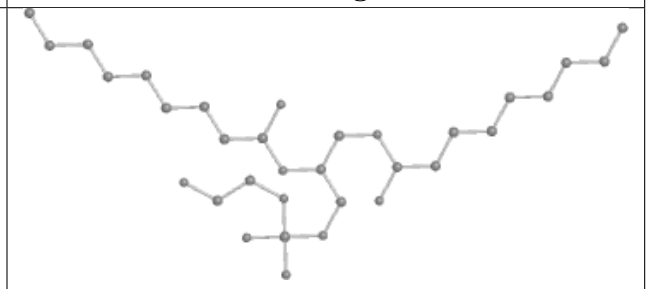
Bond lengths



Bond angles

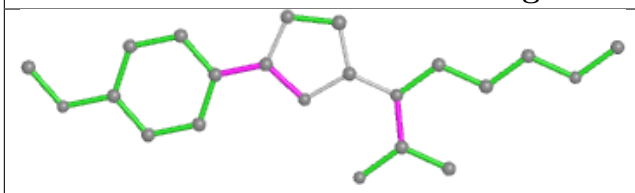


Torsions

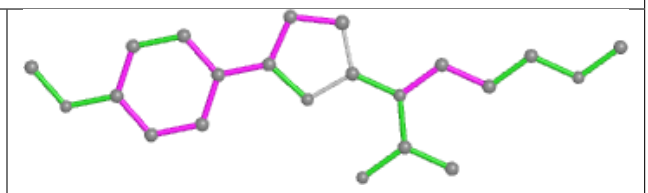


Rings

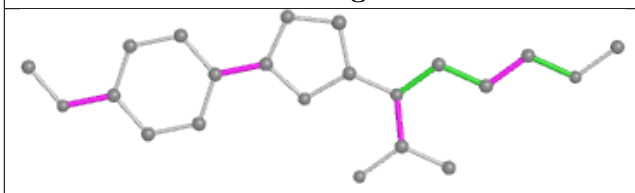
Ligand JT0 A 1204



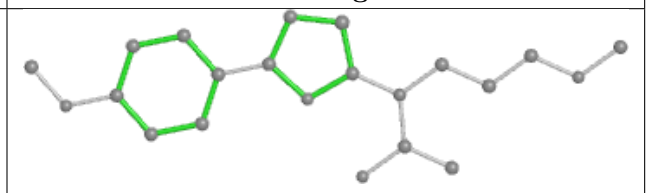
Bond lengths



Bond angles

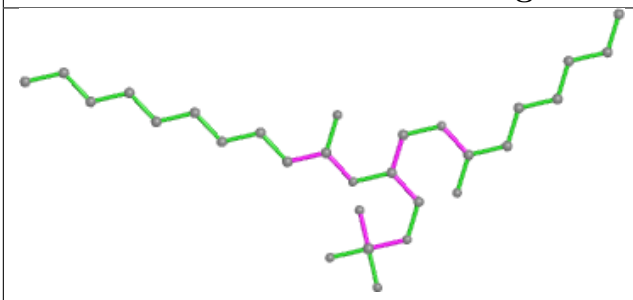


Torsions

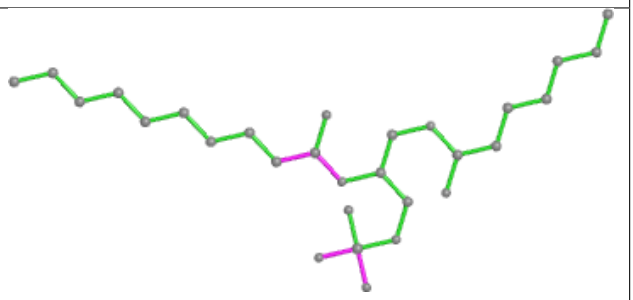


Rings

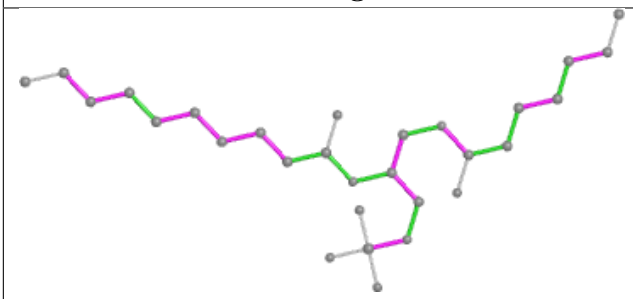
Ligand 6OU A 1208



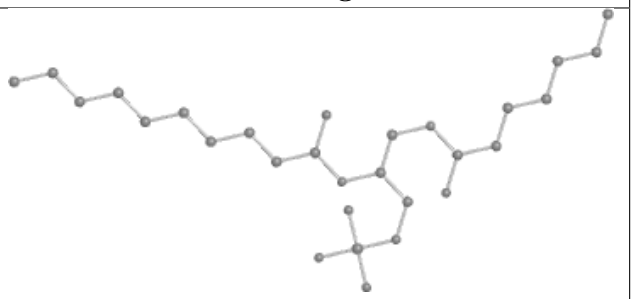
Bond lengths



Bond angles

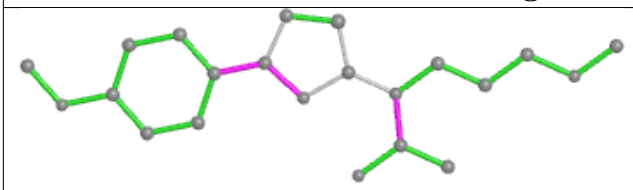


Torsions

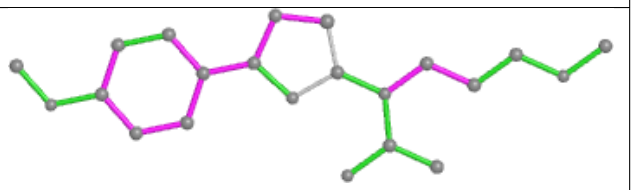


Rings

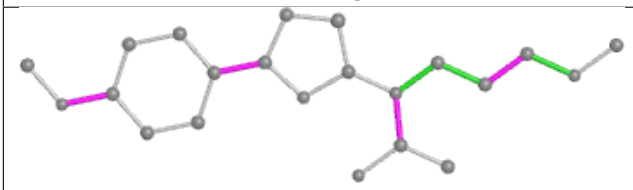
Ligand JT0 C 1205



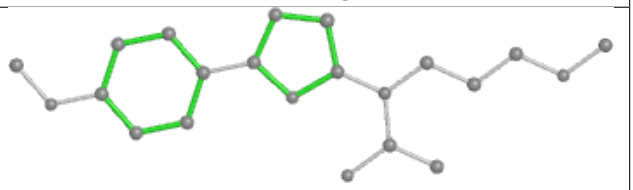
Bond lengths



Bond angles

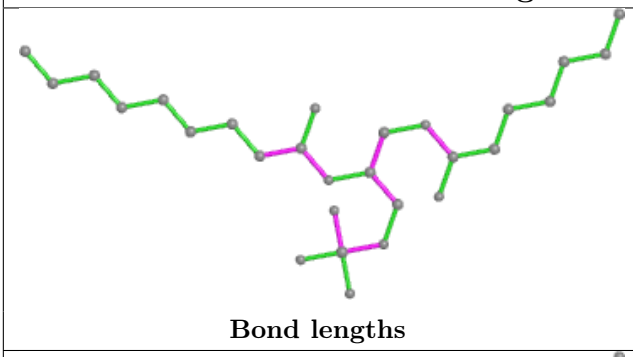


Torsions

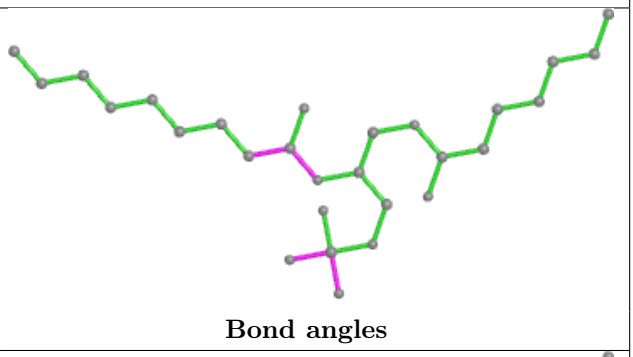


Rings

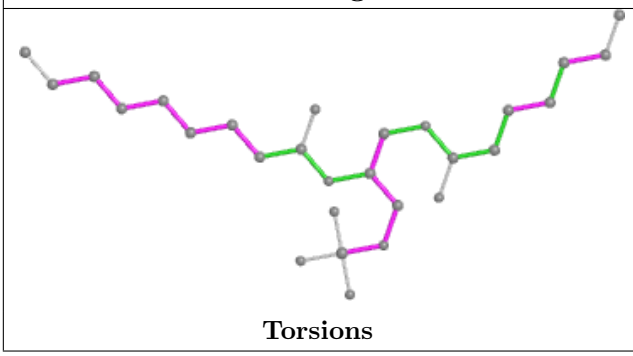
Ligand 6OU B 1208



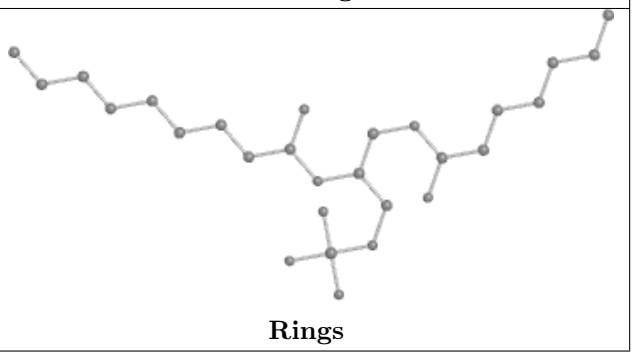
Bond lengths



Bond angles

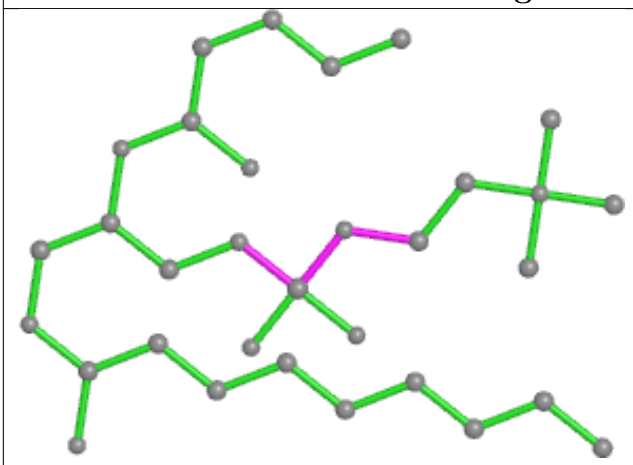


Torsions

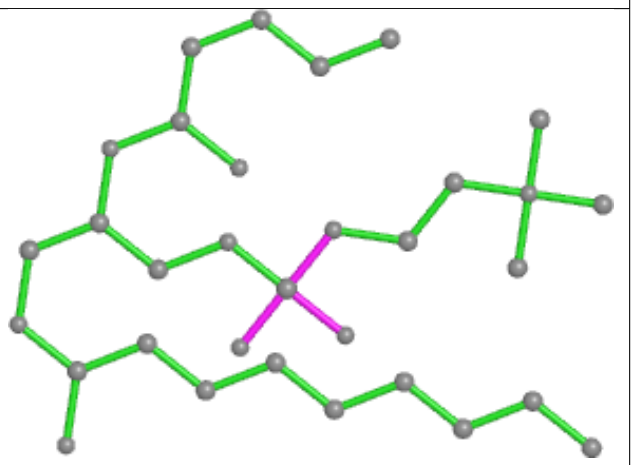


Rings

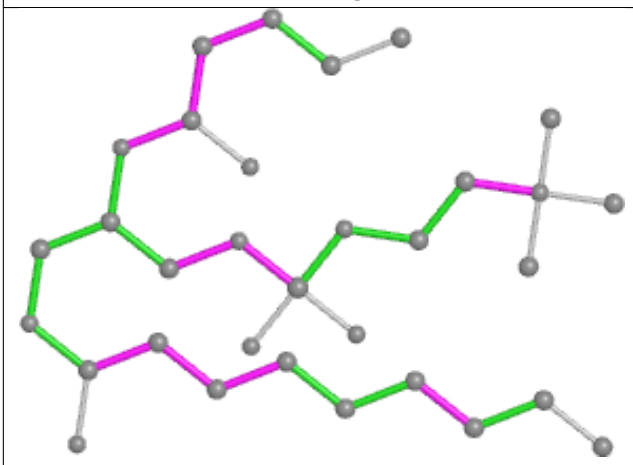
Ligand LBN A 1205



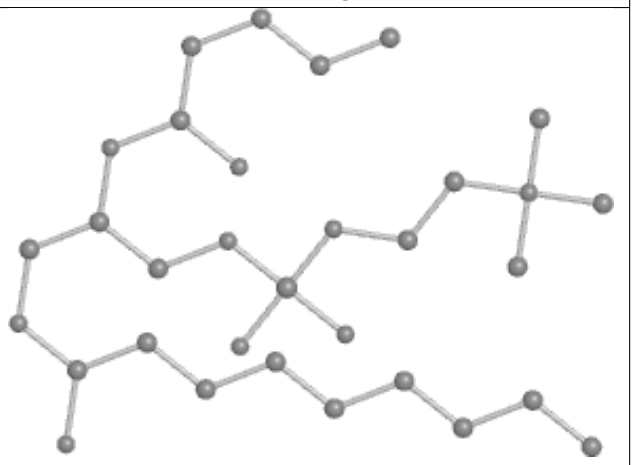
Bond lengths



Bond angles

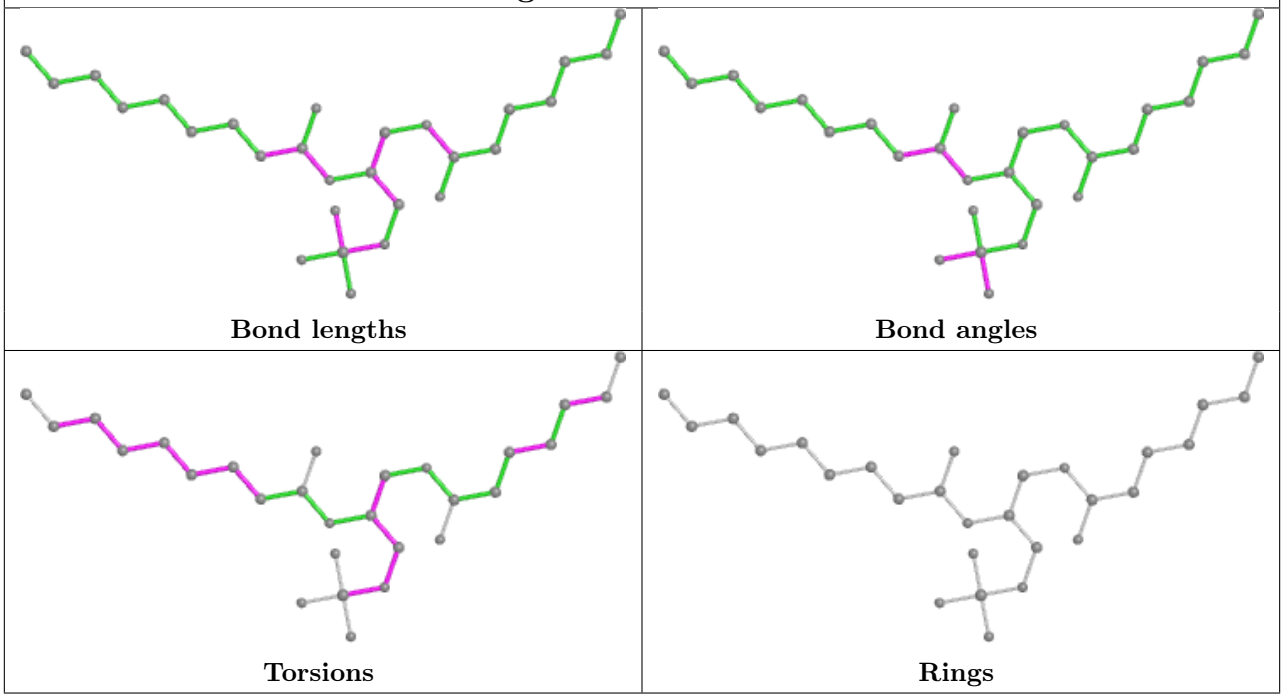


Torsions

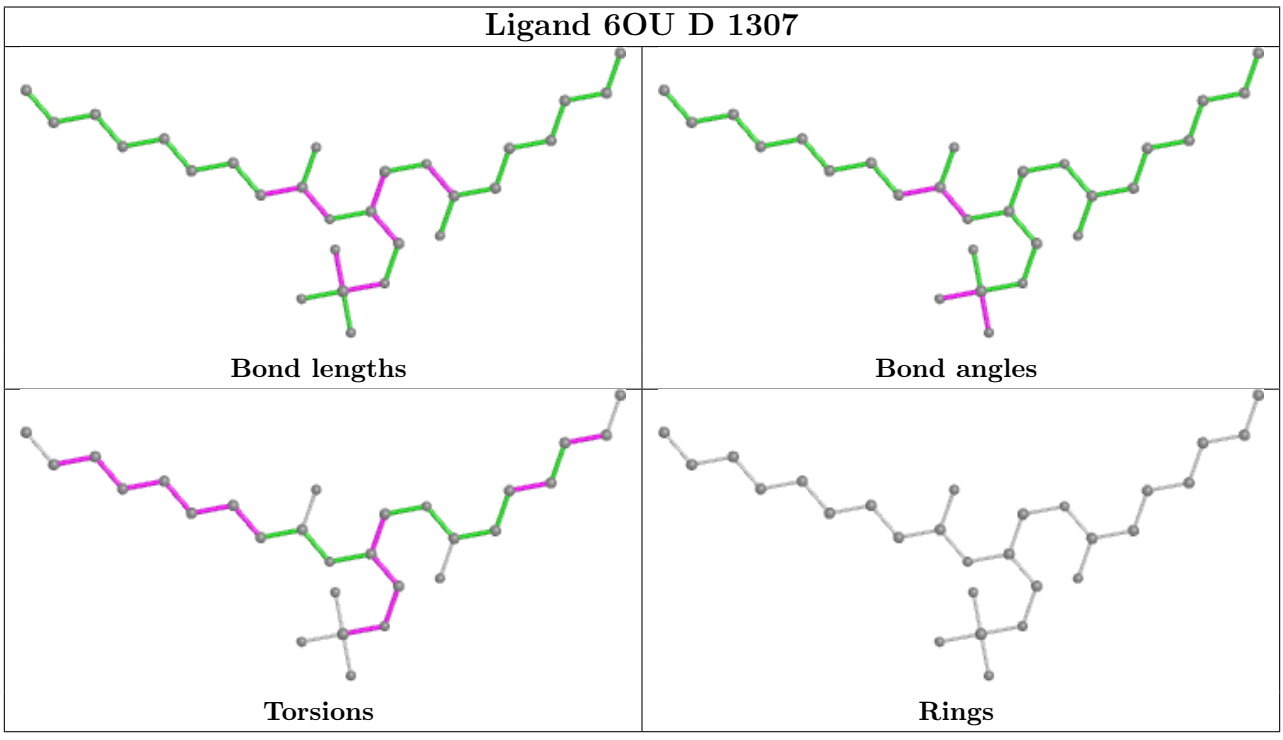


Rings

Ligand 6OU C 1209



Ligand 6OU D 1307



5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

6 Map visualisation

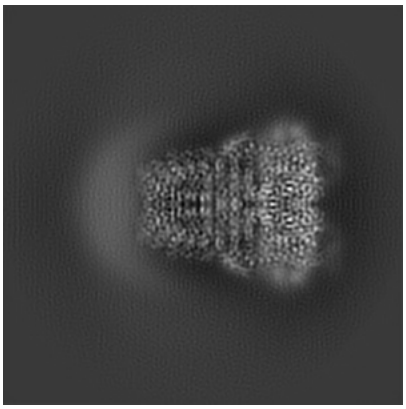
This section contains visualisations of the EMDB entry EMD-20449. These allow visual inspection of the internal detail of the map and identification of artifacts.

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.

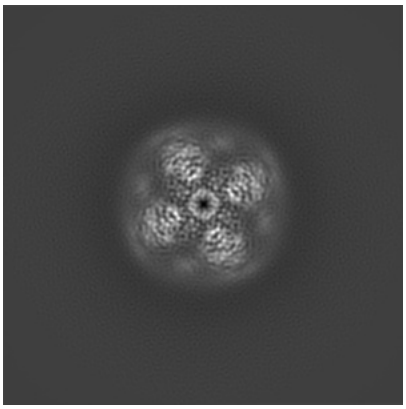
6.1 Orthogonal projections

6.1.1 Primary map

X

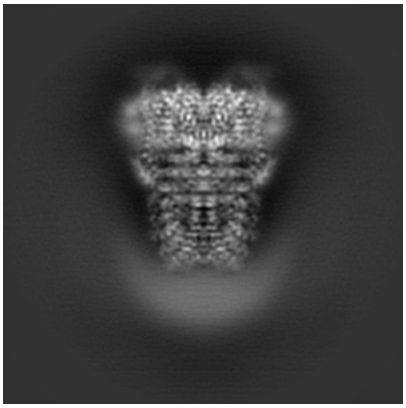


Y

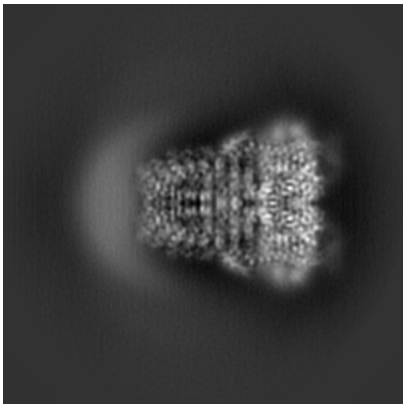


Z

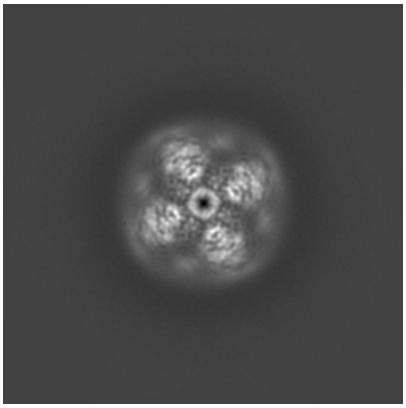
6.1.2 Raw map



X



Y

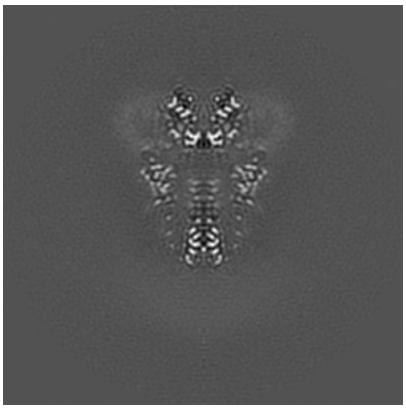


Z

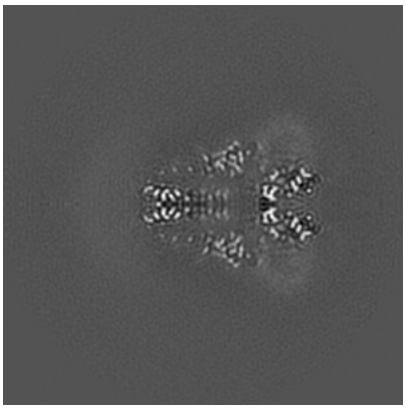
The images above show the map projected in three orthogonal directions.

6.2 Central slices (i)

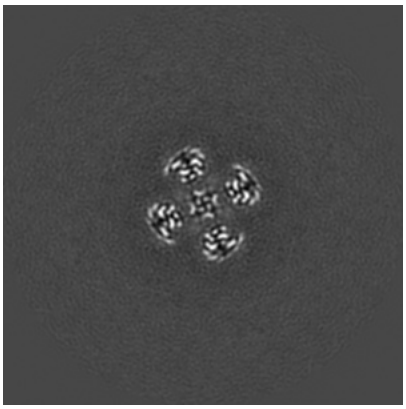
6.2.1 Primary map



X Index: 128

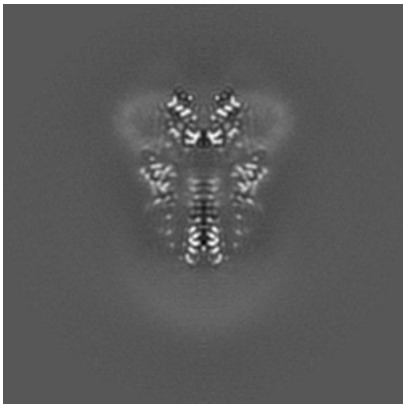


Y Index: 128

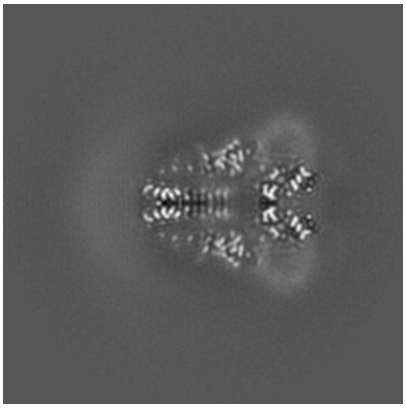


Z Index: 128

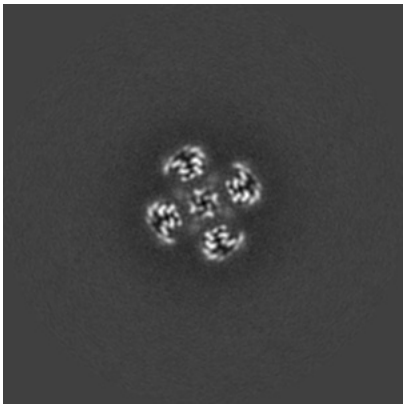
6.2.2 Raw map



X Index: 128



Y Index: 128

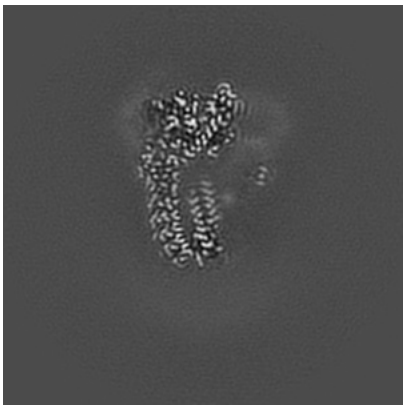


Z Index: 128

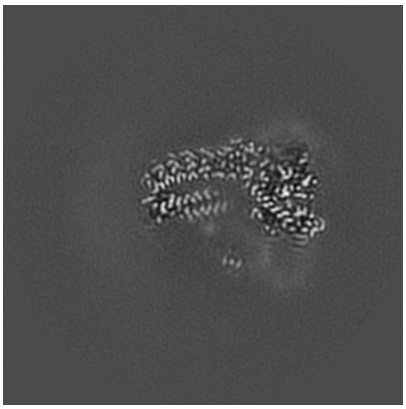
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

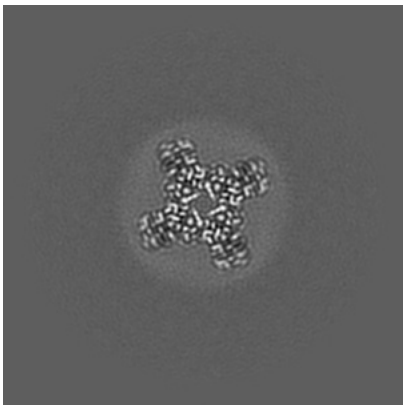
6.3.1 Primary map



X Index: 134

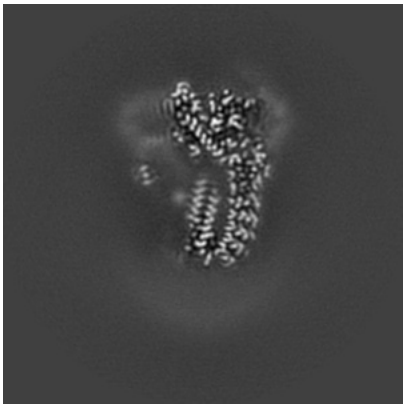


Y Index: 134

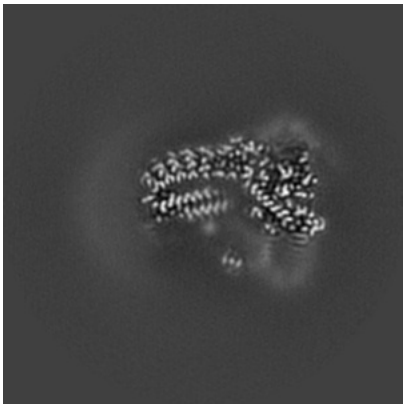


Z Index: 192

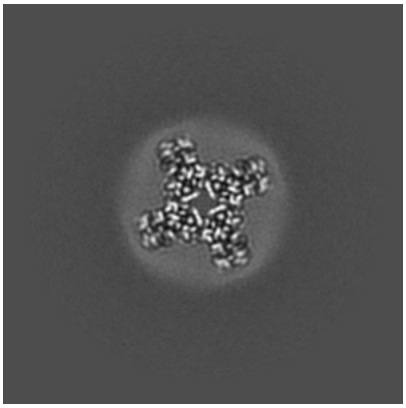
6.3.2 Raw map



X Index: 122



Y Index: 134

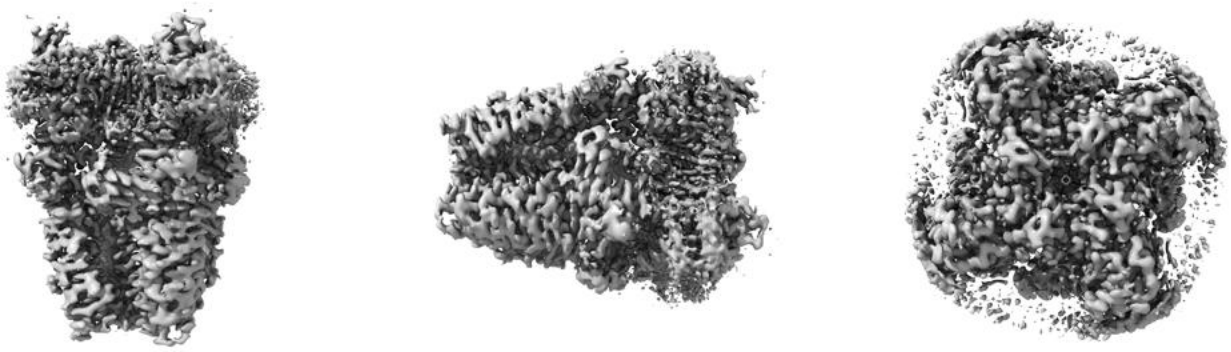


Z Index: 192

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

6.4 Orthogonal surface views (i)

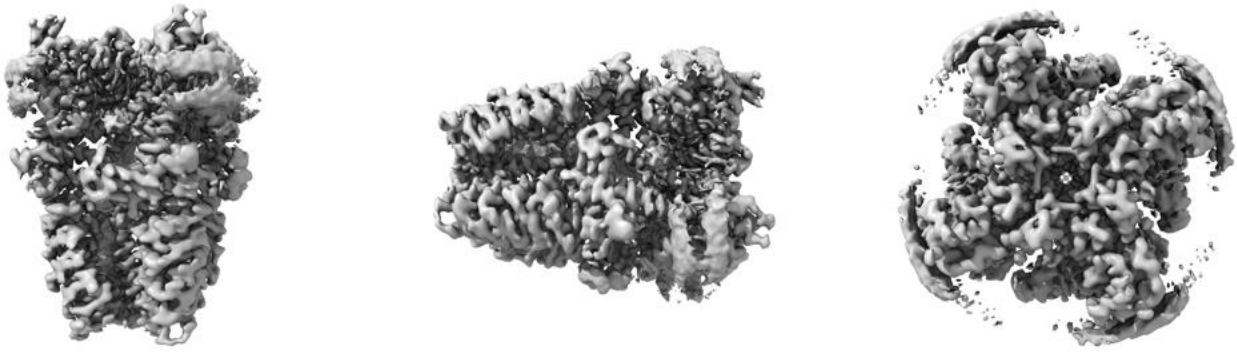
6.4.1 Primary map



X Y Z

The images above show the 3D surface view of the map at the recommended contour level 0.025. 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.

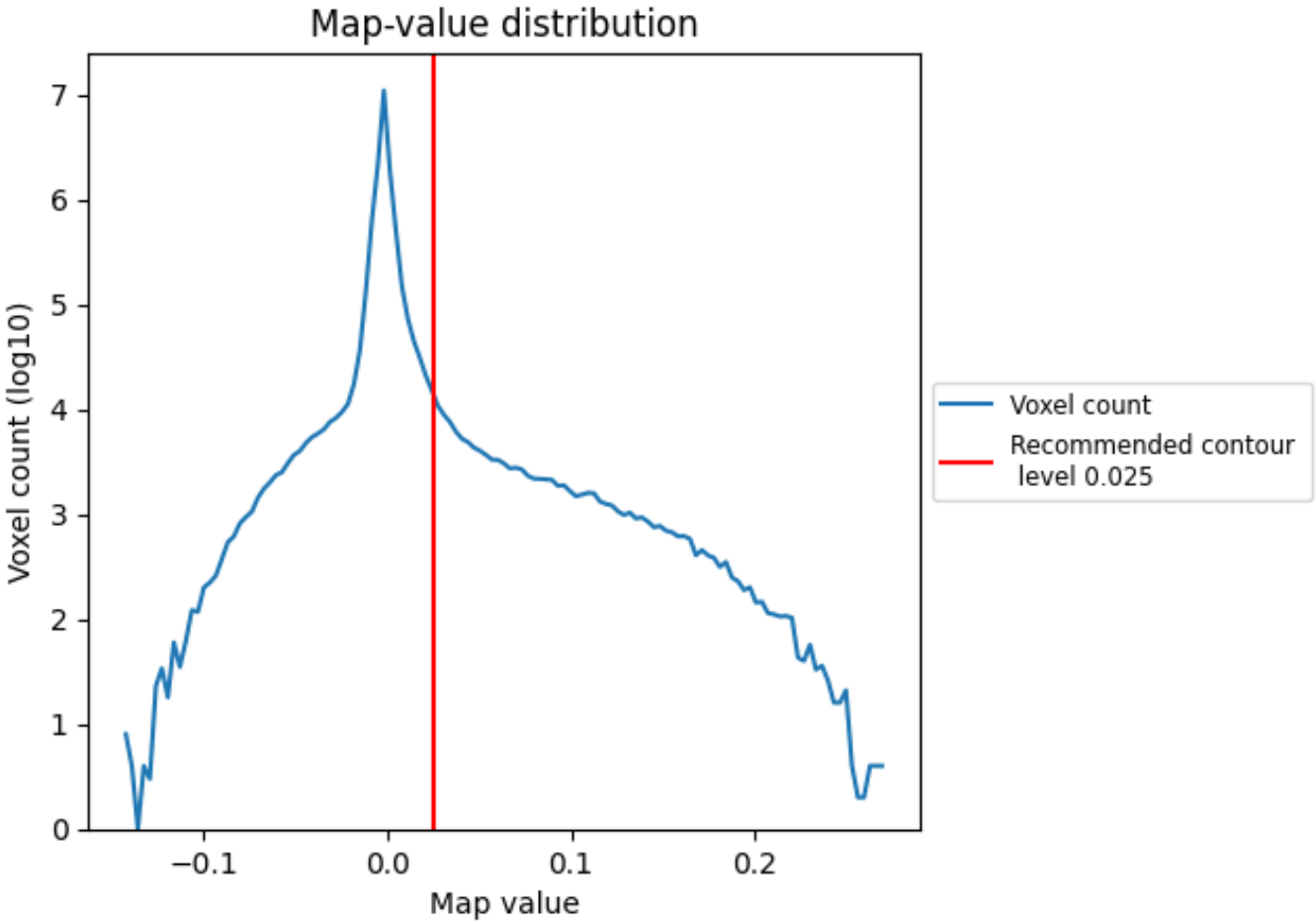
6.5 Mask visualisation (i)

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

7 Map analysis

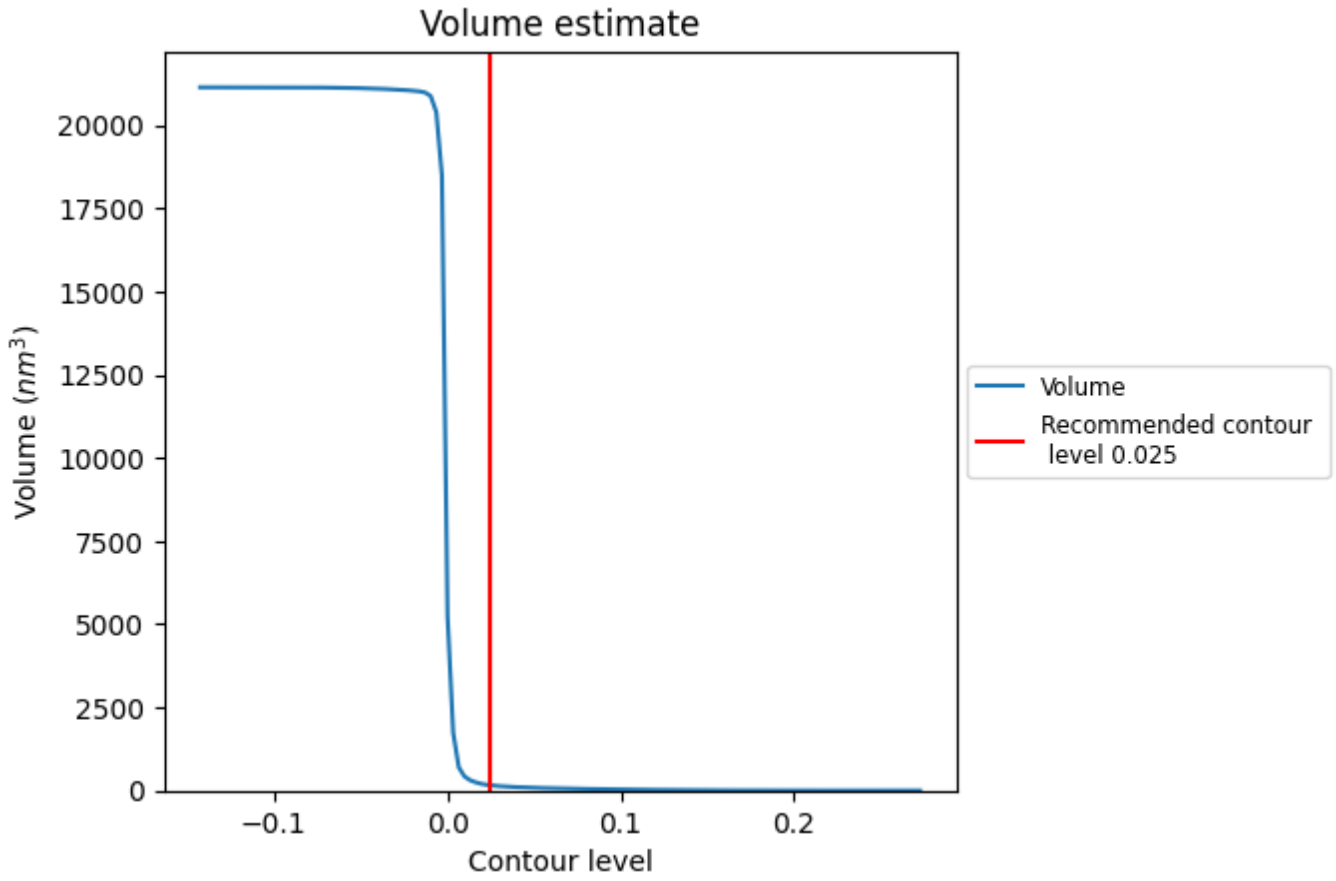
This section contains the results of statistical analysis of the map.

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.

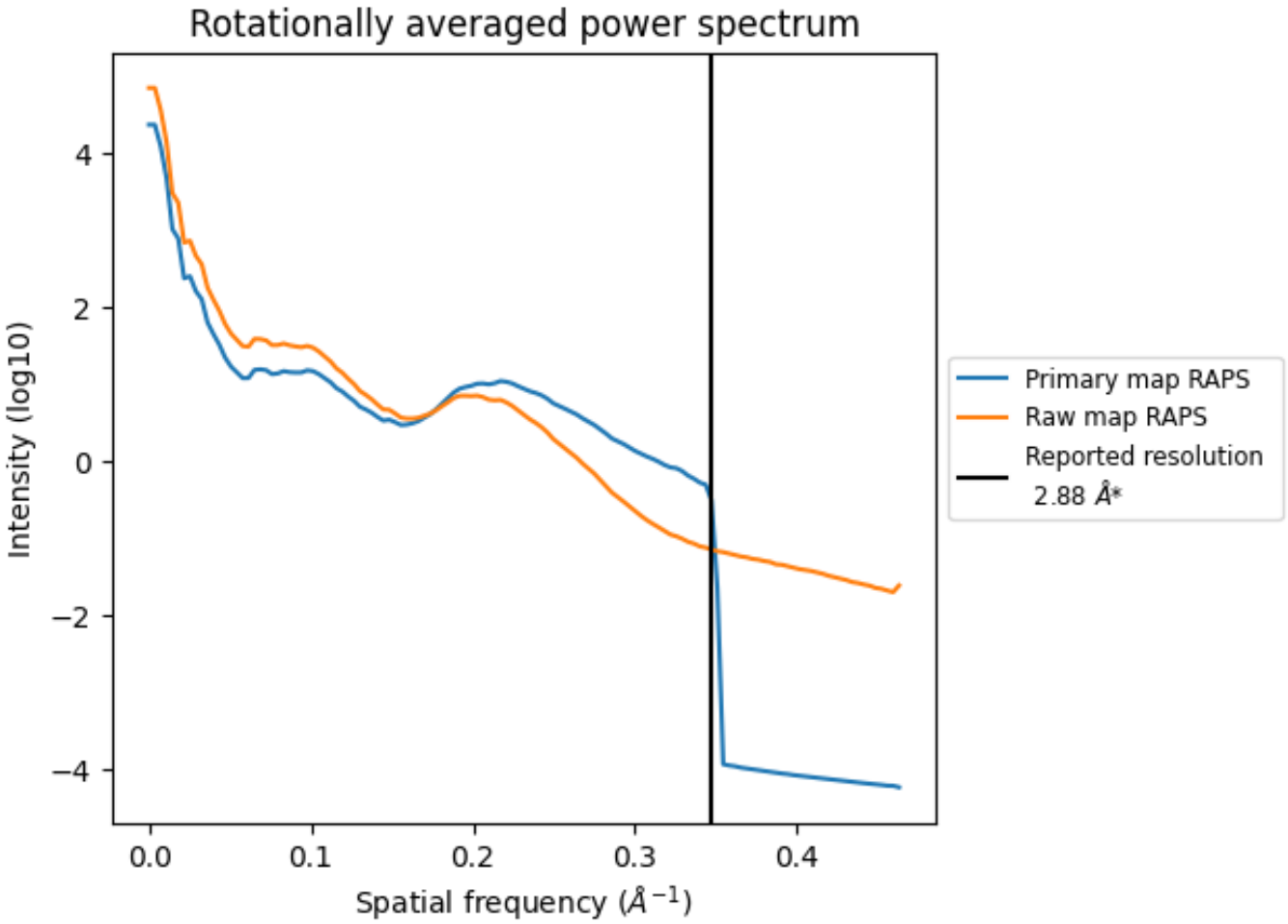
7.2 Volume estimate



The volume at the recommended contour level is 158 nm^3; this corresponds to an approximate mass of 143 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)

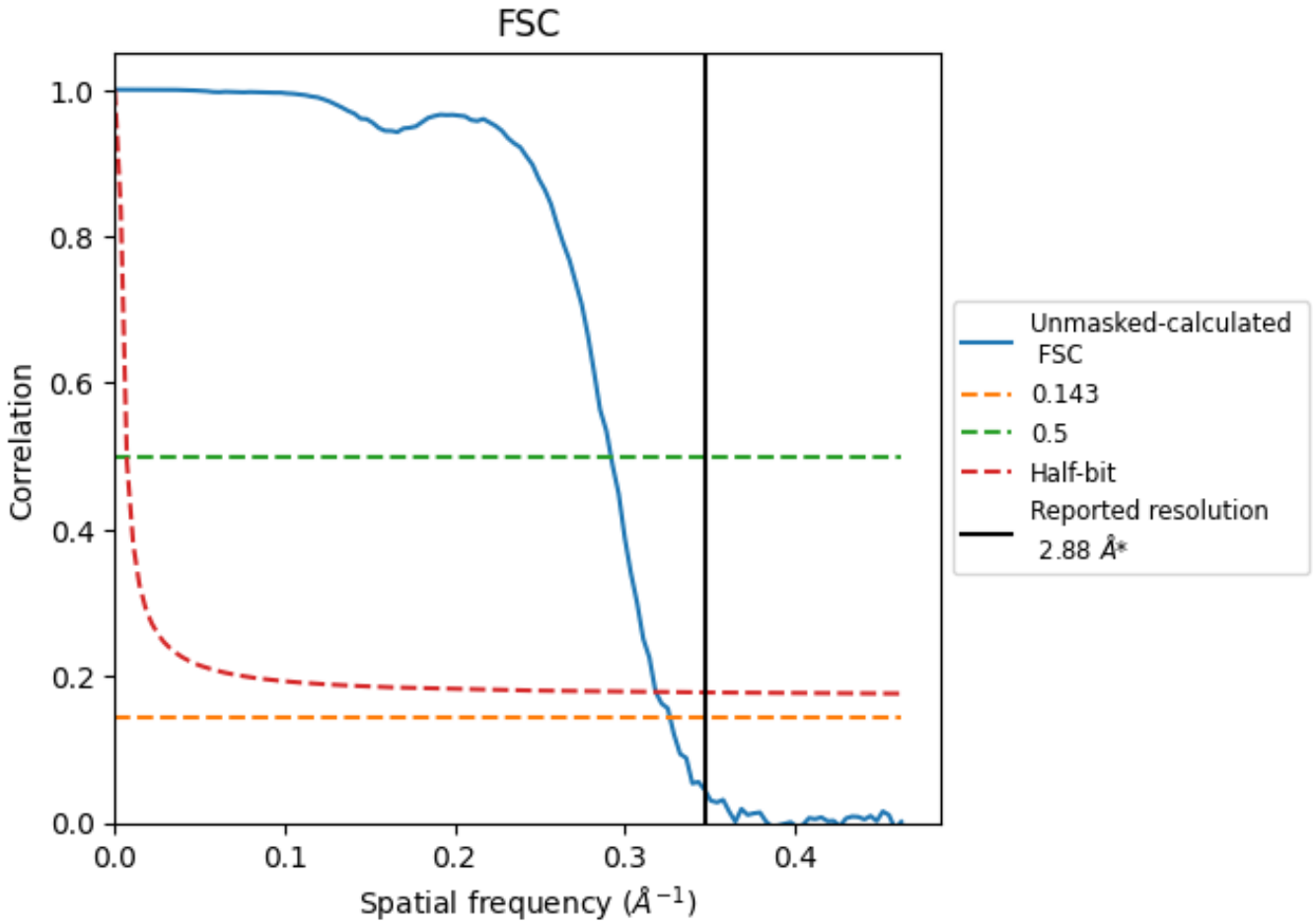


*Reported resolution corresponds to spatial frequency of 0.347 Å^{-1}

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 0.347 Å^{-1}

8.2 Resolution estimates (i)

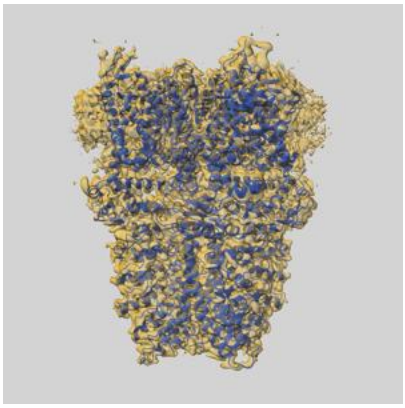
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	2.88	-	-
Author-provided FSC curve	-	-	-
Unmasked-calculated*	3.06	3.42	3.14

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

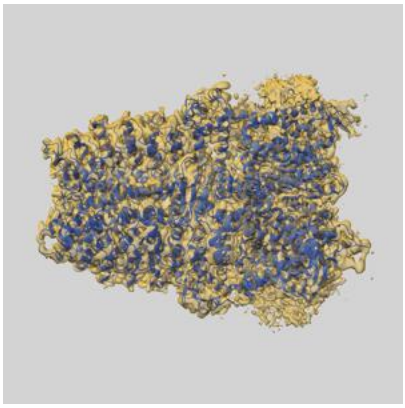
9 Map-model fit

This section contains information regarding the fit between EMDB map EMD-20449 and PDB model 6PQO. Per-residue inclusion information can be found in section 3 on page 12.

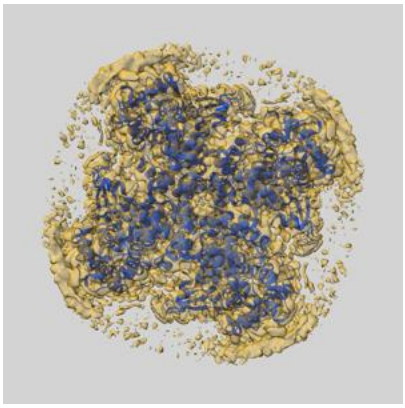
9.1 Map-model overlay



X



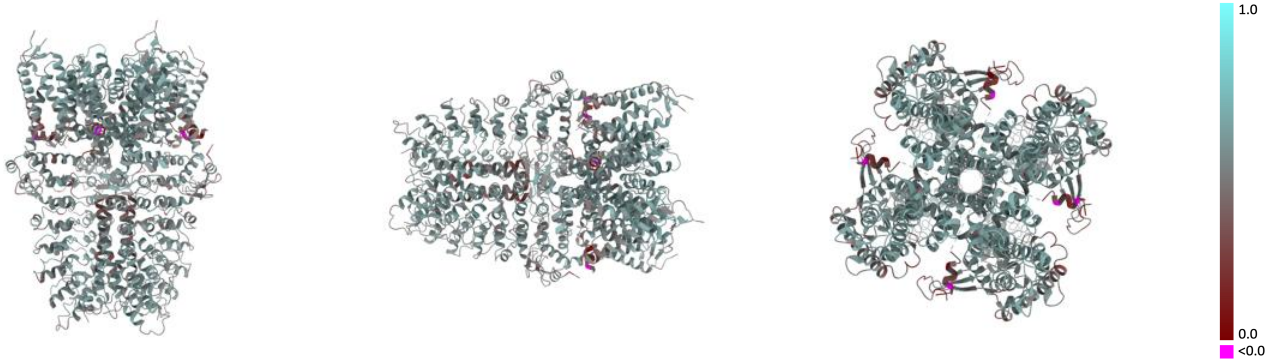
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.025 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.

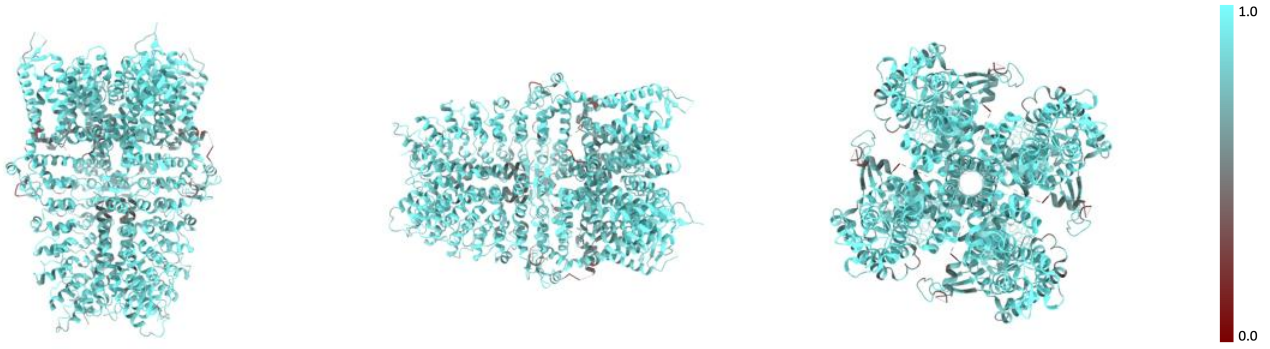
9.2 Q-score mapped to coordinate model (i)



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.

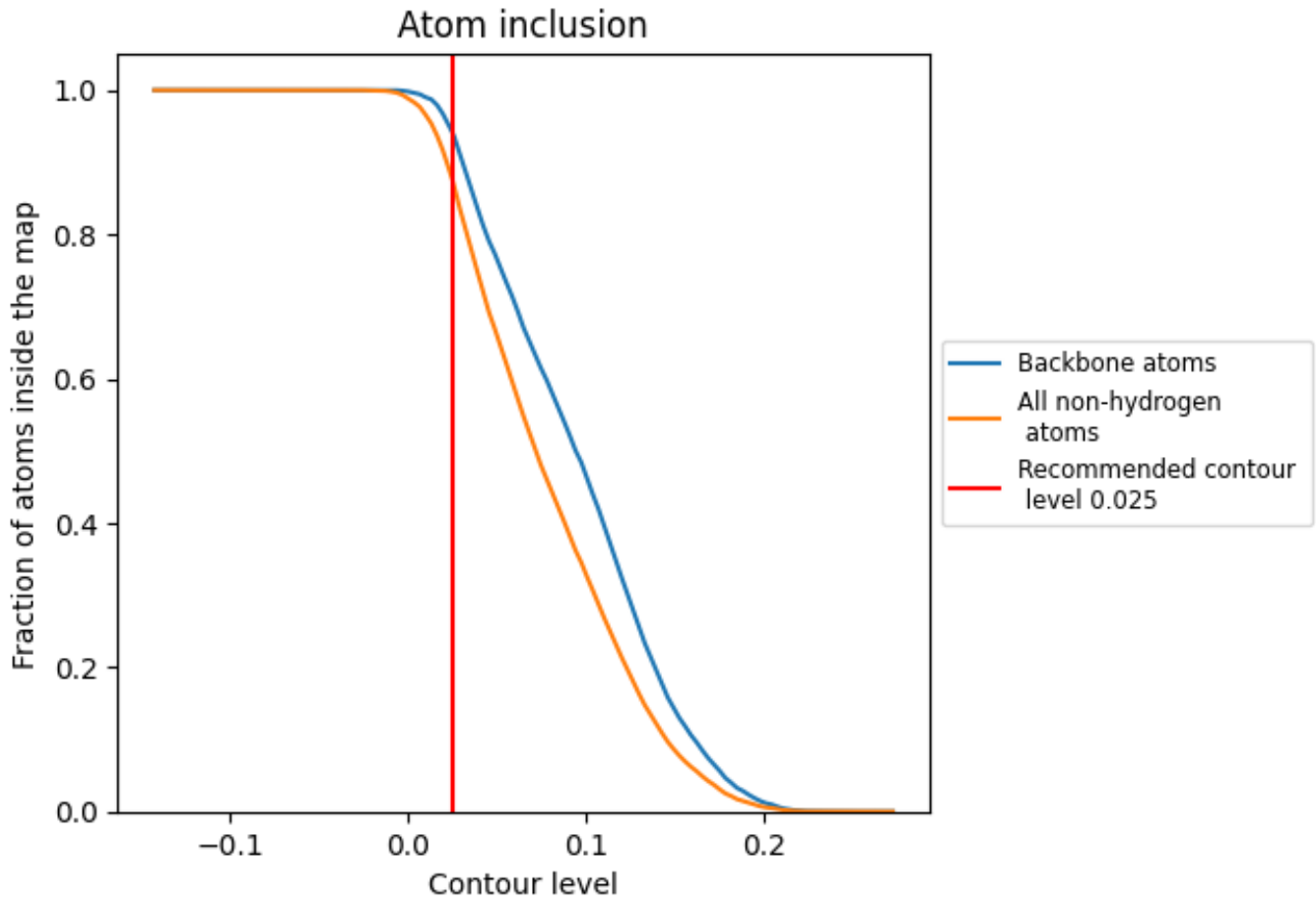
9.3 Atom inclusion mapped to coordinate model (i)



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 (0.025).

9.4 Atom inclusion (i)



At the recommended contour level, 94% of all backbone atoms, 88% 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 (0.025) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.8756	0.5330
A	0.8789	0.5360
B	0.8793	0.5360
C	0.8707	0.5270
D	0.8779	0.5350
E	0.6786	0.4110
F	0.6786	0.4210
G	0.6786	0.4220
H	0.6786	0.3890