Full wwPDB EM Validation Report ⓘ

Mar 11, 2024 – 12:32 PM JST

PDB ID	:	8WOQ
EMDB ID	:	EMD-37695
Title	:	Cryo-EM structure of human SIDT1 protein with C1 symmetry at neutral pH
Authors	:	Liu, W.; Tang, M.; Wang, J.; Zhang, X.; Wu, S.; Ru, H.
Deposited on	:	2023-10-07
Resolution	:	2.85 Å(reported)

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:

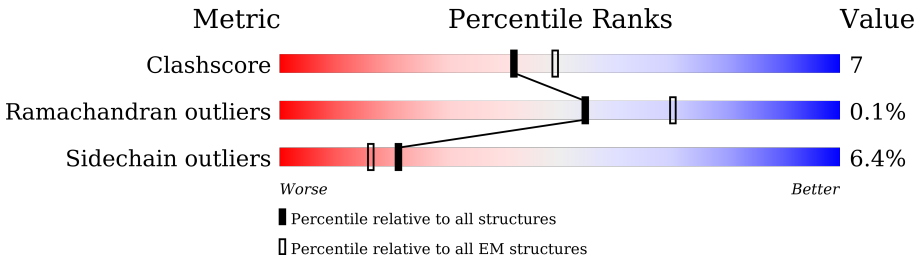
EMDB validation analysis	:	0.0.1.dev70
Mogul	:	1.8.5 (274361), CSD as541be (2020)
MolProbity	:	4.02b-467
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ	:	1.9.13
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

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 2.85 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	881	14% 59% 12% • 27%
1	B	881	13% 58% 15% • 27%
2	C	2	50% 100%
2	D	2	50% 100%
2	E	2	50% 100%
2	F	2	50% 100%

2 Entry composition

There are 9 unique types of molecules in this entry. The entry contains 11218 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 SID1 transmembrane family member 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	647	Total	C	N	O	S	1	0
			5261	3475	841	915	30		
1	B	647	Total	C	N	O	S	1	0
			5261	3475	841	915	30		

There are 98 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	833	SER	-	expression tag	UNP Q9NXL6
A	834	ARG	-	expression tag	UNP Q9NXL6
A	835	GLU	-	expression tag	UNP Q9NXL6
A	836	ASN	-	expression tag	UNP Q9NXL6
A	837	LEU	-	expression tag	UNP Q9NXL6
A	838	TYR	-	expression tag	UNP Q9NXL6
A	839	PHE	-	expression tag	UNP Q9NXL6
A	840	GLN	-	expression tag	UNP Q9NXL6
A	841	GLY	-	expression tag	UNP Q9NXL6
A	842	SER	-	expression tag	UNP Q9NXL6
A	843	GLY	-	expression tag	UNP Q9NXL6
A	844	TRP	-	expression tag	UNP Q9NXL6
A	845	SER	-	expression tag	UNP Q9NXL6
A	846	HIS	-	expression tag	UNP Q9NXL6
A	847	PRO	-	expression tag	UNP Q9NXL6
A	848	GLN	-	expression tag	UNP Q9NXL6
A	849	PHE	-	expression tag	UNP Q9NXL6
A	850	GLU	-	expression tag	UNP Q9NXL6
A	851	LYS	-	expression tag	UNP Q9NXL6
A	852	GLY	-	expression tag	UNP Q9NXL6
A	853	GLY	-	expression tag	UNP Q9NXL6
A	854	GLY	-	expression tag	UNP Q9NXL6
A	855	SER	-	expression tag	UNP Q9NXL6
A	856	GLY	-	expression tag	UNP Q9NXL6
A	857	GLY	-	expression tag	UNP Q9NXL6
A	858	GLY	-	expression tag	UNP Q9NXL6

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Chain	Residue	Modelled	Actual	Comment	Reference
A	859	SER	-	expression tag	UNP Q9NXL6
A	860	GLY	-	expression tag	UNP Q9NXL6
A	861	GLY	-	expression tag	UNP Q9NXL6
A	862	SER	-	expression tag	UNP Q9NXL6
A	863	ALA	-	expression tag	UNP Q9NXL6
A	864	TRP	-	expression tag	UNP Q9NXL6
A	865	SER	-	expression tag	UNP Q9NXL6
A	866	HIS	-	expression tag	UNP Q9NXL6
A	867	PRO	-	expression tag	UNP Q9NXL6
A	868	GLN	-	expression tag	UNP Q9NXL6
A	869	PHE	-	expression tag	UNP Q9NXL6
A	870	GLU	-	expression tag	UNP Q9NXL6
A	871	LYS	-	expression tag	UNP Q9NXL6
A	872	GLY	-	expression tag	UNP Q9NXL6
A	873	SER	-	expression tag	UNP Q9NXL6
A	874	ASP	-	expression tag	UNP Q9NXL6
A	875	TYR	-	expression tag	UNP Q9NXL6
A	876	LYS	-	expression tag	UNP Q9NXL6
A	877	ASP	-	expression tag	UNP Q9NXL6
A	878	ASP	-	expression tag	UNP Q9NXL6
A	879	ASP	-	expression tag	UNP Q9NXL6
A	880	ASP	-	expression tag	UNP Q9NXL6
A	881	LYS	-	expression tag	UNP Q9NXL6
B	833	SER	-	expression tag	UNP Q9NXL6
B	834	ARG	-	expression tag	UNP Q9NXL6
B	835	GLU	-	expression tag	UNP Q9NXL6
B	836	ASN	-	expression tag	UNP Q9NXL6
B	837	LEU	-	expression tag	UNP Q9NXL6
B	838	TYR	-	expression tag	UNP Q9NXL6
B	839	PHE	-	expression tag	UNP Q9NXL6
B	840	GLN	-	expression tag	UNP Q9NXL6
B	841	GLY	-	expression tag	UNP Q9NXL6
B	842	SER	-	expression tag	UNP Q9NXL6
B	843	GLY	-	expression tag	UNP Q9NXL6
B	844	TRP	-	expression tag	UNP Q9NXL6
B	845	SER	-	expression tag	UNP Q9NXL6
B	846	HIS	-	expression tag	UNP Q9NXL6
B	847	PRO	-	expression tag	UNP Q9NXL6
B	848	GLN	-	expression tag	UNP Q9NXL6
B	849	PHE	-	expression tag	UNP Q9NXL6
B	850	GLU	-	expression tag	UNP Q9NXL6
B	851	LYS	-	expression tag	UNP Q9NXL6

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Chain	Residue	Modelled	Actual	Comment	Reference
B	852	GLY	-	expression tag	UNP Q9NXL6
B	853	GLY	-	expression tag	UNP Q9NXL6
B	854	GLY	-	expression tag	UNP Q9NXL6
B	855	SER	-	expression tag	UNP Q9NXL6
B	856	GLY	-	expression tag	UNP Q9NXL6
B	857	GLY	-	expression tag	UNP Q9NXL6
B	858	GLY	-	expression tag	UNP Q9NXL6
B	859	SER	-	expression tag	UNP Q9NXL6
B	860	GLY	-	expression tag	UNP Q9NXL6
B	861	GLY	-	expression tag	UNP Q9NXL6
B	862	SER	-	expression tag	UNP Q9NXL6
B	863	ALA	-	expression tag	UNP Q9NXL6
B	864	TRP	-	expression tag	UNP Q9NXL6
B	865	SER	-	expression tag	UNP Q9NXL6
B	866	HIS	-	expression tag	UNP Q9NXL6
B	867	PRO	-	expression tag	UNP Q9NXL6
B	868	GLN	-	expression tag	UNP Q9NXL6
B	869	PHE	-	expression tag	UNP Q9NXL6
B	870	GLU	-	expression tag	UNP Q9NXL6
B	871	LYS	-	expression tag	UNP Q9NXL6
B	872	GLY	-	expression tag	UNP Q9NXL6
B	873	SER	-	expression tag	UNP Q9NXL6
B	874	ASP	-	expression tag	UNP Q9NXL6
B	875	TYR	-	expression tag	UNP Q9NXL6
B	876	LYS	-	expression tag	UNP Q9NXL6
B	877	ASP	-	expression tag	UNP Q9NXL6
B	878	ASP	-	expression tag	UNP Q9NXL6
B	879	ASP	-	expression tag	UNP Q9NXL6
B	880	ASP	-	expression tag	UNP Q9NXL6
B	881	LYS	-	expression tag	UNP Q9NXL6

- 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	C	2	Total	C	N	O	0	0
			28	16	2	10		

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

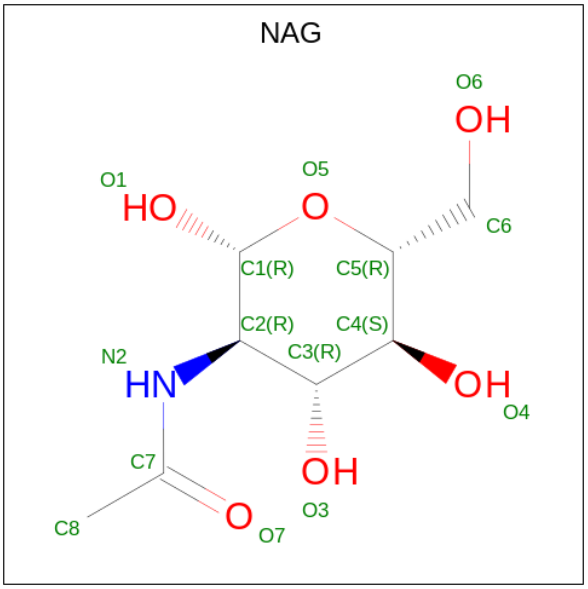
- Molecule 3 is ZINC ION (three-letter code: ZN) (formula: Zn) (labeled as "Ligand of Interest" by depositor).

Mol	Chain	Residues	Atoms	AltConf
3	A	1	Total Zn 1 1	0
3	B	1	Total Zn 1 1	0

- Molecule 4 is CALCIUM ION (three-letter code: CA) (formula: Ca) (labeled as "Ligand of Interest" by depositor).

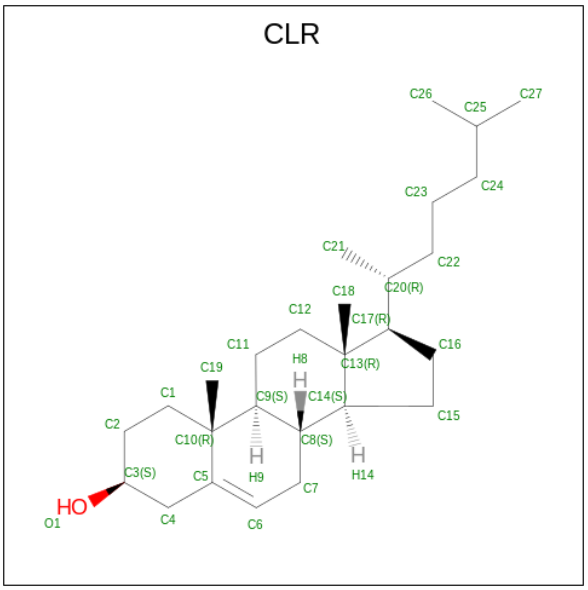
Mol	Chain	Residues	Atoms	AltConf
4	A	1	Total Ca 1 1	0
4	B	1	Total Ca 1 1	0

- Molecule 5 is 2-acetamido-2-deoxy-beta-D-glucopyranose (three-letter code: NAG) (formula: $C_8H_{15}NO_6$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms	AltConf
5	A	1	Total C N O 14 8 1 5	0
5	A	1	Total C N O 14 8 1 5	0
5	B	1	Total C N O 14 8 1 5	0
5	B	1	Total C N O 14 8 1 5	0

- Molecule 6 is CHOLESTEROL (three-letter code: CLR) (formula: $C_{27}H_{46}O$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms	AltConf
6	A	1	Total C O 28 27 1	0
6	A	1	Total C O 28 27 1	0
6	A	1	Total C O 28 27 1	0
6	A	1	Total C O 28 27 1	0
6	A	1	Total C O 28 27 1	0
6	A	1	Total C O 28 27 1	0
6	A	1	Total C O 28 27 1	0

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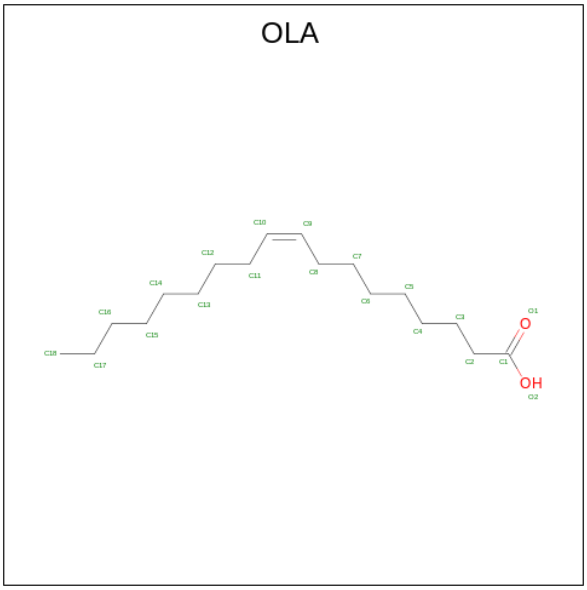
Mol	Chain	Residues	Atoms	AltConf
6	B	1	Total C O 28 27 1	0
6	B	1	Total C O 28 27 1	0
6	B	1	Total C O 28 27 1	0
6	B	1	Total C O 28 27 1	0
6	B	1	Total C O 28 27 1	0
6	B	1	Total C O 28 27 1	0
6	B	1	Total C O 28 27 1	0
6	B	1	Total C O 28 27 1	0

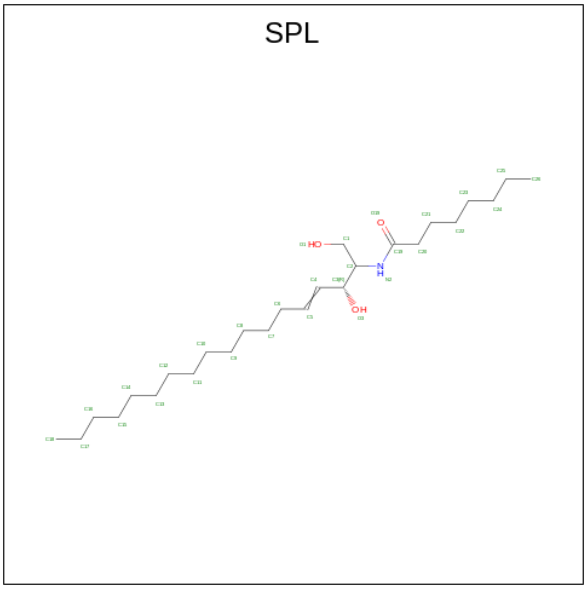
- Molecule 7 is OLEIC ACID (three-letter code: OLA) (formula: $C_{18}H_{34}O_2$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms	AltConf
7	A	1	Total C O 20 18 2	0
7	B	1	Total C O 20 18 2	0

- Molecule 8 is OCTANOIC ACID (2-HYDROXY-1-HYDROXYMETHYL-HEPTADEC-

3-ENYL)-AMIDE (three-letter code: SPL) (formula: $C_{26}H_{51}NO_3$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms				AltConf
8	A	1	Total	C	N	O	0
			30	26	1	3	
8	B	1	Total	C	N	O	0
			30	26	1	3	

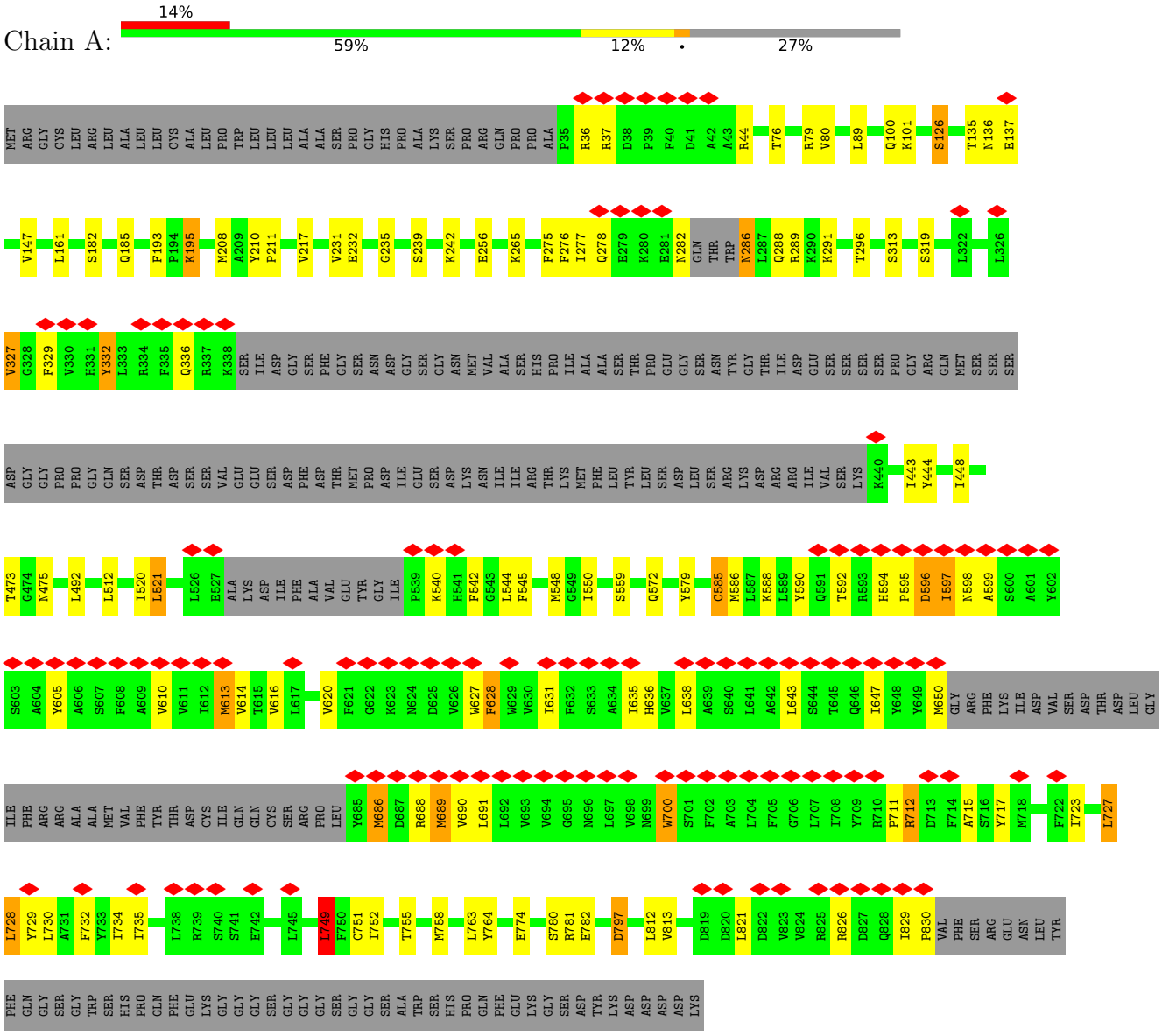
- Molecule 9 is water.

Mol	Chain	Residues	Atoms		AltConf
9	A	2	Total	O	0
			2	2	
9	B	2	Total	O	0
			2	2	

3 Residue-property plots (i)

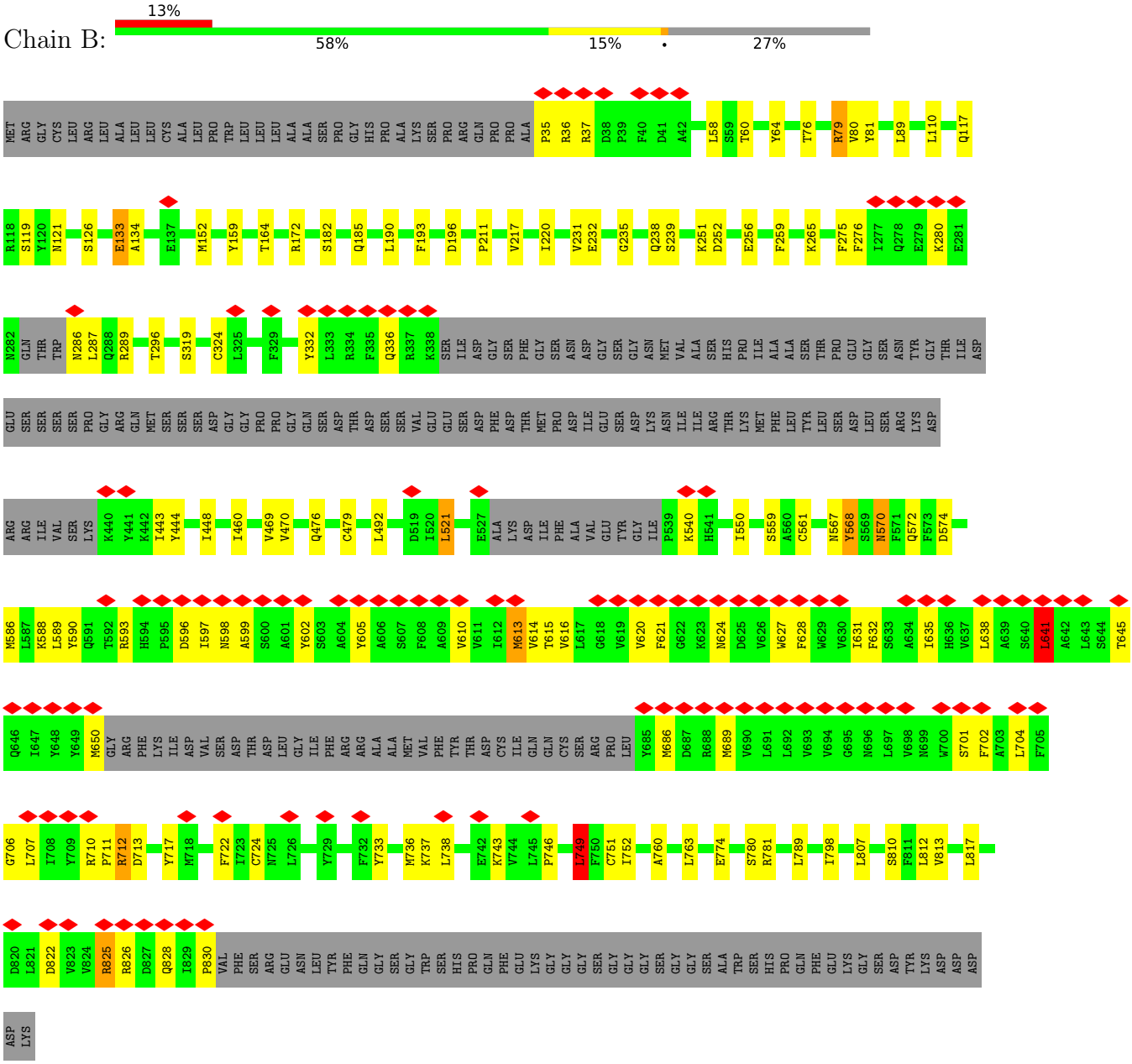
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion 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: SID1 transmembrane family member 1



• Molecule 1: SID1 transmembrane family member 1

Chain B:

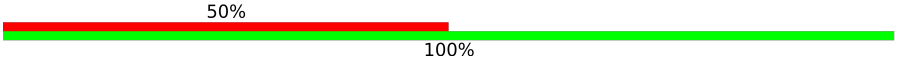


• Molecule 2: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain C:

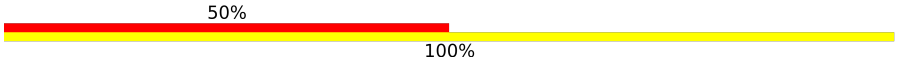
• Molecule 2: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain D:



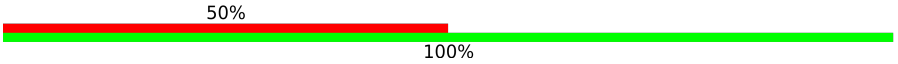
• Molecule 2: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain E:



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

Chain F:



4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	503286	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 ($e^-/Å^2$)	52.52	Depositor
Minimum defocus (nm)	1000	Depositor
Maximum defocus (nm)	1500	Depositor
Magnification	Not provided	
Image detector	GATAN K3 BIOQUANTUM (6k x 4k)	Depositor
Maximum map value	0.558	Depositor
Minimum map value	-0.229	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.013	Depositor
Recommended contour level	0.1	Depositor
Map size (Å)	306.36002, 306.36002, 306.36002	wwPDB
Map dimensions	360, 360, 360	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	0.8510001, 0.8510001, 0.8510001	Depositor

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: ZN, OLA, CLR, NAG, SPL, CA

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\#\|Z\| > 5$	RMSZ	$\#\|Z\| > 5$
1	A	0.28	0/5408	0.54	3/7351 (0.0%)
1	B	0.28	0/5408	0.53	4/7351 (0.1%)
All	All	0.28	0/10816	0.53	7/14702 (0.0%)

There are no bond length outliers.

All (7) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	728	LEU	CA-CB-CG	9.23	136.52	115.30
1	B	738	LEU	CA-CB-CG	7.45	132.43	115.30
1	B	613	MET	CA-CB-CG	6.33	124.06	113.30
1	A	749	LEU	CA-CB-CG	5.84	128.73	115.30
1	A	613	MET	CA-CB-CG	5.72	123.03	113.30
1	B	641	LEU	CA-CB-CG	5.54	128.03	115.30
1	B	749	LEU	CA-CB-CG	5.43	127.80	115.30

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	5261	0	5242	85	0
1	B	5261	0	5242	73	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	C	28	0	25	0	0
2	D	28	0	25	0	0
2	E	28	0	25	2	0
2	F	28	0	25	0	0
3	A	1	0	0	0	0
3	B	1	0	0	0	0
4	A	1	0	0	0	0
4	B	1	0	0	0	0
5	A	28	0	26	0	0
5	B	28	0	26	0	0
6	A	196	0	322	8	0
6	B	224	0	368	9	0
7	A	20	0	33	2	0
7	B	20	0	33	1	0
8	A	30	0	51	2	0
8	B	30	0	51	2	0
9	A	2	0	0	0	0
9	B	2	0	0	0	0
All	All	11218	0	11494	166	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 7.

All (166) 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:602:TYR:HB3	1:B:605:TYR:HE2	1.45	0.80
1:B:265:LYS:O	1:B:289:ARG:NH1	2.20	0.75
1:B:217:VAL:O	1:B:235:GLY:HA3	1.91	0.70
1:A:473:THR:HG23	1:A:475:ASN:H	1.57	0.69
1:B:749:LEU:HA	1:B:752:ILE:HG22	1.73	0.68
1:A:282:ASN:ND2	1:A:288:GLN:O	2.27	0.68
1:A:749:LEU:HA	1:A:752:ILE:HG22	1.77	0.67
1:B:712:ARG:HD2	1:B:712:ARG:H	1.58	0.67
1:B:182:SER:HB3	1:B:185:GLN:HG3	1.80	0.64
1:A:691:LEU:HD13	1:A:732:PHE:HB3	1.78	0.64
1:A:728:LEU:HD13	1:A:732:PHE:CE1	2.32	0.63
1:A:217:VAL:O	1:A:235:GLY:HA3	1.99	0.63
1:B:632:PHE:HZ	1:B:706:GLY:HA3	1.62	0.63
1:B:743:LYS:HE3	1:B:743:LYS:HA	1.81	0.62
1:B:443:ILE:HD12	1:B:444:TYR:H	1.65	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:239:SER:O	1:B:781:ARG:NH1	2.32	0.61
1:A:239:SER:O	1:A:781:ARG:NH1	2.34	0.61
1:A:627:TRP:O	1:A:631:ILE:HG13	2.01	0.61
1:A:821:LEU:HD11	1:A:829:ILE:HG22	1.83	0.61
1:B:602:TYR:HB3	1:B:605:TYR:CE2	2.30	0.60
1:B:710:ARG:HE	1:B:711:PRO:HD3	1.67	0.60
1:A:610:VAL:HG11	1:A:638:LEU:HG	1.84	0.60
1:B:280:LYS:HE3	1:B:280:LYS:HA	1.85	0.59
1:A:135:THR:OG1	1:A:137:GLU:OE1	2.13	0.59
1:A:540:LYS:HE2	1:A:592:THR:HG21	1.85	0.59
1:B:774:GLU:N	1:B:774:GLU:OE1	2.35	0.59
1:B:443:ILE:HD12	1:B:444:TYR:N	2.19	0.58
1:B:825:ARG:NE	1:B:825:ARG:HA	2.19	0.57
1:A:286:ASN:HD22	1:A:286:ASN:N	2.03	0.57
1:A:723:ILE:HD11	8:A:913:SPL:H102	1.86	0.56
1:B:193:PHE:HB2	1:B:256:GLU:HB3	1.88	0.56
1:B:822:ASP:OD1	1:B:828:GLN:NE2	2.39	0.56
1:A:686:MET:H	1:A:686:MET:CE	2.17	0.55
1:A:729:TYR:HA	1:A:732:PHE:HD1	1.71	0.55
1:A:774:GLU:OE1	1:A:774:GLU:N	2.39	0.55
1:B:568:TYR:H	1:B:568:TYR:HD1	1.55	0.55
1:A:732:PHE:HA	1:A:735:ILE:HG22	1.89	0.55
1:A:36:ARG:HH21	2:E:2:NAG:H4	1.73	0.54
1:B:717:TYR:HA	6:B:912:CLR:H222	1.90	0.54
1:A:650:MET:O	1:A:688:ARG:NH2	2.40	0.53
1:A:278:GLN:NE2	1:A:282:ASN:O	2.40	0.53
1:A:327:VAL:HG11	6:A:905:CLR:H121	1.90	0.53
1:A:182:SER:HB3	1:A:185:GLN:HG3	1.89	0.53
1:B:567:ASN:H	1:B:570:ASN:ND2	2.06	0.53
1:B:567:ASN:H	1:B:570:ASN:HD21	1.55	0.53
1:A:730:LEU:O	1:A:734:ILE:HG22	2.09	0.53
1:B:540:LYS:HB2	1:B:830:PRO:HB2	1.91	0.53
1:A:614:VAL:HG11	1:A:635:ILE:HG21	1.91	0.53
1:A:723:ILE:O	1:A:727:LEU:HD23	2.08	0.53
1:A:597:ILE:HD12	1:A:598:ASN:H	1.74	0.52
1:A:751:CYS:HB3	1:A:813:VAL:HG23	1.91	0.52
1:B:238:GLN:NE2	1:B:476:GLN:OE1	2.36	0.52
1:B:713:ASP:H	6:B:912:CLR:H271	1.74	0.52
1:A:763:LEU:HD21	6:A:910:CLR:H11	1.92	0.52
1:B:64:TYR:OH	1:B:159:TYR:OH	2.25	0.52
1:A:544:LEU:O	1:A:548:MET:HG3	2.10	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:448:ILE:HG22	1:A:550:ILE:HG21	1.92	0.51
6:A:909:CLR:H21	6:A:911:CLR:H12	1.92	0.51
6:B:911:CLR:H21	6:B:913:CLR:H12	1.93	0.51
1:B:789:LEU:HD22	1:B:798:ILE:HD11	1.93	0.50
1:B:807:LEU:HD11	8:B:906:SPL:H61	1.94	0.50
1:A:44:ARG:HB3	1:B:35:PRO:HG3	1.94	0.50
1:B:760:ALA:HB1	6:B:909:CLR:H213	1.94	0.50
1:A:712:ARG:HH11	6:A:910:CLR:H262	1.77	0.49
1:A:616:VAL:O	1:A:620:VAL:HG23	2.13	0.49
1:A:443:ILE:HD12	1:A:444:TYR:N	2.28	0.49
1:A:749:LEU:HA	1:A:752:ILE:CG2	2.42	0.49
1:A:231:VAL:HG13	1:A:232:GLU:HG3	1.94	0.49
1:A:797:ASP:N	1:A:797:ASP:OD1	2.45	0.49
1:B:231:VAL:HG13	1:B:232:GLU:HG3	1.95	0.49
1:A:631:ILE:O	1:A:635:ILE:HG13	2.13	0.49
1:B:79:ARG:HG2	1:B:81[A]:TYR:CZ	2.48	0.48
1:B:597:ILE:HG23	1:B:598:ASN:H	1.78	0.48
1:A:717:TYR:HA	6:A:910:CLR:H222	1.95	0.48
1:A:635:ILE:HD12	1:A:636:HIS:N	2.29	0.48
1:A:826:ARG:HA	1:A:826:ARG:HD2	1.62	0.48
1:B:616:VAL:O	1:B:620:VAL:HG23	2.14	0.47
1:A:628:PHE:CZ	1:A:711:PRO:HD2	2.48	0.47
1:B:825:ARG:HE	1:B:828:GLN:HE22	1.61	0.47
1:A:752:ILE:HA	1:A:755:THR:HG22	1.97	0.47
1:A:444:TYR:HE1	1:A:588:LYS:HG2	1.79	0.47
1:B:641:LEU:O	1:B:645:THR:HG22	2.14	0.47
1:B:763:LEU:HD21	6:B:912:CLR:H11	1.97	0.47
1:A:80:VAL:O	1:A:126:SER:HA	2.15	0.47
1:B:211:PRO:HB3	1:B:289:ARG:NH1	2.30	0.47
1:B:598:ASN:H	1:B:599:ALA:HA	1.80	0.46
1:A:595:PRO:O	1:A:597:ILE:N	2.49	0.46
1:A:89:LEU:HD12	1:A:89:LEU:HA	1.81	0.46
1:A:136:ASN:OD1	1:A:137:GLU:N	2.49	0.46
1:A:444:TYR:CE1	1:A:588:LYS:HG2	2.51	0.46
1:A:597:ILE:HD12	1:A:599:ALA:HA	1.97	0.46
1:B:492:LEU:HD23	1:B:492:LEU:HA	1.85	0.45
1:B:812:LEU:HD23	1:B:812:LEU:HA	1.80	0.45
1:B:632:PHE:O	1:B:635:ILE:HG13	2.16	0.45
1:A:36:ARG:NH1	2:E:1:NAG:O7	2.49	0.45
1:B:460:ILE:HG12	1:B:561:CYS:SG	2.57	0.45
1:B:631:ILE:O	1:B:635:ILE:HG23	2.16	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:826:ARG:HA	1:B:826:ARG:HD2	1.64	0.45
1:A:729:TYR:HA	1:A:732:PHE:CD1	2.49	0.45
1:B:89:LEU:HD23	1:B:89:LEU:HA	1.80	0.45
6:B:908:CLR:H22	7:B:914:OLA:H132	2.00	0.44
1:A:147:VAL:HG11	1:A:161:LEU:HD11	1.99	0.44
1:B:58:LEU:HD13	1:B:152:MET:HG2	1.98	0.44
1:A:444:TYR:O	1:A:448:ILE:HG12	2.17	0.44
1:A:712:ARG:HD2	1:A:712:ARG:H	1.82	0.44
1:A:598:ASN:H	1:A:599:ALA:HA	1.82	0.44
1:A:636:HIS:NE2	1:A:717:TYR:OH	2.44	0.44
1:A:689:MET:SD	1:A:690:VAL:N	2.91	0.44
1:A:764:TYR:CZ	6:A:908:CLR:H122	2.53	0.43
6:B:912:CLR:H213	6:B:912:CLR:H231	1.86	0.43
1:B:521:LEU:HD22	1:B:521:LEU:HA	1.86	0.43
1:A:492:LEU:HD23	1:A:492:LEU:HA	1.84	0.43
1:A:700:TRP:HA	1:A:700:TRP:CE3	2.54	0.43
7:A:912:OLA:H9	7:A:912:OLA:H62	1.75	0.43
8:A:913:SPL:H212	8:A:913:SPL:H4	2.00	0.43
1:A:265:LYS:O	1:A:289:ARG:NH2	2.34	0.43
1:A:812:LEU:HD23	1:A:812:LEU:HA	1.76	0.43
1:B:751:CYS:HB3	1:B:813:VAL:HG23	2.00	0.43
1:A:195:LYS:HE2	1:A:195:LYS:HB2	1.84	0.43
1:B:251:LYS:NZ	1:B:252:ASP:OD1	2.50	0.43
1:B:80:VAL:O	1:B:126:SER:HA	2.19	0.43
1:B:133:GLU:OE1	1:B:134:ALA:N	2.50	0.43
1:B:702:PHE:HZ	1:B:724:CYS:HG	1.64	0.43
1:A:242:LYS:HB2	1:A:782:GLU:HG2	2.01	0.42
1:B:469:VAL:HG11	6:B:905:CLR:H183	2.01	0.42
1:A:691:LEU:HD22	1:A:732:PHE:HD2	1.85	0.42
1:A:520:ILE:HD13	1:A:520:ILE:HA	1.94	0.42
1:B:110:LEU:O	1:B:121:ASN:HA	2.19	0.42
1:B:701:SER:O	1:B:704:LEU:HG	2.19	0.42
1:B:710:ARG:HE	1:B:711:PRO:CD	2.31	0.42
1:A:540:LYS:HB2	1:A:830:PRO:HB2	2.01	0.42
1:A:193:PHE:HB2	1:A:256:GLU:HB3	2.01	0.42
1:A:211:PRO:O	1:A:291:LYS:NZ	2.38	0.42
1:A:579:TYR:OH	1:A:715:ALA:O	2.30	0.42
1:A:643:LEU:O	1:A:647:ILE:HG22	2.20	0.42
1:A:700:TRP:HA	1:A:700:TRP:HE3	1.85	0.42
6:A:906:CLR:H22	7:A:912:OLA:H132	2.00	0.42
6:A:910:CLR:H162	6:A:910:CLR:H221	1.87	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:585:CYS:SG	1:A:586:MET:N	2.93	0.42
1:A:594:HIS:ND1	1:A:595:PRO:HD2	2.35	0.42
1:B:332:TYR:O	1:B:336:GLN:HB2	2.20	0.42
1:A:728:LEU:HD13	1:A:732:PHE:HE1	1.79	0.41
1:B:448:ILE:HG22	1:B:550:ILE:HG21	2.01	0.41
1:B:733:TYR:O	1:B:736:MET:HG3	2.20	0.41
1:A:100:GLN:HG2	1:A:101:LYS:HG3	2.01	0.41
8:B:906:SPL:H112	8:B:906:SPL:H141	1.84	0.41
1:A:594:HIS:HB3	1:A:596:ASP:OD1	2.20	0.41
1:A:512:LEU:HD23	1:A:512:LEU:HA	1.88	0.41
1:B:737:LYS:NZ	1:B:817:LEU:O	2.52	0.41
1:B:746:PRO:O	1:B:749:LEU:HD23	2.20	0.41
1:A:332:TYR:O	1:A:336:GLN:HB2	2.21	0.41
1:A:521:LEU:HD22	1:A:521:LEU:HA	1.84	0.41
1:B:702:PHE:HE1	6:B:912:CLR:H42	1.86	0.41
1:B:190:LEU:HB2	1:B:259:PHE:HE1	1.86	0.41
1:B:614:VAL:HG21	1:B:635:ILE:HG22	2.03	0.41
1:B:621:PHE:HB3	1:B:624:ASN:HB2	2.03	0.41
1:B:704:LEU:HA	1:B:707:LEU:HD12	2.03	0.41
1:A:210:TYR:O	1:A:277:ILE:HD11	2.21	0.40
1:A:540:LYS:O	1:A:540:LYS:HD2	2.21	0.40
1:B:470:VAL:HG21	1:B:479:CYS:SG	2.60	0.40
1:A:542:PHE:HA	1:A:545:PHE:HD2	1.86	0.40
1:B:610:VAL:HG11	1:B:638:LEU:HG	2.01	0.40
1:B:172:ARG:HD2	1:B:172:ARG:HA	1.95	0.40
1:B:220:ILE:HD13	1:B:220:ILE:HA	1.95	0.40
1:B:589:LEU:O	1:B:593:ARG:HG2	2.22	0.40
1:B:763:LEU:HD12	1:B:763:LEU:HA	1.79	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	638/881 (72%)	607 (95%)	30 (5%)	1 (0%)	47 75
1	B	638/881 (72%)	607 (95%)	31 (5%)	0	100 100
All	All	1276/1762 (72%)	1214 (95%)	61 (5%)	1 (0%)	54 79

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	596	ASP

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	581/774 (75%)	548 (94%)	33 (6%)	20 47
1	B	581/774 (75%)	540 (93%)	41 (7%)	14 36
All	All	1162/1548 (75%)	1088 (94%)	74 (6%)	21 41

All (74) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	37	ARG
1	A	76	THR
1	A	79	ARG
1	A	126	SER
1	A	195	LYS
1	A	208	MET
1	A	275	PHE
1	A	276	PHE
1	A	286	ASN
1	A	296	THR
1	A	313	SER
1	A	319	SER
1	A	327	VAL
1	A	329	PHE
1	A	332	TYR

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Mol	Chain	Res	Type
1	A	521	LEU
1	A	559	SER
1	A	572	GLN
1	A	585	CYS
1	A	590	TYR
1	A	597	ILE
1	A	605	TYR
1	A	613	MET
1	A	628	PHE
1	A	686	MET
1	A	689	MET
1	A	700	TRP
1	A	712	ARG
1	A	727	LEU
1	A	749	LEU
1	A	758	MET
1	A	780	SER
1	A	797	ASP
1	B	36	ARG
1	B	37	ARG
1	B	60	THR
1	B	76	THR
1	B	79	ARG
1	B	117	GLN
1	B	119	SER
1	B	133	GLU
1	B	164	THR
1	B	196	ASP
1	B	275	PHE
1	B	276	PHE
1	B	286	ASN
1	B	287	LEU
1	B	296	THR
1	B	319	SER
1	B	324	CYS
1	B	521	LEU
1	B	559	SER
1	B	568	TYR
1	B	570	ASN
1	B	572	GLN
1	B	574	ASP
1	B	586	MET

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Mol	Chain	Res	Type
1	B	588	LYS
1	B	590	TYR
1	B	596	ASP
1	B	613	MET
1	B	615	THR
1	B	627	TRP
1	B	628	PHE
1	B	641	LEU
1	B	650	MET
1	B	686	MET
1	B	689	MET
1	B	712	ARG
1	B	722	PHE
1	B	749	LEU
1	B	780	SER
1	B	810	SER
1	B	825	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (1) such sidechains are listed below:

Mol	Chain	Res	Type
1	B	570	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	C	1	2,1	14,14,15	0.28	0	17,19,21	0.33	0
2	NAG	C	2	2	14,14,15	0.22	0	17,19,21	0.44	0
2	NAG	D	1	2,1	14,14,15	0.19	0	17,19,21	0.55	0
2	NAG	D	2	2	14,14,15	0.21	0	17,19,21	0.42	0
2	NAG	E	1	2,1	14,14,15	0.27	0	17,19,21	0.35	0
2	NAG	E	2	2	14,14,15	0.22	0	17,19,21	0.43	0
2	NAG	F	1	2,1	14,14,15	0.24	0	17,19,21	0.55	0
2	NAG	F	2	2	14,14,15	0.21	0	17,19,21	0.45	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	C	1	2,1	-	2/6/23/26	0/1/1/1
2	NAG	C	2	2	-	2/6/23/26	0/1/1/1
2	NAG	D	1	2,1	-	2/6/23/26	0/1/1/1
2	NAG	D	2	2	-	2/6/23/26	0/1/1/1
2	NAG	E	1	2,1	-	2/6/23/26	0/1/1/1
2	NAG	E	2	2	-	2/6/23/26	0/1/1/1
2	NAG	F	1	2,1	-	3/6/23/26	0/1/1/1
2	NAG	F	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 (19) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	E	2	NAG	C4-C5-C6-O6
2	C	1	NAG	O5-C5-C6-O6
2	C	1	NAG	C4-C5-C6-O6
2	E	2	NAG	O5-C5-C6-O6
2	D	2	NAG	C8-C7-N2-C2
2	D	2	NAG	O7-C7-N2-C2

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Mol	Chain	Res	Type	Atoms
2	F	2	NAG	C8-C7-N2-C2
2	F	2	NAG	O7-C7-N2-C2
2	E	1	NAG	O5-C5-C6-O6
2	F	2	NAG	C4-C5-C6-O6
2	E	1	NAG	C4-C5-C6-O6
2	F	2	NAG	O5-C5-C6-O6
2	F	1	NAG	C4-C5-C6-O6
2	F	1	NAG	O5-C5-C6-O6
2	D	1	NAG	C3-C2-N2-C7
2	F	1	NAG	C3-C2-N2-C7
2	C	2	NAG	C4-C5-C6-O6
2	D	1	NAG	C4-C5-C6-O6
2	C	2	NAG	O5-C5-C6-O6

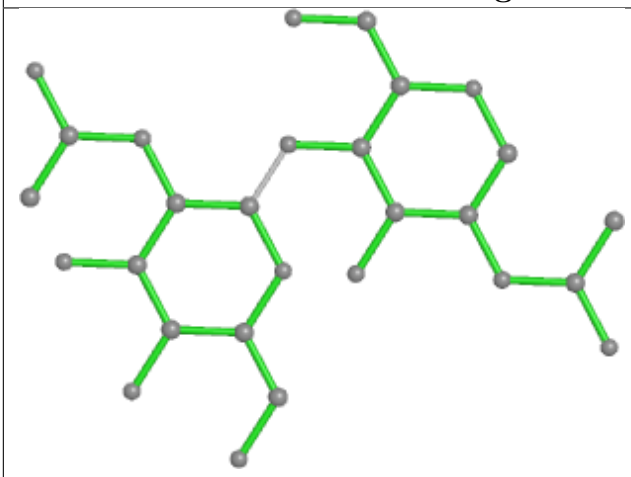
There are no ring outliers.

2 monomers are involved in 2 short contacts:

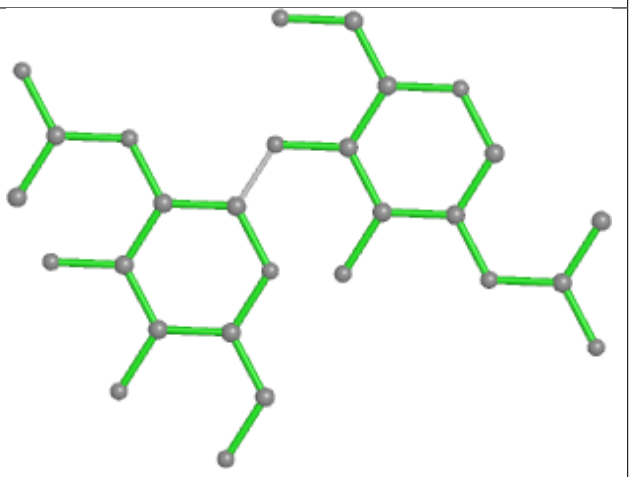
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	E	1	NAG	1	0
2	E	2	NAG	1	0

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

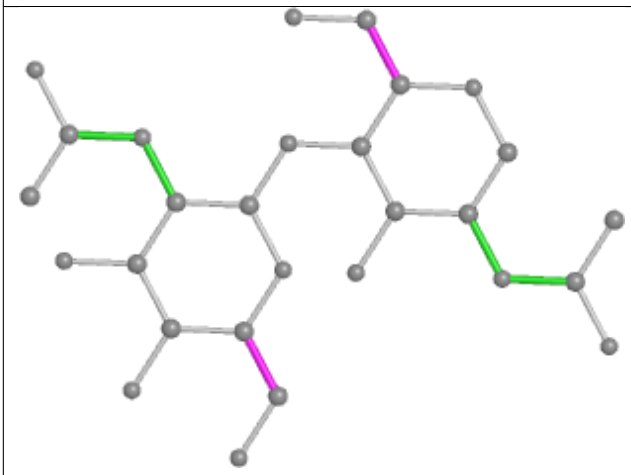
Oligosaccharide Chain C



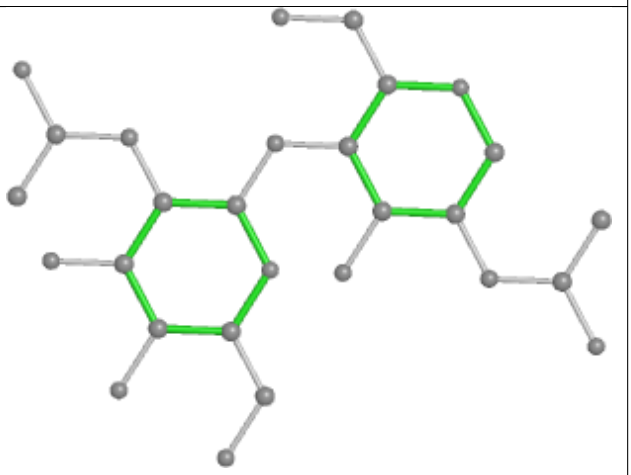
Bond lengths



Bond angles

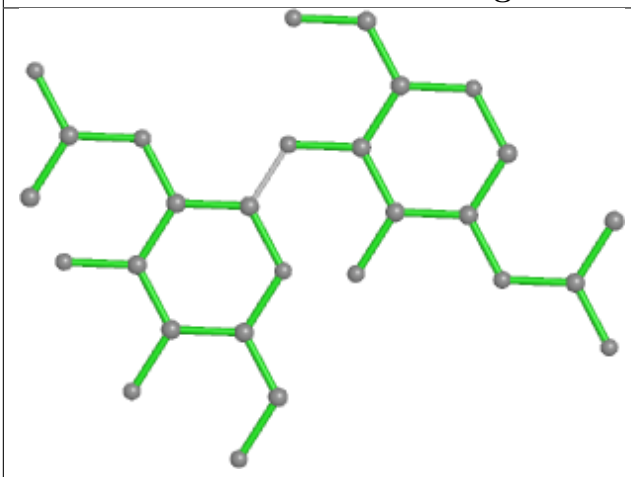


Torsions

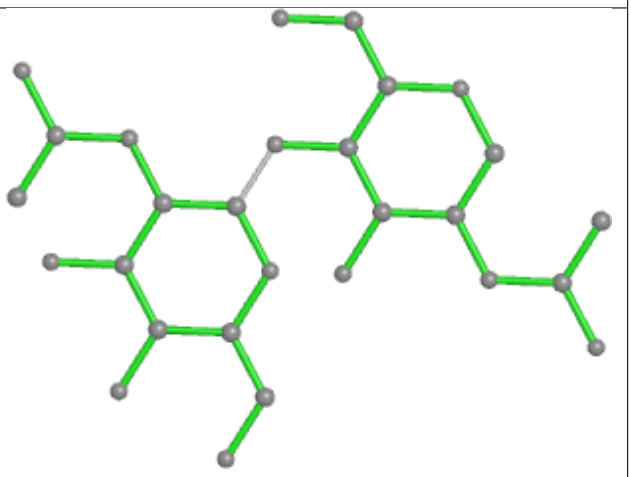


Rings

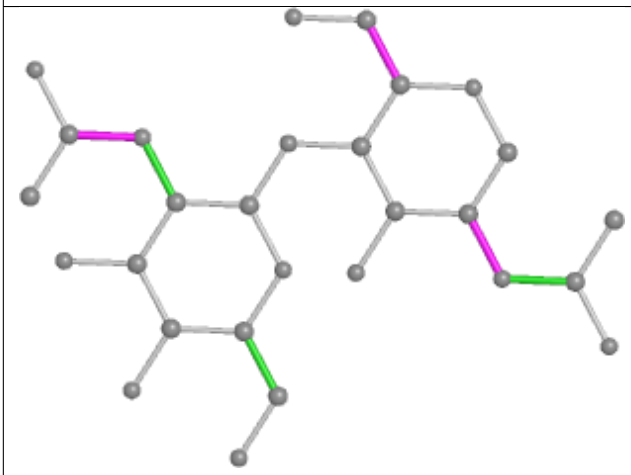
Oligosaccharide Chain D



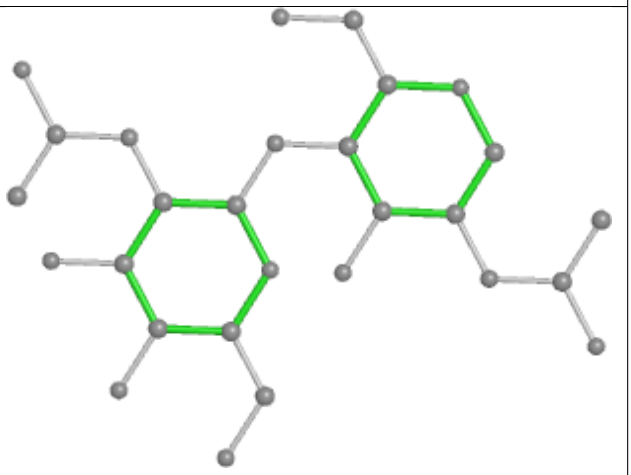
Bond lengths



Bond angles

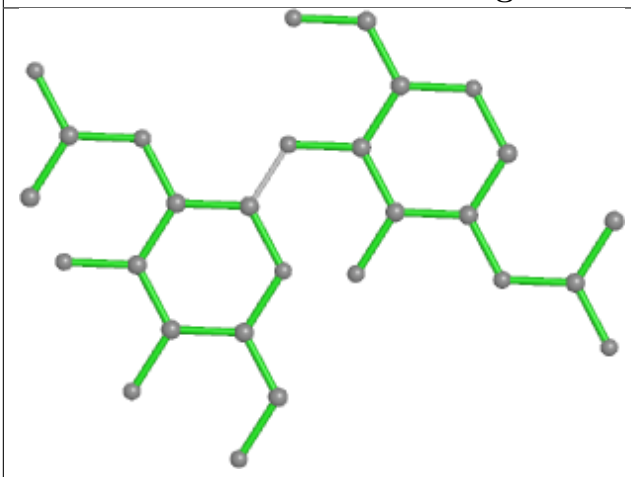


Torsions

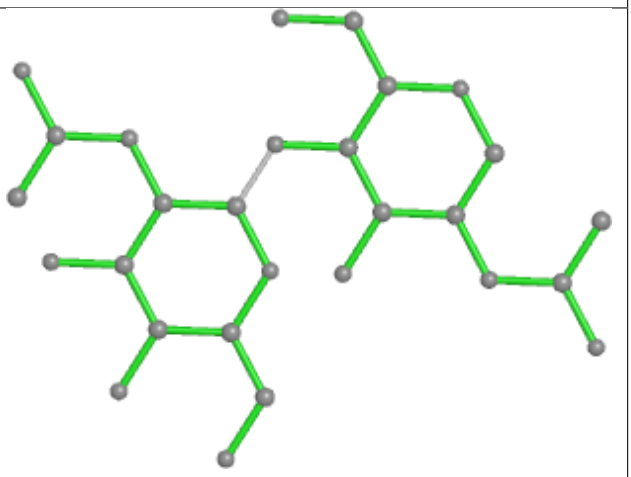


Rings

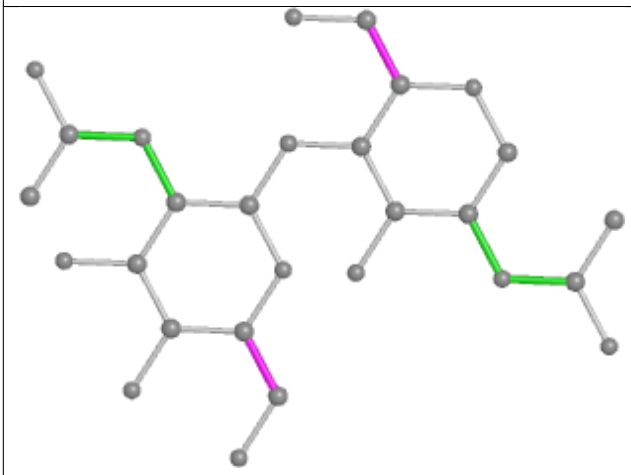
Oligosaccharide Chain E



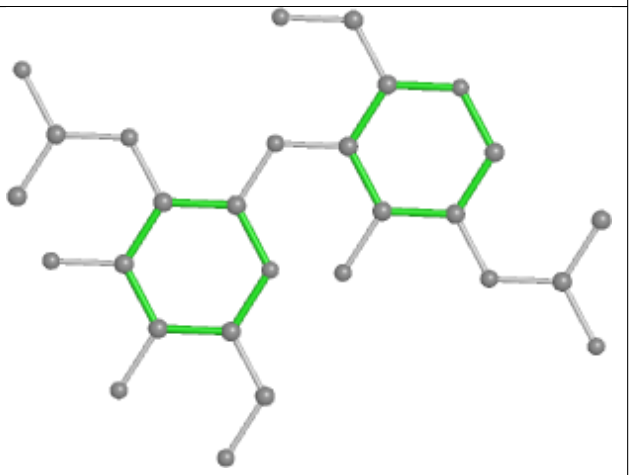
Bond lengths



Bond angles

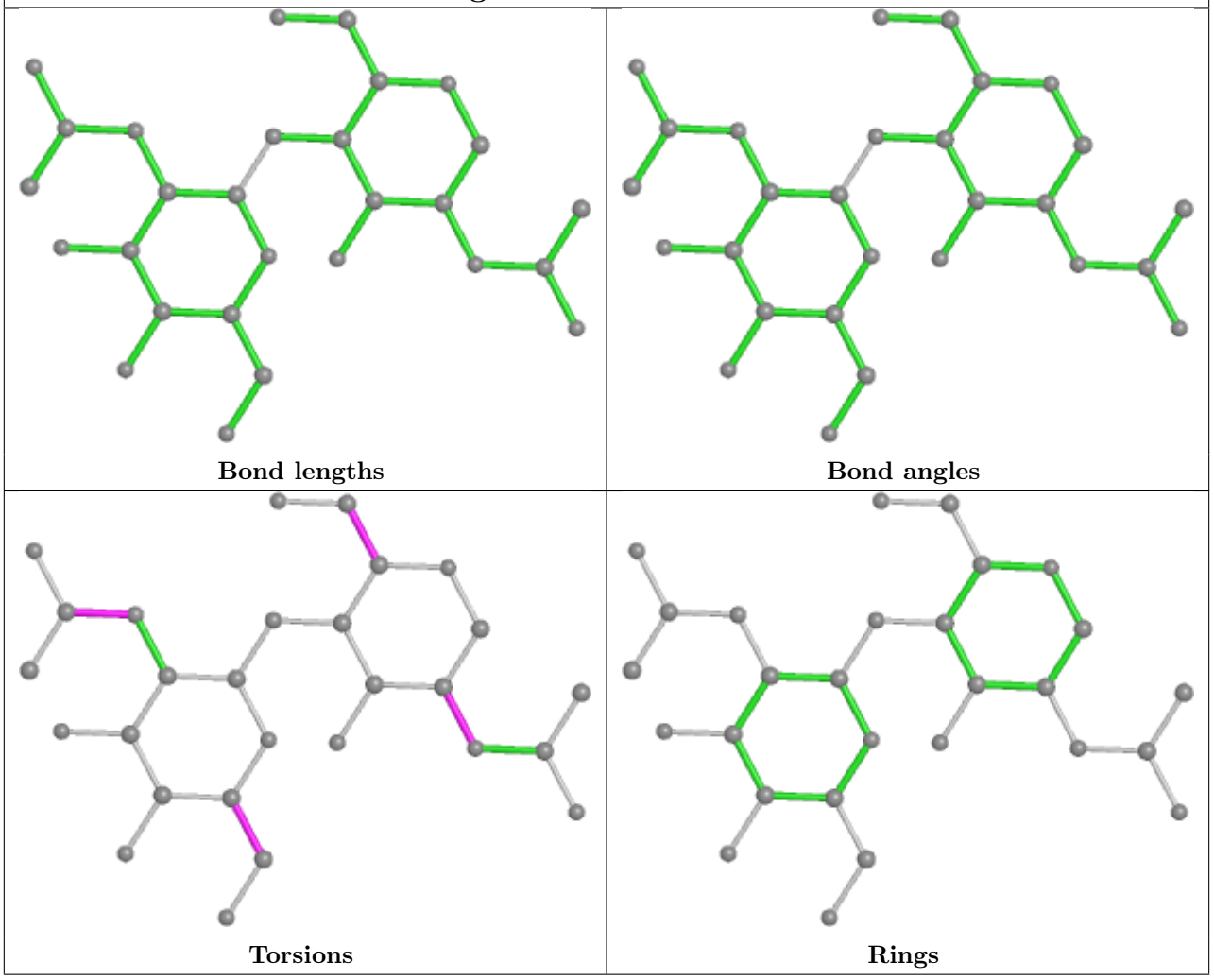


Torsions



Rings

Oligosaccharide Chain F



5.6 Ligand geometry (i)

Of 27 ligands modelled in this entry, 4 are monoatomic - leaving 23 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
5	NAG	A	904	1	14,14,15	0.21	0	17,19,21	0.41	0
6	CLR	B	913	-	31,31,31	0.36	0	48,48,48	0.58	0
5	NAG	B	904	1	14,14,15	0.21	0	17,19,21	0.41	0
6	CLR	A	909	-	31,31,31	0.38	0	48,48,48	0.48	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
6	CLR	A	911	-	31,31,31	0.37	0	48,48,48	0.52	0
6	CLR	A	910	-	31,31,31	0.38	0	48,48,48	0.60	0
6	CLR	A	908	-	31,31,31	0.38	0	48,48,48	0.54	0
6	CLR	A	906	-	31,31,31	0.38	0	48,48,48	0.53	0
6	CLR	B	907	-	31,31,31	0.38	0	48,48,48	0.63	0
7	OLA	A	912	-	19,19,19	0.77	1 (5%)	19,19,19	0.98	1 (5%)
8	SPL	A	913	-	28,29,29	0.44	0	29,31,31	1.56	4 (13%)
6	CLR	B	912	-	31,31,31	0.39	0	48,48,48	0.58	0
7	OLA	B	914	-	19,19,19	0.77	1 (5%)	19,19,19	0.98	1 (5%)
6	CLR	B	905	-	31,31,31	0.40	0	48,48,48	0.69	0
6	CLR	B	909	-	31,31,31	0.40	0	48,48,48	0.64	0
5	NAG	A	903	1	14,14,15	0.23	0	17,19,21	0.44	0
8	SPL	B	906	-	28,29,29	0.44	0	29,31,31	1.52	4 (13%)
6	CLR	A	905	-	31,31,31	0.38	0	48,48,48	0.71	0
6	CLR	A	907	-	31,31,31	0.38	0	48,48,48	0.57	0
5	NAG	B	903	1	14,14,15	0.22	0	17,19,21	0.45	0
6	CLR	B	910	-	31,31,31	0.38	0	48,48,48	0.61	0
6	CLR	B	911	-	31,31,31	0.38	0	48,48,48	0.49	0
6	CLR	B	908	-	31,31,31	0.38	0	48,48,48	0.54	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
5	NAG	A	904	1	-	2/6/23/26	0/1/1/1
6	CLR	B	913	-	-	4/10/68/68	0/4/4/4
5	NAG	B	904	1	-	2/6/23/26	0/1/1/1
6	CLR	A	909	-	-	1/10/68/68	0/4/4/4
6	CLR	A	911	-	-	1/10/68/68	0/4/4/4
6	CLR	A	910	-	-	4/10/68/68	0/4/4/4
6	CLR	A	908	-	-	1/10/68/68	0/4/4/4
6	CLR	A	906	-	-	2/10/68/68	0/4/4/4
6	CLR	B	907	-	-	3/10/68/68	0/4/4/4
7	OLA	A	912	-	-	11/17/17/17	-
8	SPL	A	913	-	-	13/32/32/32	-
6	CLR	B	912	-	-	3/10/68/68	0/4/4/4
7	OLA	B	914	-	-	12/17/17/17	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
6	CLR	B	905	-	-	4/10/68/68	0/4/4/4
6	CLR	B	909	-	-	1/10/68/68	0/4/4/4
5	NAG	A	903	1	-	2/6/23/26	0/1/1/1
8	SPL	B	906	-	-	16/32/32/32	-
6	CLR	A	905	-	-	4/10/68/68	0/4/4/4
6	CLR	A	907	-	-	0/10/68/68	0/4/4/4
5	NAG	B	903	1	-	2/6/23/26	0/1/1/1
6	CLR	B	910	-	-	1/10/68/68	0/4/4/4
6	CLR	B	911	-	-	1/10/68/68	0/4/4/4
6	CLR	B	908	-	-	2/10/68/68	0/4/4/4

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	B	914	OLA	C10-C9	2.67	1.47	1.31
7	A	912	OLA	C10-C9	2.66	1.47	1.31

All (10) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
8	A	913	SPL	C2-N2-C19	6.20	133.94	123.48
8	B	906	SPL	C2-N2-C19	6.12	133.79	123.48
8	A	913	SPL	C3-C4-C5	3.07	131.62	124.79
8	B	906	SPL	C3-C4-C5	2.80	131.04	124.79
8	B	906	SPL	C1-C2-N2	2.43	113.13	109.27
8	A	913	SPL	C1-C2-N2	2.24	112.84	109.27
7	B	914	OLA	C3-C2-C1	-2.24	108.83	114.47
7	A	912	OLA	C3-C2-C1	-2.20	108.92	114.47
8	A	913	SPL	C20-C19-N2	2.11	119.49	115.83
8	B	906	SPL	C20-C19-N2	2.04	119.38	115.83

There are no chirality outliers.

All (92) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
8	A	913	SPL	N2-C2-C3-C4
8	B	906	SPL	N2-C2-C3-C4
5	B	904	NAG	C4-C5-C6-O6
6	B	905	CLR	C21-C20-C22-C23
8	A	913	SPL	C20-C19-N2-C2

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Mol	Chain	Res	Type	Atoms
8	B	906	SPL	C20-C19-N2-C2
5	A	904	NAG	C4-C5-C6-O6
5	B	904	NAG	O5-C5-C6-O6
8	A	913	SPL	O19-C19-N2-C2
8	B	906	SPL	O19-C19-N2-C2
6	B	905	CLR	C17-C20-C22-C23
6	B	907	CLR	C17-C20-C22-C23
5	A	904	NAG	O5-C5-C6-O6
5	B	903	NAG	C4-C5-C6-O6
6	B	912	CLR	C17-C20-C22-C23
7	B	914	OLA	C3-C4-C5-C6
6	A	910	CLR	C17-C20-C22-C23
7	A	912	OLA	C3-C4-C5-C6
6	B	907	CLR	C21-C20-C22-C23
6	A	906	CLR	C20-C22-C23-C24
6	A	905	CLR	C20-C22-C23-C24
6	B	908	CLR	C20-C22-C23-C24
7	A	912	OLA	C1-C2-C3-C4
6	B	905	CLR	C22-C23-C24-C25
7	B	914	OLA	C1-C2-C3-C4
6	B	905	CLR	C20-C22-C23-C24
6	B	910	CLR	C20-C22-C23-C24
5	B	903	NAG	O5-C5-C6-O6
6	A	909	CLR	C21-C20-C22-C23
7	A	912	OLA	C4-C5-C6-C7
7	B	914	OLA	C4-C5-C6-C7
6	A	911	CLR	C21-C20-C22-C23
8	B	906	SPL	C5-C6-C7-C8
8	B	906	SPL	C20-C21-C22-C23
8	A	913	SPL	C1-C2-N2-C19
8	B	906	SPL	O1-C1-C2-C3
8	B	906	SPL	C1-C2-N2-C19
8	A	913	SPL	C10-C11-C12-C13
8	B	906	SPL	C10-C11-C12-C13
6	A	905	CLR	C17-C20-C22-C23
8	B	906	SPL	O1-C1-C2-N2
7	A	912	OLA	C11-C12-C13-C14
7	B	914	OLA	C2-C3-C4-C5
7	B	914	OLA	C11-C12-C13-C14
8	B	906	SPL	C6-C7-C8-C9
6	B	907	CLR	C20-C22-C23-C24
6	A	908	CLR	C20-C22-C23-C24

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Mol	Chain	Res	Type	Atoms
5	A	903	NAG	C4-C5-C6-O6
6	B	913	CLR	C21-C20-C22-C23
7	B	914	OLA	C11-C10-C9-C8
7	A	912	OLA	C12-C13-C14-C15
7	A	912	OLA	C11-C10-C9-C8
6	A	905	CLR	C21-C20-C22-C23
6	A	906	CLR	C21-C20-C22-C23
6	B	911	CLR	C21-C20-C22-C23
8	B	906	SPL	C19-C20-C21-C22
6	B	912	CLR	C21-C20-C22-C23
8	A	913	SPL	C9-C10-C11-C12
8	A	913	SPL	N2-C2-C3-O3
8	B	906	SPL	N2-C2-C3-O3
8	A	913	SPL	C3-C2-N2-C19
8	B	906	SPL	C3-C2-N2-C19
8	A	913	SPL	C1-C2-C3-C4
5	A	903	NAG	O5-C5-C6-O6
7	B	914	OLA	C12-C13-C14-C15
8	B	906	SPL	C2-C3-C4-C5
8	A	913	SPL	C20-C21-C22-C23
7	A	912	OLA	C9-C10-C11-C12
7	B	914	OLA	C9-C10-C11-C12
6	A	910	CLR	C21-C20-C22-C23
7	A	912	OLA	C14-C15-C16-C17
7	B	914	OLA	C6-C7-C8-C9
7	B	914	OLA	C5-C6-C7-C8
6	B	913	CLR	C13-C17-C20-C21
6	A	905	CLR	C23-C24-C25-C27
6	A	910	CLR	C23-C24-C25-C26
7	B	914	OLA	C14-C15-C16-C17
6	B	912	CLR	C20-C22-C23-C24
7	B	914	OLA	C7-C8-C9-C10
6	B	913	CLR	C13-C17-C20-C22
7	A	912	OLA	C7-C8-C9-C10
8	A	913	SPL	C4-C5-C6-C7
6	B	909	CLR	C22-C23-C24-C25
8	A	913	SPL	O1-C1-C2-N2
7	A	912	OLA	C6-C7-C8-C9
8	B	906	SPL	C15-C16-C17-C18
6	B	908	CLR	C21-C20-C22-C23
6	B	913	CLR	C16-C17-C20-C22
8	A	913	SPL	C19-C20-C21-C22

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Mol	Chain	Res	Type	Atoms
7	A	912	OLA	C5-C6-C7-C8
6	A	910	CLR	C20-C22-C23-C24
8	B	906	SPL	C11-C12-C13-C14

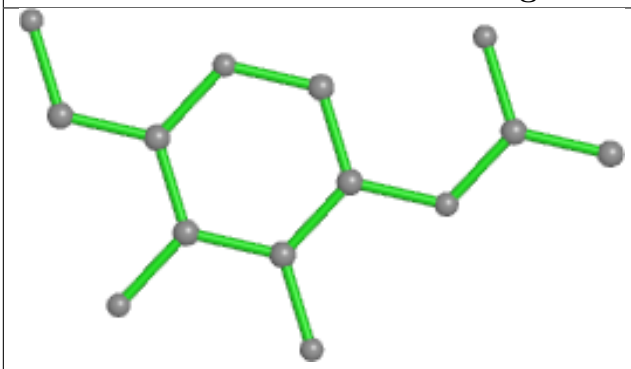
There are no ring outliers.

16 monomers are involved in 22 short contacts:

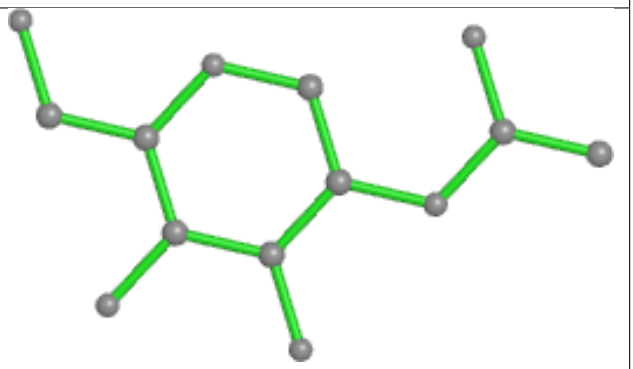
Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	B	913	CLR	1	0
6	A	909	CLR	1	0
6	A	911	CLR	1	0
6	A	910	CLR	4	0
6	A	908	CLR	1	0
6	A	906	CLR	1	0
7	A	912	OLA	2	0
8	A	913	SPL	2	0
6	B	912	CLR	5	0
7	B	914	OLA	1	0
6	B	905	CLR	1	0
6	B	909	CLR	1	0
8	B	906	SPL	2	0
6	A	905	CLR	1	0
6	B	911	CLR	1	0
6	B	908	CLR	1	0

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.

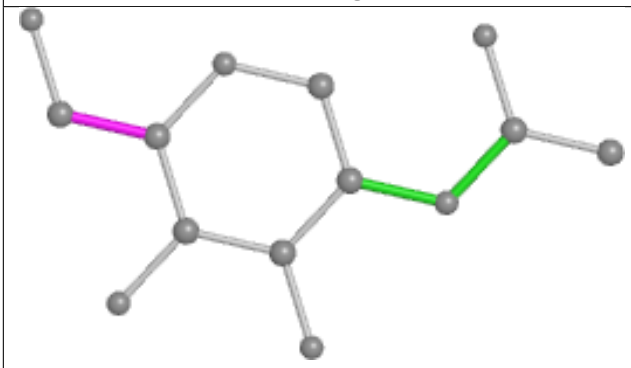
Ligand NAG A 904



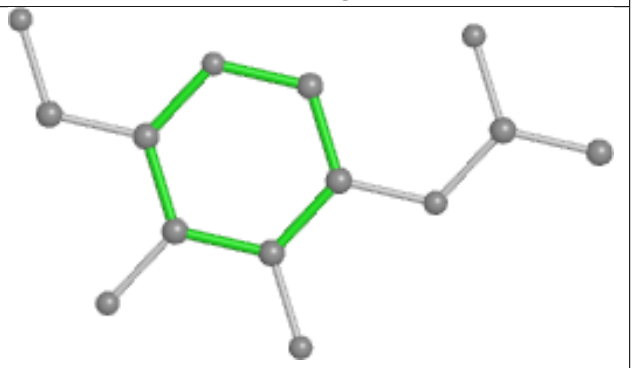
Bond lengths



Bond angles

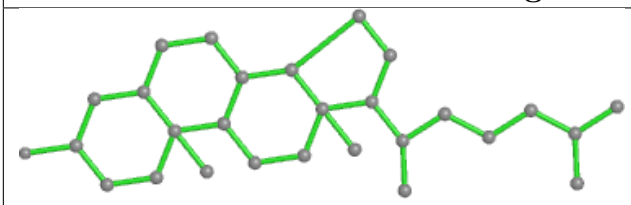


Torsions

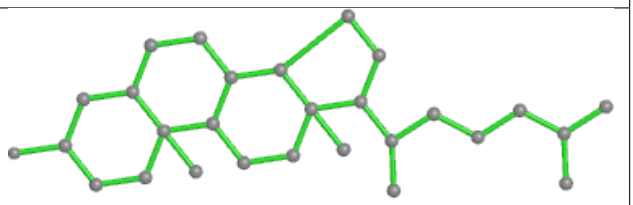


Rings

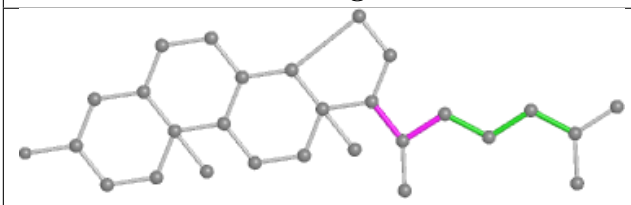
Ligand CLR B 913



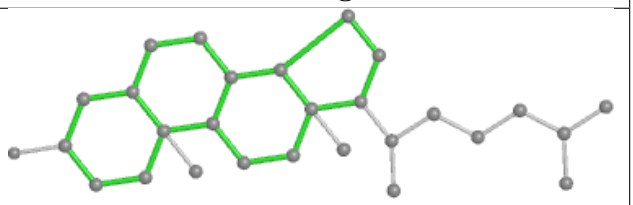
Bond lengths



Bond angles

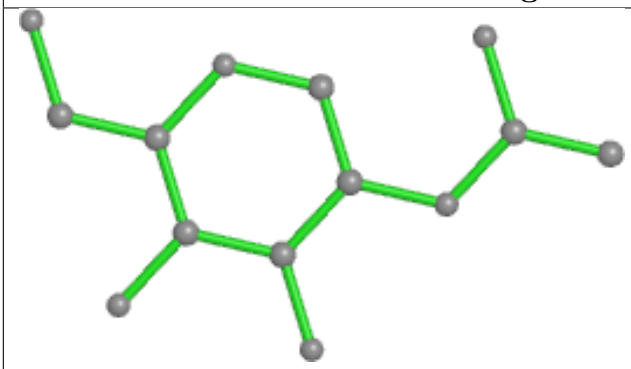


Torsions

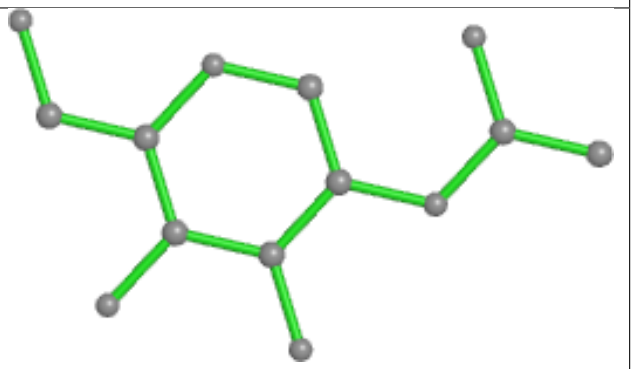


Rings

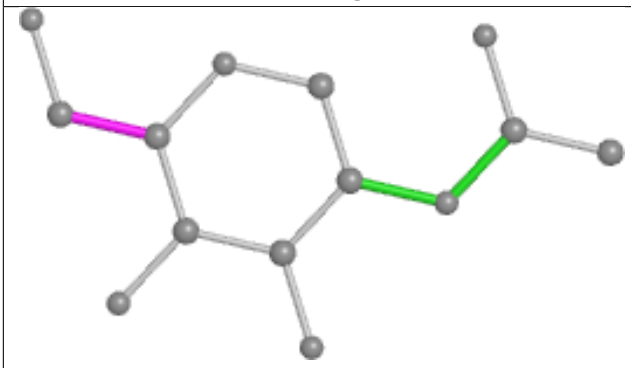
Ligand NAG B 904



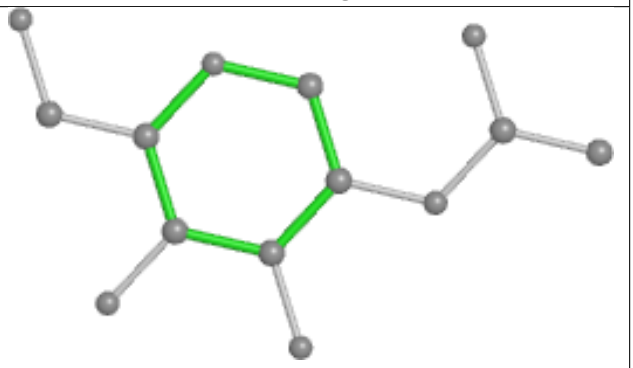
Bond lengths



Bond angles

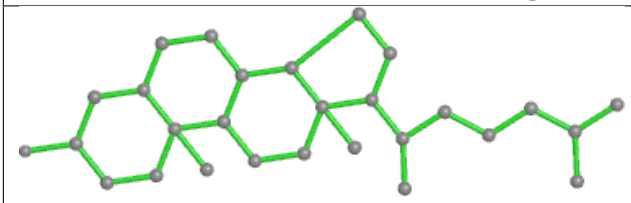


Torsions

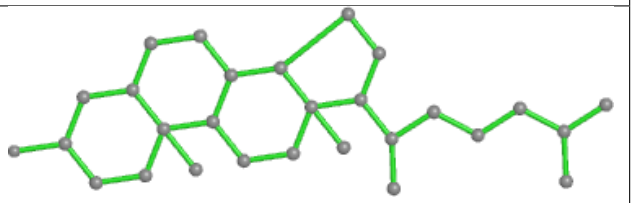


Rings

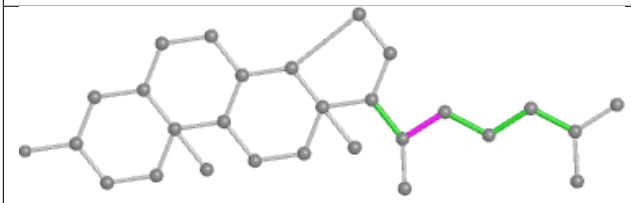
Ligand CLR A 909



Bond lengths



Bond angles



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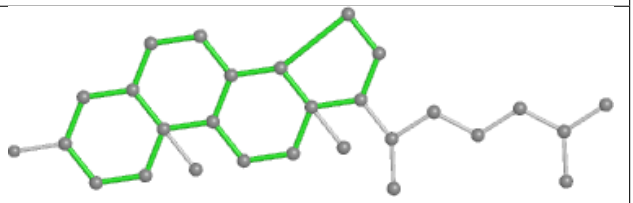
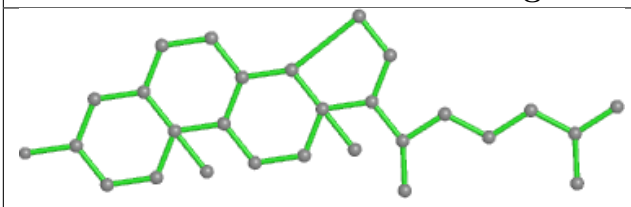


Rings

Ligand CLR A 911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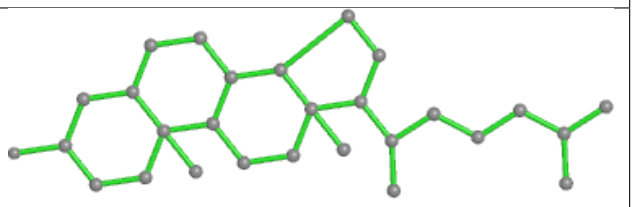
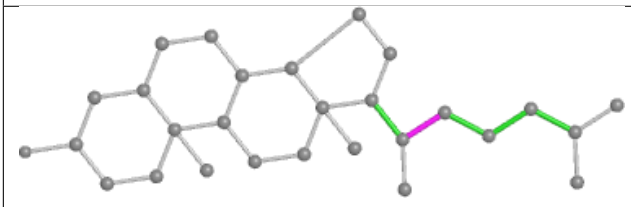
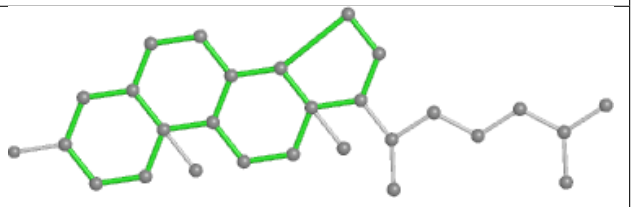
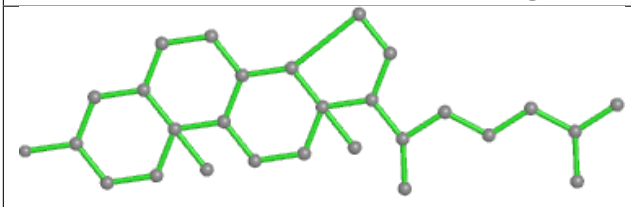

Bond angles


Torsions


Rings

Ligand CLR A 910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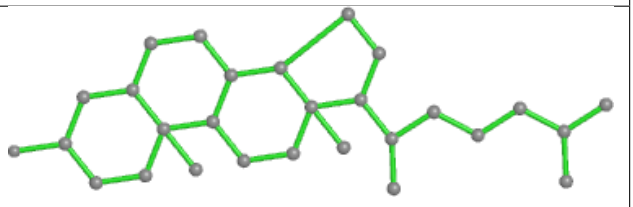
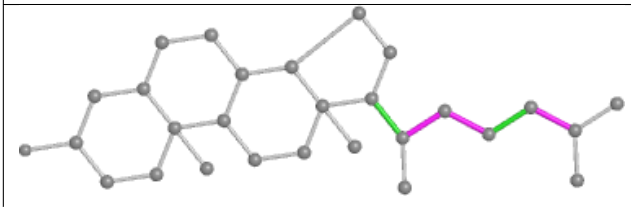
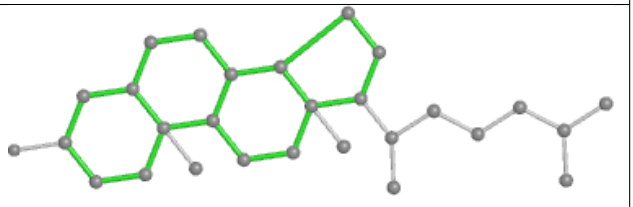
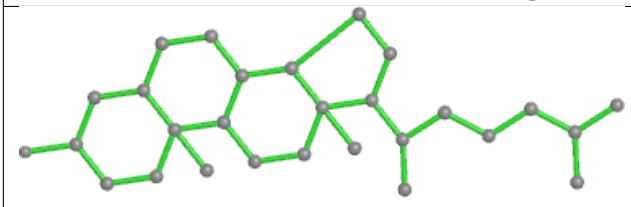

Bond angles


Torsions


Rings

Ligand CLR A 908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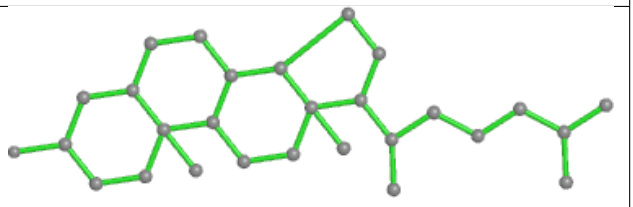
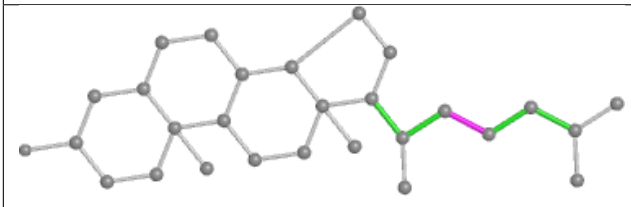

Bond angles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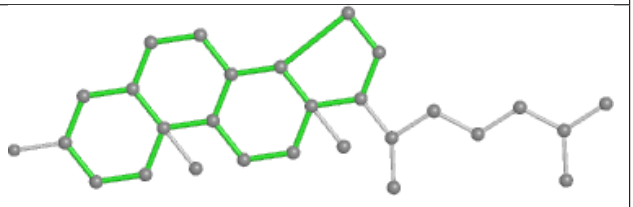
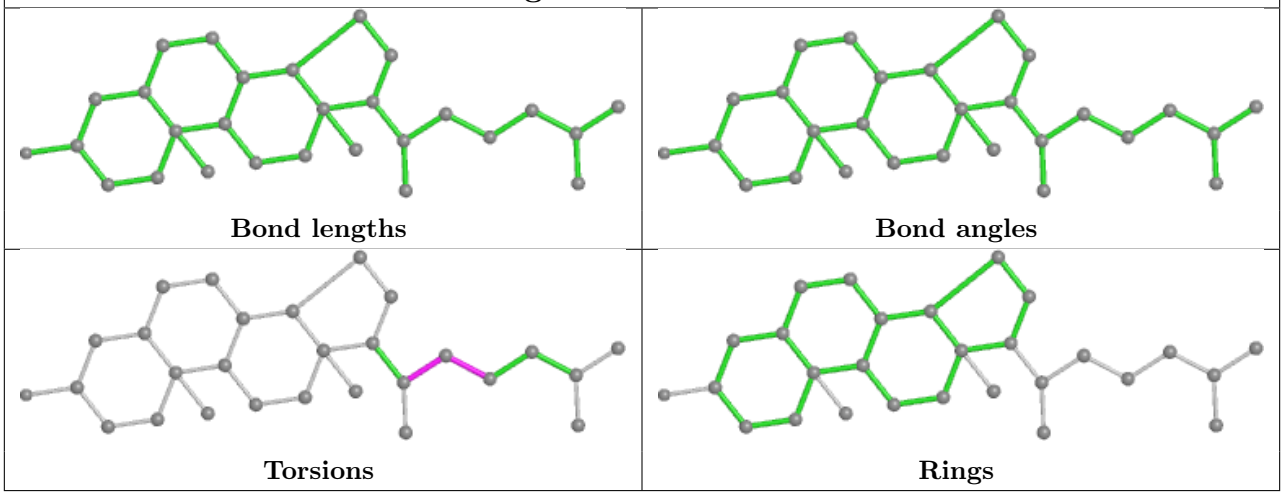
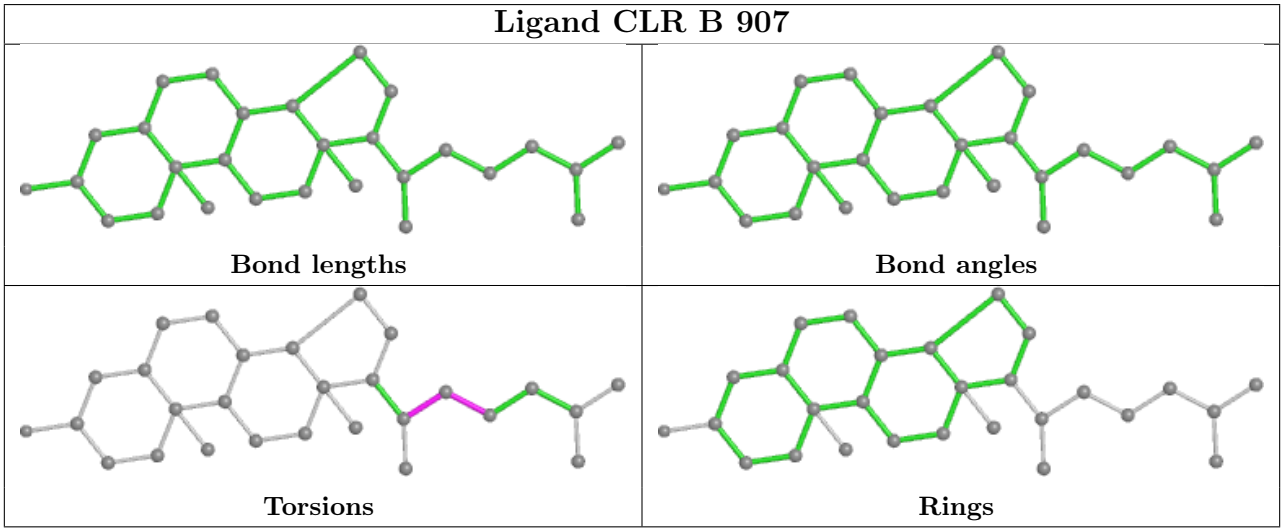

Rings

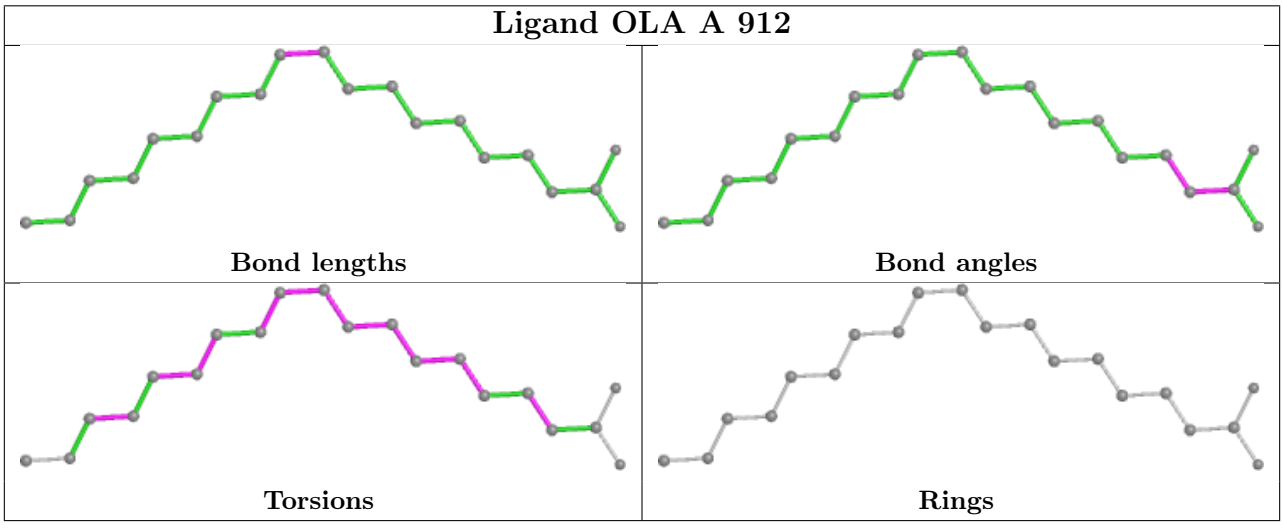
Ligand CLR A 906



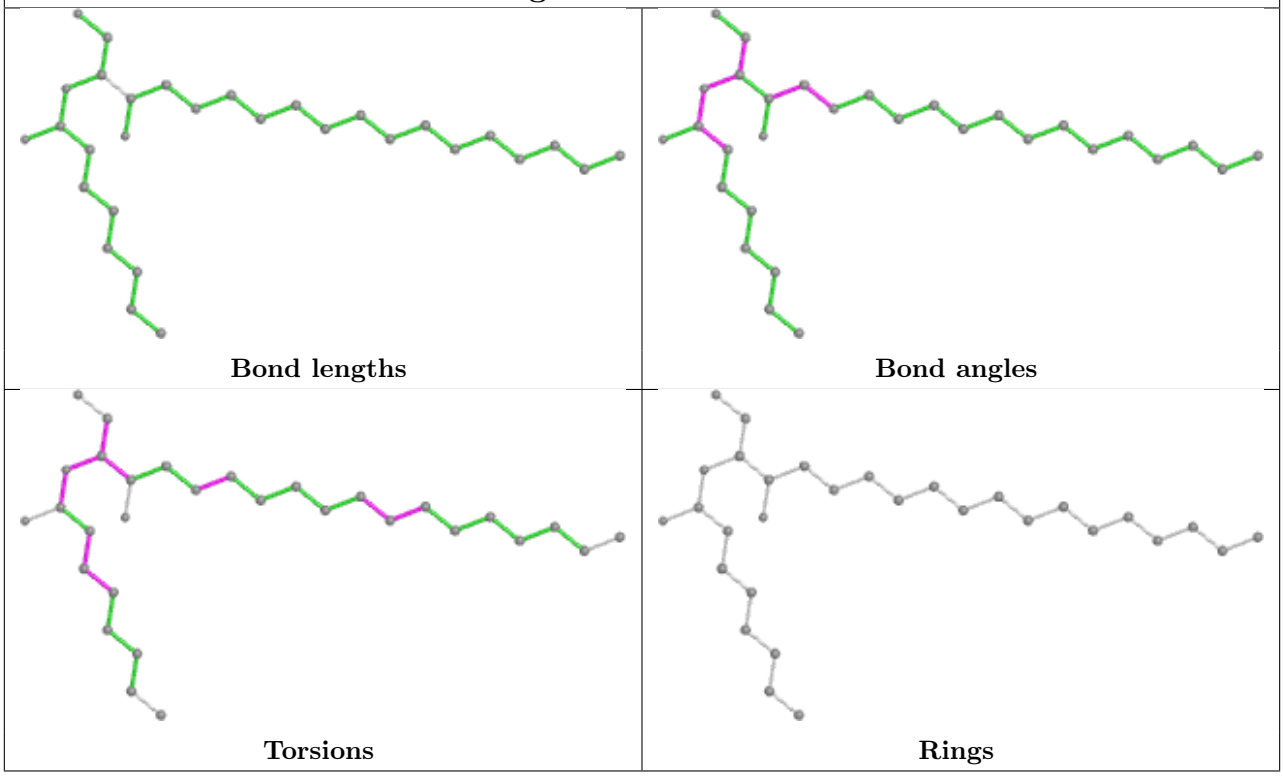
Ligand CLR B 907



Ligand OLA A 912



Ligand SPL A 913



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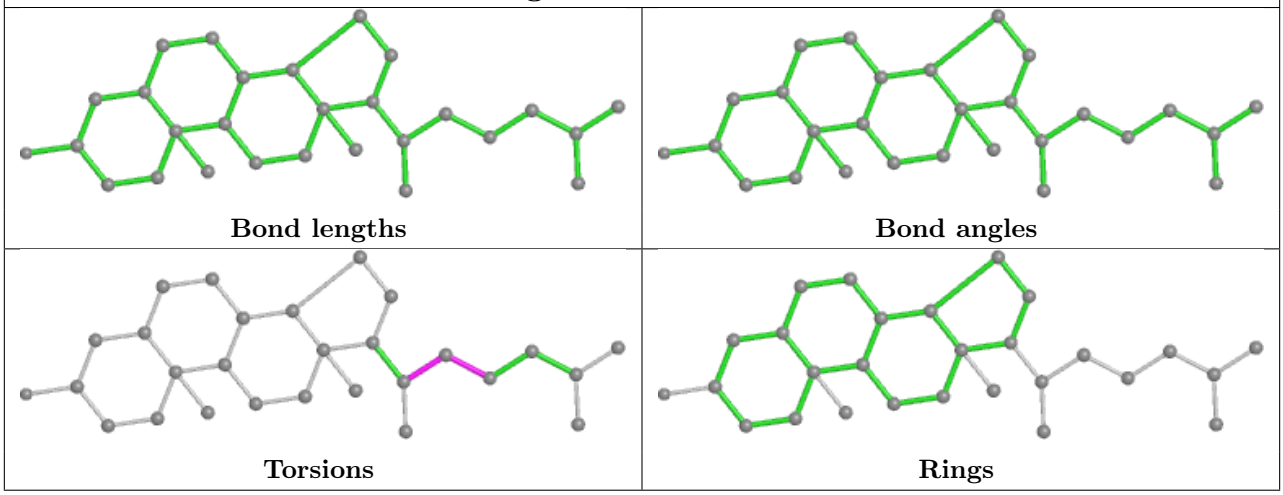
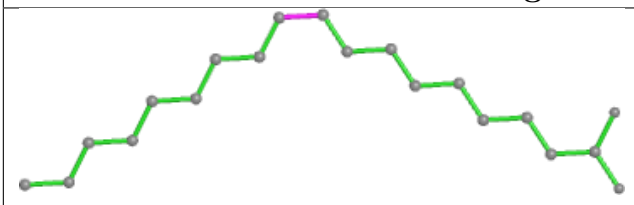
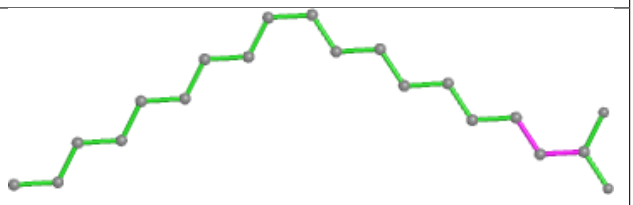
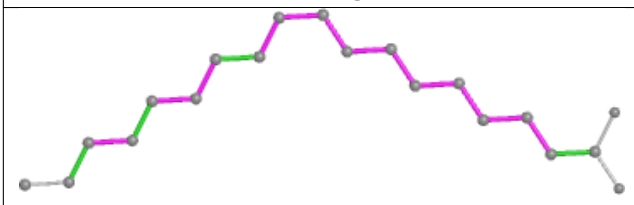
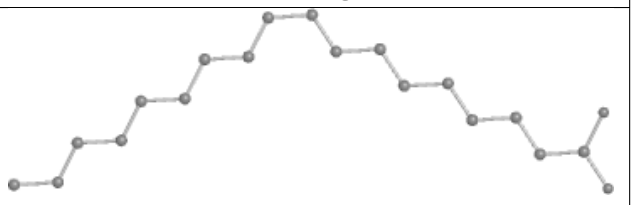


Ligand OLA B 914

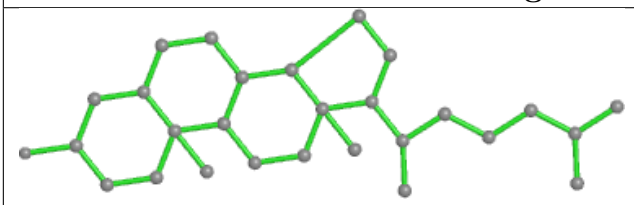

Bond lengths

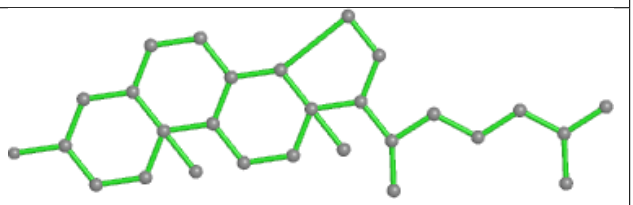

Bond angles

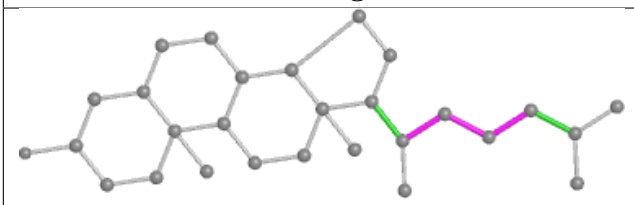

Torsions

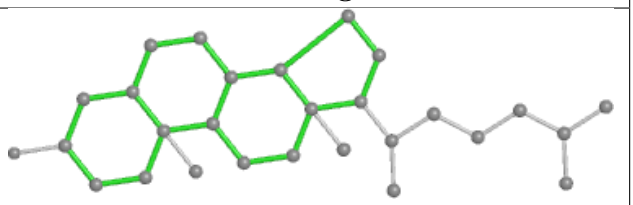

Rings

Ligand CLR B 905

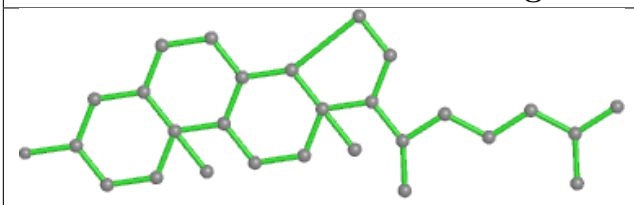

Bond lengths

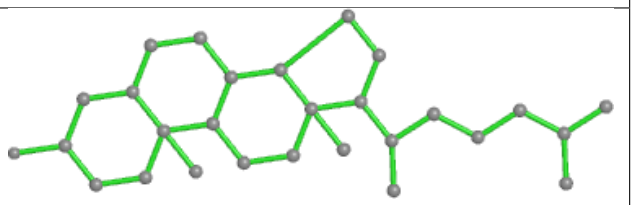

Bond angles

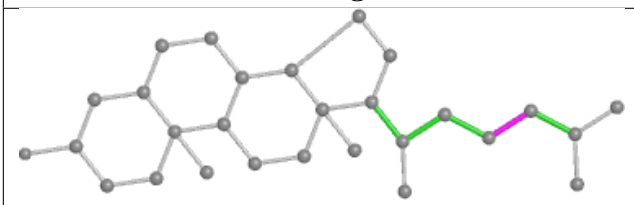

Torsions

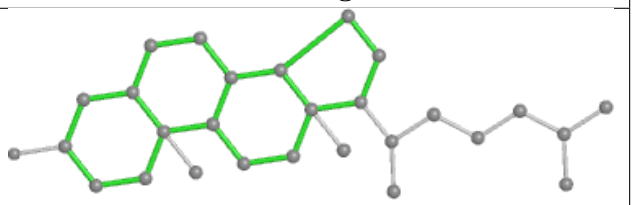

Rings

Ligand CLR B 909

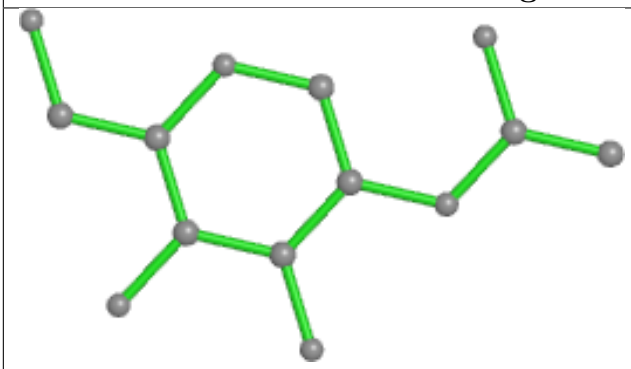

Bond lengths


Bond angles


Torsions


Rings

Ligand NAG A 903



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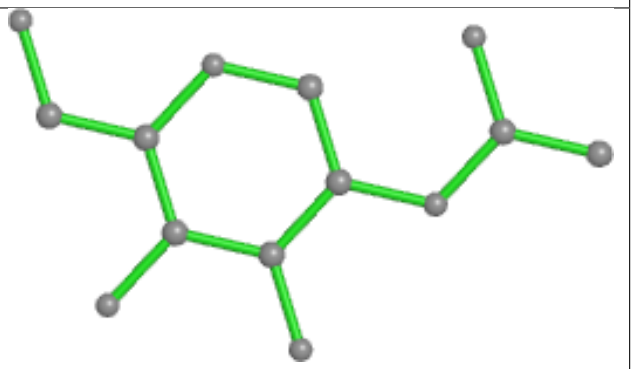
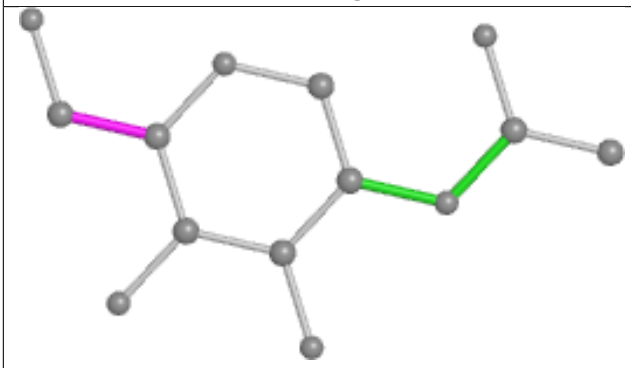
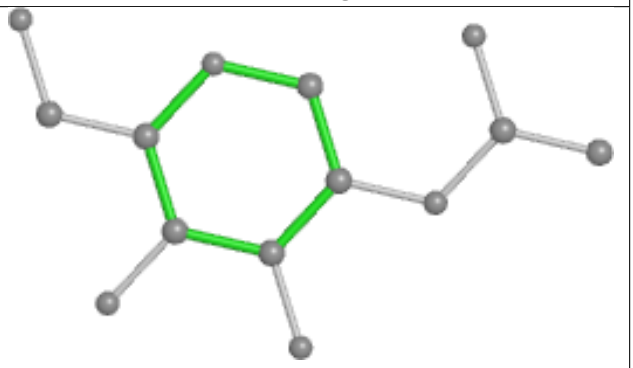


Bond angles

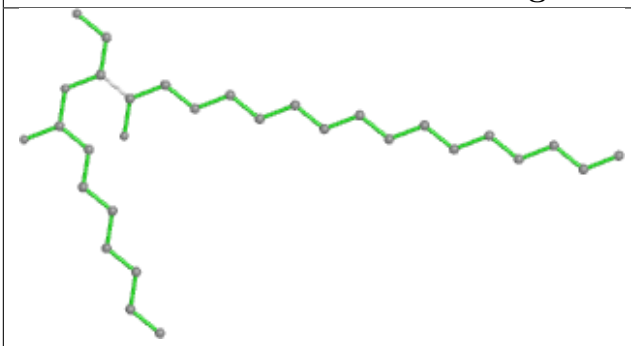


Torsions

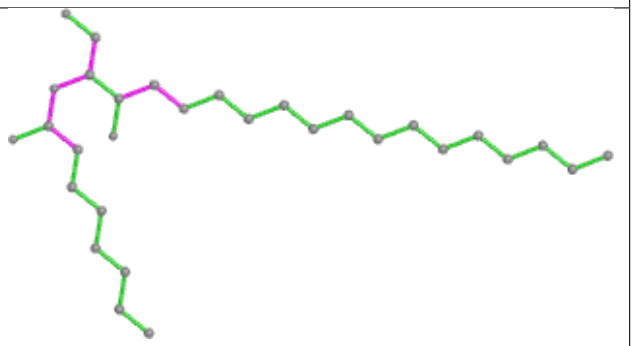


Rings

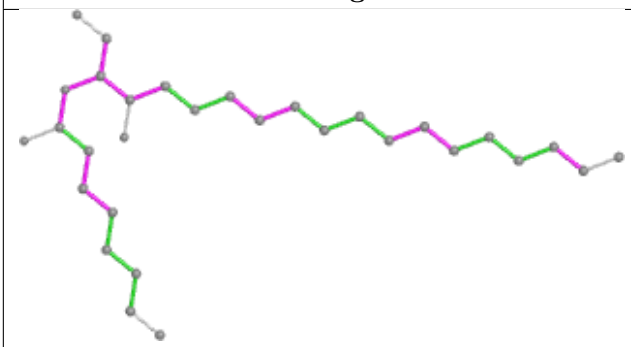
Ligand SPL B 906



Bond lengths



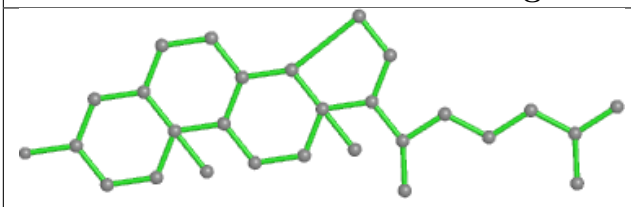
Bond angles



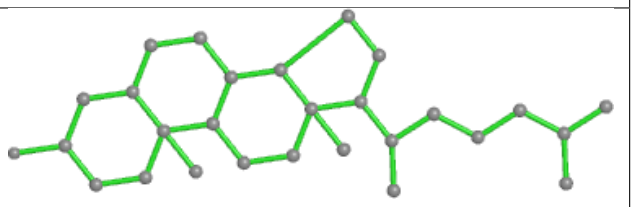
Torsions

Rings

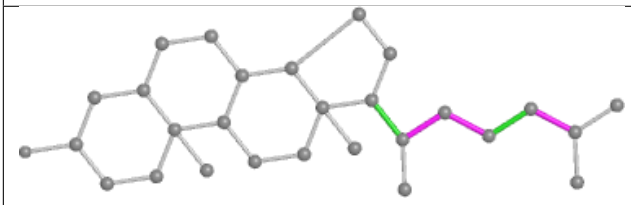
Ligand CLR A 905



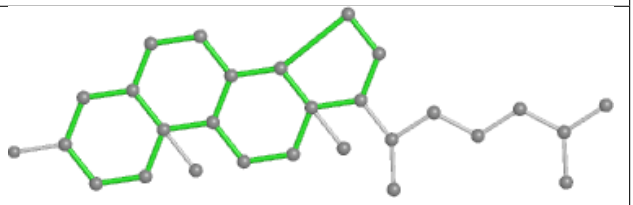
Bond lengths



Bond angles

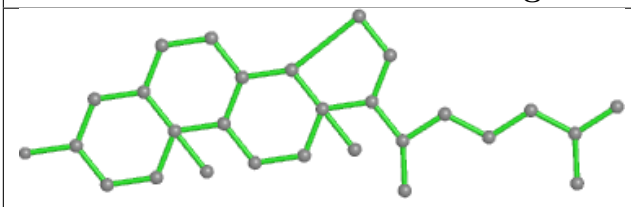


Torsions

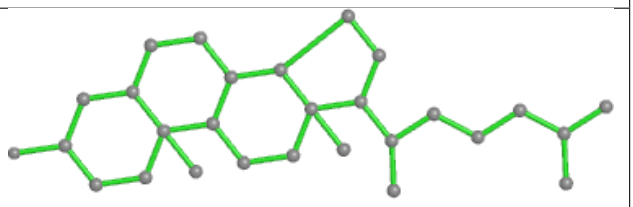


Rings

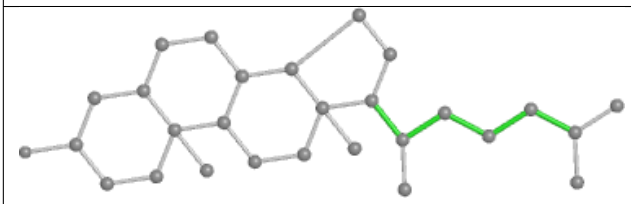
Ligand CLR A 907



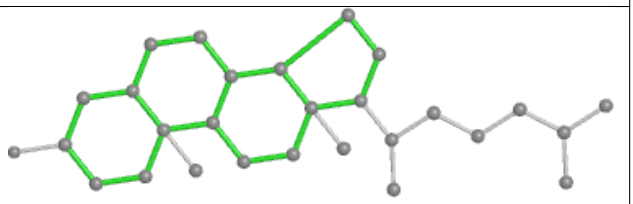
Bond lengths



Bond angles

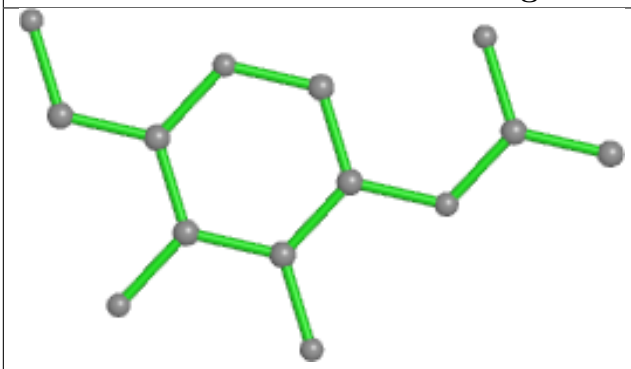


Torsions

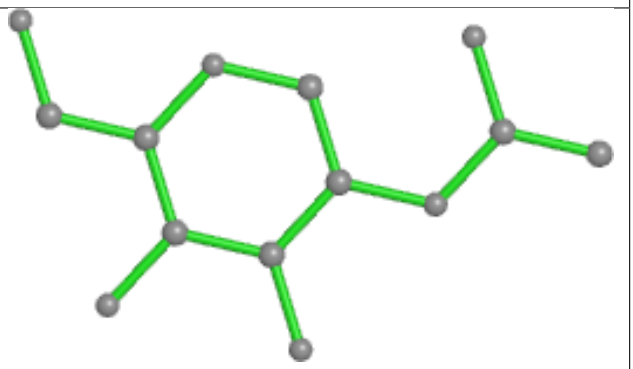


Rings

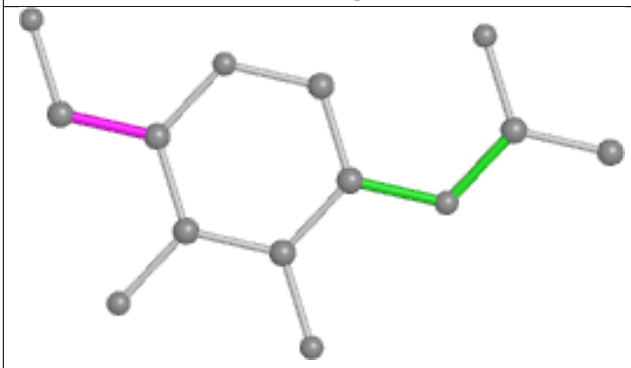
Ligand NAG B 903



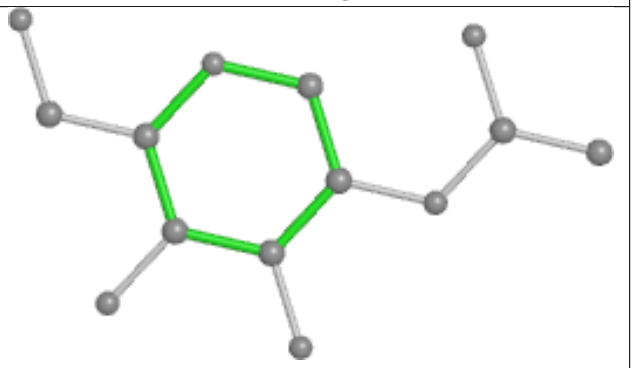
Bond lengths



Bond angles

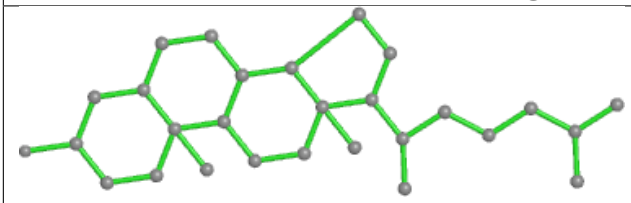


Torsions

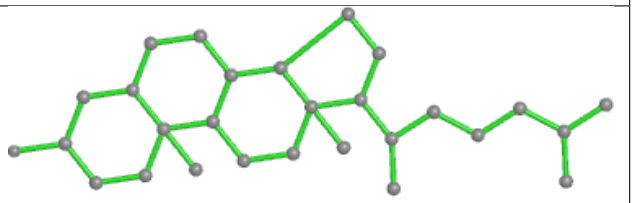


Rings

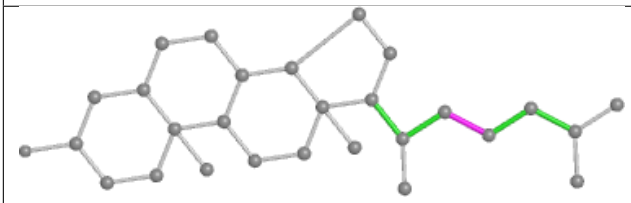
Ligand CLR B 910



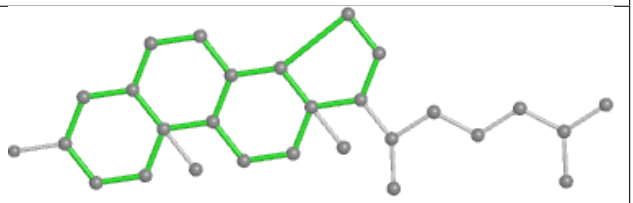
Bond lengths



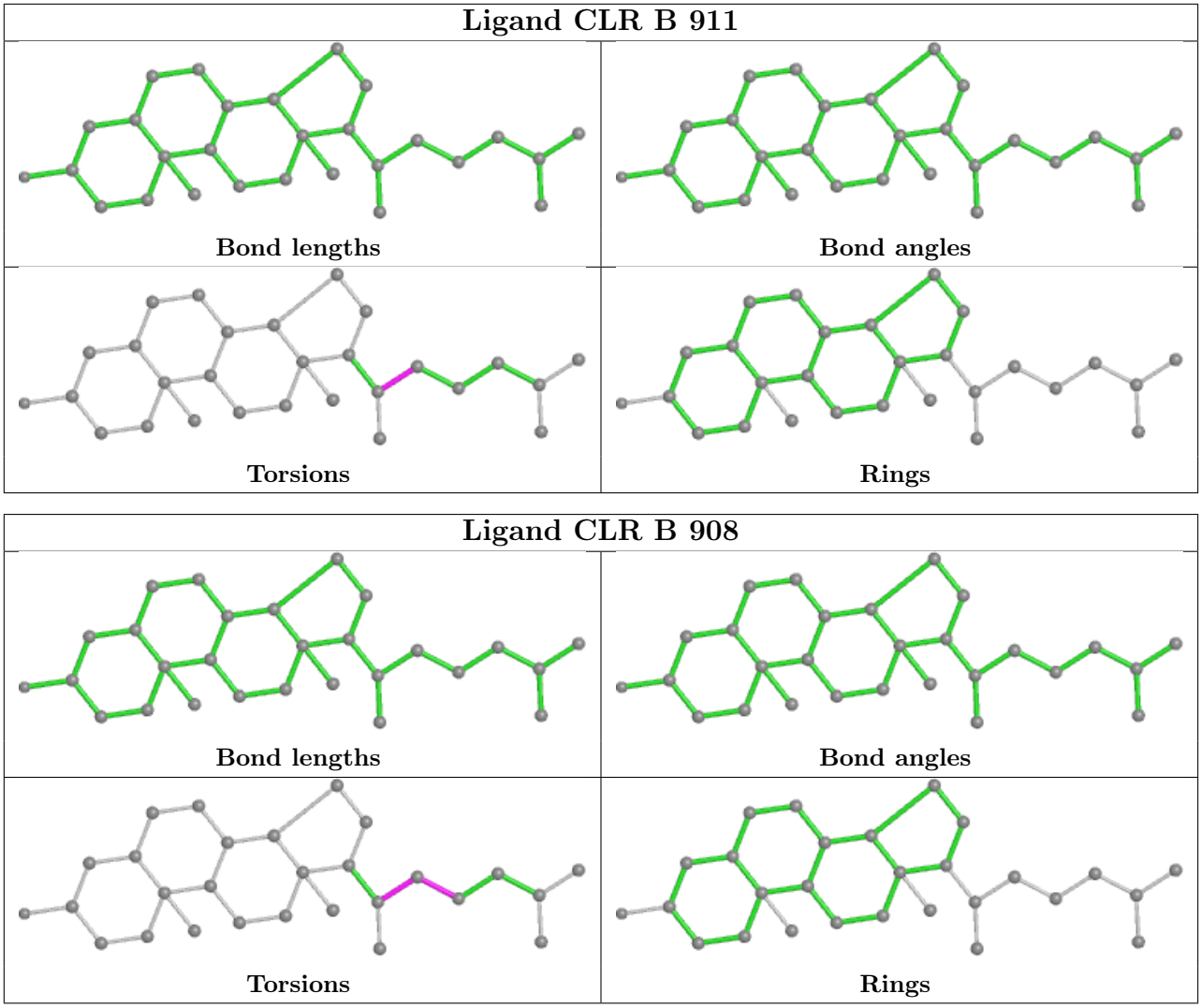
Bond angles



Torsions



Rings



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.

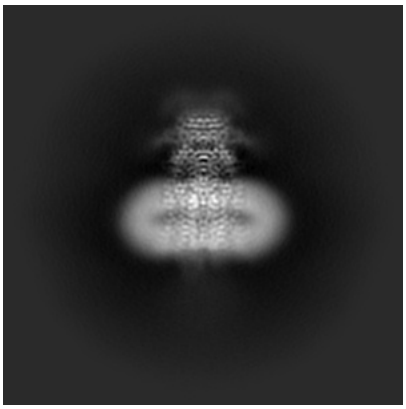
6 Map visualisation

This section contains visualisations of the EMDB entry EMD-37695. These allow visual inspection of the internal detail of the map and identification of artifacts.

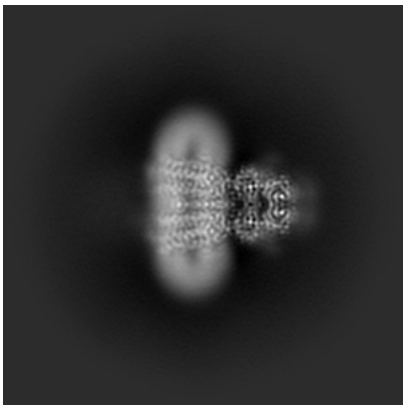
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections

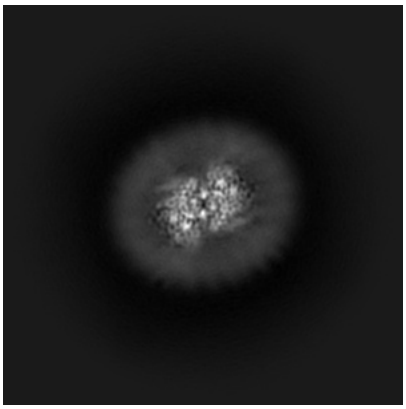
6.1.1 Primary map



X

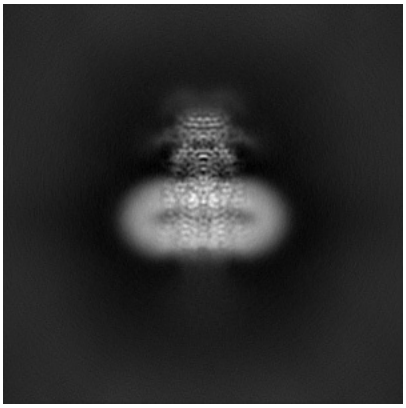


Y

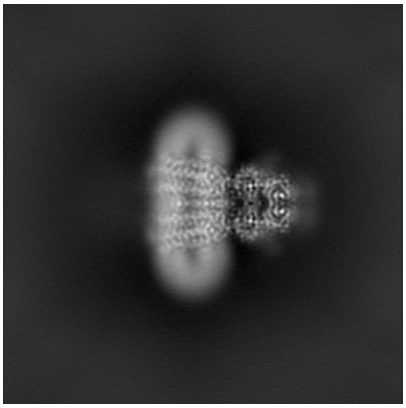


Z

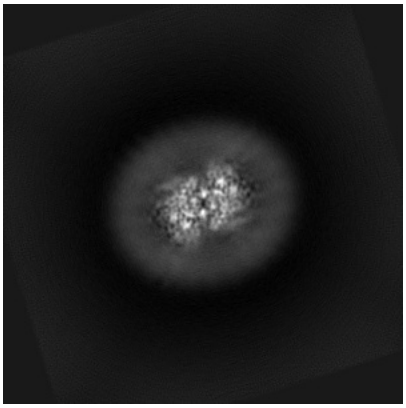
6.1.2 Raw map



X



Y



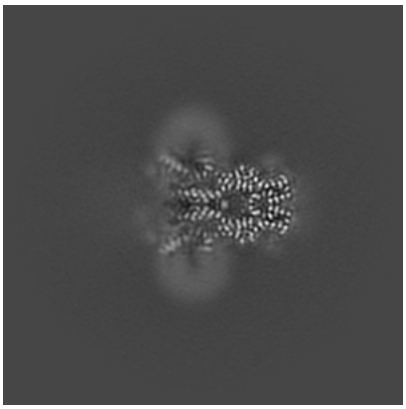
Z

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

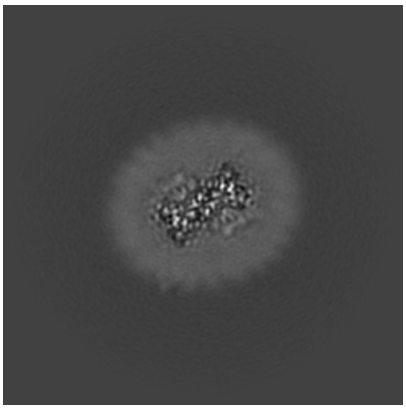
6.2 Central slices (i)

6.2.1 Primary map

X Index: 180

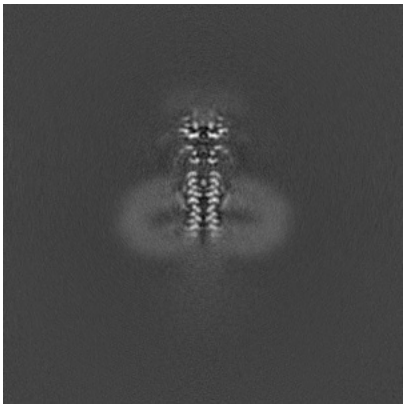


Y Index: 180

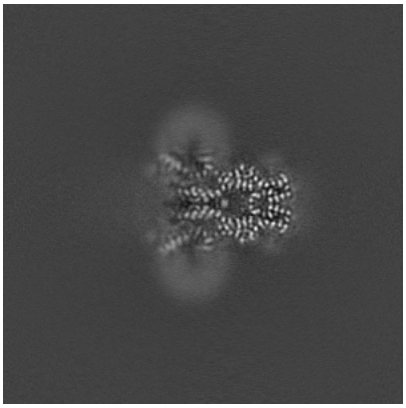


Z Index: 180

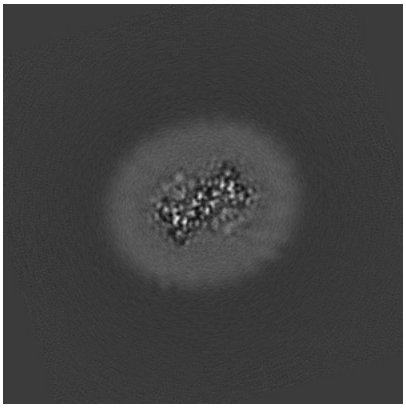
6.2.2 Raw map



X Index: 180



Y Index: 180

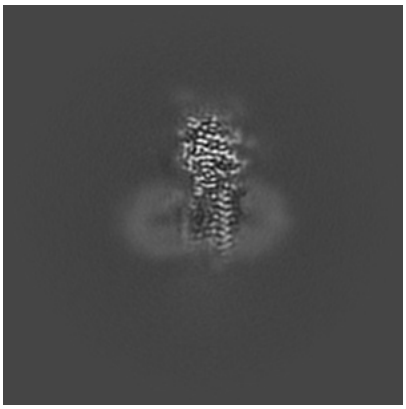


Z Index: 180

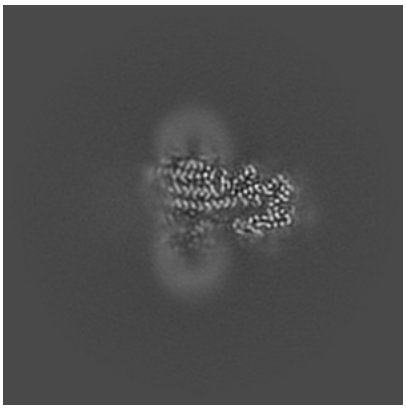
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

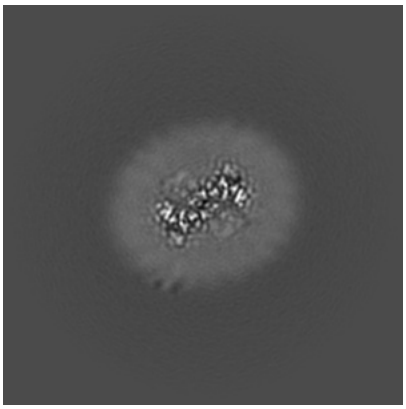
6.3.1 Primary map



X Index: 196

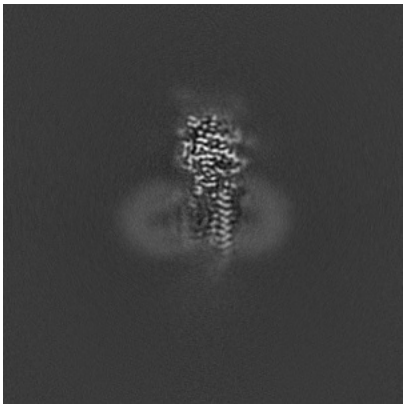


Y Index: 190

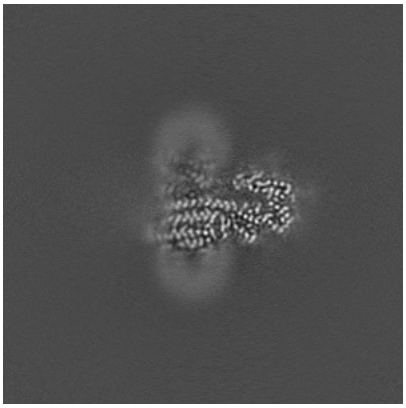


Z Index: 184

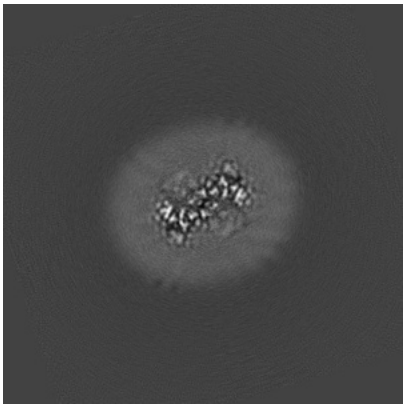
6.3.2 Raw map



X Index: 196



Y Index: 170

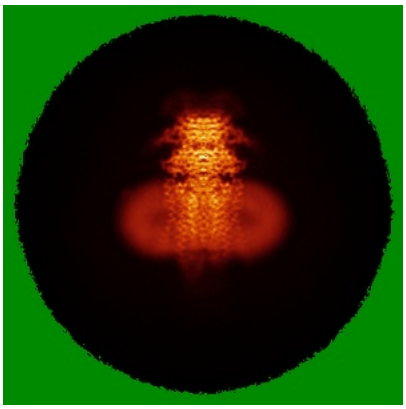


Z Index: 184

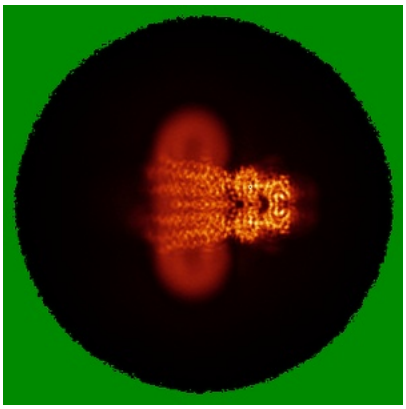
The images above show the largest variance slices of the map in three orthogonal directions.

6.4 Orthogonal standard-deviation projections (False-color) (i)

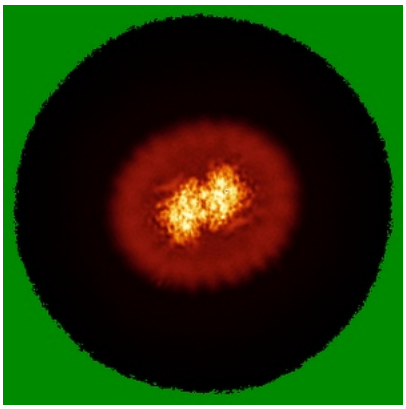
6.4.1 Primary map



X

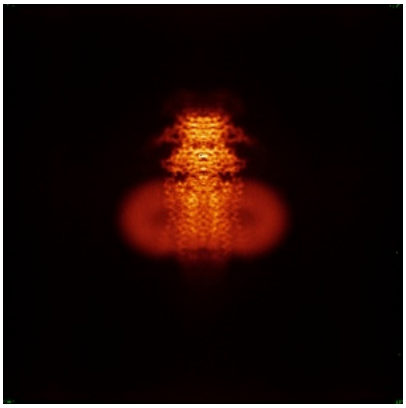


Y

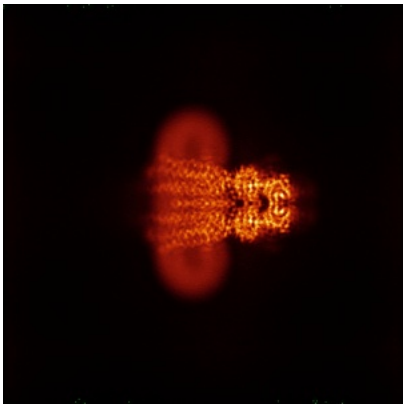


Z

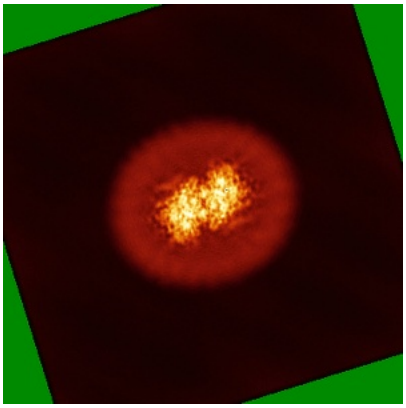
6.4.2 Raw map



X



Y



Z

The images above show the map standard deviation projections with false color in three orthogonal directions. Minimum values are shown in green, max in blue, and dark to light orange shades represent small to large values respectively.

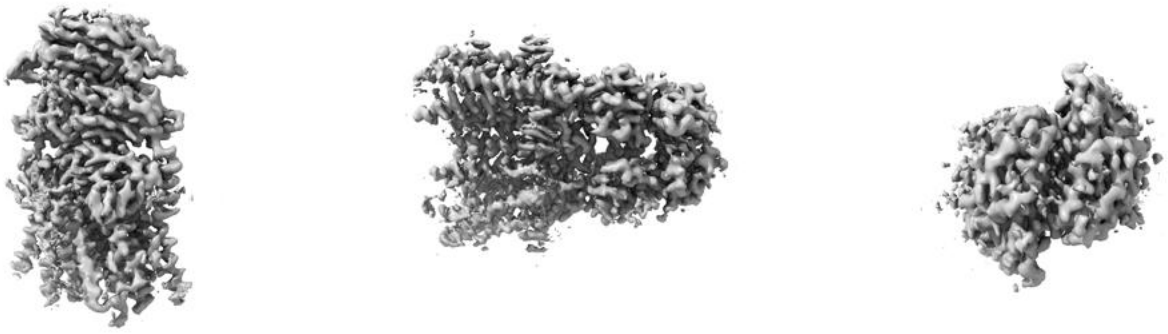
6.5 Orthogonal surface views (i)

6.5.1 Primary map

X Y Z

The images above show the 3D surface view of the map at the recommended contour level 0.1. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

6.5.2 Raw map



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.

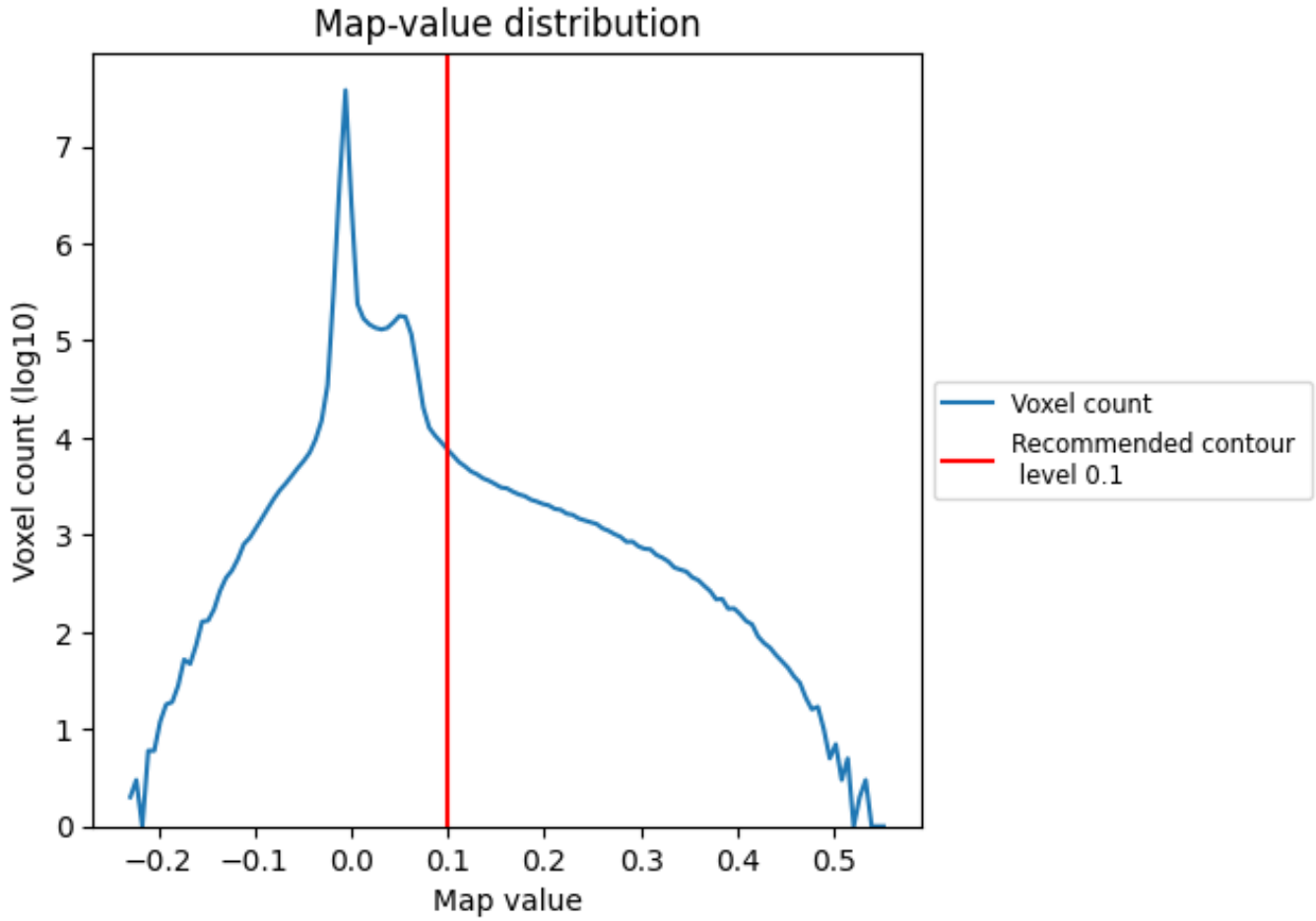
6.6 Mask visualisation (i)

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

7 Map analysis

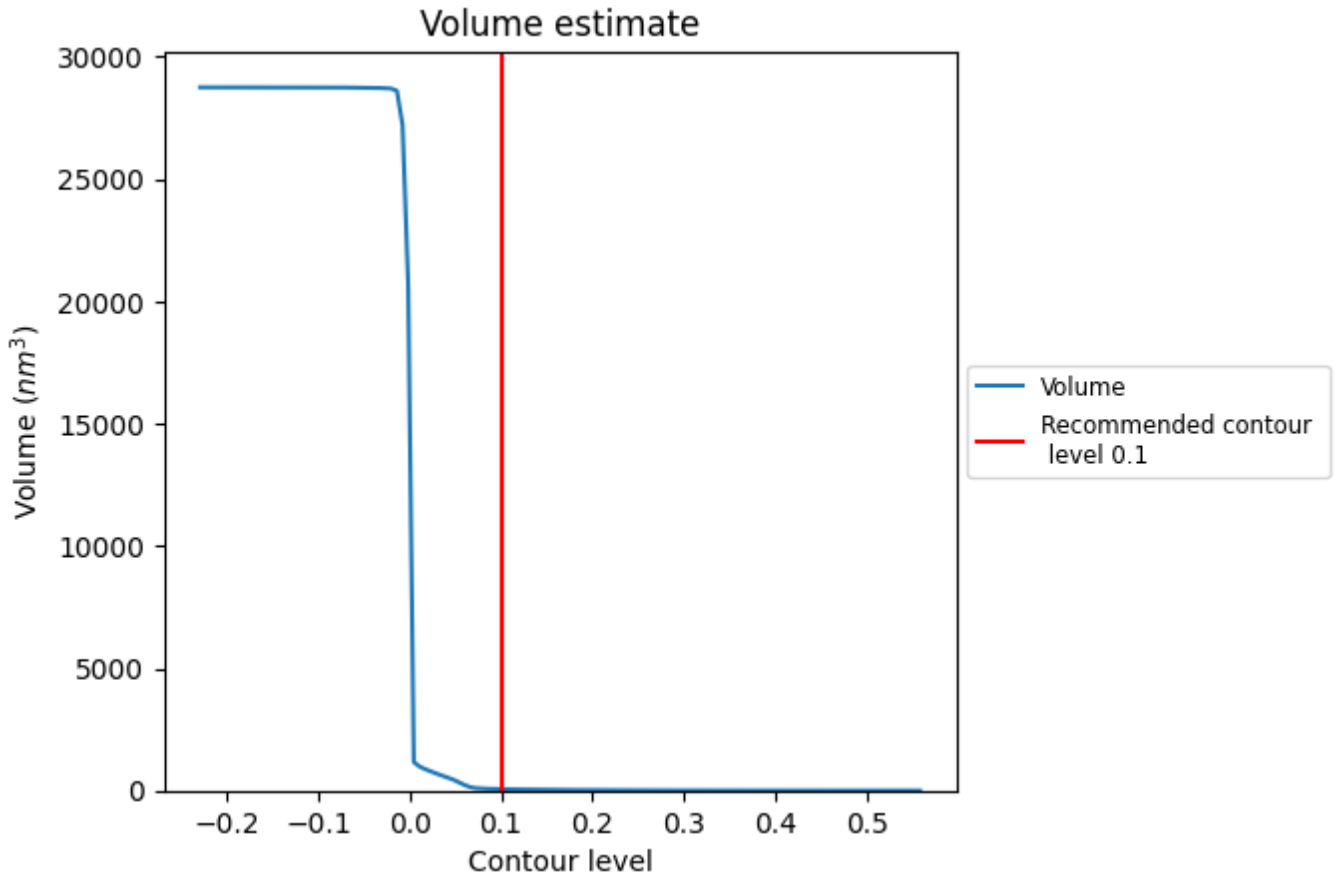
This section contains the results of statistical analysis of the map.

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.

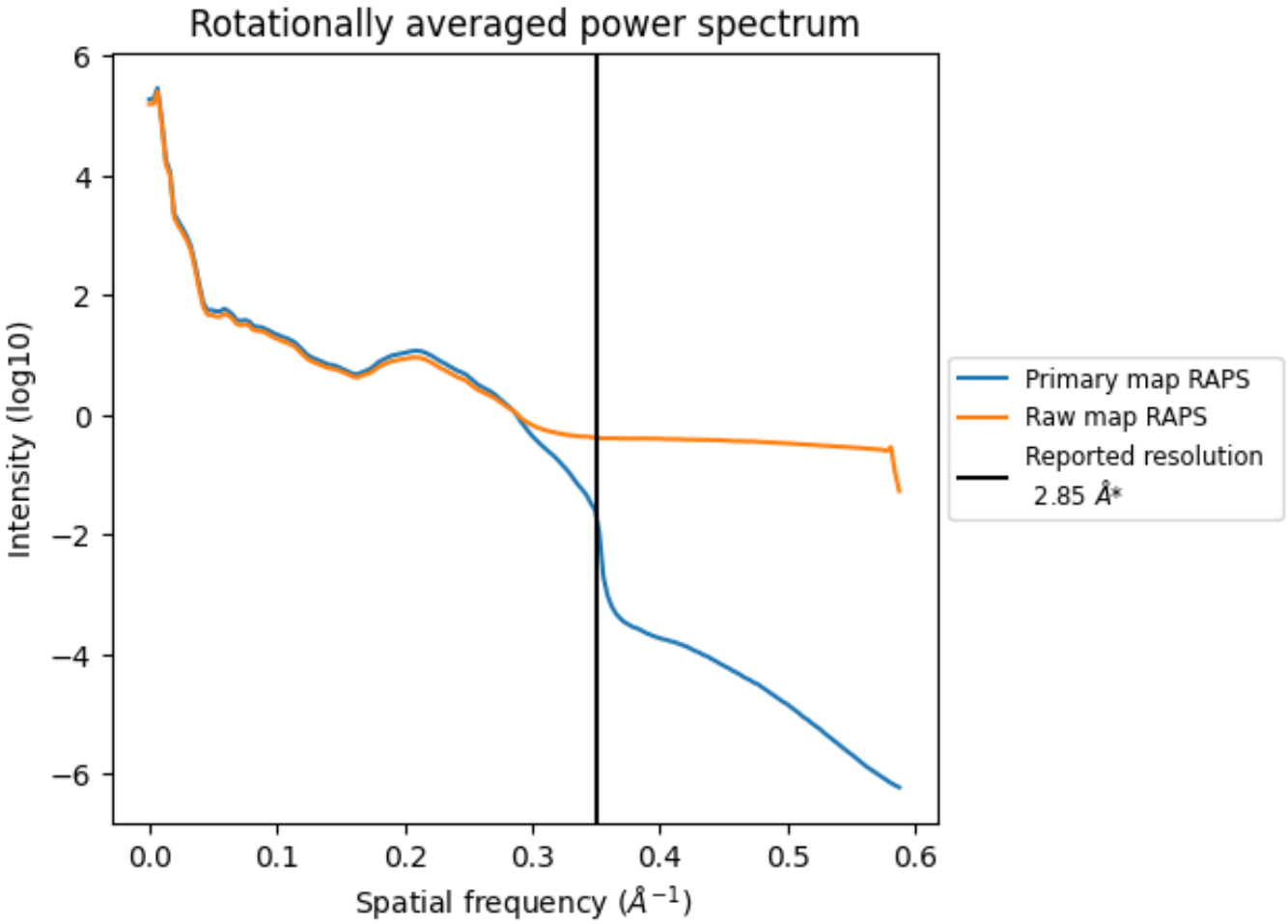
7.2 Volume estimate



The volume at the recommended contour level is 57 nm^3; this corresponds to an approximate mass of 52 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)

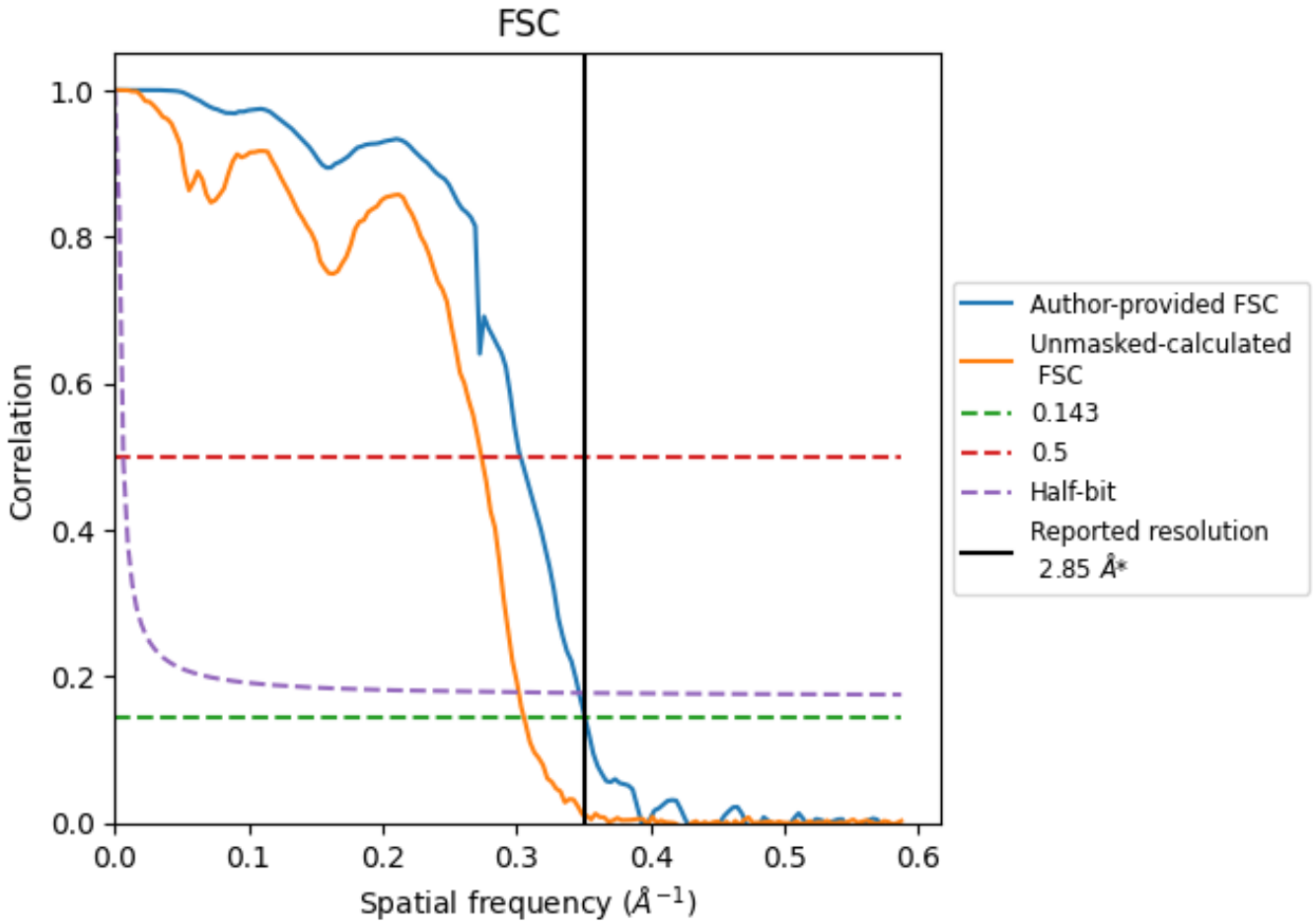


*Reported resolution corresponds to spatial frequency of 0.351 Å^{-1}

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 0.351 Å^{-1}

8.2 Resolution estimates (i)

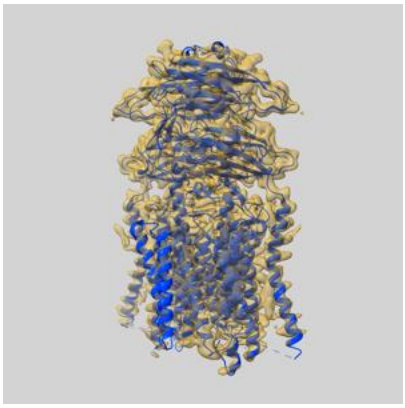
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	2.85	-	-
Author-provided FSC curve	2.85	3.30	2.88
Unmasked-calculated*	3.27	3.65	3.31

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 3.27 differs from the reported value 2.85 by more than 10 %

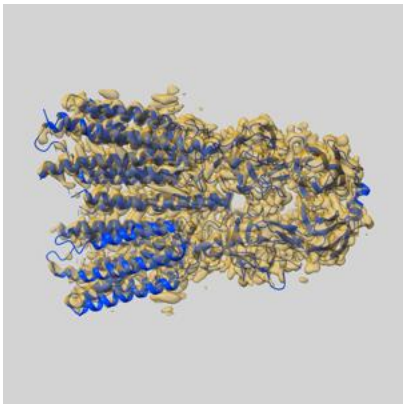
9 Map-model fit

This section contains information regarding the fit between EMDB map EMD-37695 and PDB model 8WOQ. Per-residue inclusion information can be found in section 3 on page 10.

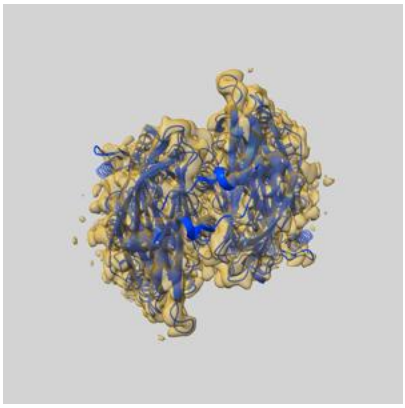
9.1 Map-model overlay



X



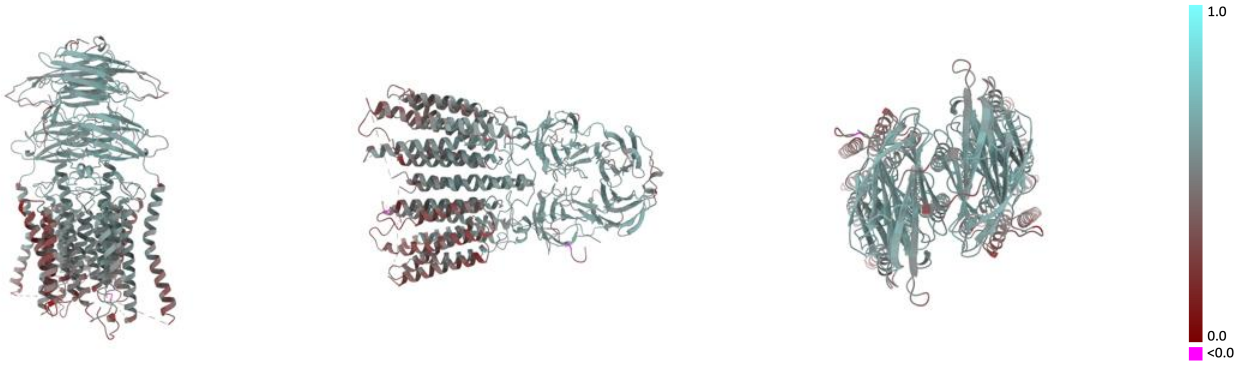
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.1 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.

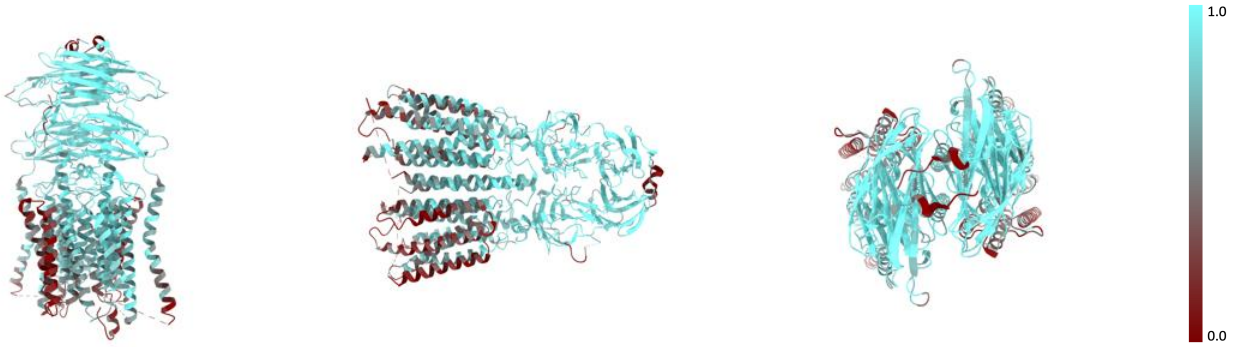
9.2 Q-score mapped to coordinate model (i)



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.

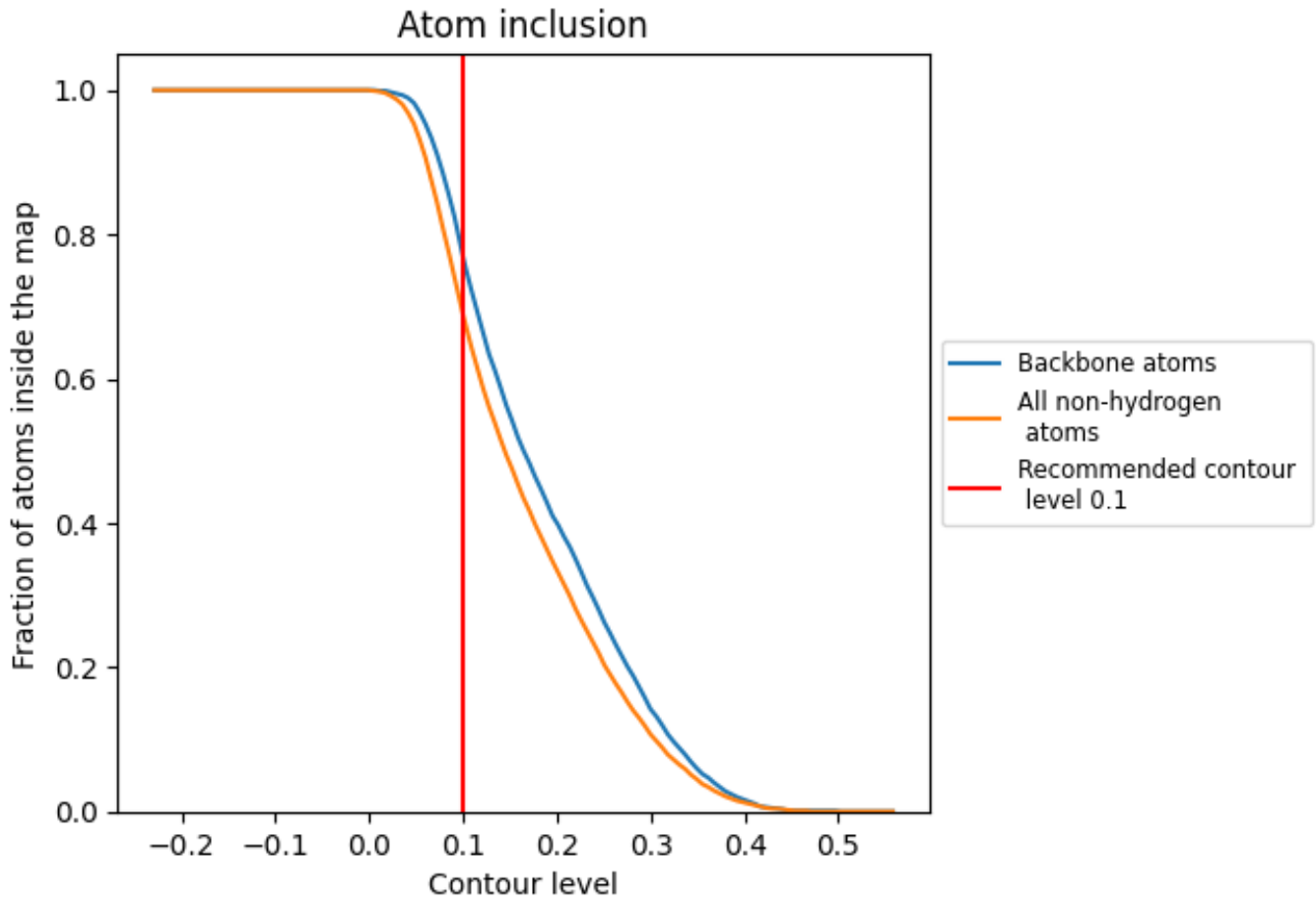
9.3 Atom inclusion mapped to coordinate model (i)



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 (0.1).

9.4 Atom inclusion (i)



At the recommended contour level, 77% of all backbone atoms, 69% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary (i)

The table lists the average atom inclusion at the recommended contour level (0.1) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.6880	0.5010
A	0.6910	0.4990
B	0.7020	0.5050
C	0.2500	0.2740
D	0.4640	0.4020
E	0.2500	0.3950
F	0.4640	0.4420