



wwPDB X-ray Structure Validation Summary Report ⓘ

Apr 26, 2026 – 08:13 AM EDT

PDB ID : 7T1X / pdb_00007t1x
Title : Crystal structure of human Fab A194-01 in complex with its synthetic heptasaccharide Ara6-Man epitope (BSI110888)
Authors : Seattle Structural Genomics Center for Infectious Disease (SSGCID)
Deposited on : 2021-12-02
Resolution : 2.60 Å(reported)

This is a wwPDB X-ray Structure 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/XrayValidationReportHelp>

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:

MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

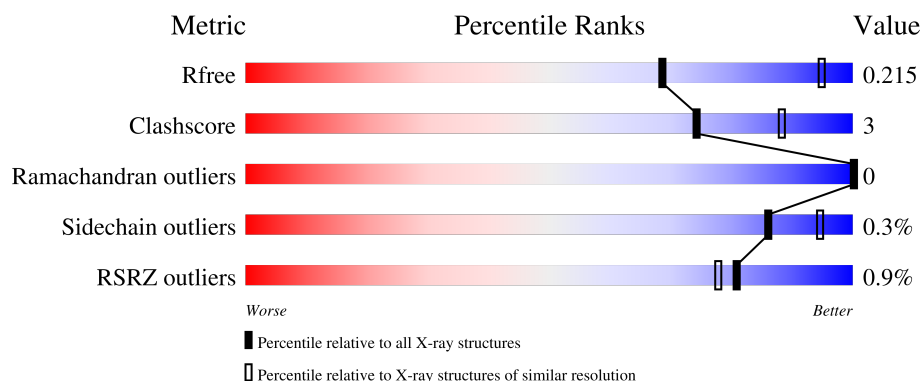
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.60 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)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	4008 (2.60-2.60)
Clashscore	190562	4347 (2.60-2.60)
Ramachandran outliers	187476	4277 (2.60-2.60)
Sidechain outliers	187428	4277 (2.60-2.60)
RSRZ outliers	180081	4008 (2.60-2.60)

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

Mol	Chain	Length	Quality of chain
1	H	228	% 86% 8% 5%
1	H2	228	87% 7% 5%
1	H3	228	4% 83% 11% 6%
1	H4	228	86% 10% 5%
1	H5	228	% 82% 11% 6%

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Mol	Chain	Length	Quality of chain
2	L	213	95%
2	L2	213	91% 9%
2	L3	213	92% 7%
2	L4	213	95% 5%
2	L5	213	92% 7%
3	A	7	29% 71%
3	B	7	14% 86%
3	C	7	29% 71%
3	D	7	43% 14% 43%
3	E	7	14% 86%

2 Entry composition [i](#)

There are 5 unique types of molecules in this entry. The entry contains 17365 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, 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.

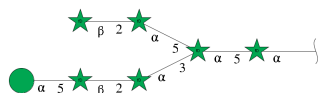
- Molecule 1 is a protein called Fab A194-01 heavy chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	H	216	Total	C	N	O	S	0	2	0
			1638	1037	277	317	7			
1	H2	217	Total	C	N	O	S	0	0	0
			1612	1021	269	315	7			
1	H3	215	Total	C	N	O	S	0	0	0
			1590	1006	265	312	7			
1	H4	217	Total	C	N	O	S	0	0	0
			1631	1031	276	317	7			
1	H5	215	Total	C	N	O	S	0	1	0
			1614	1021	272	314	7			

- Molecule 2 is a protein called Fab A194-01 light chain.

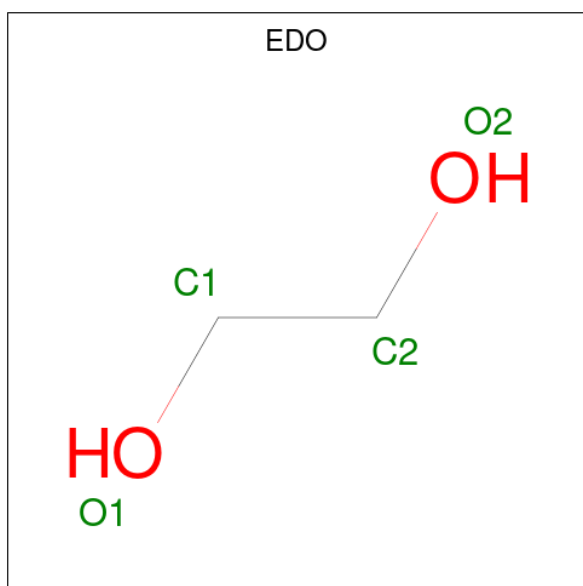
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	L	212	Total	C	N	O	S	0	0	0
			1619	1013	279	322	5			
2	L2	213	Total	C	N	O	S	0	0	0
			1616	1010	279	322	5			
2	L3	212	Total	C	N	O	S	0	1	0
			1592	996	275	316	5			
2	L4	212	Total	C	N	O	S	0	0	0
			1609	1005	277	322	5			
2	L5	212	Total	C	N	O	S	0	1	0
			1613	1008	279	321	5			

- Molecule 3 is an oligosaccharide called alpha-D-mannopyranose-(1-5)-beta-D-arabinofuranose-(1-2)-alpha-D-arabinofuranose-(1-3)-[beta-D-arabinofuranose-(1-2)-alpha-D-arabinofuranose-(1-5)]alpha-D-arabinofuranose-(1-5)-alpha-D-arabinofuranose.



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf	Trace
3	A	7	Total	C	O	0	0	0
			66	36	30			
3	B	7	Total	C	O	0	0	0
			66	36	30			
3	C	7	Total	C	O	0	0	0
			66	36	30			
3	D	7	Total	C	O	0	0	0
			66	36	30			
3	E	7	Total	C	O	0	0	0
			66	36	30			

- Molecule 4 is 1,2-ETHANEDIOL (CCD ID: EDO) (formula: C₂H₆O₂).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	H	1	Total	C	O	0	0
			4	2	2		
4	H	1	Total	C	O	0	0
			4	2	2		
4	L	1	Total	C	O	0	0
			4	2	2		
4	L3	1	Total	C	O	0	0
			4	2	2		
4	H4	1	Total	C	O	0	0
			4	2	2		
4	H5	1	Total	C	O	0	0
			4	2	2		

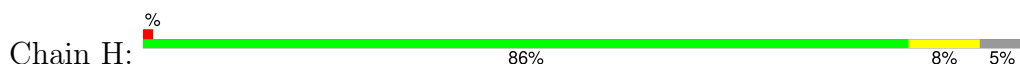
- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	H	109	Total 111	O 111	0	2
5	L	130	Total 131	O 131	0	1
5	H2	62	Total 62	O 62	0	0
5	L2	68	Total 68	O 68	0	0
5	H3	50	Total 50	O 50	0	0
5	L3	92	Total 92	O 92	0	0
5	H4	128	Total 128	O 128	0	0
5	L4	91	Total 91	O 91	0	0
5	H5	85	Total 85	O 85	0	0
5	L5	58	Total 59	O 59	0	1

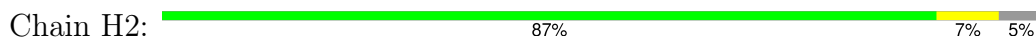
3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron 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 dot above a residue indicates a poor fit to the electron density ($RSRZ > 2$). 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.

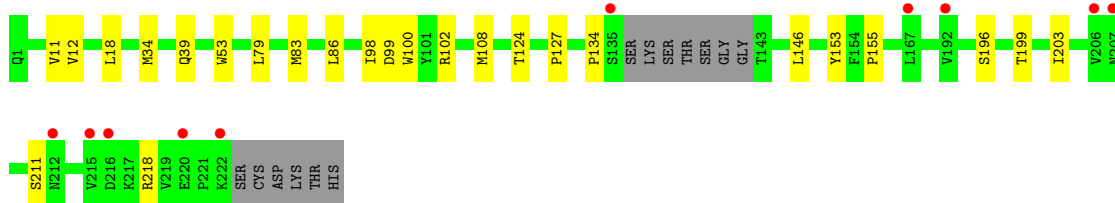
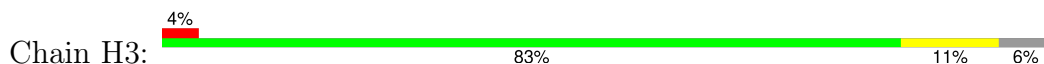
- Molecule 1: Fab A194-01 heavy chain



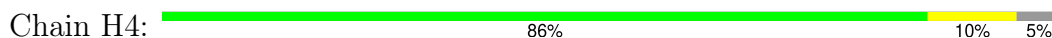
- Molecule 1: Fab A194-01 heavy chain



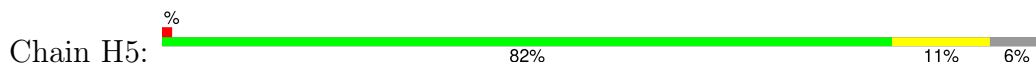
- Molecule 1: Fab A194-01 heavy chain

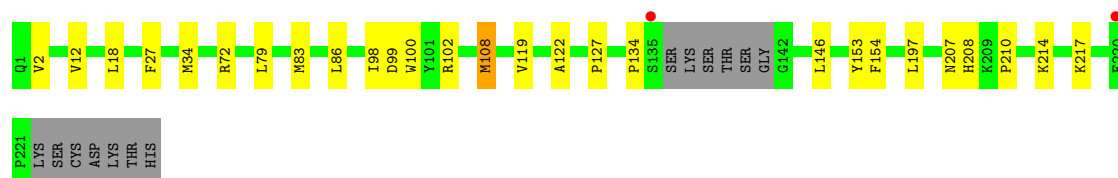


- Molecule 1: Fab A194-01 heavy chain



- Molecule 1: Fab A194-01 heavy chain





- Molecule 2: Fab A194-01 light chain

Chain L: 95%



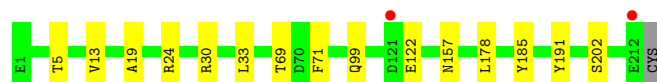
- Molecule 2: Fab A194-01 light chain

Chain L2: 91%



- Molecule 2: Fab A194-01 light chain

Chain L3: 92%



- Molecule 2: Fab A194-01 light chain

Chain L4: 95%



- Molecule 2: Fab A194-01 light chain

Chain L5: 92%

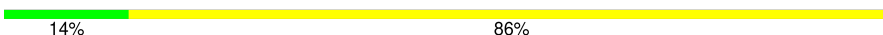


- Molecule 3: alpha-D-mannopyranose-(1-5)-beta-D-arabinofuranose-(1-2)-alpha-D-arabinofuranose-(1-3)-[beta-D-arabinofuranose-(1-2)-alpha-D-arabinofuranose-(1-5)]alpha-D-arabinofuranose-(1-5)-alpha-D-arabinofuranose

Chain A: 29%

BXY1	BXY2	BXY3	BXY4	MAN5	BXY6	BXY7
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- Molecule 3: alpha-D-mannopyranose-(1-5)-beta-D-arabinofuranose-(1-2)-alpha-D-arabinofuranose-(1-3)-[beta-D-arabinofuranose-(1-2)-alpha-D-arabinofuranose-(1-5)]alpha-D-arabinofuranose-(1-5)-alpha-D-arabinofuranose

Chain B:  14% 86%

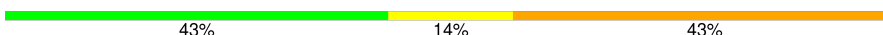
BXY1	BXY2	BXY3	BXY4	MAN5	BXY6	BXY7
------	------	------	------	------	------	------

- Molecule 3: alpha-D-mannopyranose-(1-5)-beta-D-arabinofuranose-(1-2)-alpha-D-arabinofuranose-(1-3)-[beta-D-arabinofuranose-(1-2)-alpha-D-arabinofuranose-(1-5)]alpha-D-arabinofuranose-(1-5)-alpha-D-arabinofuranose

Chain C:  29% 71%

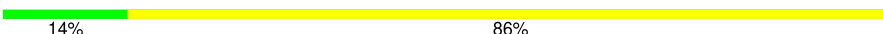
BXY1	BXY2	BXY3	BXY4	MAN5	BXY6	BXY7
------	------	------	------	------	------	------

- Molecule 3: alpha-D-mannopyranose-(1-5)-beta-D-arabinofuranose-(1-2)-alpha-D-arabinofuranose-(1-3)-[beta-D-arabinofuranose-(1-2)-alpha-D-arabinofuranose-(1-5)]alpha-D-arabinofuranose-(1-5)-alpha-D-arabinofuranose

Chain D:  43% 14% 43%

BXY1	BXY2	BXY3	BXY4	MAN5	BXY6	BXY7
------	------	------	------	------	------	------

- Molecule 3: alpha-D-mannopyranose-(1-5)-beta-D-arabinofuranose-(1-2)-alpha-D-arabinofuranose-(1-3)-[beta-D-arabinofuranose-(1-2)-alpha-D-arabinofuranose-(1-5)]alpha-D-arabinofuranose-(1-5)-alpha-D-arabinofuranose

Chain E:  14% 86%

BXY1	BXY2	BXY3	BXY4	MAN5	BXY6	BXY7
------	------	------	------	------	------	------

4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	85.93Å 149.26Å 115.36Å 90.00° 99.31° 90.00°	Depositor
Resolution (Å)	28.03 – 2.60 28.03 – 2.60	Depositor EDS
% Data completeness (in resolution range)	99.4 (28.03-2.60) 99.4 (28.03-2.60)	Depositor EDS
R_{merge}	0.11	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.88 (at 2.61Å)	Xtriage
Refinement program	PHENIX 1.18rc1 3776	Depositor
R, R_{free}	0.159 , 0.216 0.163 , 0.215	Depositor DCC
R_{free} test set	2039 reflections (2.31%)	wwPDB-VP
Wilson B-factor (Å ²)	37.4	Xtriage
Anisotropy	0.200	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 59.3	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.34$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	17365	wwPDB-VP
Average B, all atoms (Å ²)	48.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.20% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: BXX, BXY, EDO, MAN

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	H	0.29	0/1684	0.54	0/2295
1	H2	0.27	0/1652	0.52	0/2255
1	H3	0.25	0/1630	0.48	0/2229
1	H4	0.30	0/1671	0.54	0/2277
1	H5	0.28	0/1657	0.52	1/2261 (0.0%)
2	L	0.30	0/1655	0.54	0/2249
2	L2	0.26	0/1652	0.50	0/2248
2	L3	0.30	0/1631	0.52	0/2223
2	L4	0.27	0/1645	0.51	0/2238
2	L5	0.25	0/1652	0.48	0/2248
All	All	0.28	0/16529	0.51	1/22523 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	H5	102	ARG	CB-CA-C	-5.57	110.14	116.54

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

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	H	1638	0	1586	10	0
1	H2	1612	0	1533	10	0
1	H3	1590	0	1494	13	0
1	H4	1631	0	1574	13	0
1	H5	1614	0	1547	17	0
2	L	1619	0	1561	6	0
2	L2	1616	0	1543	10	0
2	L3	1592	0	1502	8	0
2	L4	1609	0	1532	7	0
2	L5	1613	0	1537	8	0
3	A	66	0	54	0	0
3	B	66	0	54	0	0
3	C	66	0	54	0	0
3	D	66	0	54	3	0
3	E	66	0	54	0	0
4	H	8	0	12	0	0
4	H4	4	0	6	1	0
4	H5	4	0	6	0	0
4	L	4	0	6	0	0
4	L3	4	0	6	0	0
5	H	111	0	0	0	0
5	H2	62	0	0	1	0
5	H3	50	0	0	1	0
5	H4	128	0	0	0	0
5	H5	85	0	0	0	0
5	L	131	0	0	1	0
5	L2	68	0	0	0	0
5	L3	92	0	0	1	0
5	L4	91	0	0	1	0
5	L5	59	0	0	0	0
All	All	17365	0	15715	101	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 3.

The worst 5 of 101 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:H5:134:PRO:HG3	1:H5:146:LEU:HB3	1.60	0.83
1:H:134:PRO:HG3	1:H:146:LEU:HB3	1.63	0.81
1:H3:11:VAL:HG22	1:H3:155:PRO:HG3	1.61	0.80
1:H3:134:PRO:HG3	1:H3:146:LEU:HB3	1.71	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H2:40:ALA:HB3	1:H2:43:LYS:HD2	1.73	0.71

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 X-ray entries followed by that with respect to entries of similar resolution.

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	H	214/228 (94%)	208 (97%)	6 (3%)	0	100	100
1	H2	213/228 (93%)	208 (98%)	5 (2%)	0	100	100
1	H3	211/228 (92%)	208 (99%)	3 (1%)	0	100	100
1	H4	213/228 (93%)	209 (98%)	4 (2%)	0	100	100
1	H5	212/228 (93%)	207 (98%)	5 (2%)	0	100	100
2	L	210/213 (99%)	203 (97%)	7 (3%)	0	100	100
2	L2	211/213 (99%)	206 (98%)	5 (2%)	0	100	100
2	L3	211/213 (99%)	204 (97%)	7 (3%)	0	100	100
2	L4	210/213 (99%)	203 (97%)	7 (3%)	0	100	100
2	L5	211/213 (99%)	204 (97%)	7 (3%)	0	100	100
All	All	2116/2205 (96%)	2060 (97%)	56 (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 X-ray entries followed by that with respect to entries of similar resolution.

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	H	180/192 (94%)	180 (100%)	0	100	100
1	H2	174/192 (91%)	173 (99%)	1 (1%)	78	91
1	H3	170/192 (88%)	170 (100%)	0	100	100
1	H4	179/192 (93%)	179 (100%)	0	100	100
1	H5	176/192 (92%)	174 (99%)	2 (1%)	65	84
2	L	178/183 (97%)	178 (100%)	0	100	100
2	L2	176/183 (96%)	175 (99%)	1 (1%)	78	91
2	L3	170/183 (93%)	169 (99%)	1 (1%)	78	91
2	L4	175/183 (96%)	175 (100%)	0	100	100
2	L5	175/183 (96%)	174 (99%)	1 (1%)	78	91
All	All	1753/1875 (94%)	1747 (100%)	6 (0%)	86	94

5 of 6 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	H5	108	MET
1	H5	217	LYS
2	L5	146	GLN
2	L2	24	ARG
1	H2	89	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 13 such sidechains are listed below:

Mol	Chain	Res	Type
2	L3	123	GLN
2	L3	198	GLN
2	L5	188	HIS
1	H4	84	ASN
2	L4	188	HIS

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 ⓘ

35 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	BXY	A	1	3	10,10,10	0.69	0	13,14,14	2.80	4 (30%)
3	BXY	A	2	3	9,9,10	0.62	0	11,12,14	1.78	3 (27%)
3	BXY	A	3	3	9,9,10	0.57	0	11,12,14	2.21	4 (36%)
3	BXX	A	4	3	9,9,10	0.43	0	11,12,14	0.79	0
3	MAN	A	5	3	11,11,12	0.45	0	15,15,17	0.74	0
3	BXY	A	6	3	9,9,10	1.00	1 (11%)	11,12,14	2.39	3 (27%)
3	BXX	A	7	3	9,9,10	0.52	0	11,12,14	0.99	1 (9%)
3	BXY	B	1	3	10,10,10	0.69	0	13,14,14	4.02	4 (30%)
3	BXY	B	2	3	9,9,10	0.58	0	11,12,14	1.65	3 (27%)
3	BXY	B	3	3	9,9,10	0.48	0	11,12,14	1.27	1 (9%)
3	BXX	B	4	3	9,9,10	0.45	0	11,12,14	0.83	0
3	MAN	B	5	3	11,11,12	0.57	0	15,15,17	1.31	1 (6%)
3	BXY	B	6	3	9,9,10	0.98	1 (11%)	11,12,14	2.48	4 (36%)
3	BXX	B	7	3	9,9,10	0.43	0	11,12,14	1.04	1 (9%)
3	BXY	C	1	3	10,10,10	0.65	0	13,14,14	1.83	2 (15%)
3	BXY	C	2	3	9,9,10	0.84	0	11,12,14	1.60	3 (27%)
3	BXY	C	3	3	9,9,10	0.38	0	11,12,14	1.18	1 (9%)
3	BXX	C	4	3	9,9,10	0.44	0	11,12,14	0.90	0
3	MAN	C	5	3	11,11,12	0.62	0	15,15,17	0.76	0
3	BXY	C	6	3	9,9,10	1.03	1 (11%)	11,12,14	3.65	3 (27%)
3	BXX	C	7	3	9,9,10	0.57	0	11,12,14	1.06	1 (9%)
3	BXY	D	1	3	10,10,10	0.66	0	13,14,14	2.15	4 (30%)
3	BXY	D	2	3	9,9,10	0.76	0	11,12,14	1.62	3 (27%)
3	BXY	D	3	3	9,9,10	0.52	0	11,12,14	1.61	1 (9%)
3	BXX	D	4	3	9,9,10	0.46	0	11,12,14	0.90	0
3	MAN	D	5	3	11,11,12	0.80	0	15,15,17	0.80	0
3	BXY	D	6	3	9,9,10	0.91	1 (11%)	11,12,14	1.74	2 (18%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
3	BXX	D	7	3	9,9,10	0.47	0	11,12,14	0.71	0
3	BXY	E	1	3	10,10,10	0.75	0	13,14,14	3.55	6 (46%)
3	BXY	E	2	3	9,9,10	0.54	0	11,12,14	1.52	2 (18%)
3	BXY	E	3	3	9,9,10	0.64	0	11,12,14	1.99	2 (18%)
3	BXX	E	4	3	9,9,10	0.53	0	11,12,14	0.93	0
3	MAN	E	5	3	11,11,12	0.61	0	15,15,17	1.00	1 (6%)
3	BXY	E	6	3	9,9,10	1.06	2 (22%)	11,12,14	3.38	5 (45%)
3	BXX	E	7	3	9,9,10	0.49	0	11,12,14	1.04	1 (9%)

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	BXY	A	1	3	-	2/2/18/18	0/1/1/1
3	BXY	A	2	3	-	0/2/15/18	0/1/1/1
3	BXY	A	3	3	-	2/2/15/18	0/1/1/1
3	BXX	A	4	3	-	0/2/15/18	0/1/1/1
3	MAN	A	5	3	-	2/2/19/22	0/1/1/1
3	BXY	A	6	3	-	0/2/15/18	0/1/1/1
3	BXX	A	7	3	-	0/2/15/18	0/1/1/1
3	BXY	B	1	3	-	2/2/18/18	0/1/1/1
3	BXY	B	2	3	-	0/2/15/18	0/1/1/1
3	BXY	B	3	3	-	2/2/15/18	0/1/1/1
3	BXX	B	4	3	-	0/2/15/18	0/1/1/1
3	MAN	B	5	3	-	2/2/19/22	0/1/1/1
3	BXY	B	6	3	-	0/2/15/18	0/1/1/1
3	BXX	B	7	3	-	0/2/15/18	0/1/1/1
3	BXY	C	1	3	-	0/2/18/18	0/1/1/1
3	BXY	C	2	3	-	1/2/15/18	0/1/1/1
3	BXY	C	3	3	-	2/2/15/18	0/1/1/1
3	BXX	C	4	3	-	0/2/15/18	0/1/1/1
3	MAN	C	5	3	-	2/2/19/22	0/1/1/1
3	BXY	C	6	3	-	0/2/15/18	0/1/1/1
3	BXX	C	7	3	-	0/2/15/18	0/1/1/1
3	BXY	D	1	3	-	0/2/18/18	0/1/1/1
3	BXY	D	2	3	-	0/2/15/18	0/1/1/1
3	BXY	D	3	3	-	2/2/15/18	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	BXX	D	4	3	-	0/2/15/18	0/1/1/1
3	MAN	D	5	3	-	2/2/19/22	0/1/1/1
3	BXY	D	6	3	-	0/2/15/18	0/1/1/1
3	BXX	D	7	3	-	0/2/15/18	0/1/1/1
3	BXY	E	1	3	-	2/2/18/18	0/1/1/1
3	BXY	E	2	3	-	1/2/15/18	0/1/1/1
3	BXY	E	3	3	-	2/2/15/18	0/1/1/1
3	BXX	E	4	3	-	0/2/15/18	0/1/1/1
3	MAN	E	5	3	-	2/2/19/22	0/1/1/1
3	BXY	E	6	3	-	0/2/15/18	0/1/1/1
3	BXX	E	7	3	-	2/2/15/18	0/1/1/1

The worst 5 of 6 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	6	BXY	O2-C2	-2.59	1.37	1.43
3	C	6	BXY	O2-C2	-2.55	1.38	1.43
3	B	6	BXY	O2-C2	-2.53	1.38	1.43
3	D	6	BXY	O2-C2	-2.36	1.38	1.43
3	E	6	BXY	O2-C2	-2.26	1.38	1.43

The worst 5 of 66 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	1	BXY	O5-C5-C4	13.02	155.67	111.33
3	E	1	BXY	O5-C5-C4	9.76	144.55	111.33
3	C	6	BXY	O2-C2-C3	9.39	129.93	111.43
3	A	1	BXY	O5-C5-C4	8.13	139.02	111.33
3	E	6	BXY	O2-C2-C3	-6.83	97.98	111.43

There are no chirality outliers.

5 of 30 torsion outliers are listed below:

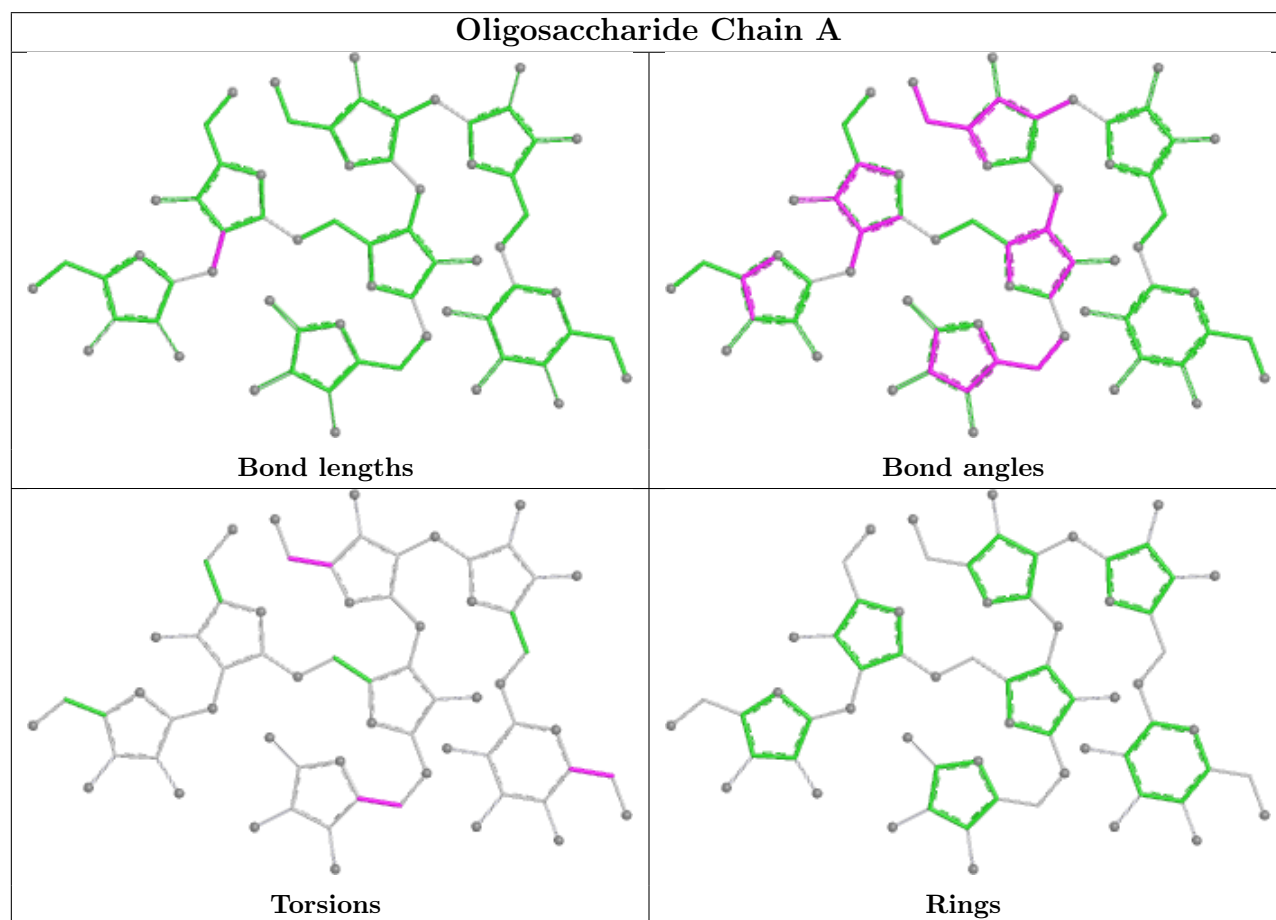
Mol	Chain	Res	Type	Atoms
3	E	3	BXY	C3-C4-C5-O5
3	A	3	BXY	C3-C4-C5-O5
3	D	5	MAN	O5-C5-C6-O6
3	D	5	MAN	C4-C5-C6-O6
3	A	3	BXY	O4-C4-C5-O5

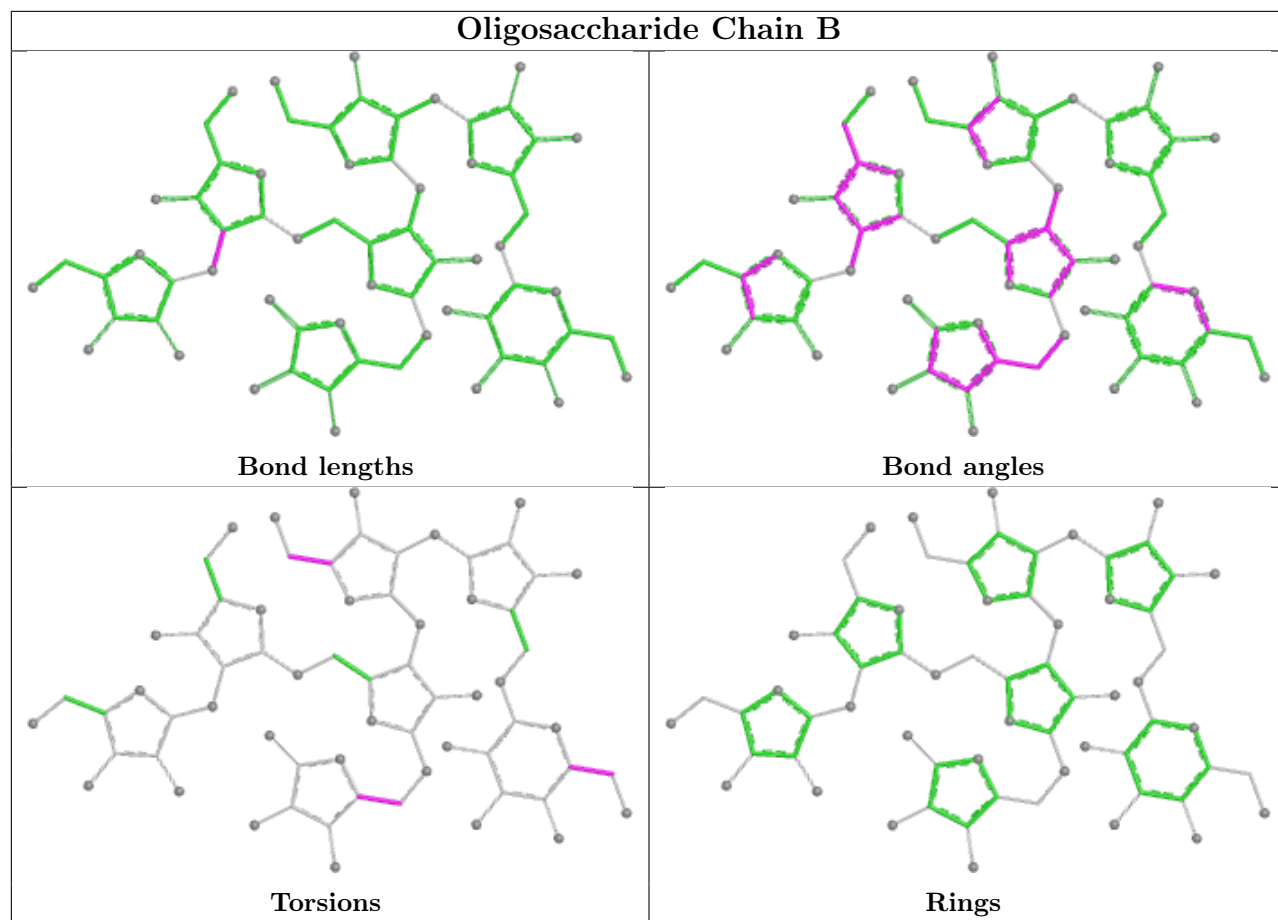
There are no ring outliers.

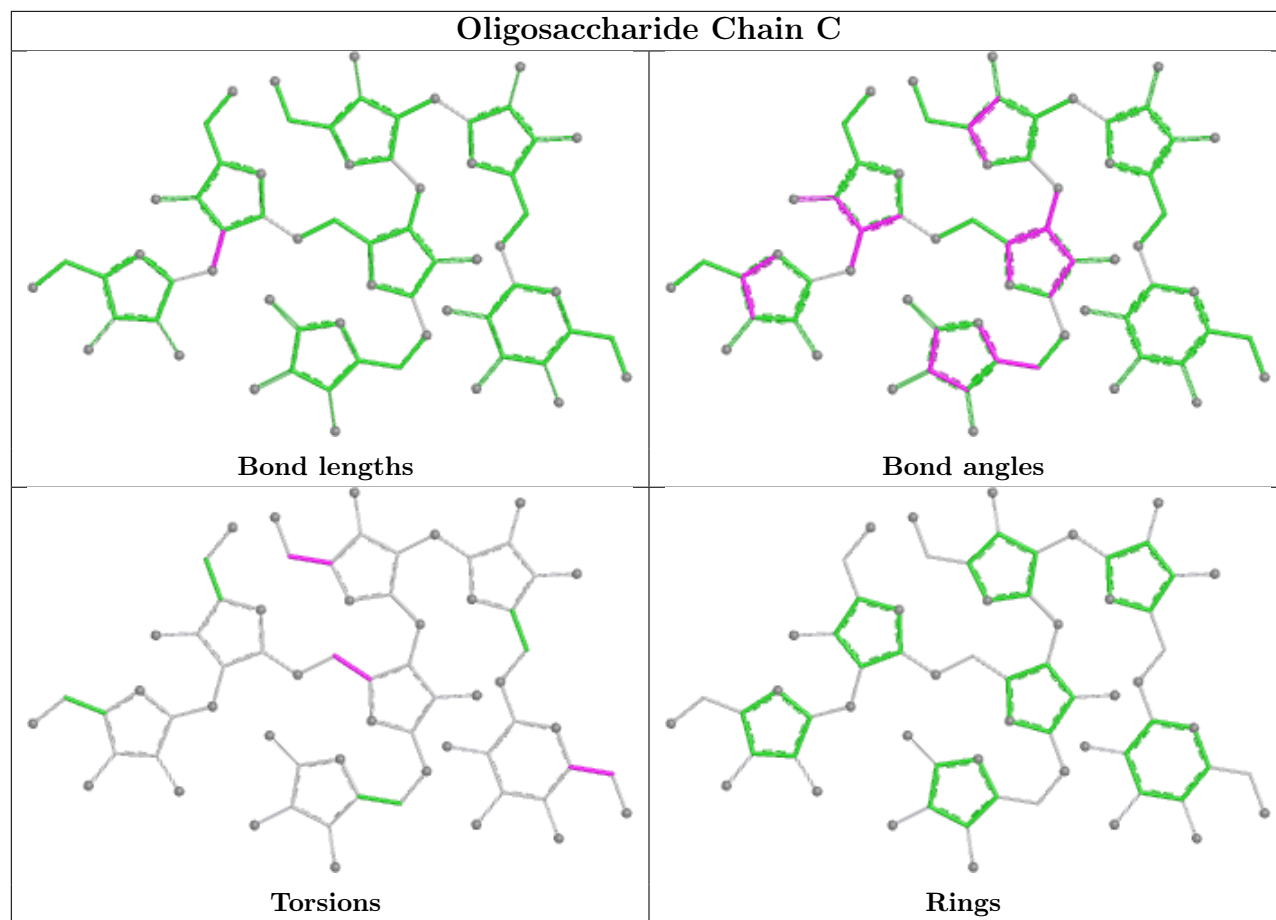
3 monomers are involved in 3 short contacts:

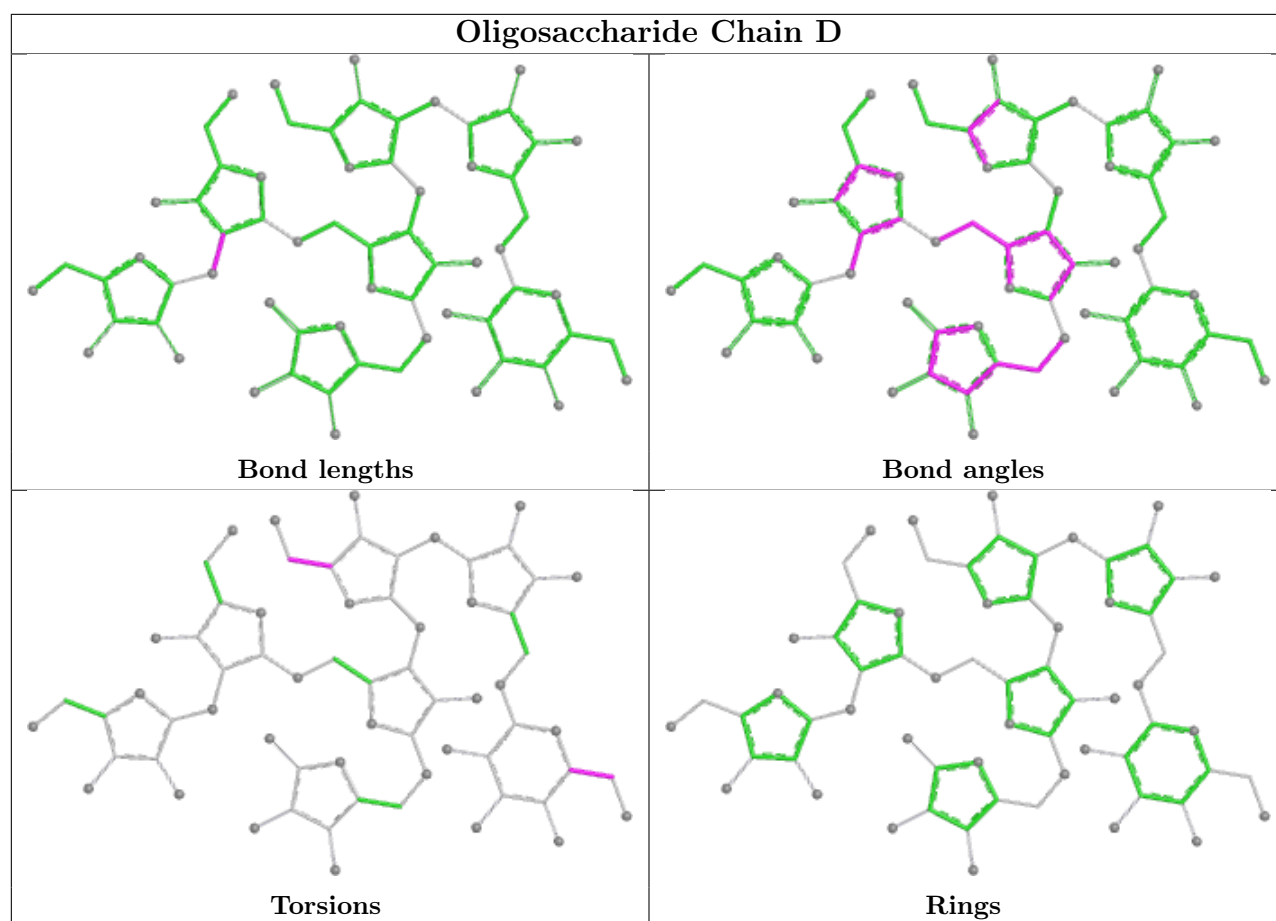
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	D	1	BXY	2	0
3	D	2	BXY	1	0
3	D	3	BXY	1	0

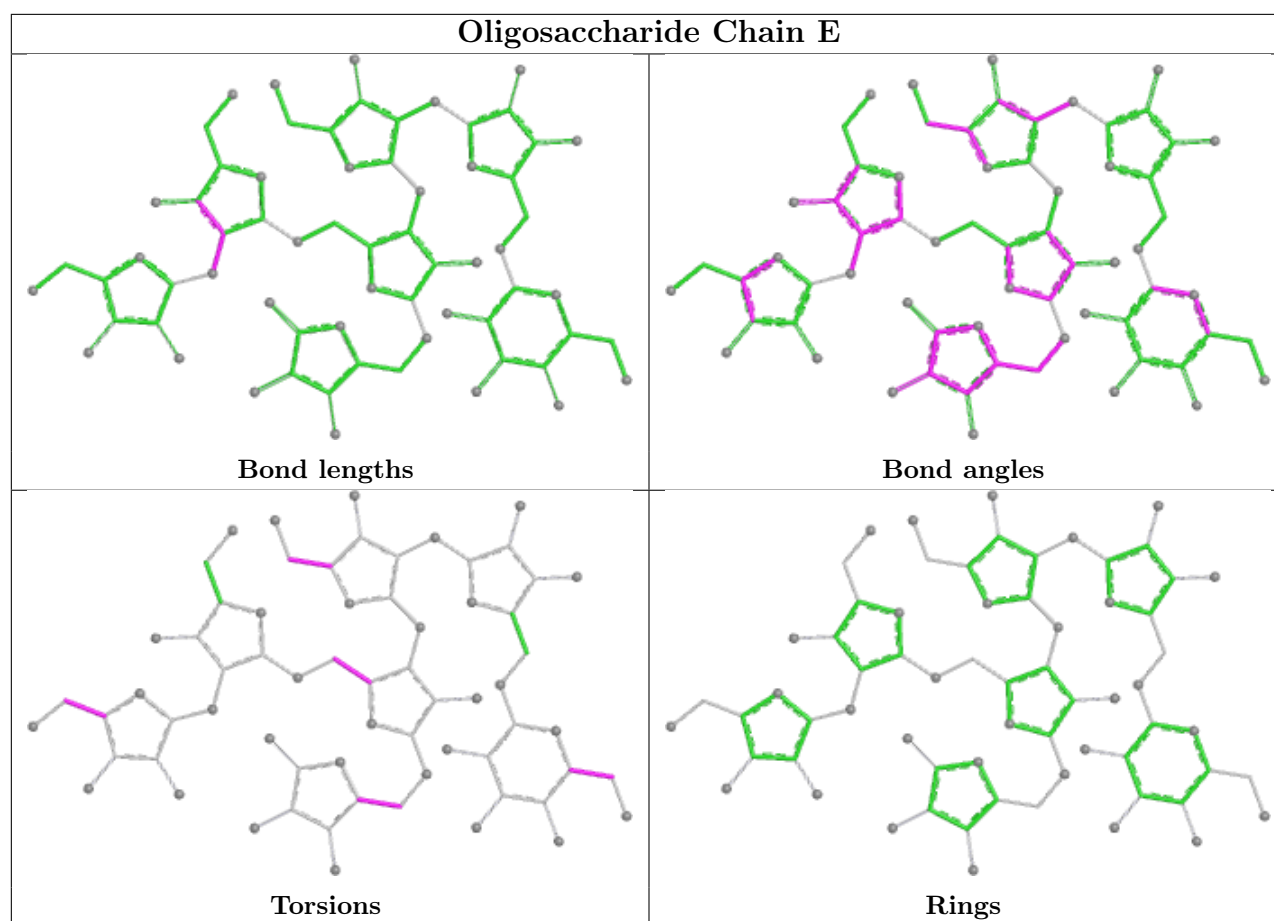
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for oligosaccharide.











5.6 Ligand geometry [i](#)

6 ligands are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
4	EDO	H	501	-	3,3,3	0.46	0	2,2,2	0.27	0
4	EDO	H4	501	-	3,3,3	0.48	0	2,2,2	0.37	0
4	EDO	L3	301	-	3,3,3	0.48	0	2,2,2	0.34	0
4	EDO	L	301	-	3,3,3	0.51	0	2,2,2	0.22	0
4	EDO	H	502	-	3,3,3	0.47	0	2,2,2	0.51	0
4	EDO	H5	501	-	3,3,3	0.51	0	2,2,2	0.28	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
4	EDO	H	501	-	-	0/1/1/1	-
4	EDO	H4	501	-	-	1/1/1/1	-
4	EDO	L3	301	-	-	0/1/1/1	-
4	EDO	L	301	-	-	0/1/1/1	-
4	EDO	H	502	-	-	1/1/1/1	-
4	EDO	H5	501	-	-	0/1/1/1	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (2) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	H4	501	EDO	O1-C1-C2-O2
4	H	502	EDO	O1-C1-C2-O2

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	H4	501	EDO	1	0

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 Fit of model and data [i](#)

6.1 Protein, DNA and RNA chains [i](#)

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	H	216/228 (94%)	-0.74	2 (0%) 81 78	17, 36, 70, 103	2 (0%)
1	H2	217/228 (95%)	-0.50	0 100 100	31, 45, 83, 110	0
1	H3	215/228 (94%)	0.06	10 (4%) 36 30	29, 59, 113, 138	0
1	H4	217/228 (95%)	-0.67	0 100 100	20, 36, 83, 101	0
1	H5	215/228 (94%)	-0.35	2 (0%) 81 78	21, 46, 98, 130	1 (0%)
2	L	212/213 (99%)	-0.82	0 100 100	20, 34, 62, 87	0
2	L2	213/213 (100%)	-0.52	1 (0%) 87 85	29, 46, 75, 98	0
2	L3	212/213 (99%)	-0.39	2 (0%) 81 78	20, 42, 93, 114	1 (0%)
2	L4	212/213 (99%)	-0.61	0 100 100	20, 40, 88, 105	0
2	L5	212/213 (99%)	-0.38	2 (0%) 81 78	25, 50, 90, 104	1 (0%)
All	All	2141/2205 (97%)	-0.49	19 (0%) 81 78	17, 44, 92, 138	5 (0%)

The worst 5 of 19 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	H3	212	ASN	4.2
2	L3	212	GLU	3.7
2	L2	213	CYS	3.1
1	H	222	LYS	2.9
1	H3	222	LYS	2.9

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

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

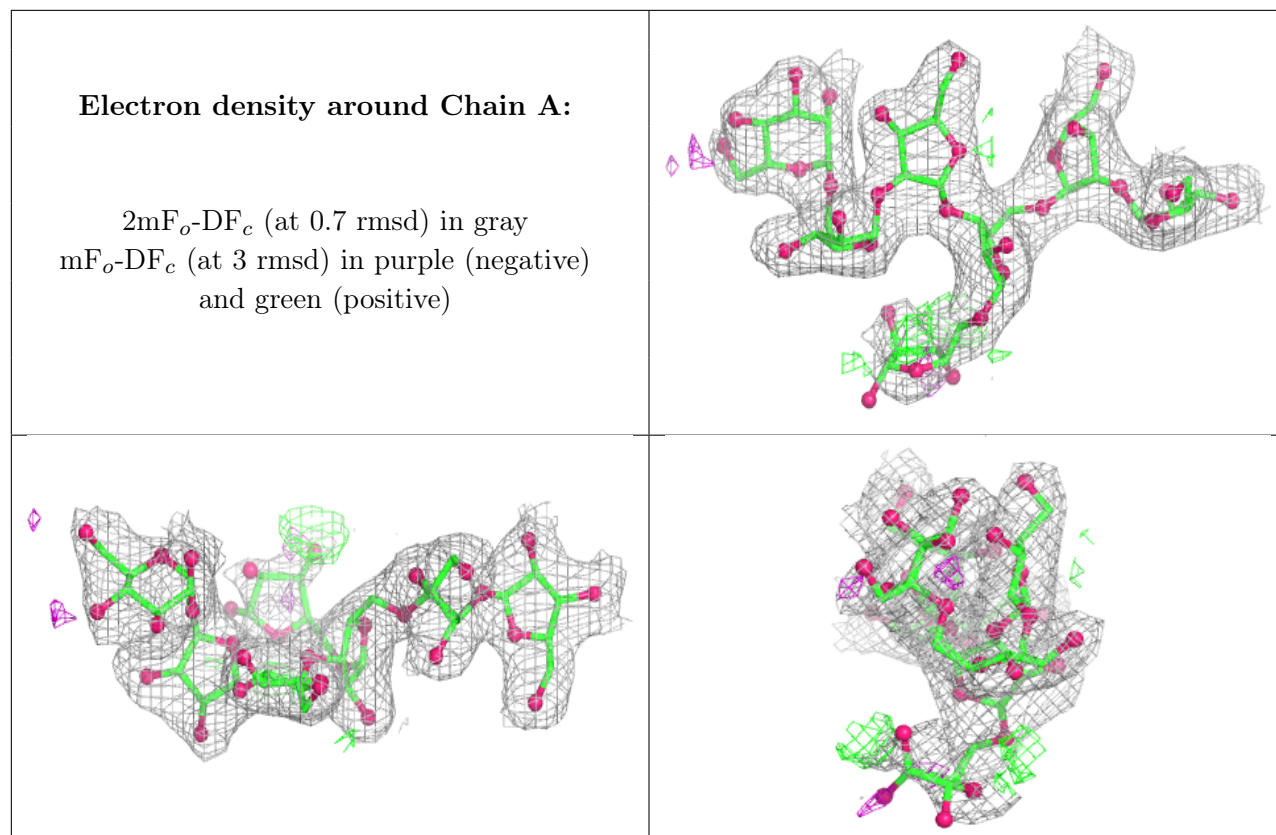
6.3 Carbohydrates ⓘ

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
3	BXY	A	1	10/10	-	-	79,109,113,119	0
3	BXY	A	2	9/10	-	-	33,43,50,56	0
3	BXY	A	3	9/10	-	-	47,50,56,56	0
3	BXX	A	4	9/10	-	-	51,53,57,66	0
3	MAN	A	5	11/12	-	-	43,58,64,65	0
3	BXY	A	6	9/10	-	-	25,27,32,33	0
3	BXX	A	7	9/10	-	-	23,26,35,36	0
3	BXY	B	1	10/10	-	-	82,105,112,116	0
3	BXY	B	2	9/10	-	-	53,58,68,68	0
3	BXY	B	3	9/10	-	-	53,58,67,72	0
3	BXX	B	4	9/10	-	-	77,81,83,88	0
3	MAN	B	5	11/12	-	-	61,70,75,84	0
3	BXY	B	6	9/10	-	-	29,36,45,49	0
3	BXX	B	7	9/10	-	-	32,38,40,41	0
3	BXY	C	1	10/10	-	-	77,108,114,114	0
3	BXY	C	2	9/10	-	-	45,64,71,74	0
3	BXY	C	3	9/10	-	-	77,83,85,87	0
3	BXX	C	4	9/10	-	-	88,95,102,103	0
3	MAN	C	5	11/12	-	-	86,95,99,101	0
3	BXY	C	6	9/10	-	-	30,41,44,45	0
3	BXX	C	7	9/10	-	-	30,38,43,44	0
3	BXY	D	1	10/10	-	-	88,115,122,125	0
3	BXY	D	2	9/10	-	-	28,48,66,69	0
3	BXY	D	3	9/10	-	-	59,72,83,90	0
3	BXX	D	4	9/10	-	-	109,114,116,118	0
3	MAN	D	5	11/12	-	-	113,117,121,122	0
3	BXY	D	6	9/10	-	-	24,27,36,38	0
3	BXX	D	7	9/10	-	-	21,25,27,33	0
3	BXY	E	1	10/10	-	-	78,101,106,108	0
3	BXY	E	2	9/10	-	-	42,46,54,59	0
3	BXY	E	3	9/10	-	-	59,69,74,74	0
3	BXX	E	4	9/10	-	-	78,84,88,90	0
3	MAN	E	5	11/12	-	-	79,91,100,101	0
3	BXY	E	6	9/10	-	-	19,34,39,44	0
3	BXX	E	7	9/10	-	-	25,27,34,34	0

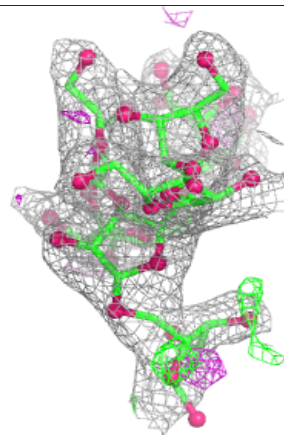
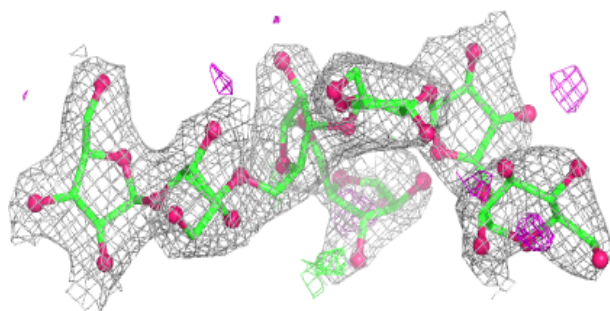
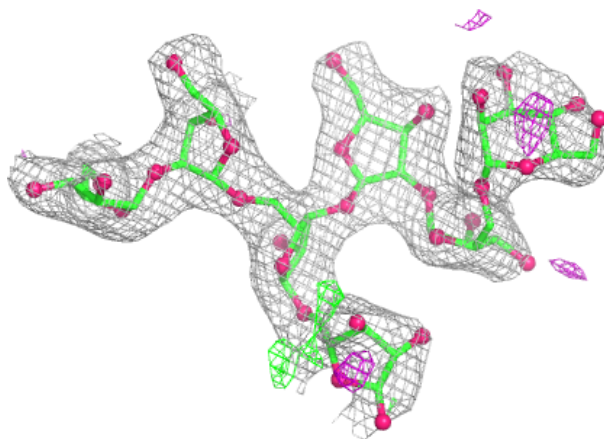
The following is a graphical depiction of the model fit to experimental electron density for oligosac-

charide. Each fit is shown from different orientation to approximate a three-dimensional view.

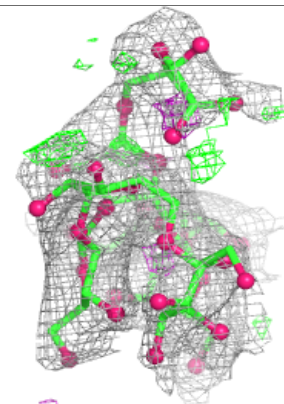
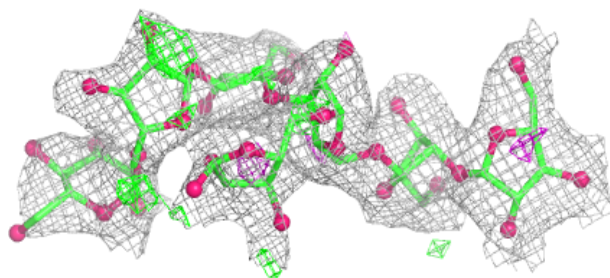
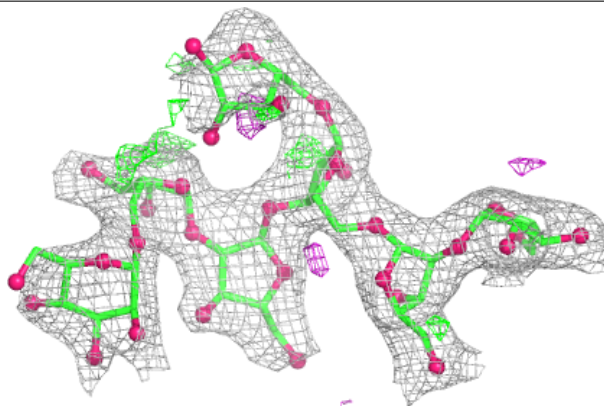


Electron density around Chain B:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

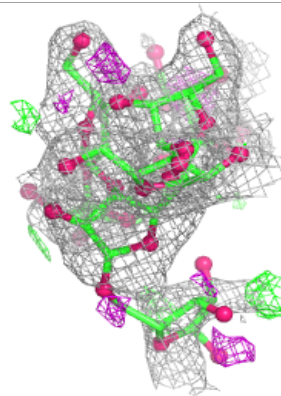
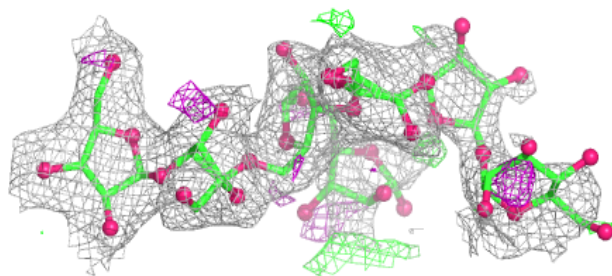
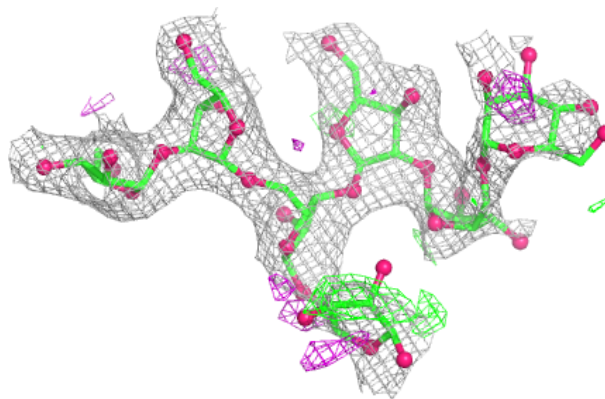
**Electron density around Chain C:**

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

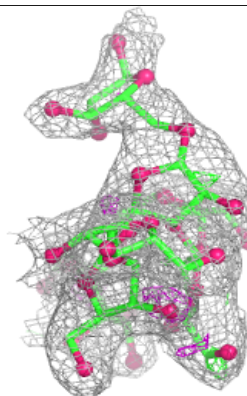
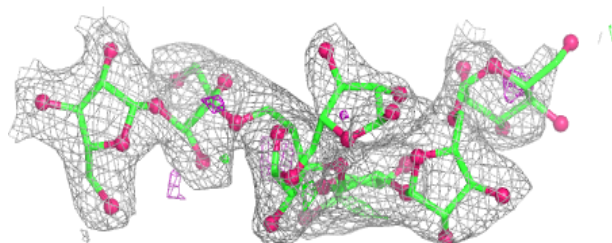
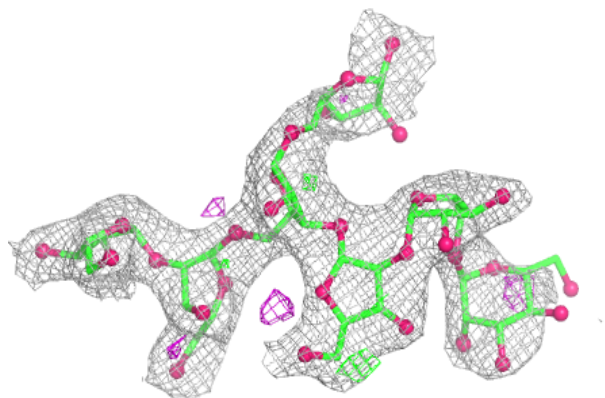


Electron density around Chain D:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

**Electron density around Chain E:**

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q<0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
4	EDO	H	502	4/4	0.54	0.24	71,73,75,76	0
4	EDO	L3	301	4/4	0.77	0.30	83,83,83,85	0
4	EDO	H5	501	4/4	0.85	0.14	54,55,55,57	0
4	EDO	H	501	4/4	0.89	0.16	72,72,72,73	0
4	EDO	L	301	4/4	0.90	0.13	41,45,45,53	0
4	EDO	H4	501	4/4	0.92	0.17	62,68,74,76	0

6.5 Other polymers [i](#)

There are no such residues in this entry.