wwPDB EM Validation Summary Report

Nov 9, 2026 – 06:08 pm GMT

PDB ID	:	34OE / pdb_000034oe
EMDB ID	:	EMD-100053
Title	:	Structure of occluded B0AT1-ACE2 complex bound to Leucine
Authors	:	Pedersen, C.N.; Christensen, M.E.; Heger, T.; Shahsavar, A.; Nissen, P.; Stock, C.
Deposited on	:	2026-09-23
Resolution	:	3.05 Å(reported)
Based on initial model	:	6M18

This is a wwPDB EM Validation Summary 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 (i) 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 (i)) were used in the production of this report:

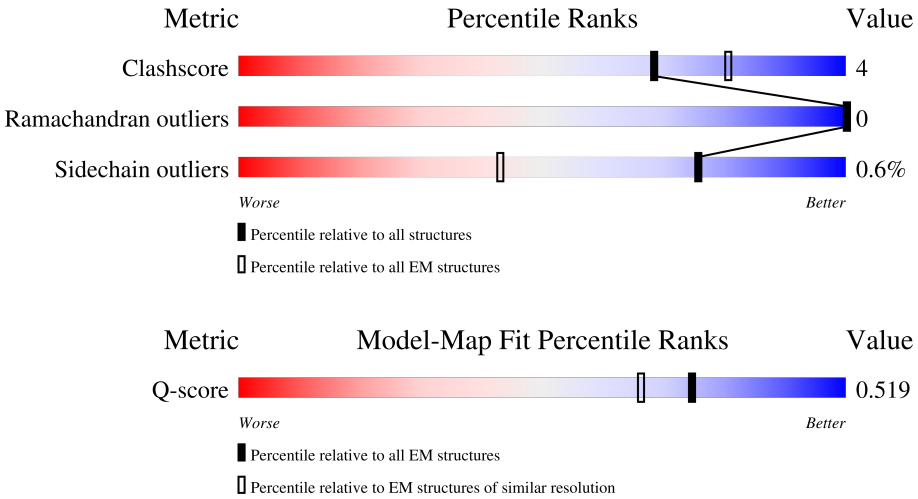
EMDB validation analysis	:	0.0.1.dev133
Mogul	:	1.8.4, CSD as541be (2020)
MolProbity	:	4-5-2 with Phenix2.2
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics	:	202505.v01 (Using data in the EMDB archive up until May 2025)
MapQ	:	1.9.13
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.51

1 Overall quality at a glance

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

The reported resolution of this entry is 3.05 Å.

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



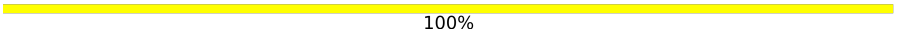
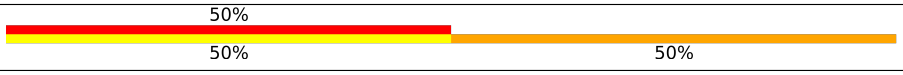
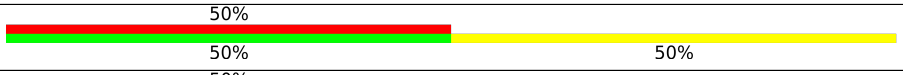
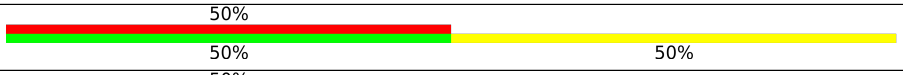
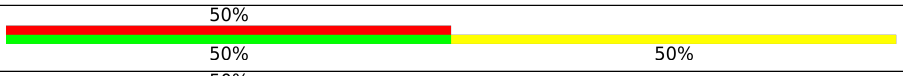
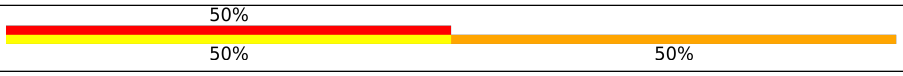
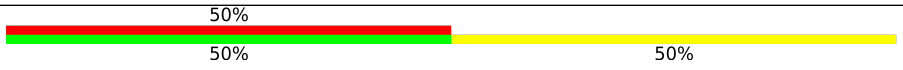
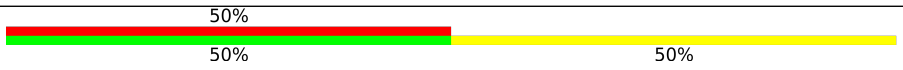
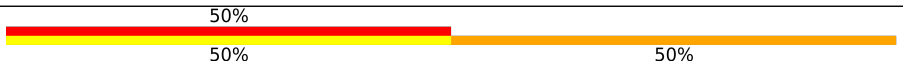
Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
Q-score	-	25397	13971 (2.55 - 3.55)

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	643	82% 13% 6%
1	B	643	86% 9% 6%
2	C	813	5% 84% 9% 7%
2	D	813	5% 87% 6% 7%

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
3	E	2	
3	F	2	
3	G	2	
3	H	2	
3	I	2	
3	K	2	
3	L	2	
3	M	2	
3	N	2	
3	P	2	
3	Q	2	
3	R	2	
4	J	3	
4	O	3	

2 Entry composition (i)

There are 9 unique types of molecules in this entry. The entry contains 45544 atoms, of which 22676 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 Sodium-dependent neutral amino acid transporter B(0)AT1.

Mol	Chain	Residues	Atoms						AltConf	Trace
1	A	606	Total	C	H	N	O	S	0	0
			9573	3174	4768	745	855	31		
1	B	606	Total	C	H	N	O	S	0	0
			9573	3174	4768	745	855	31		

There are 18 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	635	GLY	-	expression tag	UNP Q695T7
A	636	GLY	-	expression tag	UNP Q695T7
A	637	ARG	-	expression tag	UNP Q695T7
A	638	LEU	-	expression tag	UNP Q695T7
A	639	GLU	-	expression tag	UNP Q695T7
A	640	VAL	-	expression tag	UNP Q695T7
A	641	LEU	-	expression tag	UNP Q695T7
A	642	PHE	-	expression tag	UNP Q695T7
A	643	GLN	-	expression tag	UNP Q695T7
B	635	GLY	-	expression tag	UNP Q695T7
B	636	GLY	-	expression tag	UNP Q695T7
B	637	ARG	-	expression tag	UNP Q695T7
B	638	LEU	-	expression tag	UNP Q695T7
B	639	GLU	-	expression tag	UNP Q695T7
B	640	VAL	-	expression tag	UNP Q695T7
B	641	LEU	-	expression tag	UNP Q695T7
B	642	PHE	-	expression tag	UNP Q695T7
B	643	GLN	-	expression tag	UNP Q695T7

- Molecule 2 is a protein called Angiotensin-converting enzyme 2.

Mol	Chain	Residues	Atoms						AltConf	Trace
2	C	753	Total	C	H	N	O	S	0	0
			12085	3932	5952	1029	1138	34		

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms						AltConf	Trace
2	D	753	Total	C	H	N	O	S	0	0
			12085	3932	5952	1029	1138	34		

There are 18 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
C	631	ARG	LYS	engineered mutation	UNP Q9BYF1
C	806	SER	-	expression tag	UNP Q9BYF1
C	807	ARG	-	expression tag	UNP Q9BYF1
C	808	LEU	-	expression tag	UNP Q9BYF1
C	809	GLU	-	expression tag	UNP Q9BYF1
C	810	VAL	-	expression tag	UNP Q9BYF1
C	811	LEU	-	expression tag	UNP Q9BYF1
C	812	PHE	-	expression tag	UNP Q9BYF1
C	813	GLN	-	expression tag	UNP Q9BYF1
D	631	ARG	LYS	engineered mutation	UNP Q9BYF1
D	806	SER	-	expression tag	UNP Q9BYF1
D	807	ARG	-	expression tag	UNP Q9BYF1
D	808	LEU	-	expression tag	UNP Q9BYF1
D	809	GLU	-	expression tag	UNP Q9BYF1
D	810	VAL	-	expression tag	UNP Q9BYF1
D	811	LEU	-	expression tag	UNP Q9BYF1
D	812	PHE	-	expression tag	UNP Q9BYF1
D	813	GLN	-	expression tag	UNP Q9BYF1

- Molecule 3 is an oligosaccharide called 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose.



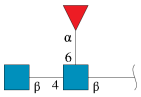
Mol	Chain	Residues	Atoms					AltConf	Trace
3	E	2	Total	C	H	N	O	0	0
			55	16	27	2	10		
3	F	2	Total	C	H	N	O	0	0
			55	16	27	2	10		
3	G	2	Total	C	H	N	O	0	0
			55	16	27	2	10		
3	H	2	Total	C	H	N	O	0	0
			55	16	27	2	10		

Continued on next page...

Continued from previous page...

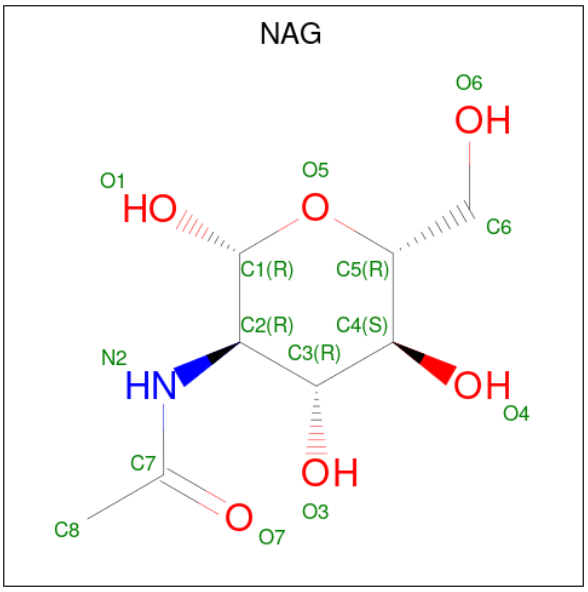
Mol	Chain	Residues	Atoms					AltConf	Trace
3	I	2	Total	C	H	N	O	0	0
			55	16	27	2	10		
3	K	2	Total	C	H	N	O	0	0
			55	16	27	2	10		
3	L	2	Total	C	H	N	O	0	0
			55	16	27	2	10		
3	M	2	Total	C	H	N	O	0	0
			55	16	27	2	10		
3	N	2	Total	C	H	N	O	0	0
			55	16	27	2	10		
3	P	2	Total	C	H	N	O	0	0
			55	16	27	2	10		
3	Q	2	Total	C	H	N	O	0	0
			55	16	27	2	10		
3	R	2	Total	C	H	N	O	0	0
			55	16	27	2	10		

- Molecule 4 is an oligosaccharide called 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-[alpha-L-fucopyranose-(1-6)]2-acetamido-2-deoxy-beta-D-glucopyranose.



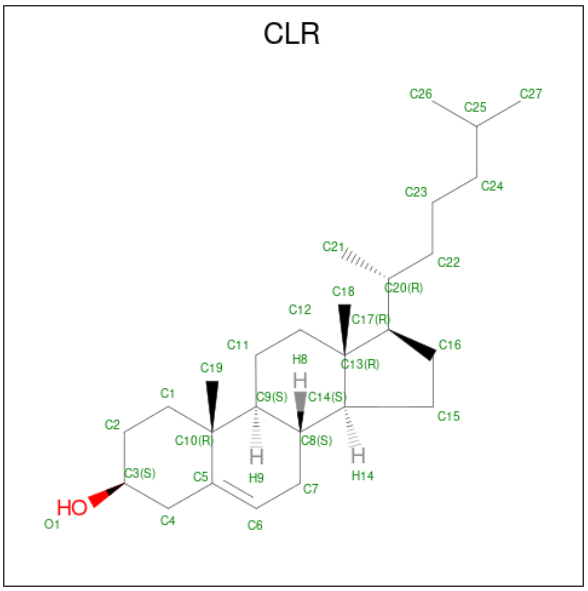
Mol	Chain	Residues	Atoms					AltConf	Trace
4	J	3	Total	C	H	N	O	0	0
			75	22	37	2	14		
4	O	3	Total	C	H	N	O	0	0
			75	22	37	2	14		

- Molecule 5 is 2-acetamido-2-deoxy-beta-D-glucopyranose (CCD ID: NAG) (formula: $C_8H_{15}NO_6$).



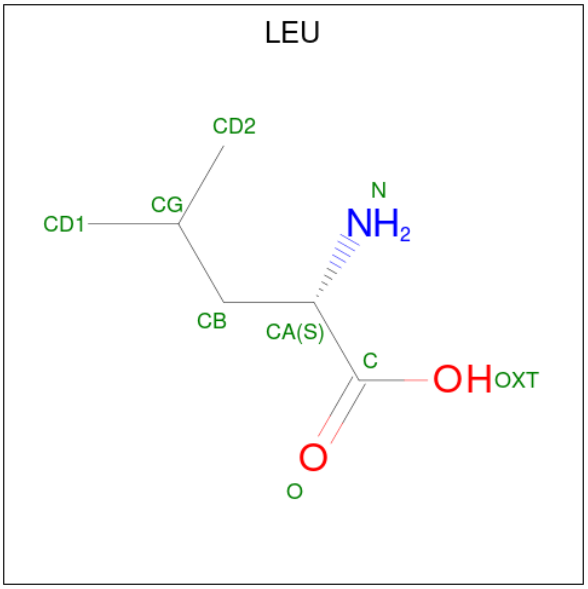
Mol	Chain	Residues	Atoms					AltConf
5	A	1	Total	C	H	N	O	0
			28	8	14	1	5	
5	A	1	Total	C	H	N	O	0
			28	8	14	1	5	
5	A	1	Total	C	H	N	O	0
			28	8	14	1	5	
5	B	1	Total	C	H	N	O	0
			28	8	14	1	5	
5	B	1	Total	C	H	N	O	0
			28	8	14	1	5	
5	B	1	Total	C	H	N	O	0
			28	8	14	1	5	
5	C	1	Total	C	H	N	O	0
			28	8	14	1	5	
5	C	1	Total	C	H	N	O	0
			28	8	14	1	5	
5	D	1	Total	C	H	N	O	0
			28	8	14	1	5	
5	D	1	Total	C	H	N	O	0
			28	8	14	1	5	

- Molecule 6 is CHOLESTEROL (CCD ID: CLR) (formula: $C_{27}H_{46}O$).



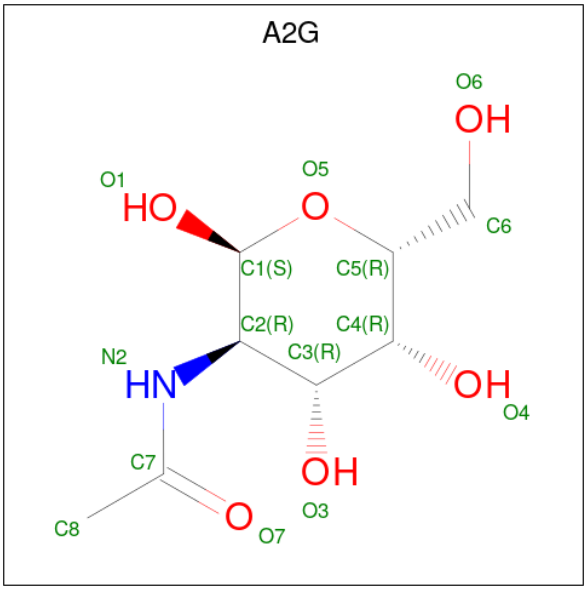
Mol	Chain	Residues	Atoms				AltConf
6	A	1	Total	C	H	O	0
			74	27	46	1	
6	A	1	Total	C	H	O	0
			74	27	46	1	
6	A	1	Total	C	H	O	0
			74	27	46	1	
6	A	1	Total	C	H	O	0
			74	27	46	1	
6	A	1	Total	C	H	O	0
			74	27	46	1	
6	A	1	Total	C	H	O	0
			74	27	46	1	
6	A	1	Total	C	H	O	0
			74	27	46	1	
6	B	1	Total	C	H	O	0
			74	27	46	1	
6	B	1	Total	C	H	O	0
			74	27	46	1	
6	B	1	Total	C	H	O	0
			74	27	46	1	
6	B	1	Total	C	H	O	0
			74	27	46	1	
6	B	1	Total	C	H	O	0
			74	27	46	1	
6	B	1	Total	C	H	O	0
			74	27	46	1	
6	B	1	Total	C	H	O	0
			74	27	46	1	

- Molecule 7 is LEUCINE (CCD ID: LEU) (formula: $C_6H_{13}NO_2$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms					AltConf
7	A	1	Total	C	H	N	O	0
			22	6	13	1	2	
7	B	1	Total	C	H	N	O	0
			22	6	13	1	2	

- Molecule 8 is 2-acetamido-2-deoxy-alpha-D-galactopyranose (CCD ID: A2G) (formula: $C_8H_{15}NO_6$).



Mol	Chain	Residues	Atoms					AltConf
8	C	1	Total	C	H	N	O	0
			28	8	14	1	5	
8	D	1	Total	C	H	N	O	0
			28	8	14	1	5	

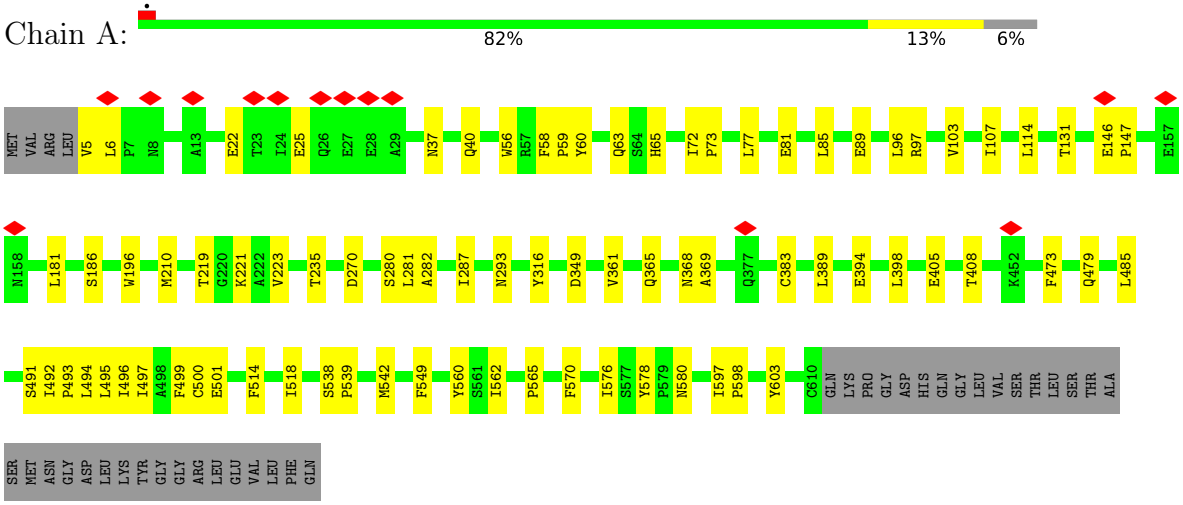
- Molecule 9 is ZINC ION (CCD ID: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		AltConf
9	C	1	Total	Zn	0
			1	1	
9	D	1	Total	Zn	0
			1	1	

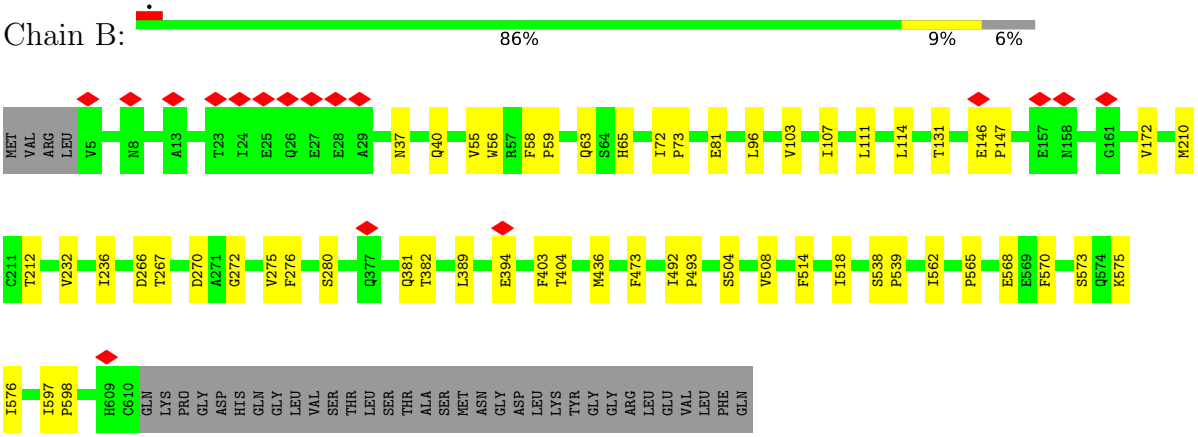
3 Residue-property plots

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

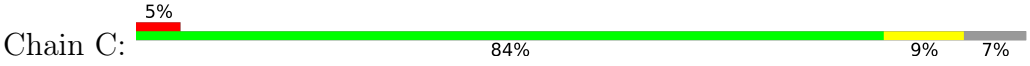
• Molecule 1: Sodium-dependent neutral amino acid transporter B(0)AT1

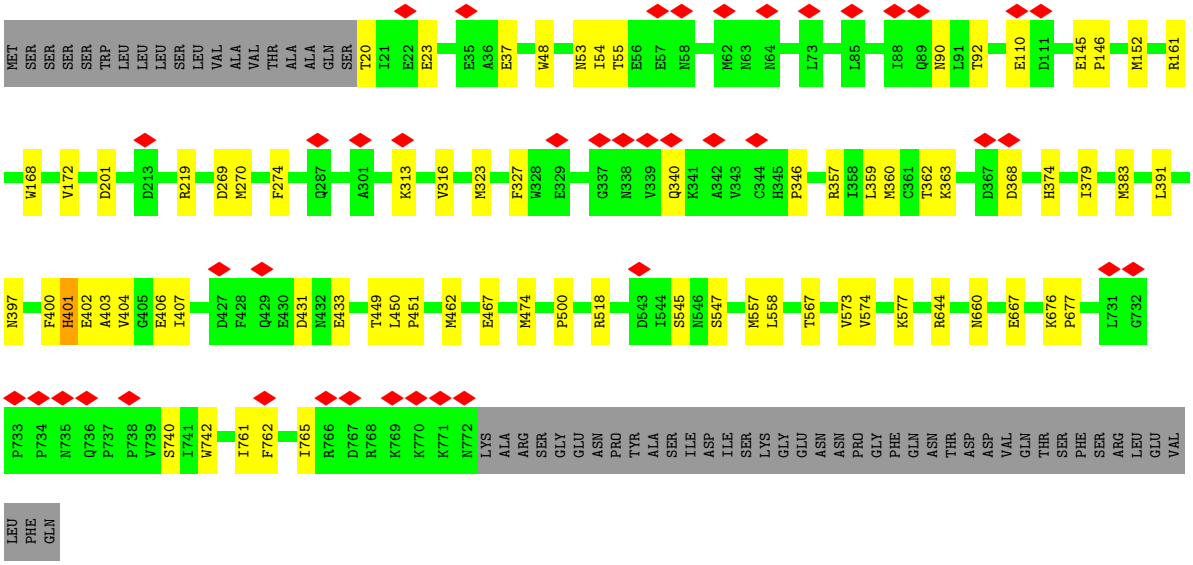


• Molecule 1: Sodium-dependent neutral amino acid transporter B(0)AT1

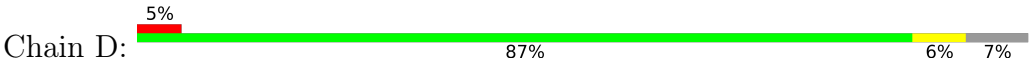


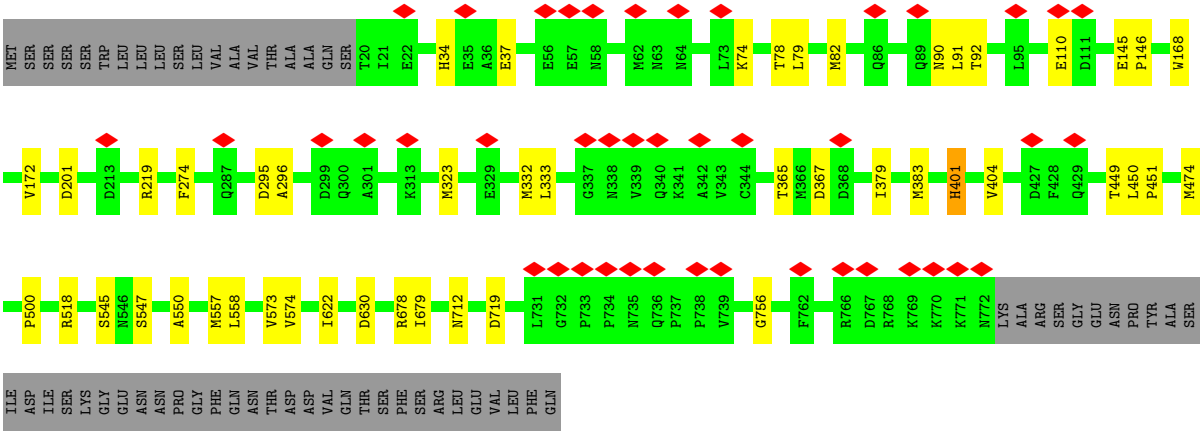
• Molecule 2: Angiotensin-converting enzyme 2





• Molecule 2: Angiotensin-converting enzyme 2





• Molecule 3: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose





• Molecule 3: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose





• Molecule 3: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain G:





• Molecule 3: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain H:





• Molecule 3: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain I:





• Molecule 3: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain K:





• Molecule 3: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain L:





• Molecule 3: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain M:





• Molecule 3: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain N:





• Molecule 3: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain P:





• Molecule 3: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain Q:





• Molecule 3: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain R:





• Molecule 4: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-[alpha-L-fucopyranose-(1-6)]2-acetamido-2-deoxy-beta-D-glucopyranose

Chain J:





• Molecule 4: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-[alpha-L-fucopyranose-(1-6)]2-acetamido-2-deoxy-beta-D-glucopyranose

Chain O:





4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	90776	Depositor
Resolution determination method	OTHER	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	TFS KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/Å^2$)	59.3	Depositor
Minimum defocus (nm)	800	Depositor
Maximum defocus (nm)	2000	Depositor
Magnification	130000	Depositor
Image detector	GATAN K3 (6k x 4k)	Depositor
Maximum map value	46.483	Depositor
Minimum map value	-32.741	Depositor
Average map value	0.003	Depositor
Map value standard deviation	1.277	Depositor
Recommended contour level	6	Depositor
Map size (Å)	310.56, 310.56, 310.56	wwPDB
Map dimensions	300, 300, 300	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.0352, 1.0352, 1.0352	Depositor

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: A2G, FUC, NAG, ZN, CLR

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	0.19	0/4946	0.42	0/6756
1	B	0.18	0/4946	0.42	0/6756
2	C	0.16	0/6296	0.41	0/8545
2	D	0.16	0/6296	0.40	0/8545
All	All	0.17	0/22484	0.41	0/30602

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	4805	4768	4767	52	0
1	B	4805	4768	4767	37	0
2	C	6133	5952	5951	47	0
2	D	6133	5952	5951	29	0
3	E	28	27	25	0	0
3	F	28	27	25	1	0
3	G	28	27	25	0	0
3	H	28	27	25	0	0
3	I	28	27	25	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	K	28	27	25	0	0
3	L	28	27	25	1	0
3	M	28	27	25	0	0
3	N	28	27	25	0	0
3	P	28	27	25	0	0
3	Q	28	27	25	1	0
3	R	28	27	25	0	0
4	J	38	37	34	0	0
4	O	38	37	34	0	0
5	A	42	42	39	2	0
5	B	42	42	39	0	0
5	C	28	28	26	1	0
5	D	28	28	26	0	0
6	A	196	322	322	7	0
6	B	196	322	322	1	0
7	A	9	13	10	0	0
7	B	9	13	10	2	0
8	C	14	14	12	0	0
8	D	14	14	12	0	0
9	C	1	0	0	0	0
9	D	1	0	0	0	0
All	All	22868	22676	22622	168	0

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

The worst 5 of 168 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)
2:D:379:ILE:O	2:D:383:MET:HG3	1.95	0.66
2:C:740:SER:HG	2:C:742:TRP:CD1	2.13	0.66
2:C:379:ILE:O	2:C:383:MET:HG3	2.00	0.62
2:C:323:MET:HE1	2:C:379:ILE:HG21	1.83	0.61
1:A:37:ASN:OD1	1:A:40:GLN:N	2.32	0.60

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	604/643 (94%)	582 (96%)	22 (4%)	0	100	100
1	B	604/643 (94%)	585 (97%)	19 (3%)	0	100	100
2	C	751/813 (92%)	730 (97%)	21 (3%)	0	100	100
2	D	751/813 (92%)	731 (97%)	20 (3%)	0	100	100
All	All	2710/2912 (93%)	2628 (97%)	82 (3%)	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	532/563 (94%)	526 (99%)	6 (1%)	65	76
1	B	532/563 (94%)	529 (99%)	3 (1%)	78	81
2	C	667/719 (93%)	665 (100%)	2 (0%)	86	85
2	D	667/719 (93%)	664 (100%)	3 (0%)	84	84
All	All	2398/2564 (94%)	2384 (99%)	14 (1%)	76	81

5 of 14 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	381	GLN
1	B	403	PHE
2	D	678	ARG

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
2	D	91	LEU
2	D	401	HIS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 38 such sidechains are listed below:

Mol	Chain	Res	Type
2	D	250	ASN
2	D	682	ASN
2	D	277	ASN
2	D	599	ASN
2	D	736	GLN

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates (i)

30 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	$\#\|Z\| > 2$
3	NAG	E	1	3,1	14,14,15	0.72	0	17,19,21	0.94	1 (5%)
3	NAG	E	2	3	14,14,15	0.71	0	17,19,21	1.00	1 (5%)
3	NAG	F	1	3,1	14,14,15	0.72	0	17,19,21	1.53	2 (11%)
3	NAG	F	2	3	14,14,15	0.66	0	17,19,21	0.88	1 (5%)
3	NAG	G	1	3,1	14,14,15	0.72	0	17,19,21	0.98	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
3	NAG	G	2	3	14,14,15	0.70	0	17,19,21	0.96	1 (5%)
3	NAG	H	1	3,1	14,14,15	0.74	0	17,19,21	0.88	1 (5%)
3	NAG	H	2	3	14,14,15	0.70	0	17,19,21	0.85	0
3	NAG	I	1	3,2	14,14,15	0.71	0	17,19,21	0.90	0
3	NAG	I	2	3	14,14,15	0.67	0	17,19,21	1.11	1 (5%)
4	NAG	J	1	4,2	14,14,15	0.81	0	17,19,21	0.94	0
4	NAG	J	2	4	14,14,15	0.67	0	17,19,21	1.11	1 (5%)
4	FUC	J	3	4	10,10,11	0.78	0	14,14,16	0.76	1 (7%)
3	NAG	K	1	3,2	14,14,15	0.73	0	17,19,21	0.90	0
3	NAG	K	2	3	14,14,15	0.67	0	17,19,21	0.98	1 (5%)
3	NAG	L	1	3,2	14,14,15	0.69	0	17,19,21	1.50	3 (17%)
3	NAG	L	2	3	14,14,15	0.71	0	17,19,21	1.60	2 (11%)
3	NAG	M	1	3,2	14,14,15	0.74	0	17,19,21	0.84	0
3	NAG	M	2	3	14,14,15	0.68	0	17,19,21	0.95	1 (5%)
3	NAG	N	1	3,2	14,14,15	0.70	0	17,19,21	0.90	0
3	NAG	N	2	3	14,14,15	0.69	0	17,19,21	1.14	1 (5%)
4	NAG	O	1	4,2	14,14,15	0.80	0	17,19,21	0.86	0
4	NAG	O	2	4	14,14,15	0.68	0	17,19,21	1.07	1 (5%)
4	FUC	O	3	4	10,10,11	0.79	0	14,14,16	0.70	1 (7%)
3	NAG	P	1	3,2	14,14,15	0.71	0	17,19,21	0.81	0
3	NAG	P	2	3	14,14,15	0.66	0	17,19,21	1.05	1 (5%)
3	NAG	Q	1	3,2	14,14,15	0.69	0	17,19,21	0.94	1 (5%)
3	NAG	Q	2	3	14,14,15	0.67	0	17,19,21	0.98	1 (5%)
3	NAG	R	1	3,2	14,14,15	0.73	0	17,19,21	0.81	0
3	NAG	R	2	3	14,14,15	0.68	0	17,19,21	0.99	1 (5%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	NAG	E	1	3,1	-	1/6/23/26	0/1/1/1
3	NAG	E	2	3	-	1/6/23/26	0/1/1/1
3	NAG	F	1	3,1	-	1/6/23/26	0/1/1/1
3	NAG	F	2	3	-	0/6/23/26	0/1/1/1
3	NAG	G	1	3,1	-	2/6/23/26	0/1/1/1
3	NAG	G	2	3	-	1/6/23/26	0/1/1/1
3	NAG	H	1	3,1	-	0/6/23/26	0/1/1/1

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	NAG	H	2	3	-	2/6/23/26	0/1/1/1
3	NAG	I	1	3,2	-	2/6/23/26	0/1/1/1
3	NAG	I	2	3	-	2/6/23/26	0/1/1/1
4	NAG	J	1	4,2	-	0/6/23/26	0/1/1/1
4	NAG	J	2	4	-	0/6/23/26	0/1/1/1
4	FUC	J	3	4	-	-	0/1/1/1
3	NAG	K	1	3,2	-	0/6/23/26	0/1/1/1
3	NAG	K	2	3	-	0/6/23/26	0/1/1/1
3	NAG	L	1	3,2	-	0/6/23/26	0/1/1/1
3	NAG	L	2	3	-	0/6/23/26	0/1/1/1
3	NAG	M	1	3,2	-	0/6/23/26	0/1/1/1
3	NAG	M	2	3	-	0/6/23/26	0/1/1/1
3	NAG	N	1	3,2	-	2/6/23/26	0/1/1/1
3	NAG	N	2	3	-	2/6/23/26	0/1/1/1
4	NAG	O	1	4,2	-	0/6/23/26	0/1/1/1
4	NAG	O	2	4	-	0/6/23/26	0/1/1/1
4	FUC	O	3	4	-	-	0/1/1/1
3	NAG	P	1	3,2	-	0/6/23/26	0/1/1/1
3	NAG	P	2	3	-	0/6/23/26	0/1/1/1
3	NAG	Q	1	3,2	-	0/6/23/26	0/1/1/1
3	NAG	Q	2	3	-	0/6/23/26	0/1/1/1
3	NAG	R	1	3,2	-	0/6/23/26	0/1/1/1
3	NAG	R	2	3	-	0/6/23/26	0/1/1/1

There are no bond length outliers.

The worst 5 of 24 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	F	1	NAG	C1-O5-C5	4.11	117.76	112.19
3	L	2	NAG	C1-O5-C5	3.79	117.32	112.19
4	J	2	NAG	C1-O5-C5	3.52	116.96	112.19
4	O	2	NAG	C1-O5-C5	3.40	116.79	112.19
3	L	1	NAG	C1-O5-C5	3.37	116.76	112.19

There are no chirality outliers.

5 of 16 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	N	1	NAG	C1-C2-N2-C7
3	E	2	NAG	C3-C2-N2-C7

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
3	G	2	NAG	C3-C2-N2-C7
3	H	2	NAG	C3-C2-N2-C7
3	I	2	NAG	C3-C2-N2-C7

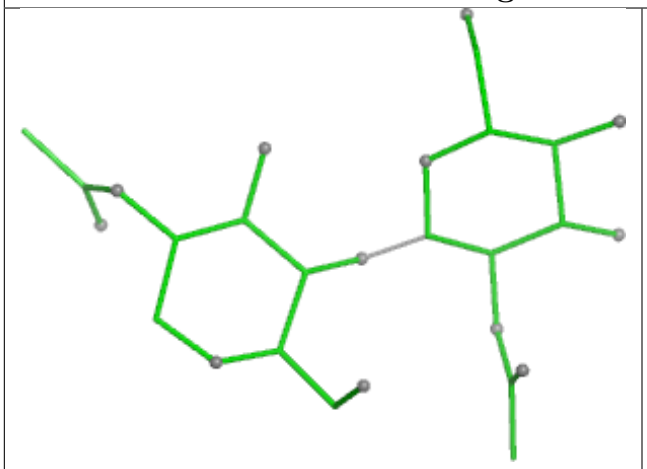
There are no ring outliers.

3 monomers are involved in 3 short contacts:

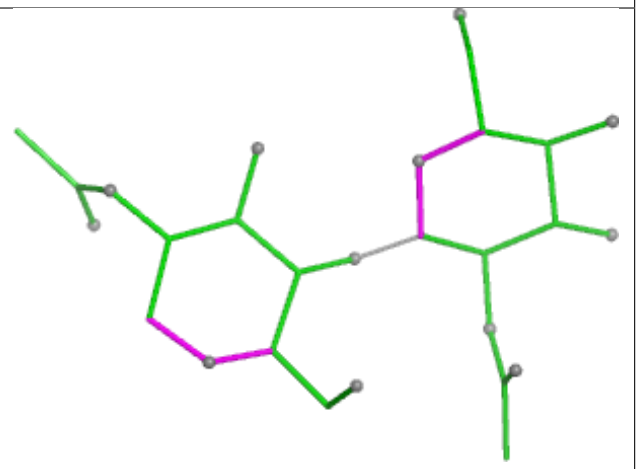
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	L	1	NAG	1	0
3	Q	1	NAG	1	0
3	F	1	NAG	1	0

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

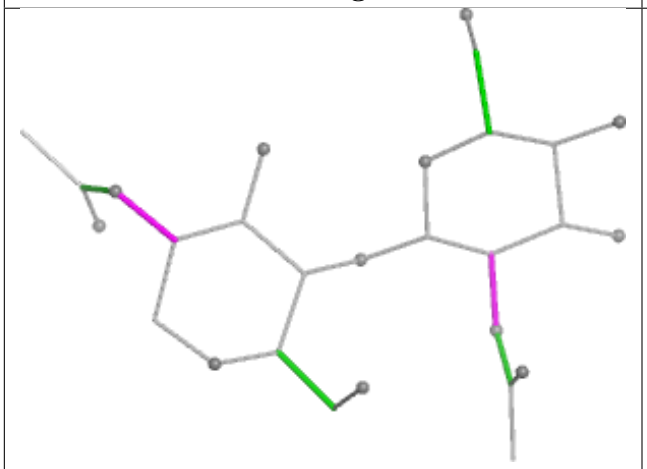
Oligosaccharide Chain E



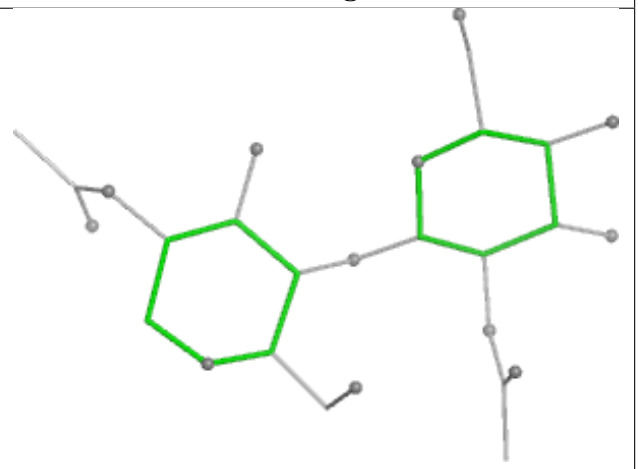
Bond lengths



Bond angles

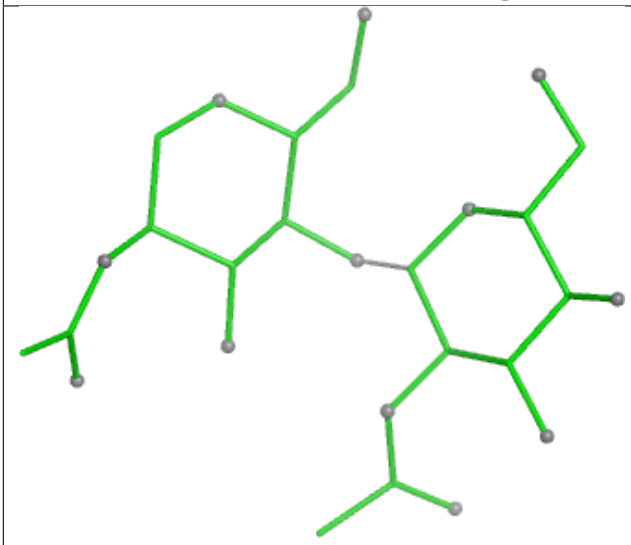


Torsions

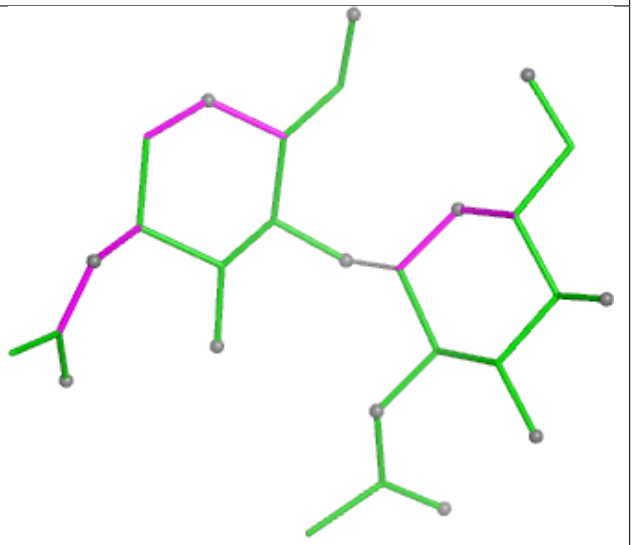


Rings

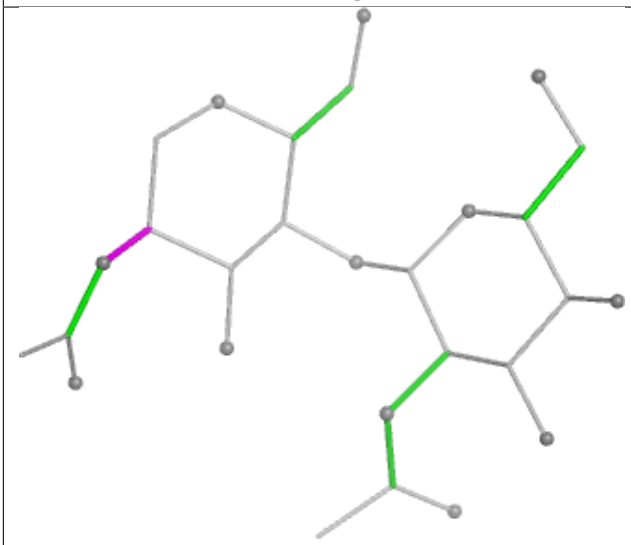
Oligosaccharide Chain F



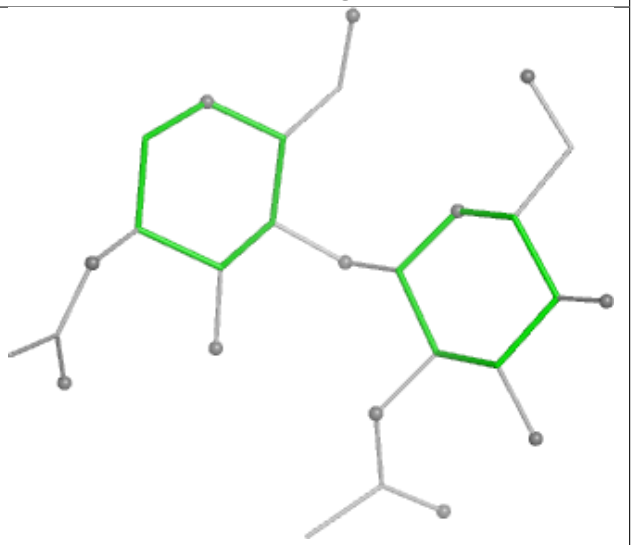
Bond lengths



Bond angles

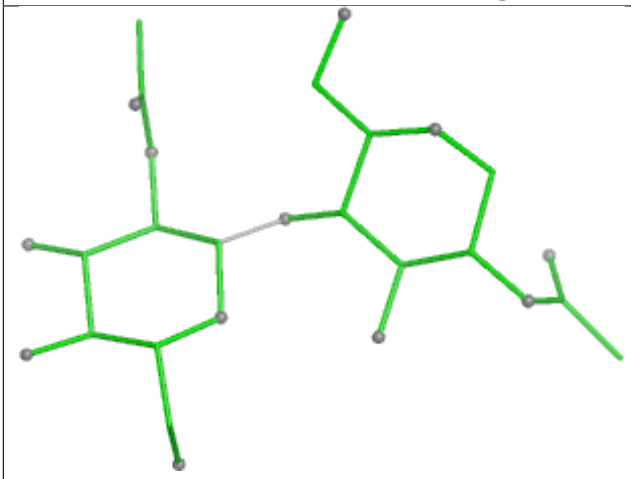


Torsions

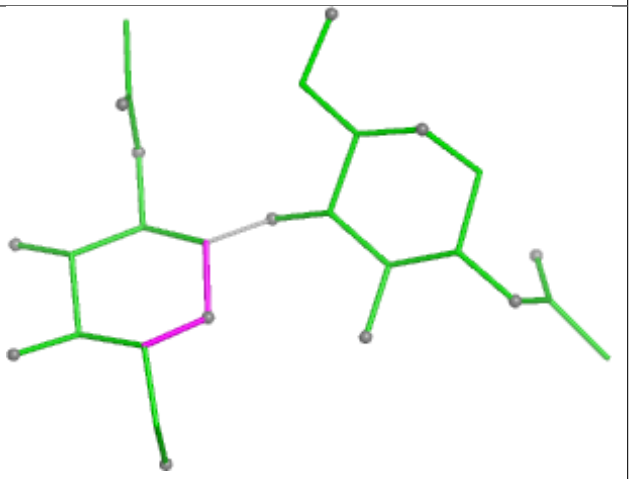


Rings

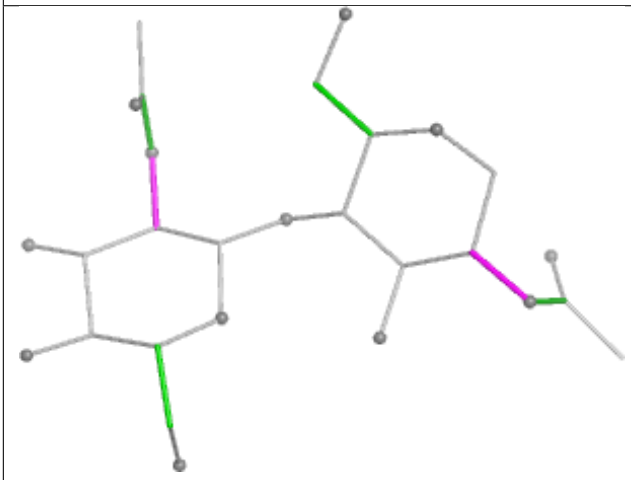
Oligosaccharide Chain G



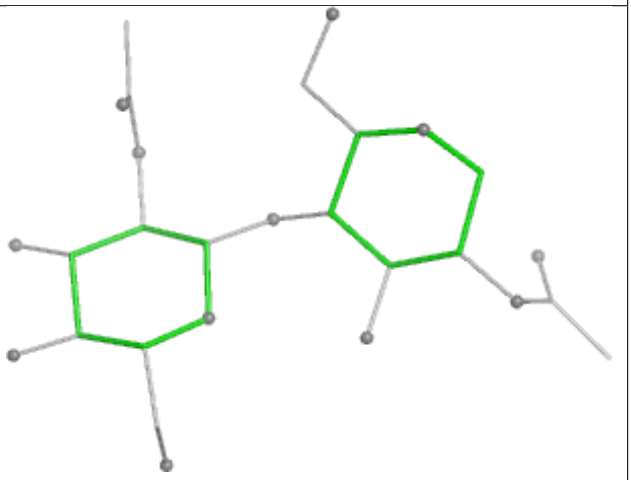
Bond lengths



Bond angles

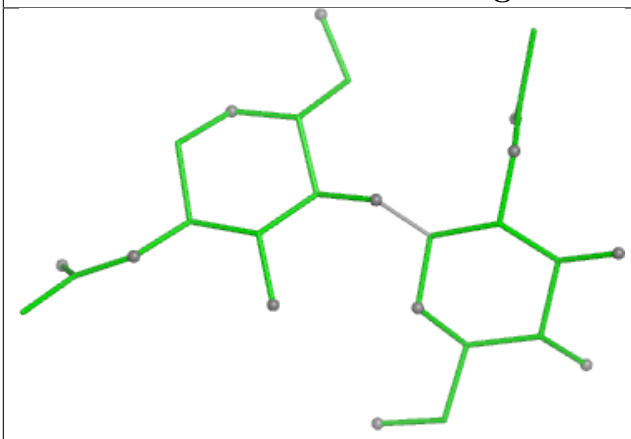


Torsions

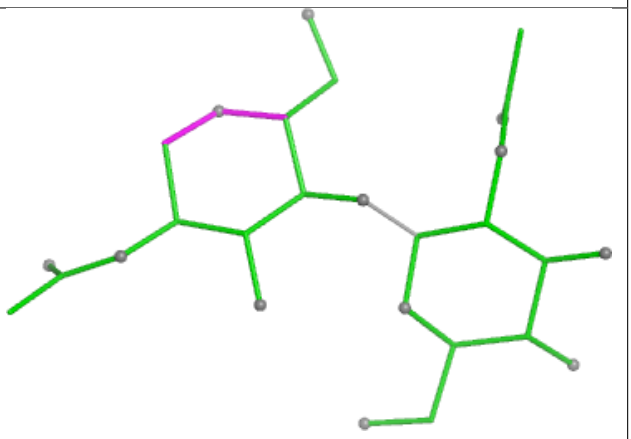


Rings

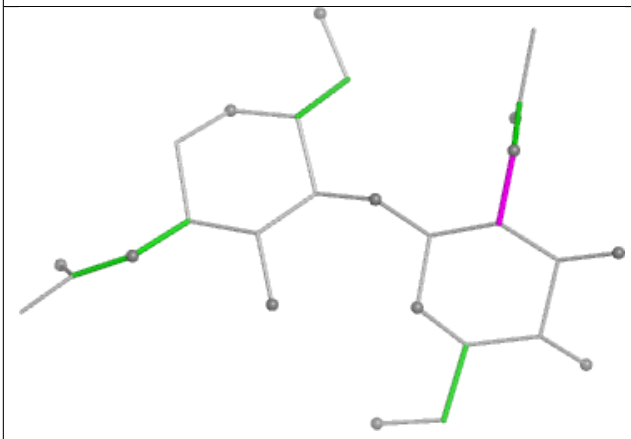
Oligosaccharide Chain H



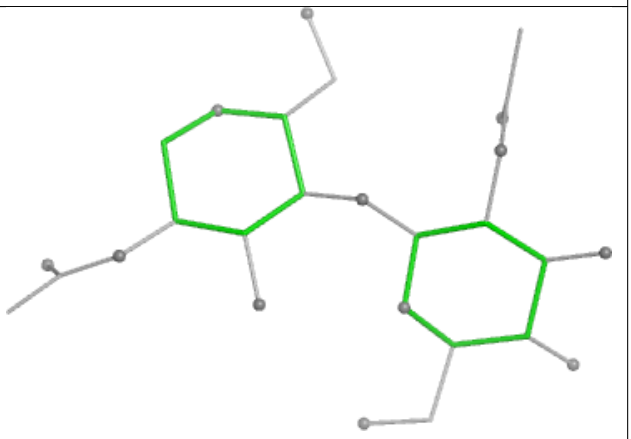
Bond lengths



Bond angles

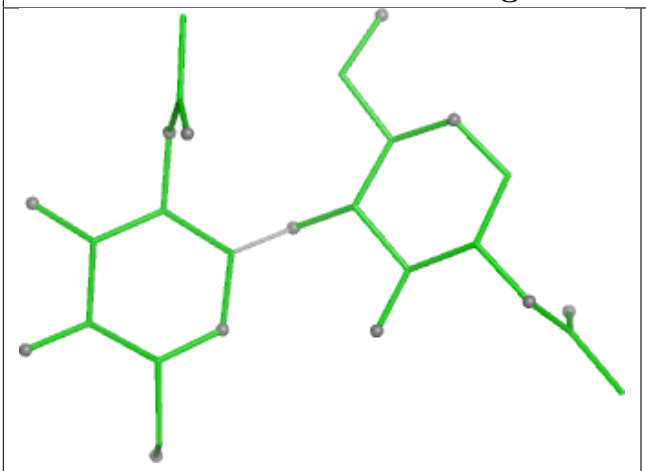


Torsions

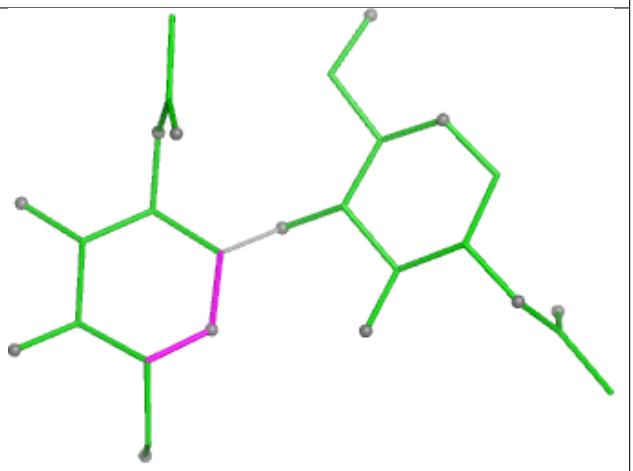


Rings

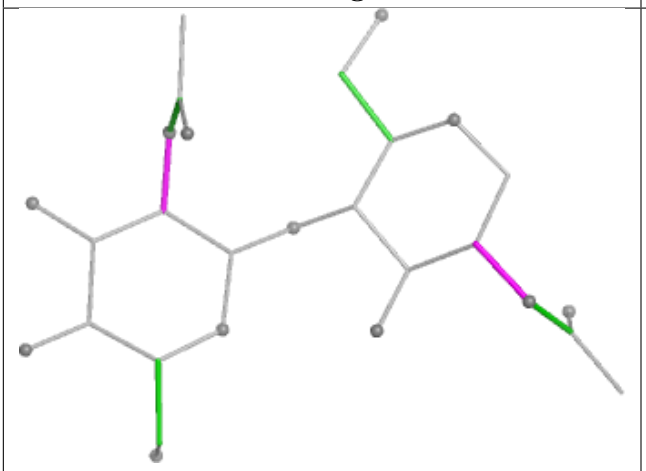
Oligosaccharide Chain I



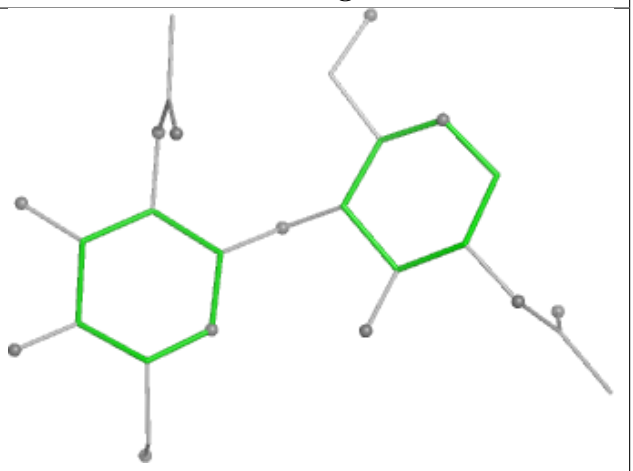
Bond lengths



Bond angles

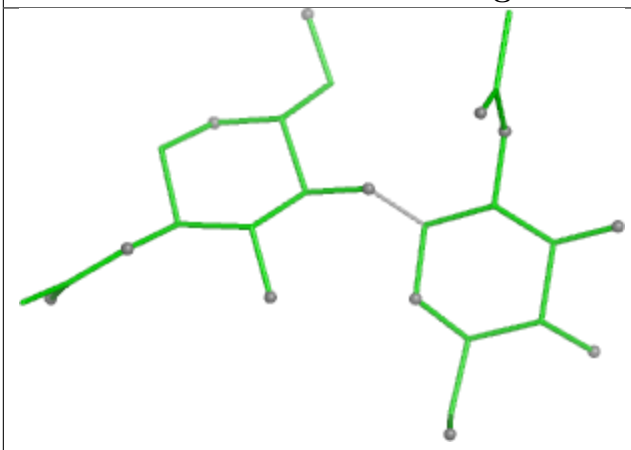


Torsions

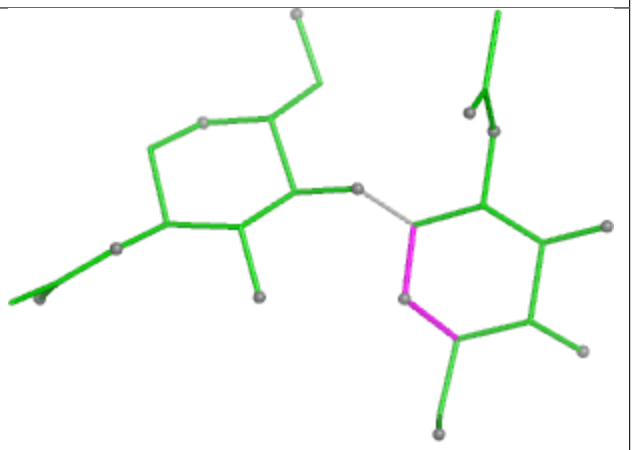


Rings

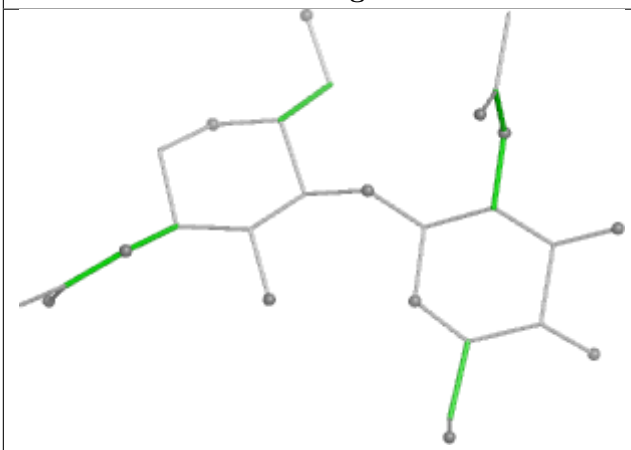
Oligosaccharide Chain K



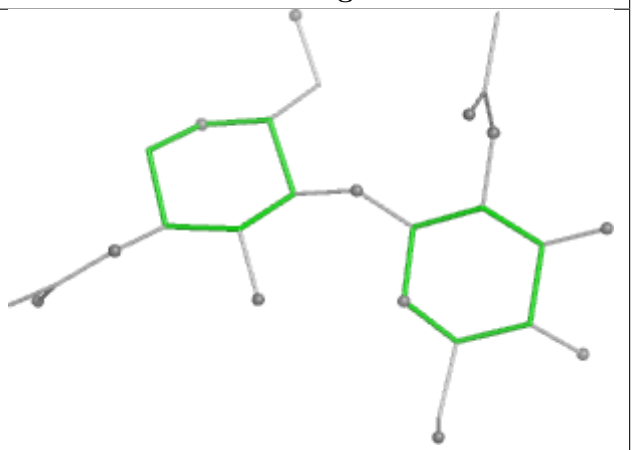
Bond lengths



Bond angles

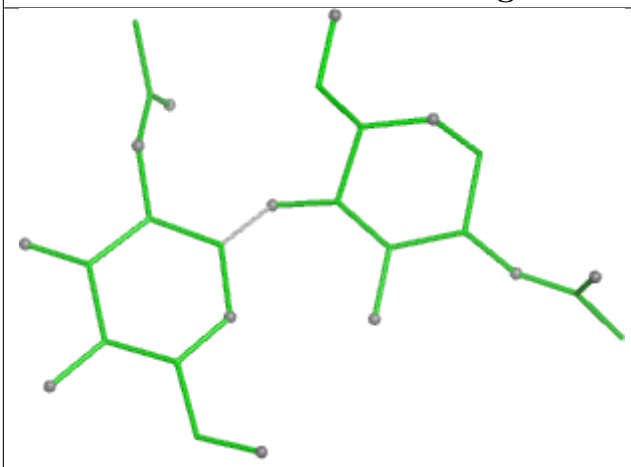


Torsions

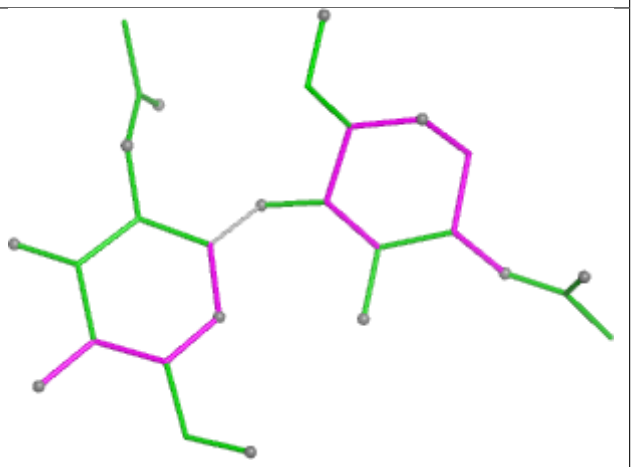


Rings

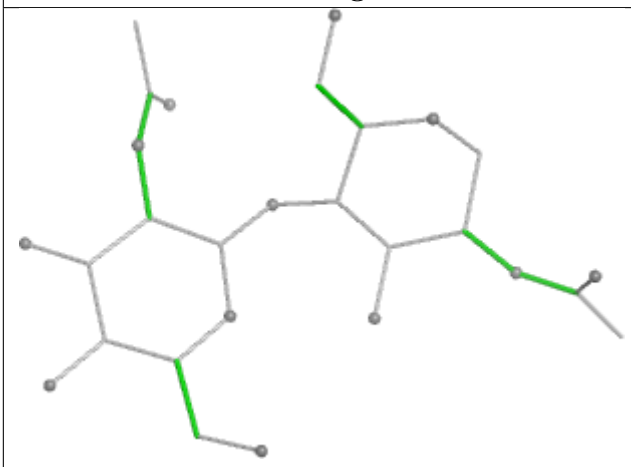
Oligosaccharide Chain L



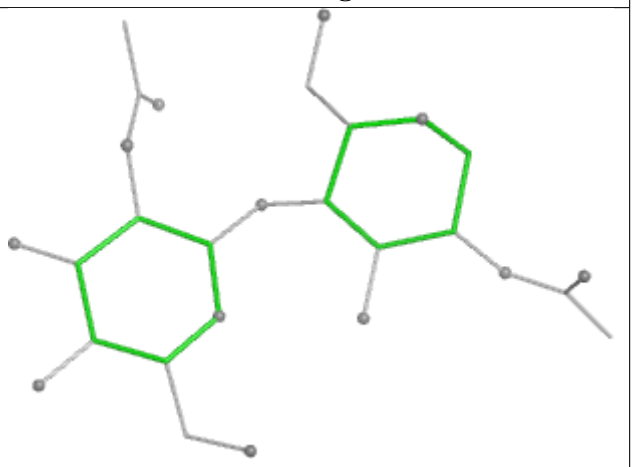
Bond lengths



Bond angles

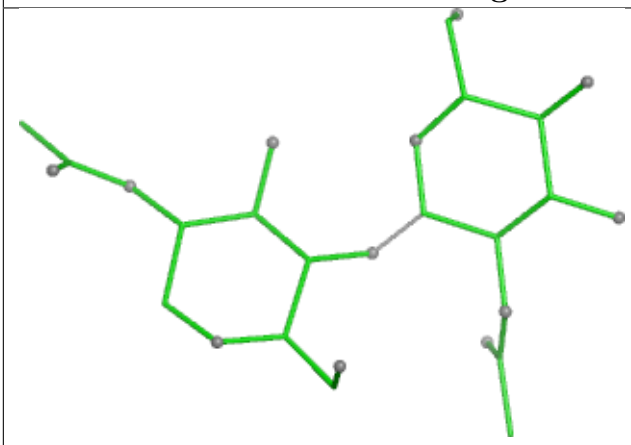


Torsions

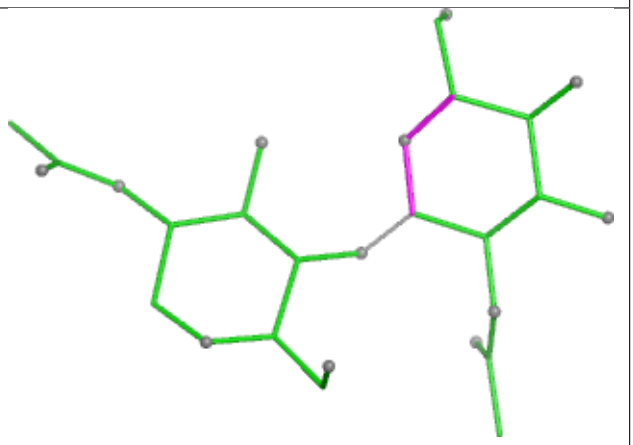


Rings

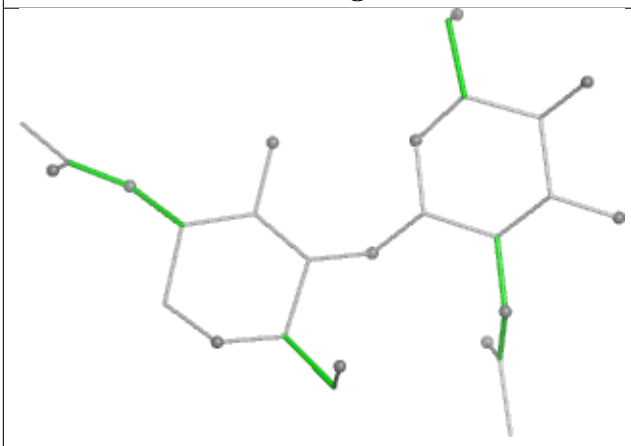
Oligosaccharide Chain M



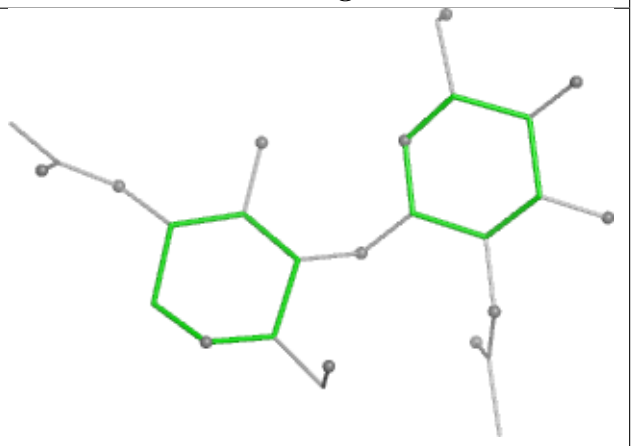
Bond lengths



Bond angles

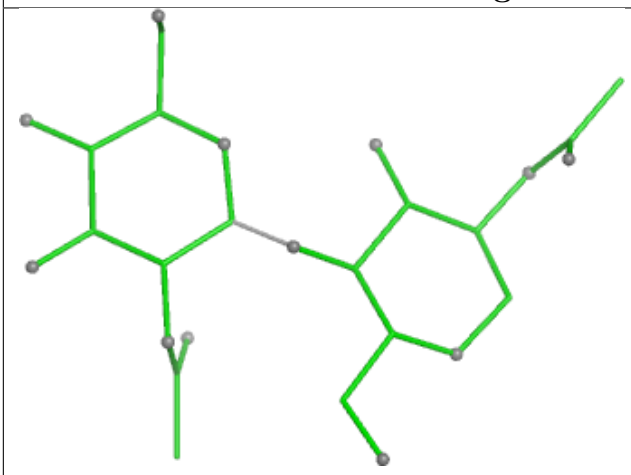


Torsions

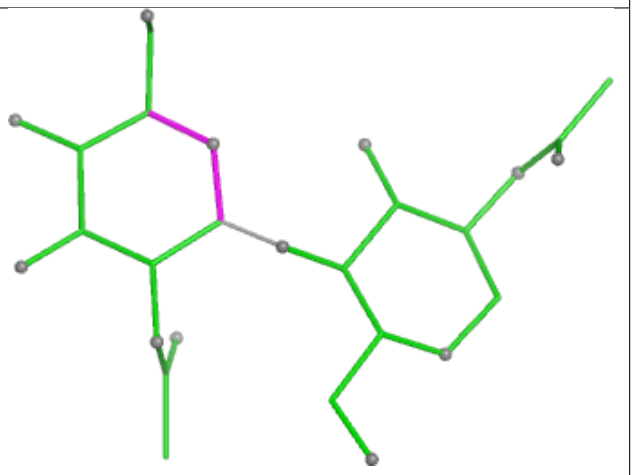


Rings

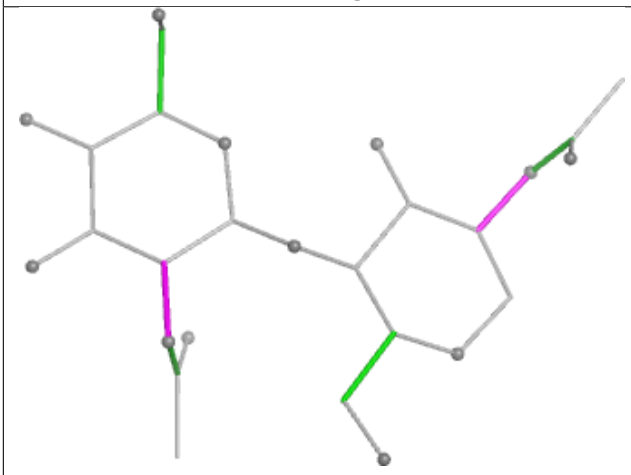
Oligosaccharide Chain N



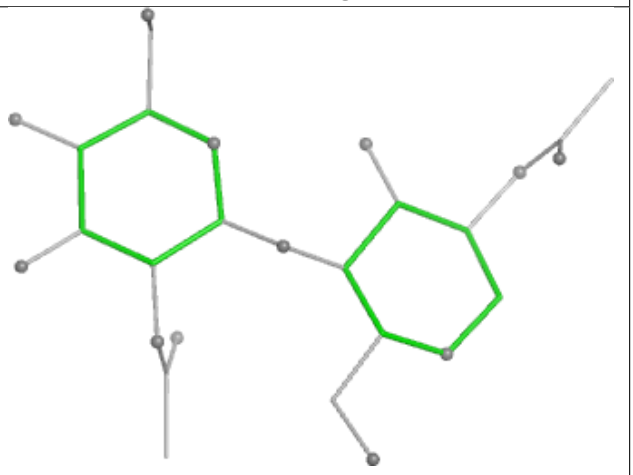
Bond lengths



Bond angles

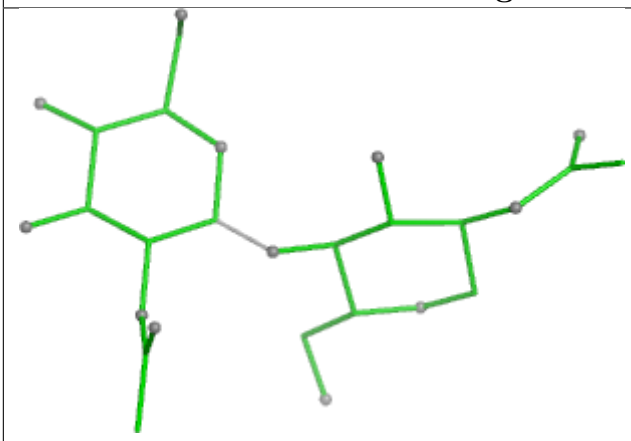


Torsions

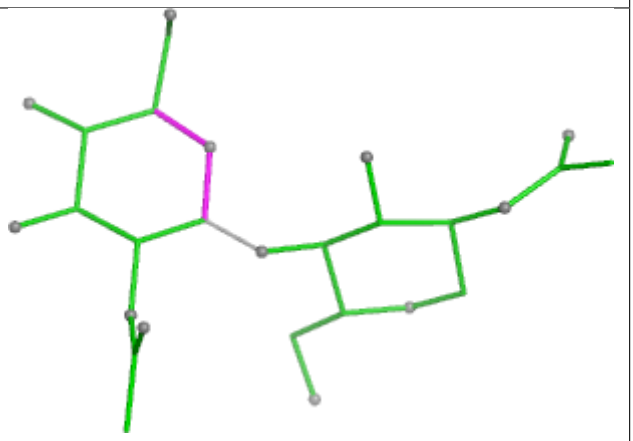


Rings

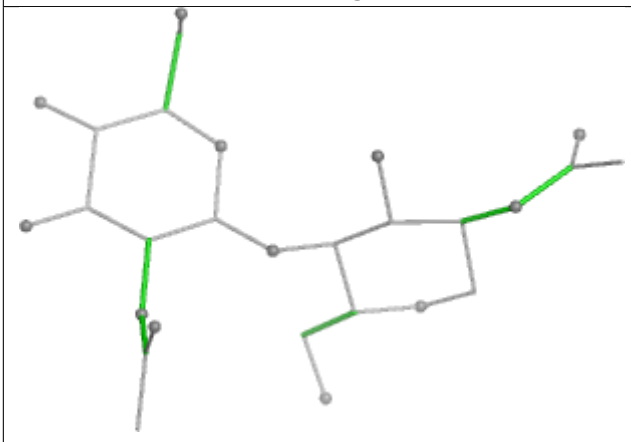
Oligosaccharide Chain P



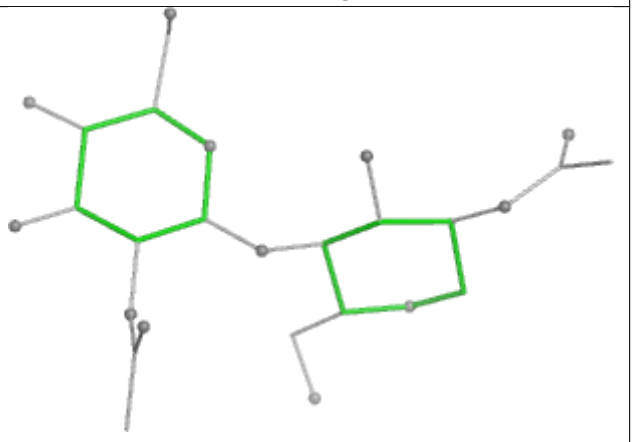
Bond lengths



Bond angles

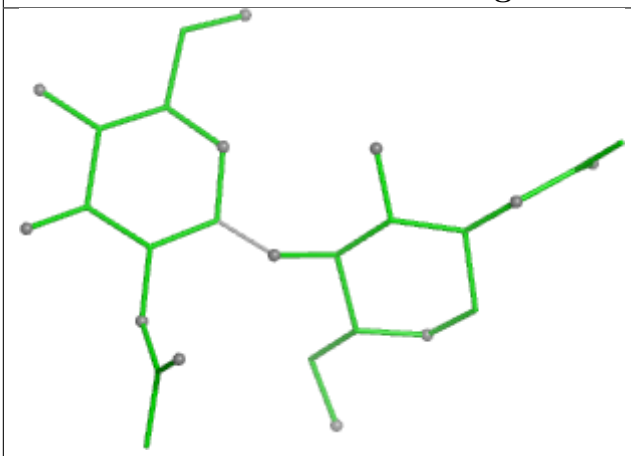


Torsions

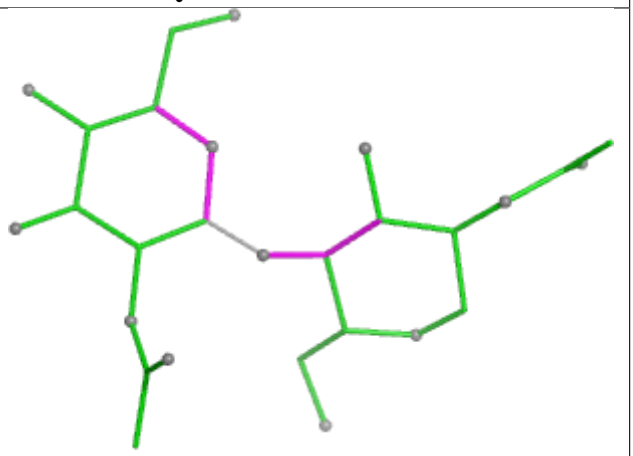


Rings

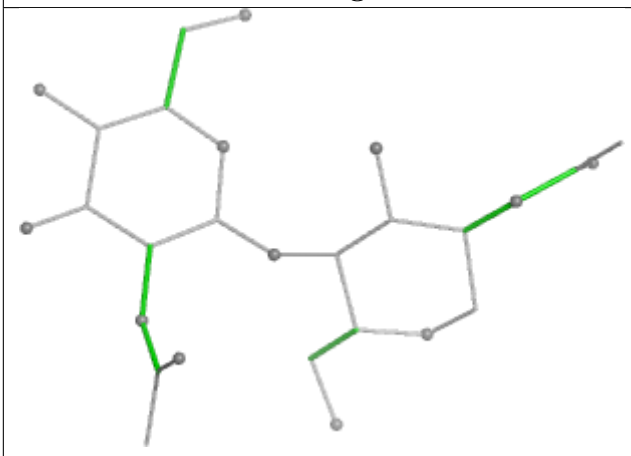
Oligosaccharide Chain Q



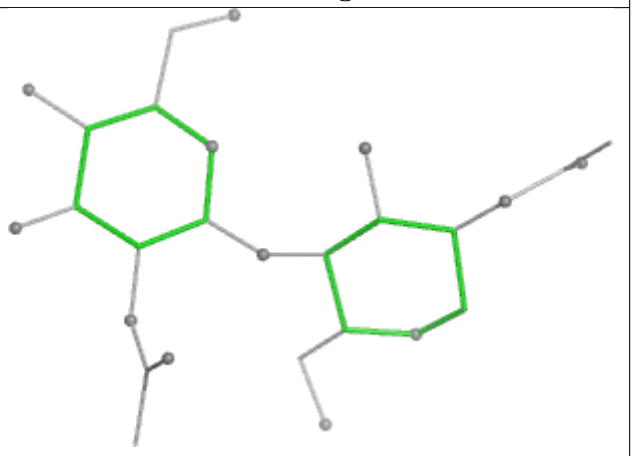
Bond lengths



Bond angles

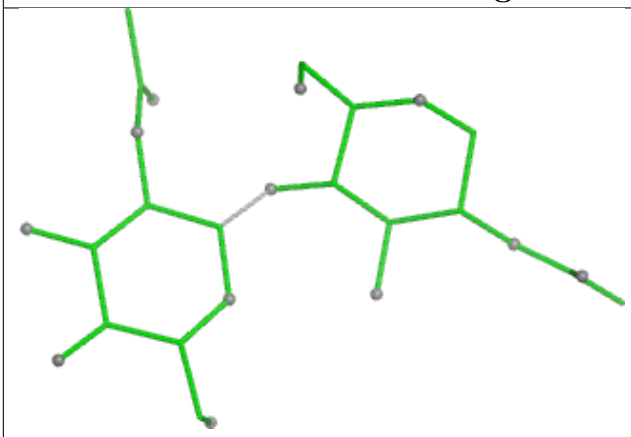


Torsions

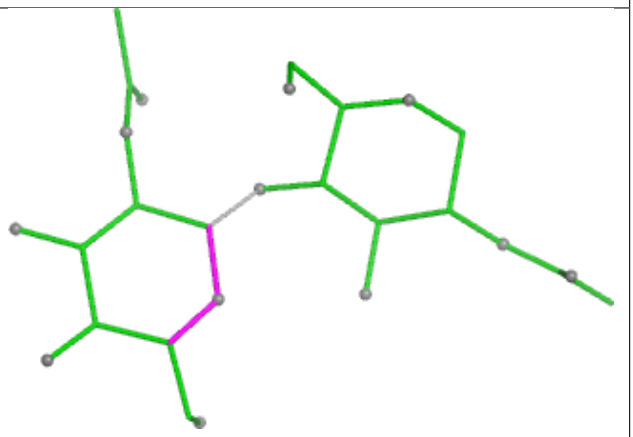


Rings

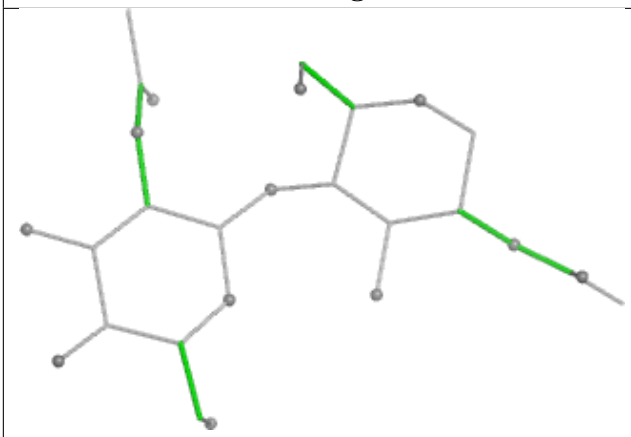
Oligosaccharide Chain R



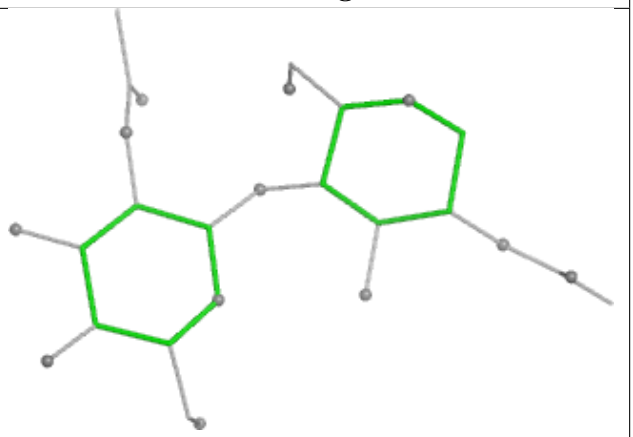
Bond lengths



Bond angles

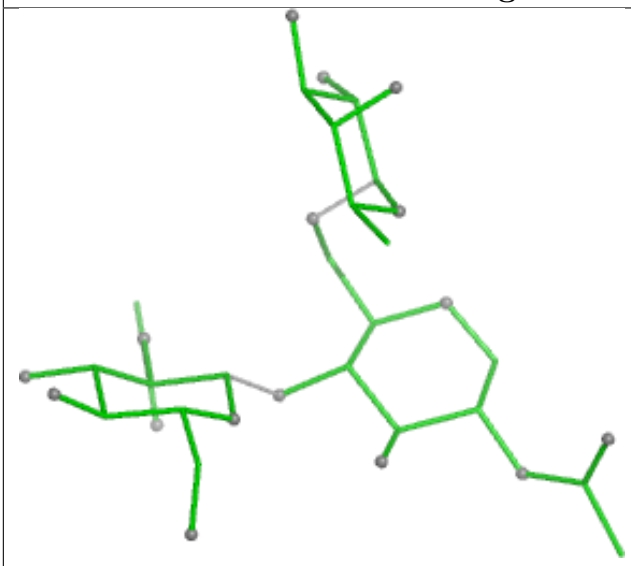


Torsions

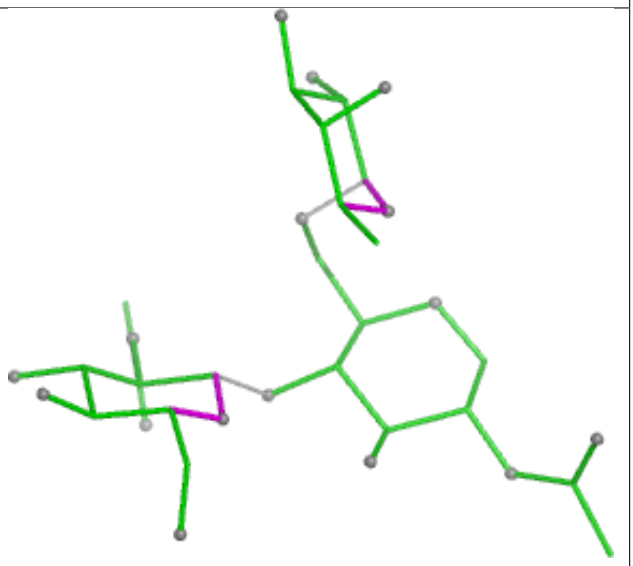


Rings

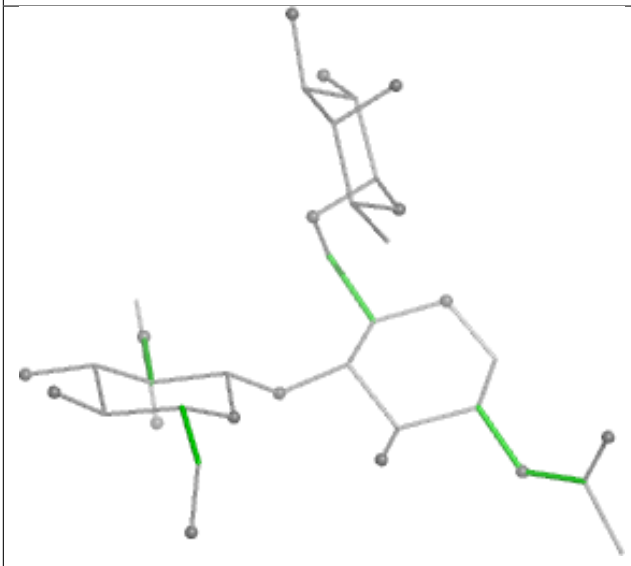
Oligosaccharide Chain J



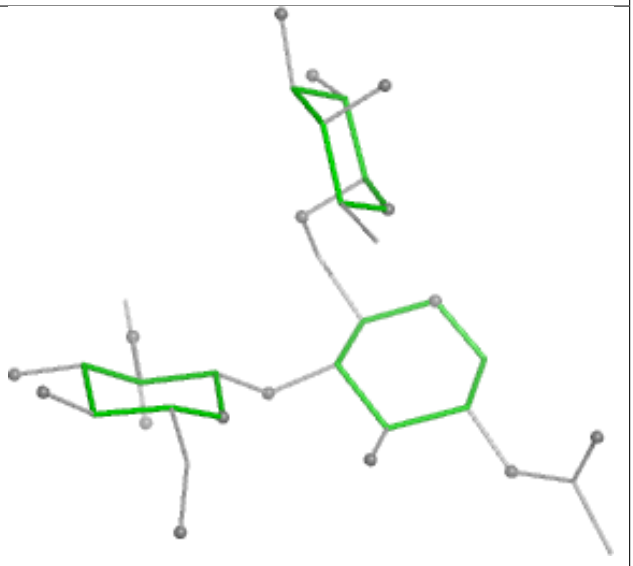
Bond lengths



Bond angles

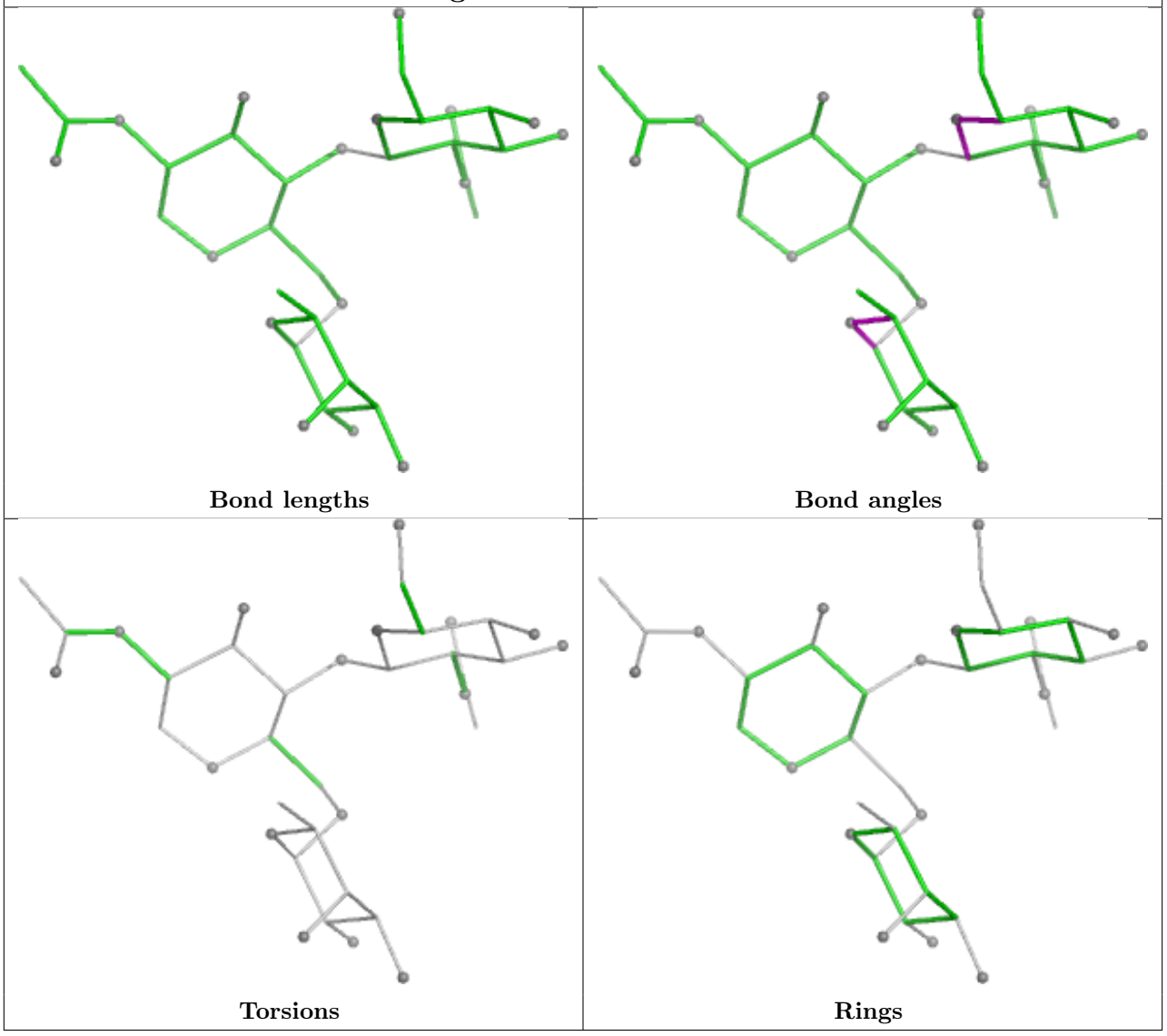


Torsions



Rings

Oligosaccharide Chain O



5.6 Ligand geometry (i)

Of 30 ligands modelled in this entry, 2 are monoatomic - leaving 28 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	$\#\|Z\| > 2$
6	CLR	A	704	-	31,31,31	0.39	0	48,48,48	0.53	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
5	NAG	C	901	2	14,14,15	0.73	0	17,19,21	0.96	1 (5%)
8	A2G	C	903	2	14,14,15	1.01	1 (7%)	17,19,21	0.87	1 (5%)
5	NAG	D	901	2	14,14,15	0.68	0	17,19,21	1.60	2 (11%)
5	NAG	B	701	1	14,14,15	0.71	0	17,19,21	0.92	1 (5%)
5	NAG	B	702	1	14,14,15	0.71	0	17,19,21	0.85	0
6	CLR	B	708	-	31,31,31	0.40	0	48,48,48	0.63	0
6	CLR	B	710	-	31,31,31	0.36	0	48,48,48	1.15	4 (8%)
6	CLR	B	709	-	31,31,31	0.45	0	48,48,48	0.84	0
7	LEU	A	711	-	7,8,8	0.88	1 (14%)	9,10,10	1.16	2 (22%)
5	NAG	A	702	1	14,14,15	0.71	0	17,19,21	1.83	3 (17%)
6	CLR	B	707	-	31,31,31	0.41	0	48,48,48	0.55	0
6	CLR	B	706	-	31,31,31	0.40	0	48,48,48	0.57	0
5	NAG	D	902	2	14,14,15	0.68	0	17,19,21	1.22	1 (5%)
6	CLR	A	708	-	31,31,31	0.40	0	48,48,48	0.60	0
6	CLR	B	705	-	31,31,31	0.38	0	48,48,48	0.55	0
6	CLR	A	710	-	31,31,31	0.35	0	48,48,48	1.16	4 (8%)
5	NAG	B	703	1	14,14,15	0.73	0	17,19,21	0.91	0
5	NAG	C	902	2	14,14,15	0.75	0	17,19,21	1.68	3 (17%)
6	CLR	A	705	-	31,31,31	0.37	0	48,48,48	0.52	0
6	CLR	A	706	-	31,31,31	0.39	0	48,48,48	0.60	0
6	CLR	A	709	-	31,31,31	0.60	0	48,48,48	0.81	2 (4%)
6	CLR	A	707	-	31,31,31	0.39	0	48,48,48	0.53	0
5	NAG	A	701	1	14,14,15	0.71	0	17,19,21	0.97	1 (5%)
8	A2G	D	903	2	14,14,15	1.02	1 (7%)	17,19,21	0.84	1 (5%)
6	CLR	B	704	-	31,31,31	0.41	0	48,48,48	0.96	3 (6%)
5	NAG	A	703	1	14,14,15	0.72	0	17,19,21	1.03	1 (5%)
7	LEU	B	711	-	7,8,8	0.88	1 (14%)	9,10,10	1.17	2 (22%)

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
6	CLR	A	704	-	-	5/10/68/68	0/4/4/4
5	NAG	C	901	2	-	1/6/23/26	0/1/1/1
8	A2G	C	903	2	-	0/6/23/26	0/1/1/1
5	NAG	D	901	2	-	0/6/23/26	0/1/1/1
5	NAG	B	701	1	-	2/6/23/26	0/1/1/1

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	NAG	B	702	1	-	0/6/23/26	0/1/1/1
6	CLR	B	708	-	-	0/10/68/68	0/4/4/4
6	CLR	B	710	-	-	2/10/68/68	0/4/4/4
6	CLR	B	709	-	-	5/10/68/68	0/4/4/4
7	LEU	A	711	-	-	0/8/8/8	-
5	NAG	A	702	1	-	2/6/23/26	0/1/1/1
6	CLR	B	707	-	-	1/10/68/68	0/4/4/4
6	CLR	B	706	-	-	1/10/68/68	0/4/4/4
5	NAG	D	902	2	-	2/6/23/26	0/1/1/1
6	CLR	A	708	-	-	0/10/68/68	0/4/4/4
6	CLR	B	705	-	-	0/10/68/68	0/4/4/4
6	CLR	A	710	-	-	3/10/68/68	0/4/4/4
5	NAG	B	703	1	-	1/6/23/26	0/1/1/1
5	NAG	C	902	2	-	0/6/23/26	0/1/1/1
6	CLR	A	705	-	-	2/10/68/68	0/4/4/4
6	CLR	A	706	-	-	0/10/68/68	0/4/4/4
6	CLR	A	709	-	-	5/10/68/68	0/4/4/4
6	CLR	A	707	-	-	1/10/68/68	0/4/4/4
5	NAG	A	701	1	-	2/6/23/26	0/1/1/1
8	A2G	D	903	2	-	0/6/23/26	0/1/1/1
6	CLR	B	704	-	-	6/10/68/68	0/4/4/4
5	NAG	A	703	1	-	1/6/23/26	0/1/1/1
7	LEU	B	711	-	-	0/8/8/8	-

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
8	D	903	A2G	O5-C1	-3.06	1.38	1.43
8	C	903	A2G	O5-C1	-3.02	1.38	1.43
7	B	711	LEU	OXT-C	-2.22	1.23	1.30
7	A	711	LEU	OXT-C	-2.21	1.23	1.30

The worst 5 of 32 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
5	A	702	NAG	C1-O5-C5	5.60	119.78	112.19
5	C	902	NAG	C1-O5-C5	5.51	119.66	112.19
5	D	901	NAG	C1-O5-C5	5.03	119.00	112.19
5	D	902	NAG	C1-O5-C5	4.07	117.70	112.19
5	A	702	NAG	O5-C1-C2	-3.17	106.28	111.29

There are no chirality outliers.

5 of 42 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
6	A	709	CLR	C13-C17-C20-C21
6	A	709	CLR	C13-C17-C20-C22
6	A	709	CLR	C16-C17-C20-C21
6	A	709	CLR	C16-C17-C20-C22
6	B	709	CLR	C13-C17-C20-C22

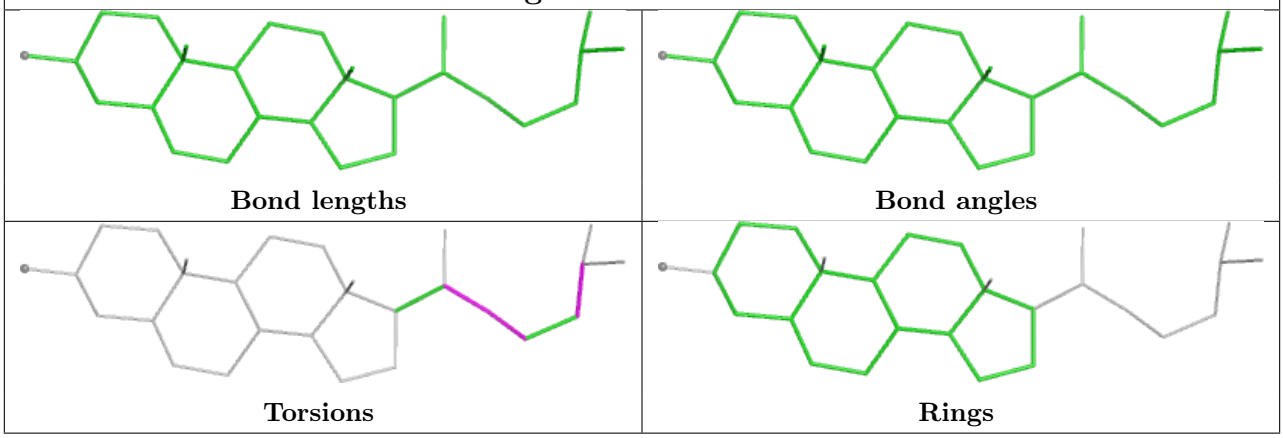
There are no ring outliers.

9 monomers are involved in 13 short contacts:

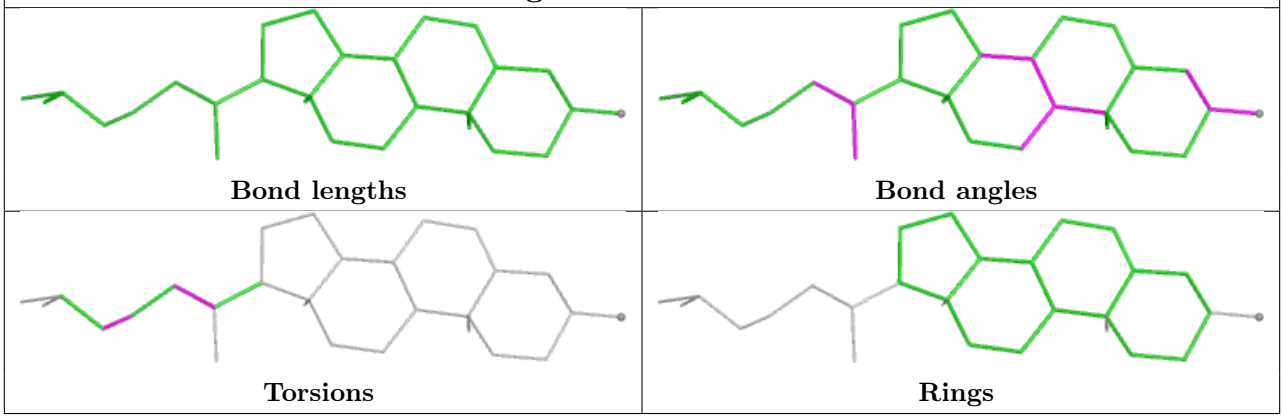
Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	C	901	NAG	1	0
5	A	702	NAG	2	0
6	B	707	CLR	1	0
6	A	708	CLR	1	0
6	A	710	CLR	1	0
6	A	705	CLR	1	0
6	A	709	CLR	3	0
6	A	707	CLR	1	0
7	B	711	LEU	2	0

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

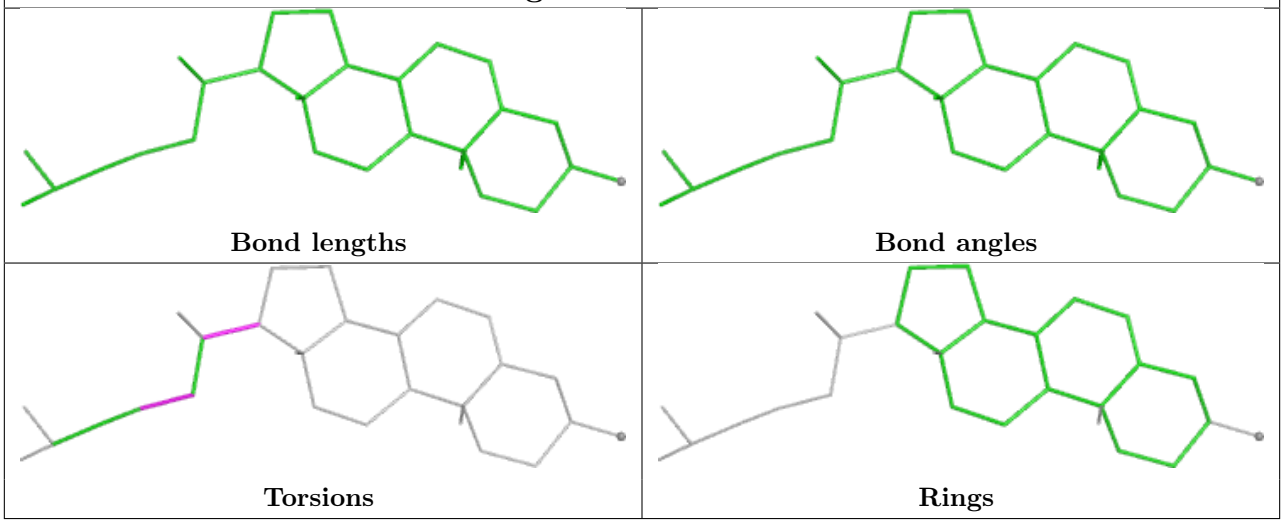
Ligand CLR A 704



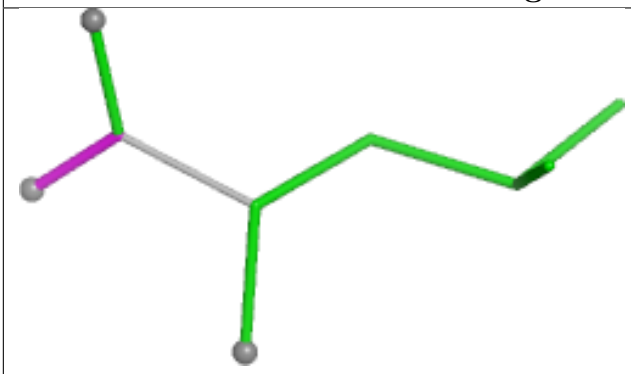
Ligand CLR B 710



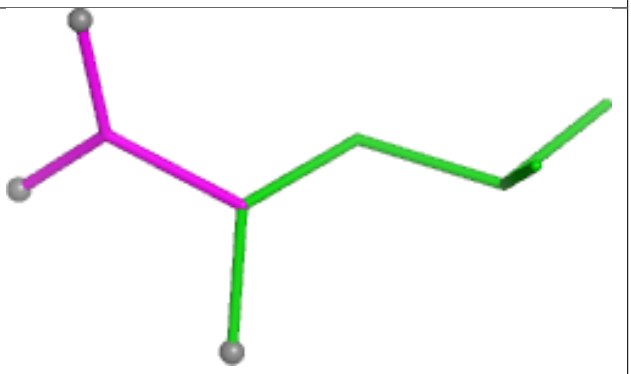
Ligand CLR B 709



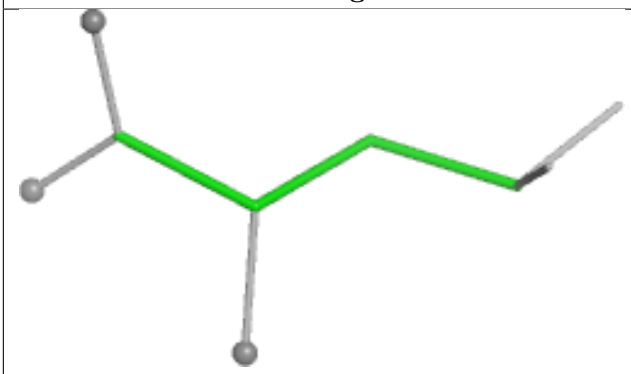
Ligand LEU A 711



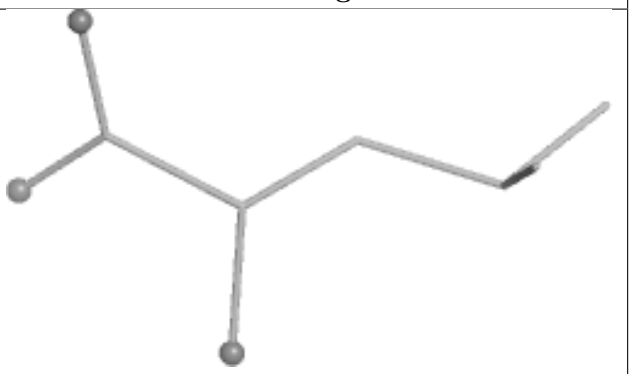
Bond lengths



Bond angles

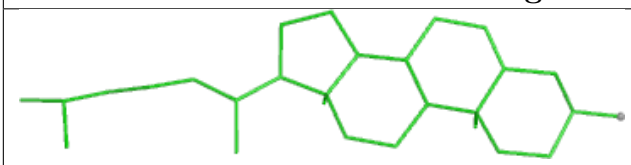


Torsions

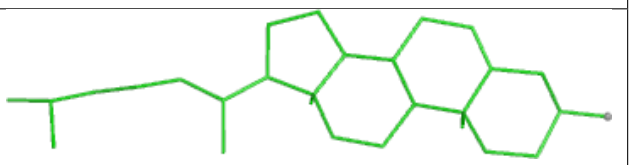


Rings

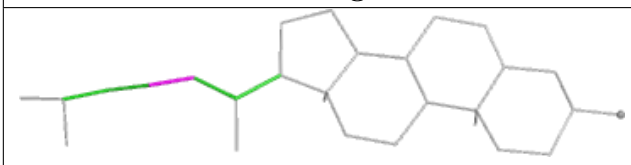
Ligand CLR B 707



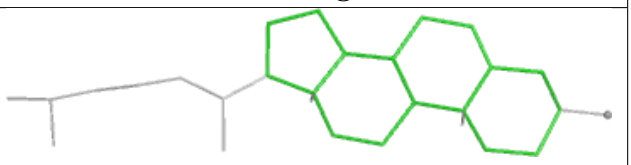
Bond lengths



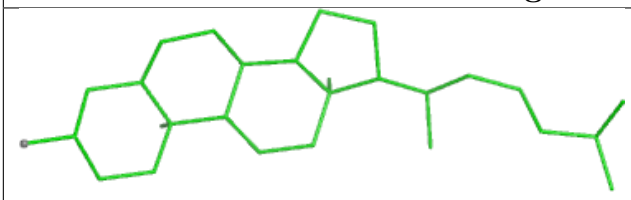
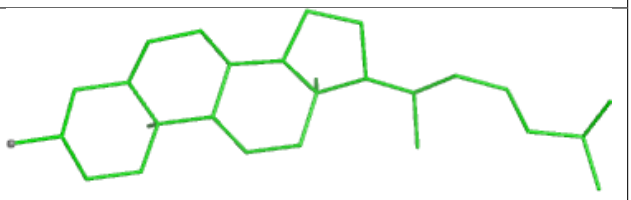
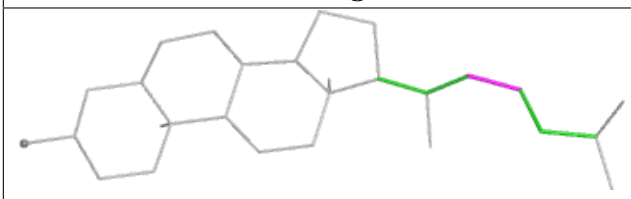
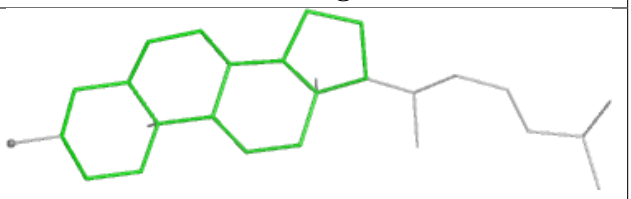
Bond angles

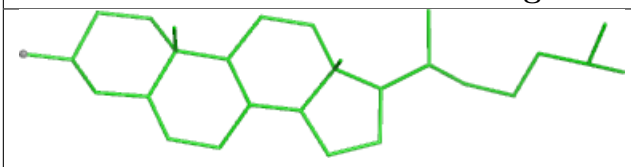
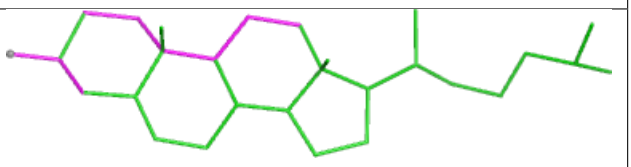
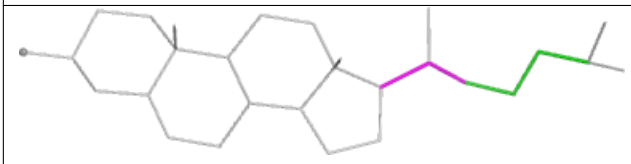
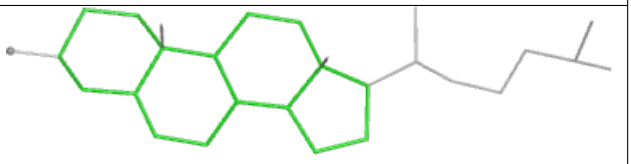


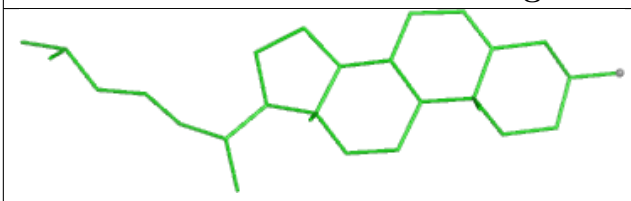
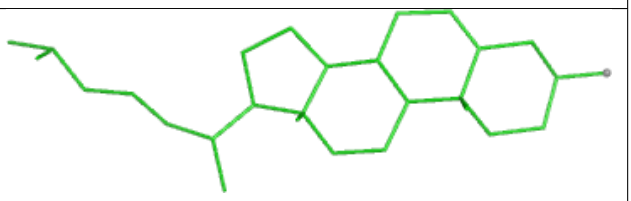
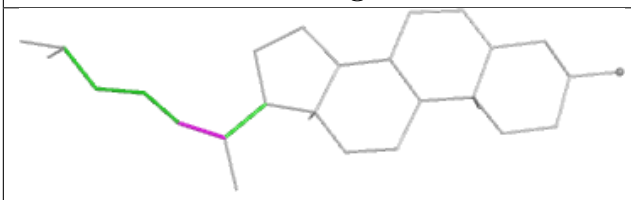
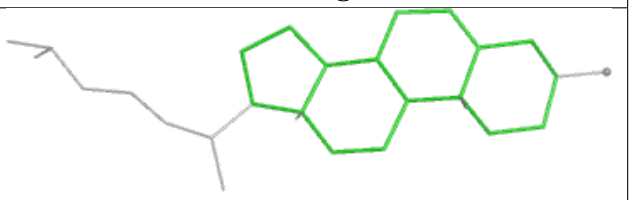
Torsions



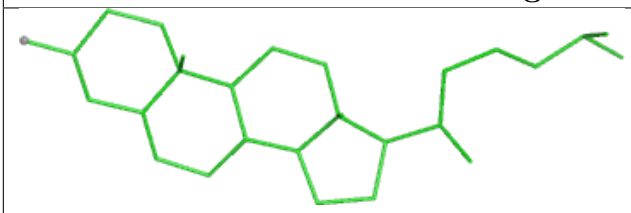
Rings

Ligand CLR B 706	
 Bond lengths	 Bond angles
 Torsions	 Rings

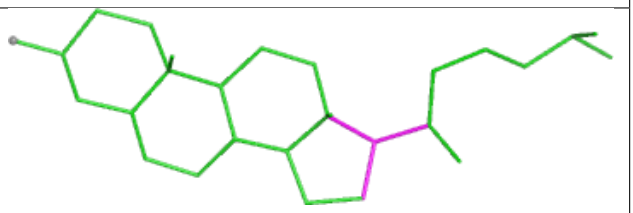
Ligand CLR A 710	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand CLR A 705	
 Bond lengths	 Bond angles
 Torsions	 Rings

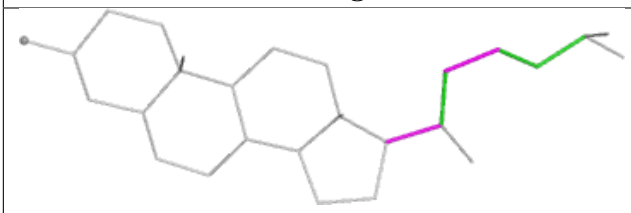
Ligand CLR A 709



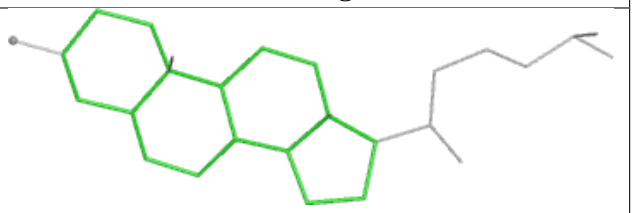
Bond lengths



Bond angles

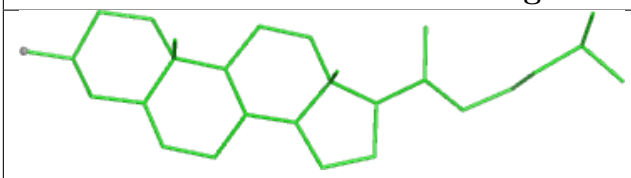


Torsions

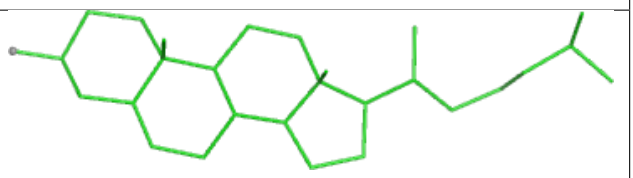


Rings

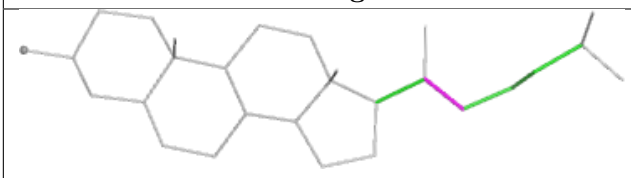
Ligand CLR A 707



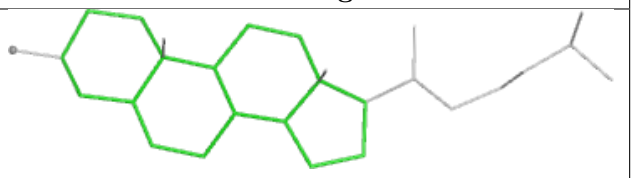
Bond lengths



Bond angles

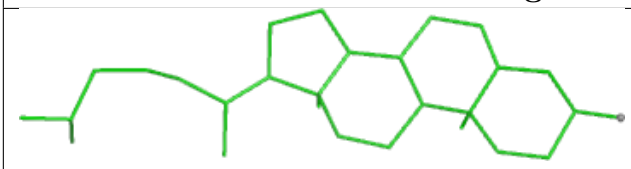


Torsions

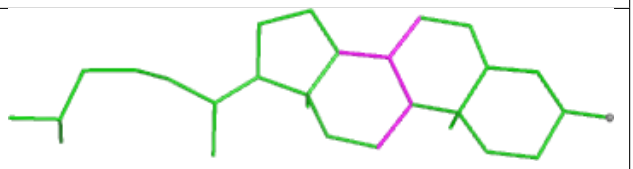


Rings

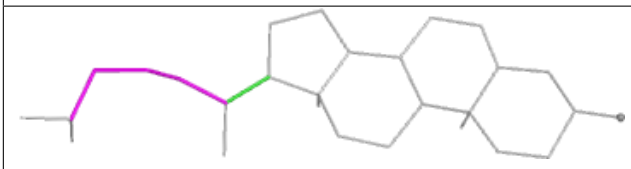
Ligand CLR B 704



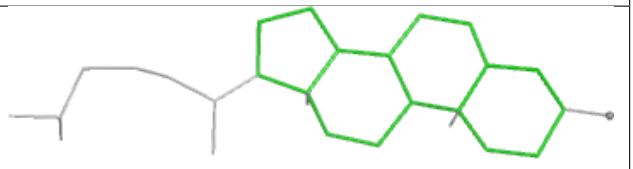
Bond lengths



Bond angles

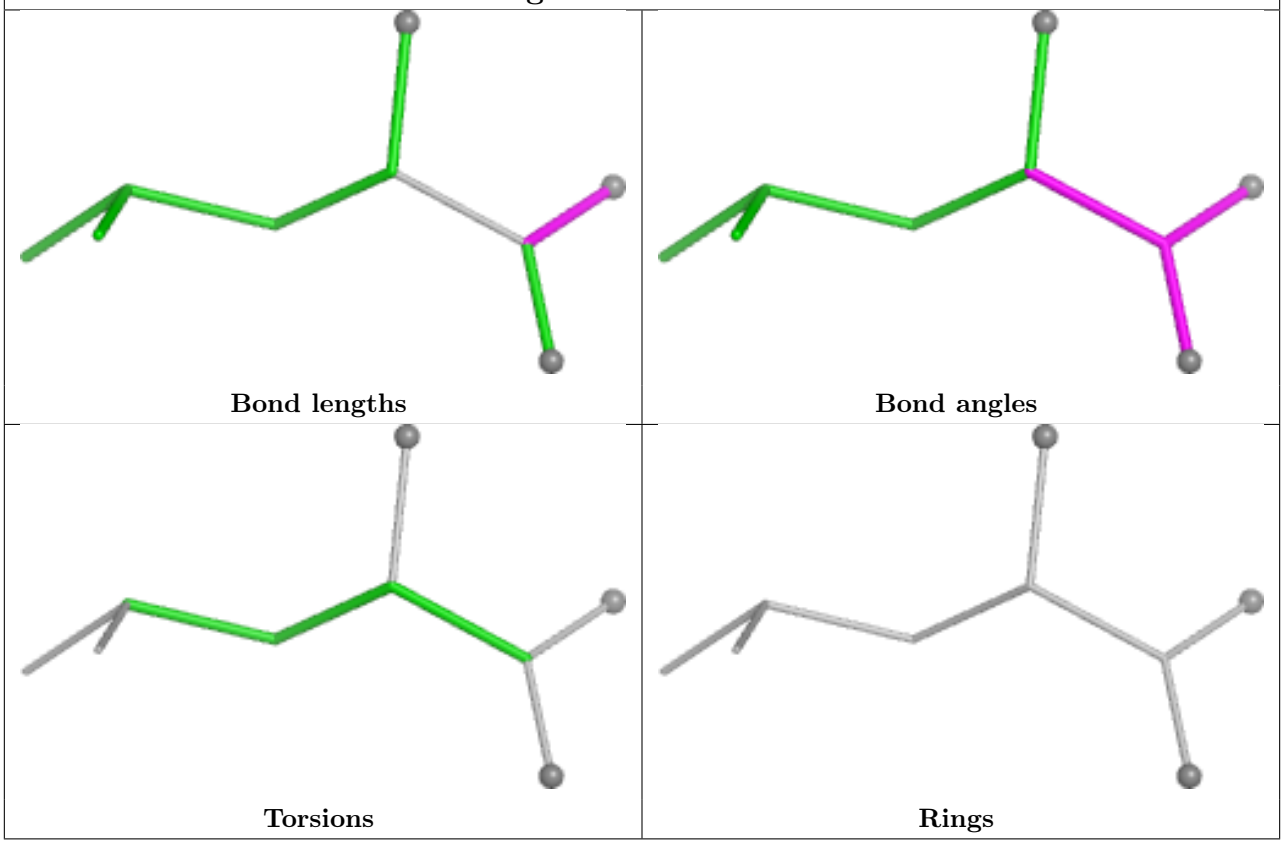


Torsions



Rings

Ligand LEU B 711



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.

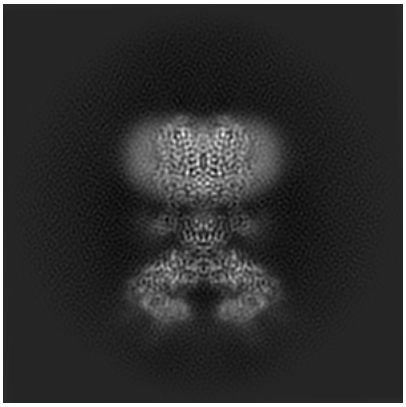
6 Map visualisation

This section contains visualisations of the EMDB entry EMD-100053. These allow visual inspection of the internal detail of the map and identification of artifacts.

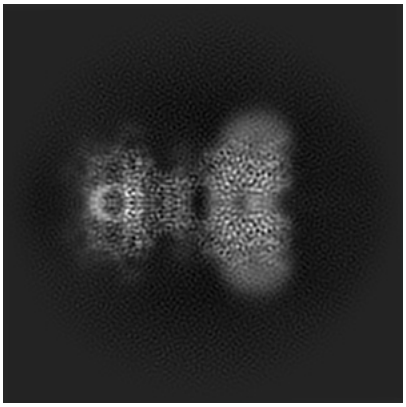
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections

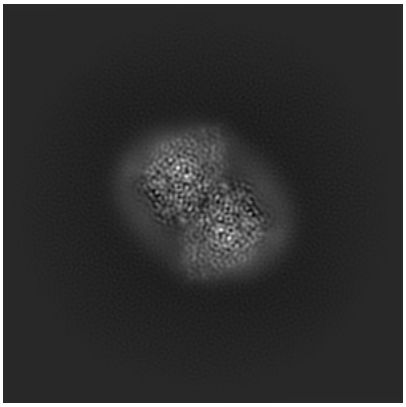
6.1.1 Primary map



X



Y

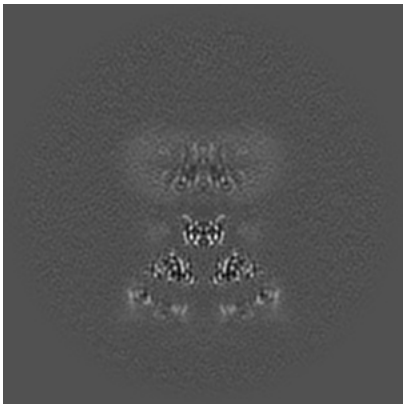


Z

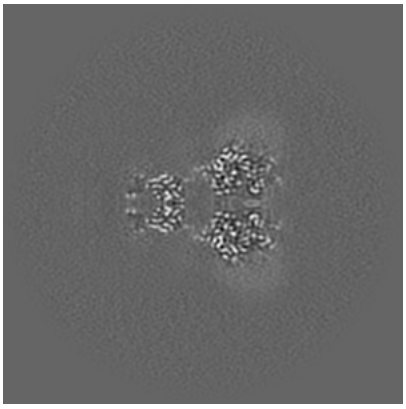
The images above show the map projected in three orthogonal directions.

6.2 Central slices

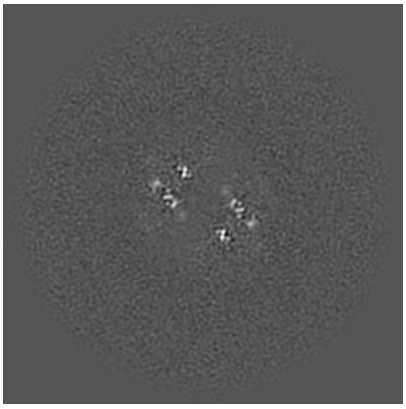
6.2.1 Primary map



X Index: 150



Y Index: 150

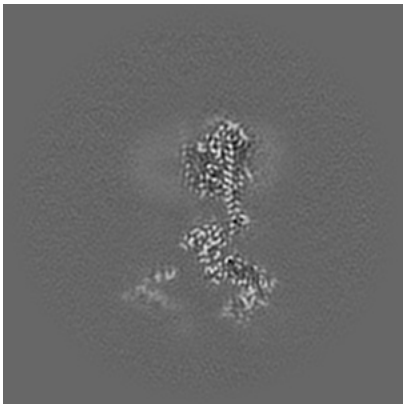


Z Index: 150

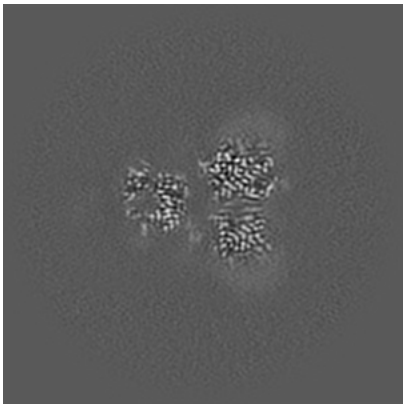
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

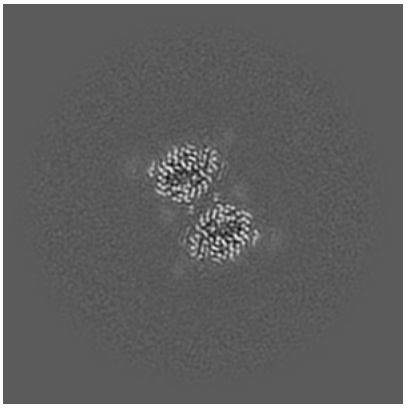
6.3.1 Primary map



X Index: 137



Y Index: 146

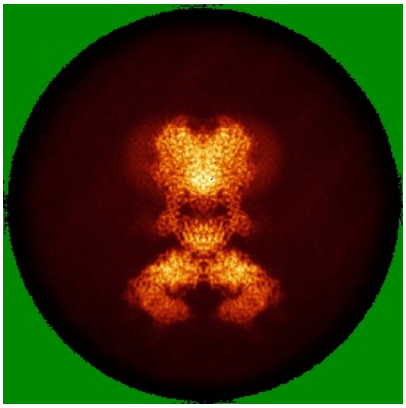


Z Index: 101

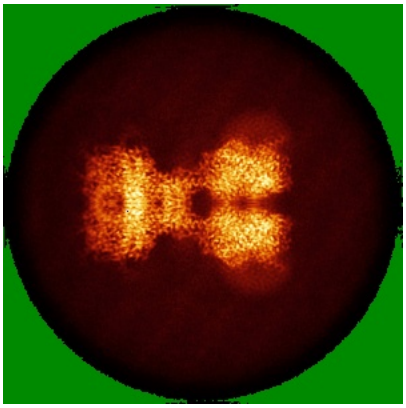
The images above show the largest variance slices of the map in three orthogonal directions.

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

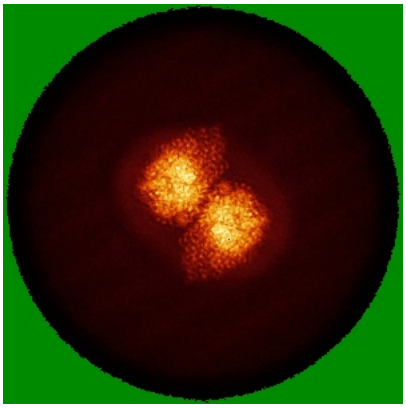
6.4.1 Primary map



X



Y

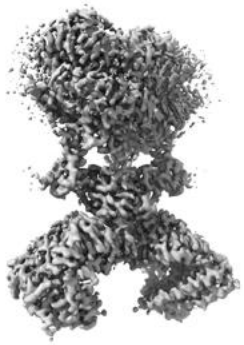


Z

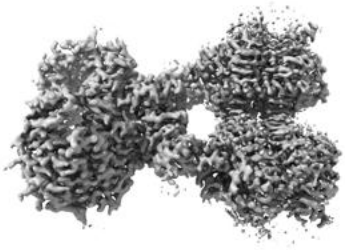
The images above show the map standard deviation projections with false color in three orthogonal directions. Minimum values are shown in green, max in blue, and dark to light orange shades represent small to large values respectively.

6.5 Orthogonal surface views (i)

6.5.1 Primary map



X



Y



Z

The images above show the 3D surface view of the map at the recommended contour level 6.0. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

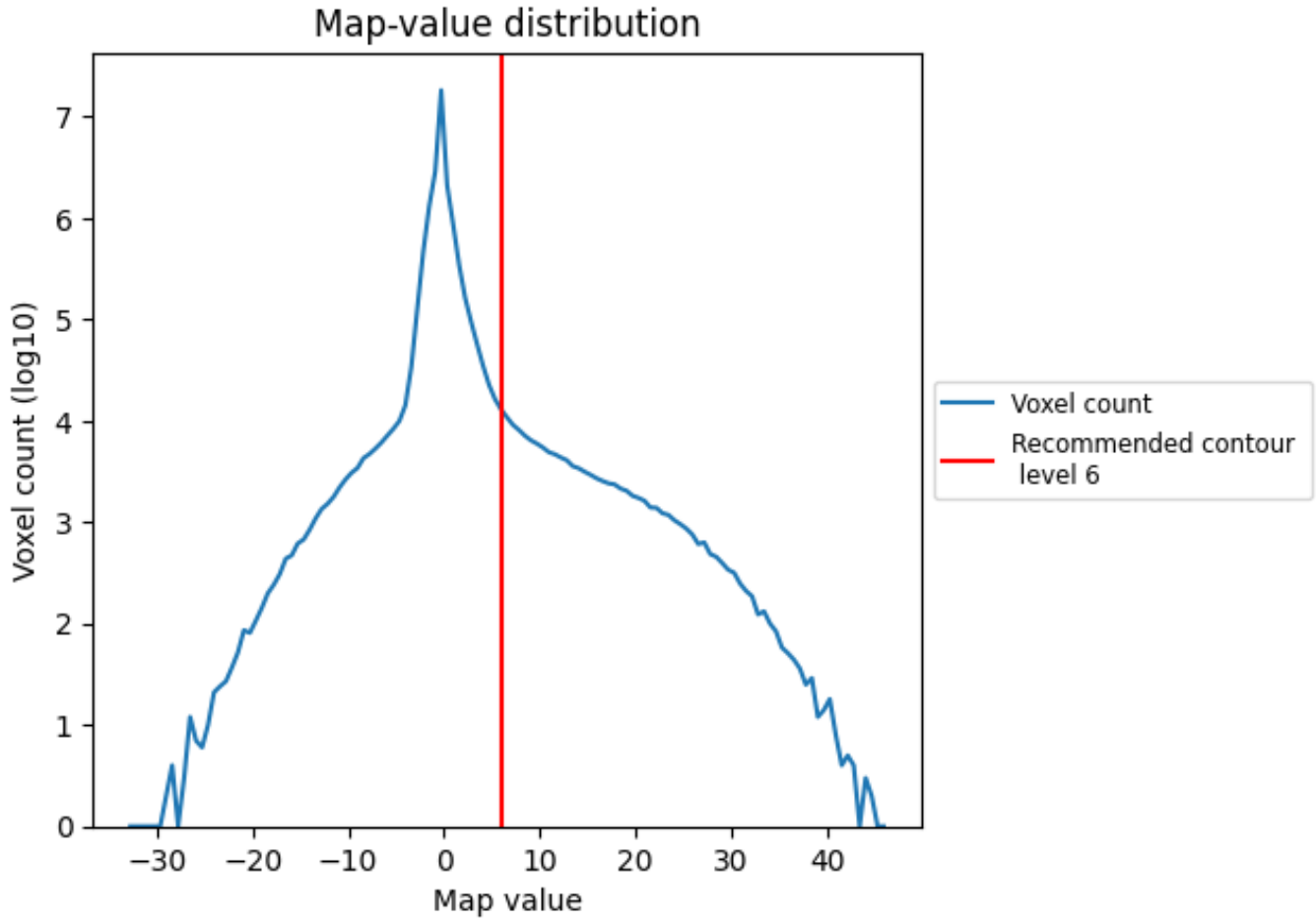
6.6 Mask visualisation (i)

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

7 Map analysis

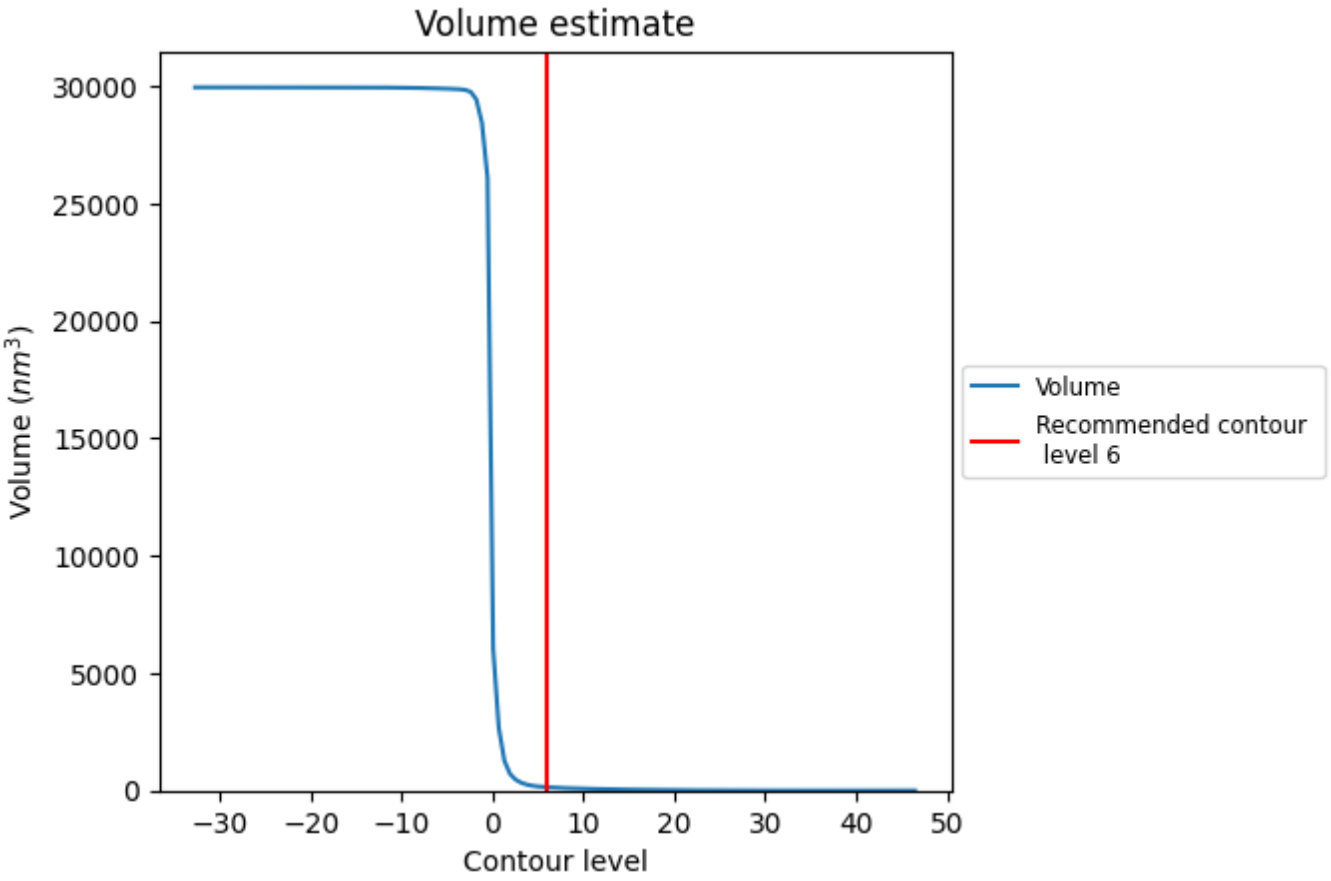
This section contains the results of statistical analysis of the map.

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.

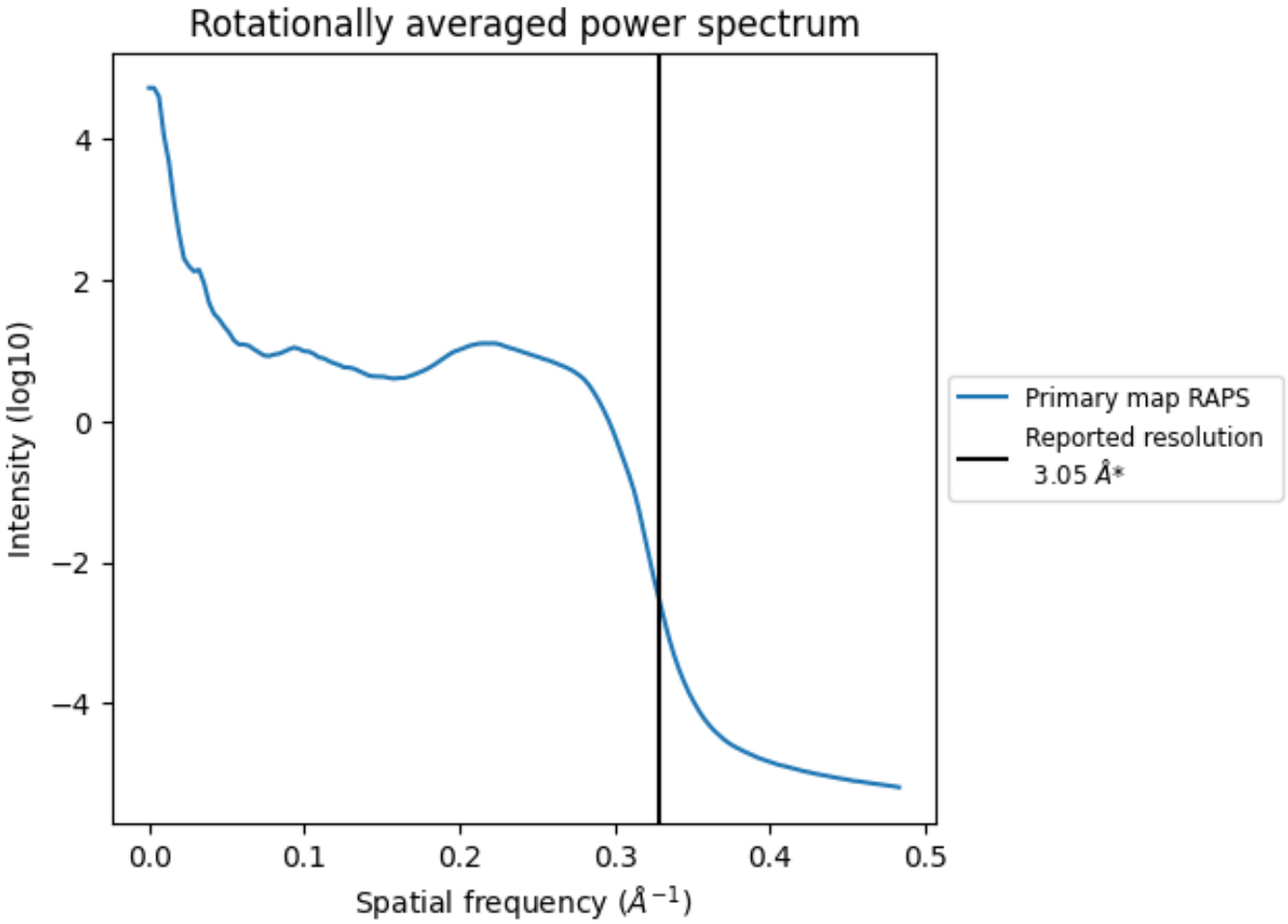
7.2 Volume estimate (i)



The volume at the recommended contour level is 143 nm^3; this corresponds to an approximate mass of 129 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 0.328 Å^{-1}

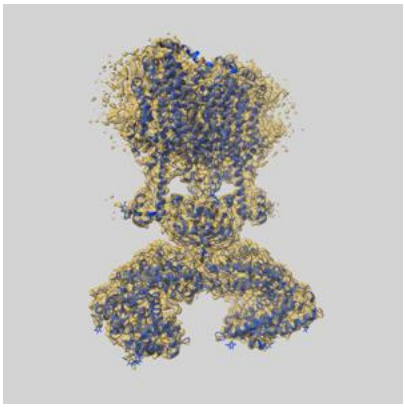
8 Fourier-Shell correlation (i)

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

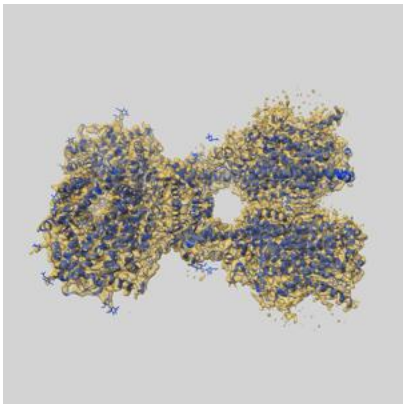
9 Map-model fit

This section contains information regarding the fit between EMDB map EMD-100053 and PDB model 34OE. Per-residue inclusion information can be found in section 3 on page 11.

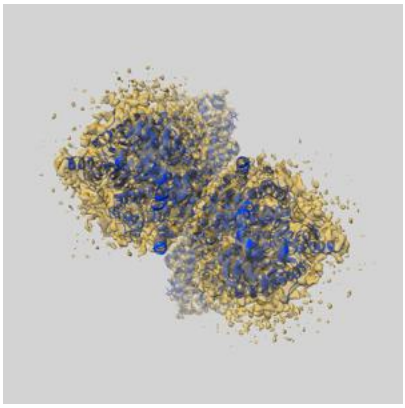
9.1 Map-model overlay



X



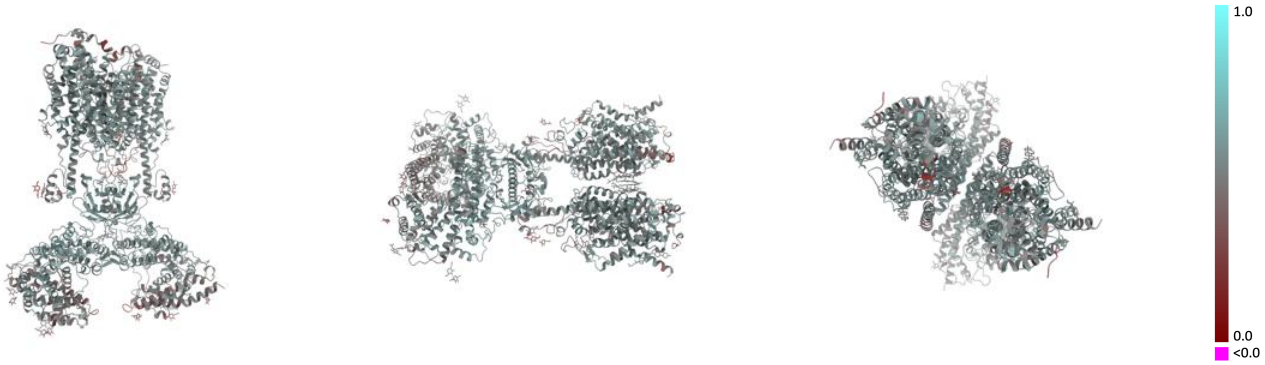
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 6.0 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.

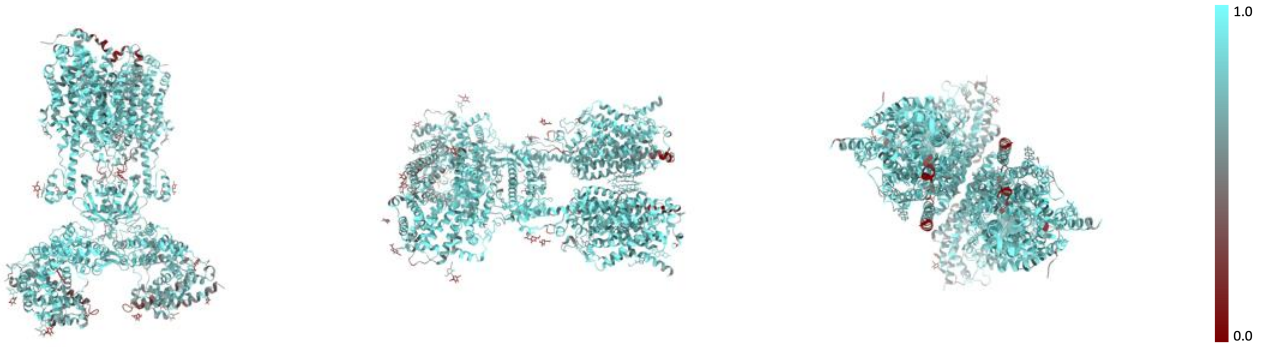
9.2 Q-score mapped to coordinate model (i)



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.

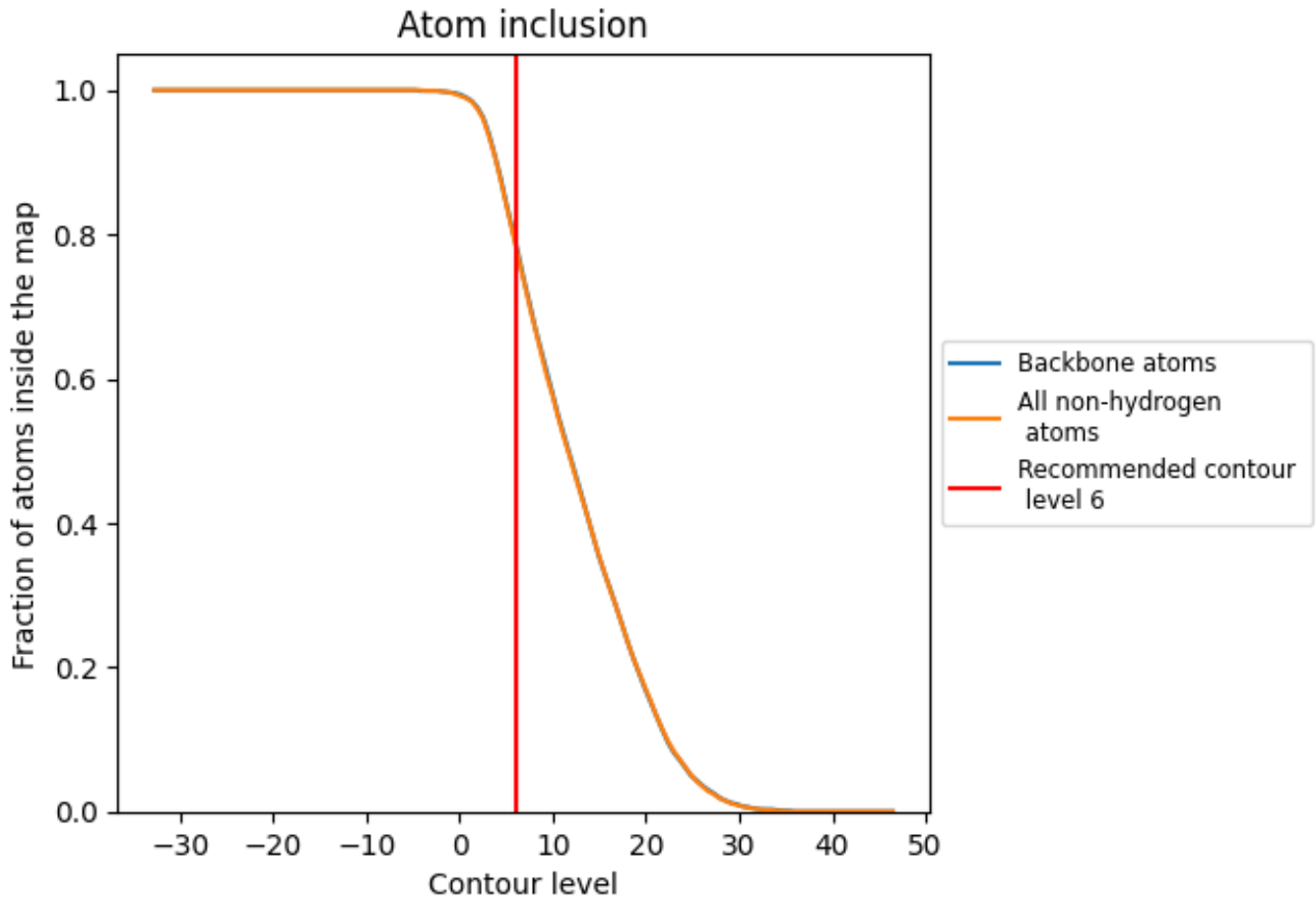
9.3 Atom inclusion mapped to coordinate model (i)



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 (6).

9.4 Atom inclusion (i)



At the recommended contour level, 79% of all backbone atoms, 79% 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 (6) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.7860	0.5190
A	0.8160	0.5200
B	0.8140	0.5180
C	0.7780	0.5200
D	0.7770	0.5230
E	0.6070	0.4460
F	0.3570	0.2260
G	0.5710	0.4160
H	0.5000	0.3470
I	0.5000	0.3990
J	0.4210	0.4650
K	0.3210	0.4400
L	0.3570	0.4260
M	0.5710	0.4710
N	0.5000	0.4270
O	0.4210	0.4560
P	0.3210	0.4640
Q	0.3930	0.4350
R	0.6070	0.4520

