wwPDB X-ray Structure Validation Summary Report (i)

Sep 25, 2023 – 12:08 AM EDT

PDB ID	:	5WB7
Title	:	Crystal structure of the epidermal growth factor receptor extracellular region in complex with epiregulin
Authors	:	Freed, D.M.; Bessman, N.J.; Ferguson, K.M.; Lemmon, M.A.
Deposited on	:	2017-06-28
Resolution	:	2.94 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 (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:

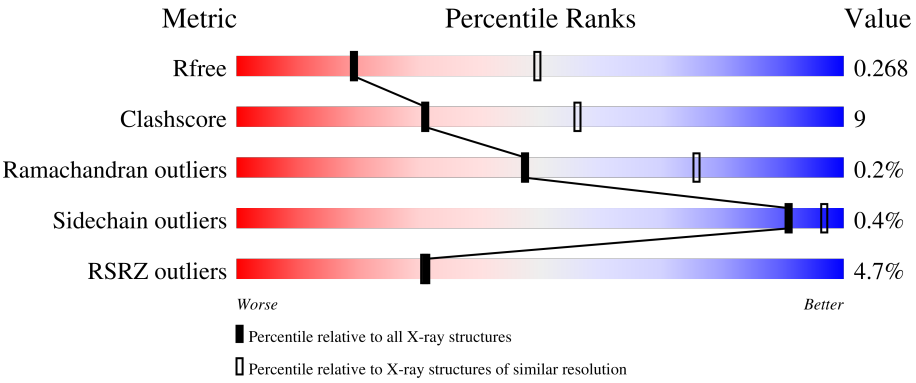
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.35.1
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.35.1

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 2.94 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}	130704	2969 (2.98-2.90)
Clashscore	141614	3218 (2.98-2.90)
Ramachandran outliers	138981	3122 (2.98-2.90)
Sidechain outliers	138945	3124 (2.98-2.90)
RSRZ outliers	127900	2902 (2.98-2.90)

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 <=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	A	507	2% 86% 12%
1	B	507	% 81% 18%
1	C	507	5% 80% 18%
1	D	507	11% 72% 26%
2	E	62	2% 69% 6% 24%

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Mol	Chain	Length	Quality of chain
2	F	62	2% 61% 11% 27%
2	G	62	5% 53% 23% 24%
2	H	62	8% 48% 23% 29%
3	I	4	50% 50%
3	M	4	50% 25% 25%
3	O	4	75% 25%
4	J	5	40% 60%
5	K	3	67% 33%
6	L	2	50% 50%
6	N	2	50% 50%

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

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
5	BMA	K	3	-	-	-	X

2 Entry composition (i)

There are 8 unique types of molecules in this entry. The entry contains 17103 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 Epidermal growth factor receptor.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	500	Total	C	N	O	S	0	0	0
			3816	2364	674	736	42			
1	B	504	Total	C	N	O	S	0	0	0
			3882	2402	694	744	42			
1	C	500	Total	C	N	O	S	0	0	0
			3791	2349	665	735	42			
1	D	499	Total	C	N	O	S	0	0	0
			3757	2331	656	728	42			

There are 24 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	502	HIS	-	expression tag	UNP P00533
A	503	HIS	-	expression tag	UNP P00533
A	504	HIS	-	expression tag	UNP P00533
A	505	HIS	-	expression tag	UNP P00533
A	506	HIS	-	expression tag	UNP P00533
A	507	HIS	-	expression tag	UNP P00533
B	502	HIS	-	expression tag	UNP P00533
B	503	HIS	-	expression tag	UNP P00533
B	504	HIS	-	expression tag	UNP P00533
B	505	HIS	-	expression tag	UNP P00533
B	506	HIS	-	expression tag	UNP P00533
B	507	HIS	-	expression tag	UNP P00533
C	502	HIS	-	expression tag	UNP P00533
C	503	HIS	-	expression tag	UNP P00533
C	504	HIS	-	expression tag	UNP P00533
C	505	HIS	-	expression tag	UNP P00533
C	506	HIS	-	expression tag	UNP P00533
C	507	HIS	-	expression tag	UNP P00533
D	502	HIS	-	expression tag	UNP P00533
D	503	HIS	-	expression tag	UNP P00533
D	504	HIS	-	expression tag	UNP P00533

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Chain	Residue	Modelled	Actual	Comment	Reference
D	505	HIS	-	expression tag	UNP P00533
D	506	HIS	-	expression tag	UNP P00533
D	507	HIS	-	expression tag	UNP P00533

- Molecule 2 is a protein called Proepiregulin.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	E	47	Total	C	N	O	S	0	0	0
			370	230	62	70	8			
2	F	45	Total	C	N	O	S	0	0	0
			347	215	58	66	8			
2	G	47	Total	C	N	O	S	0	0	0
			357	223	57	69	8			
2	H	44	Total	C	N	O	S	0	0	0
			338	209	55	66	8			

There are 4 discrepancies between the modelled and reference sequences:

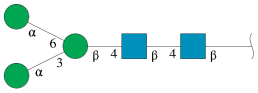
Chain	Residue	Modelled	Actual	Comment	Reference
E	-7	SER	-	expression tag	UNP O14944
F	-7	SER	-	expression tag	UNP O14944
G	-7	SER	-	expression tag	UNP O14944
H	-7	SER	-	expression tag	UNP O14944

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

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
3	I	4	Total	C	N	O	0	0	0
			50	28	2	20			
3	M	4	Total	C	N	O	0	0	0
			50	28	2	20			
3	O	4	Total	C	N	O	0	0	0
			50	28	2	20			

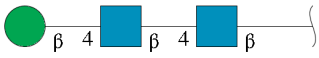
- Molecule 4 is an oligosaccharide called alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-6)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-a

cetamido-2-deoxy-beta-D-glucopyranose.



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
4	J	5	Total	C	N	O	0	0	0
			61	34	2	25			

- Molecule 5 is an oligosaccharide called beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose.

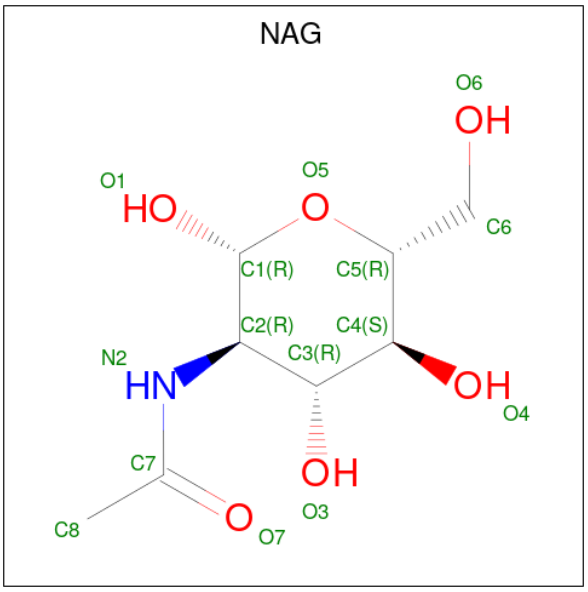


Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
5	K	3	Total	C	N	O	0	0	0
			39	22	2	15			

- Molecule 6 is an oligosaccharide called 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
6	L	2	Total	C	N	O	0	0	0
			28	16	2	10			
6	N	2	Total	C	N	O	0	0	0
			28	16	2	10			

- Molecule 7 is 2-acetamido-2-deoxy-beta-D-glucopyranose (three-letter code: NAG) (formula: $C_8H_{15}NO_6$).



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

- Molecule 8 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
8	A	5	Total O 5 5	0	0
8	B	20	Total O 20 20	0	0
8	C	9	Total O 9 9	0	0
8	D	5	Total O 5 5	0	0
8	E	1	Total O 1 1	0	0

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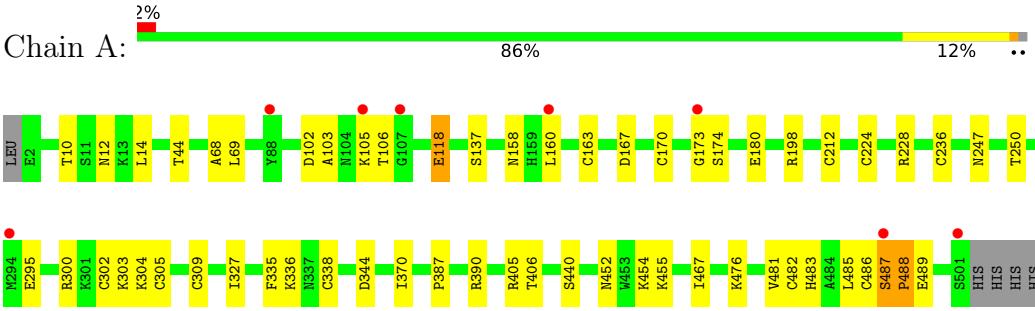
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
8	F	1	Total O 1 1	0	0

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.

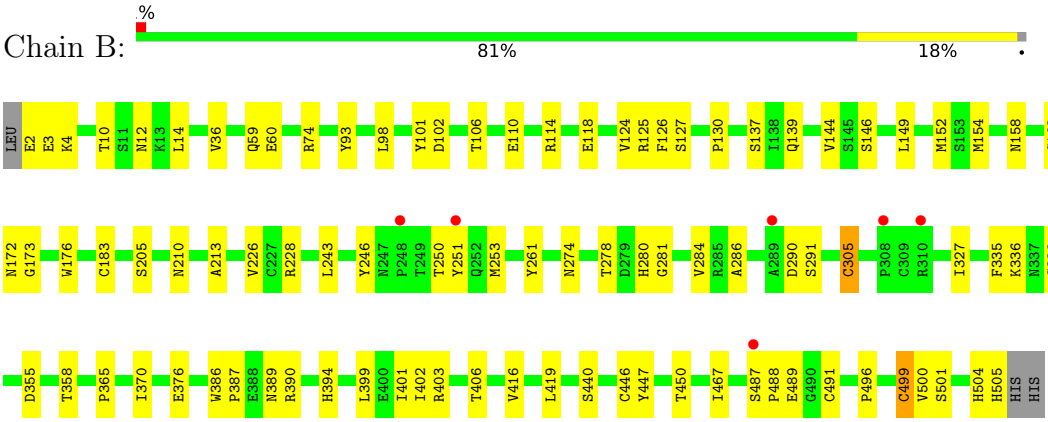
• Molecule 1: Epidermal growth factor receptor

Chain A:



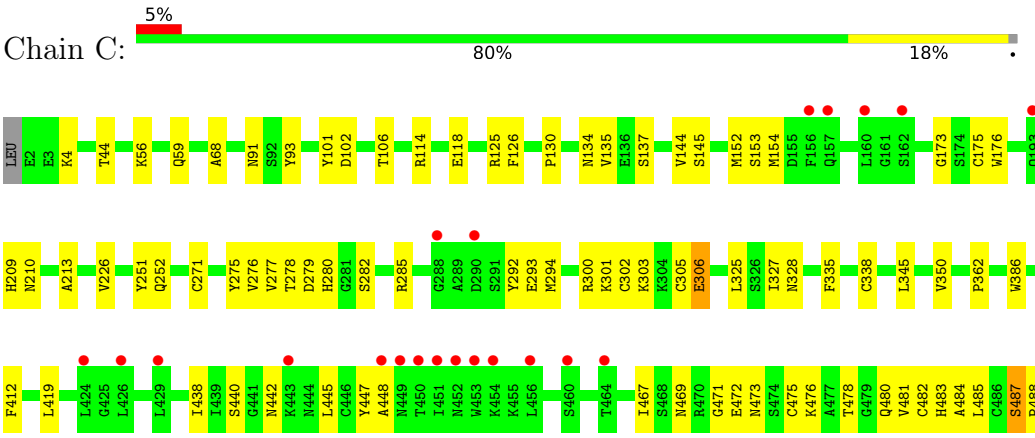
• Molecule 1: Epidermal growth factor receptor

Chain B:



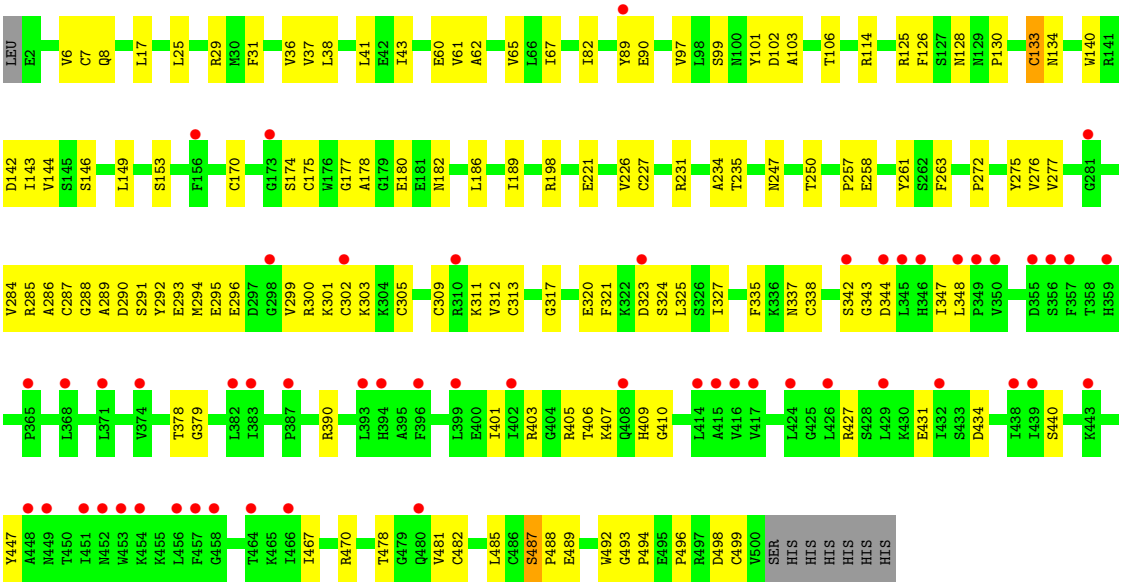
• Molecule 1: Epidermal growth factor receptor

Chain C:



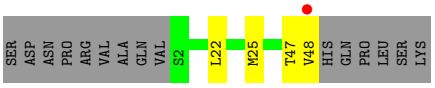
• Molecule 1: Epidermal growth factor receptor

Chain D:



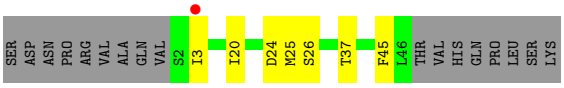
• Molecule 2: Proepiregulin

Chain E:



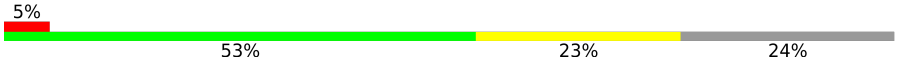
• Molecule 2: Proepiregulin

Chain F:



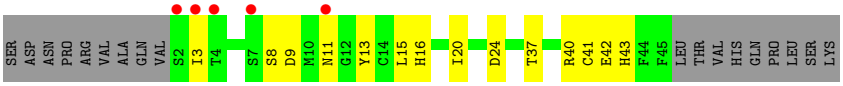
• Molecule 2: Proepiregulin

Chain G:



• Molecule 2: Proepiregulin

Chain H:



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

Chain I:

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

Chain M:

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

Chain O:

• Molecule 4: alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-6)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain J:

• Molecule 5: beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain K:

• Molecule 6: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain L:

• Molecule 6: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain N:

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	76.65Å 199.29Å 87.92Å 90.00° 96.74° 90.00°	Depositor
Resolution (Å)	47.68 – 2.94 47.68 – 2.94	Depositor EDS
% Data completeness (in resolution range)	96.5 (47.68-2.94) 96.5 (47.68-2.94)	Depositor EDS
R_{merge}	0.13	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.83 (at 2.96Å)	Xtriage
Refinement program	PHENIX 1.11.1_2575	Depositor
R, R_{free}	0.225 , 0.268 0.225 , 0.268	Depositor DCC
R_{free} test set	2596 reflections (4.85%)	wwPDB-VP
Wilson B-factor (Å^2)	71.4	Xtriage
Anisotropy	0.387	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.25 , 42.4	EDS
L-test for twinning[2]	$< \|L\| > = 0.48$, $< L^2 > = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.93	EDS
Total number of atoms	17103	wwPDB-VP
Average B, all atoms (Å^2)	92.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.50% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: MAN, NAG, BMA

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	0.27	0/3885	0.51	1/5256 (0.0%)
1	B	0.28	0/3957	0.50	0/5350
1	C	0.28	0/3861	0.50	0/5235
1	D	0.29	0/3827	0.50	0/5193
2	E	0.27	0/377	0.48	0/507
2	F	0.42	0/354	0.50	0/476
2	G	0.29	0/364	0.49	0/492
2	H	0.34	0/345	0.53	0/465
All	All	0.29	0/16970	0.50	1/22974 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	327	ILE	N-CA-C	-6.62	93.14	111.00

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	3816	0	3670	38	2
1	B	3882	0	3731	58	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	C	3791	0	3597	74	1
1	D	3757	0	3539	107	1
2	E	370	0	340	4	0
2	F	347	0	302	6	1
2	G	357	0	314	11	0
2	H	338	0	291	15	1
3	I	50	0	43	1	0
3	M	50	0	43	1	0
3	O	50	0	43	6	0
4	J	61	0	52	2	1
5	K	39	0	34	0	0
6	L	28	0	25	5	0
6	N	28	0	25	1	0
7	A	42	0	39	0	0
7	B	28	0	26	0	0
7	C	14	0	13	0	0
7	D	14	0	13	0	0
8	A	5	0	0	0	0
8	B	20	0	0	1	0
8	C	9	0	0	2	0
8	D	5	0	0	0	0
8	E	1	0	0	0	0
8	F	1	0	0	0	0
All	All	17103	0	16140	301	4

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 9.

The worst 5 of 301 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:H:13:TYR:O	2:H:40:ARG:NE	2.07	0.87
1:B:158:ASN:ND2	1:B:163:CYS:SG	2.49	0.85
1:B:327:ILE:HD11	1:B:345:LEU:HD22	1.61	0.82
1:D:31:PHE:CE2	1:D:41:LEU:HG	2.21	0.76
1:C:101:TYR:OH	2:G:24:ASP:OD2	2.03	0.76

All (4) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:180:GLU:OE2	4:J:3:BMA:O4[1_556]	1.69	0.51
1:A:489:GLU:OE2	2:F:26:SER:OG[1_656]	1.99	0.21
1:C:56:LYS:NZ	2:H:9:ASP:OD2[1_454]	2.13	0.07
1:D:180:GLU:OE2	1:D:390:ARG:NH1[1_455]	2.19	0.01

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	A	498/507 (98%)	471 (95%)	25 (5%)	2 (0%)	34 64
1	B	502/507 (99%)	475 (95%)	27 (5%)	0	100 100
1	C	498/507 (98%)	464 (93%)	32 (6%)	2 (0%)	34 64
1	D	497/507 (98%)	463 (93%)	33 (7%)	1 (0%)	47 76
2	E	45/62 (73%)	43 (96%)	2 (4%)	0	100 100
2	F	43/62 (69%)	40 (93%)	3 (7%)	0	100 100
2	G	45/62 (73%)	44 (98%)	1 (2%)	0	100 100
2	H	42/62 (68%)	39 (93%)	3 (7%)	0	100 100
All	All	2170/2276 (95%)	2039 (94%)	126 (6%)	5 (0%)	47 76

All (5) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	488	PRO
1	C	306	GLU
1	D	487	SER
1	C	487	SER
1	A	487	SER

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	A	426/446 (96%)	424 (100%)	2 (0%)	88 96
1	B	435/446 (98%)	432 (99%)	3 (1%)	84 94
1	C	419/446 (94%)	418 (100%)	1 (0%)	93 98
1	D	410/446 (92%)	409 (100%)	1 (0%)	93 98
2	E	43/57 (75%)	43 (100%)	0	100 100
2	F	38/57 (67%)	38 (100%)	0	100 100
2	G	40/57 (70%)	40 (100%)	0	100 100
2	H	38/57 (67%)	38 (100%)	0	100 100
All	All	1849/2012 (92%)	1842 (100%)	7 (0%)	91 97

5 of 7 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	446	CYS
1	B	499	CYS
1	D	133	CYS
1	C	271	CYS
1	B	305	CYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

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)

24 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	I	1	1,3	14,14,15	0.55	0	17,19,21	1.16	2 (11%)
3	NAG	I	2	3	14,14,15	0.38	0	17,19,21	0.87	1 (5%)
3	BMA	I	3	3	11,11,12	0.23	0	15,15,17	0.62	0
3	MAN	I	4	3	11,11,12	0.31	0	15,15,17	1.02	0
4	NAG	J	1	4,1	14,14,15	0.50	0	17,19,21	1.22	2 (11%)
4	NAG	J	2	4	14,14,15	0.40	0	17,19,21	0.89	0
4	BMA	J	3	4	11,11,12	0.45	0	15,15,17	1.32	2 (13%)
4	MAN	J	4	4	11,11,12	0.25	0	15,15,17	0.86	0
4	MAN	J	5	4	11,11,12	0.43	0	15,15,17	1.97	2 (13%)
5	NAG	K	1	5,1	14,14,15	0.29	0	17,19,21	1.02	2 (11%)
5	NAG	K	2	5	14,14,15	0.32	0	17,19,21	0.68	0
5	BMA	K	3	5	11,11,12	0.28	0	15,15,17	0.79	0
6	NAG	L	1	1,6	14,14,15	0.34	0	17,19,21	1.01	2 (11%)
6	NAG	L	2	6	14,14,15	0.35	0	17,19,21	0.76	0
3	NAG	M	1	1,3	14,14,15	0.44	0	17,19,21	0.88	1 (5%)
3	NAG	M	2	3	14,14,15	0.33	0	17,19,21	0.72	1 (5%)
3	BMA	M	3	3	11,11,12	0.25	0	15,15,17	0.66	0
3	MAN	M	4	3	11,11,12	0.26	0	15,15,17	0.63	0
6	NAG	N	1	1,6	14,14,15	0.35	0	17,19,21	0.91	1 (5%)
6	NAG	N	2	6	14,14,15	0.38	0	17,19,21	1.12	2 (11%)
3	NAG	O	1	1,3	14,14,15	0.42	0	17,19,21	0.71	0
3	NAG	O	2	3	14,14,15	0.36	0	17,19,21	0.88	1 (5%)
3	BMA	O	3	3	11,11,12	0.25	0	15,15,17	0.72	0
3	MAN	O	4	3	11,11,12	0.24	0	15,15,17	0.62	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
3	NAG	I	1	1,3	-	4/6/23/26	0/1/1/1
3	NAG	I	2	3	-	4/6/23/26	0/1/1/1
3	BMA	I	3	3	-	2/2/19/22	0/1/1/1
3	MAN	I	4	3	-	2/2/19/22	0/1/1/1
4	NAG	J	1	4,1	-	0/6/23/26	0/1/1/1
4	NAG	J	2	4	-	4/6/23/26	0/1/1/1
4	BMA	J	3	4	-	0/2/19/22	0/1/1/1
4	MAN	J	4	4	-	0/2/19/22	0/1/1/1
4	MAN	J	5	4	-	2/2/19/22	0/1/1/1
5	NAG	K	1	5,1	-	4/6/23/26	0/1/1/1
5	NAG	K	2	5	-	3/6/23/26	0/1/1/1
5	BMA	K	3	5	-	1/2/19/22	0/1/1/1
6	NAG	L	1	1,6	-	4/6/23/26	0/1/1/1
6	NAG	L	2	6	-	4/6/23/26	0/1/1/1
3	NAG	M	1	1,3	-	3/6/23/26	0/1/1/1
3	NAG	M	2	3	-	3/6/23/26	0/1/1/1
3	BMA	M	3	3	-	1/2/19/22	0/1/1/1
3	MAN	M	4	3	-	2/2/19/22	0/1/1/1
6	NAG	N	1	1,6	-	4/6/23/26	0/1/1/1
6	NAG	N	2	6	-	5/6/23/26	0/1/1/1
3	NAG	O	1	1,3	-	3/6/23/26	0/1/1/1
3	NAG	O	2	3	-	2/6/23/26	0/1/1/1
3	BMA	O	3	3	-	2/2/19/22	0/1/1/1
3	MAN	O	4	3	-	0/2/19/22	0/1/1/1

There are no bond length outliers.

The worst 5 of 19 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	J	5	MAN	C1-C2-C3	5.02	115.83	109.67
4	J	5	MAN	O5-C1-C2	4.45	117.64	110.77
3	O	2	NAG	O5-C1-C2	-2.99	106.57	111.29
4	J	1	NAG	C4-C3-C2	2.88	115.24	111.02
4	J	3	BMA	C1-C2-C3	2.86	113.19	109.67

There are no chirality outliers.

5 of 59 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	I	2	NAG	O7-C7-N2-C2
3	M	1	NAG	C8-C7-N2-C2
3	M	1	NAG	O7-C7-N2-C2
3	M	2	NAG	O7-C7-N2-C2
6	L	1	NAG	C1-C2-N2-C7

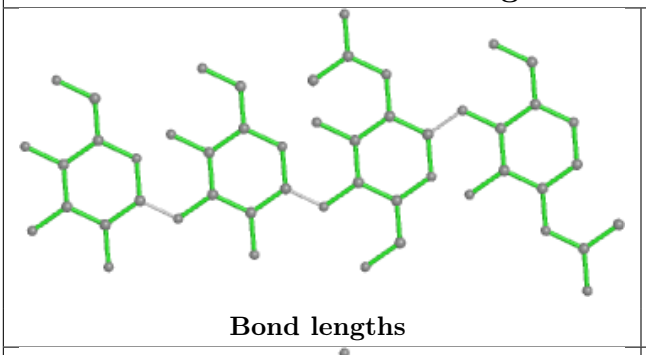
There are no ring outliers.

12 monomers are involved in 17 short contacts:

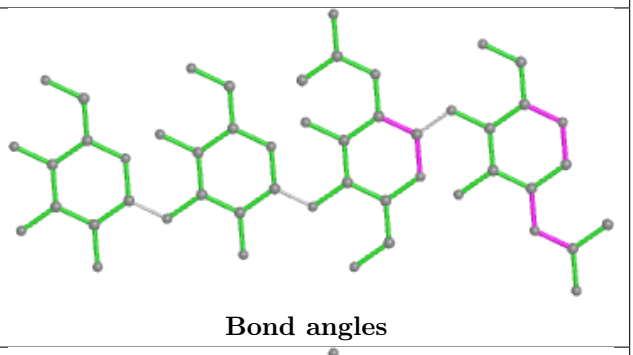
Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	N	2	NAG	1	0
4	J	3	BMA	0	1
4	J	1	NAG	1	0
3	O	4	MAN	1	0
3	O	2	NAG	2	0
3	I	2	NAG	1	0
3	M	1	NAG	1	0
6	L	1	NAG	5	0
4	J	5	MAN	1	0
3	I	1	NAG	1	0
3	O	1	NAG	3	0
3	O	3	BMA	1	0

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

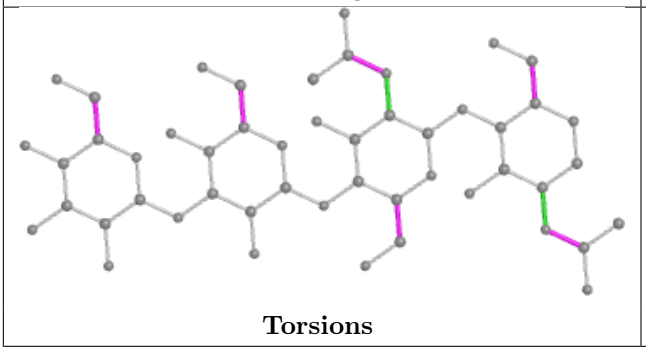
Oligosaccharide Chain I



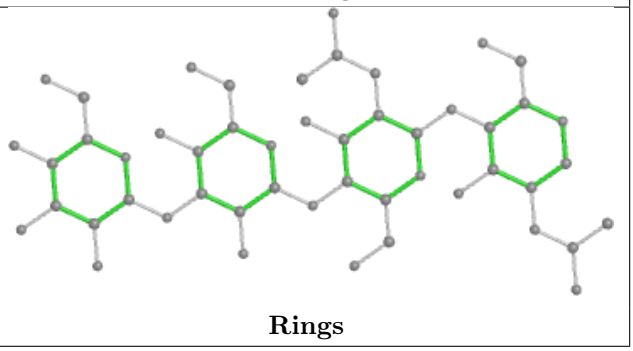
Bond lengths



Bond angles

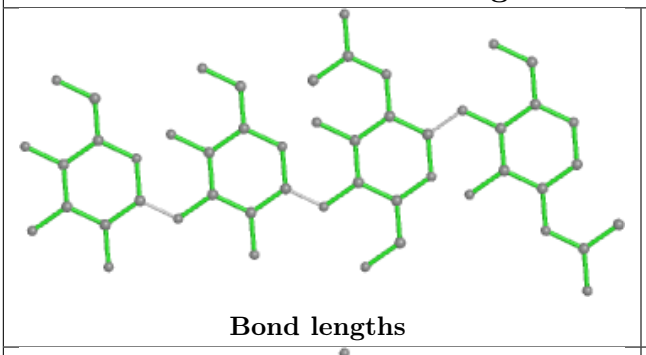


Torsions

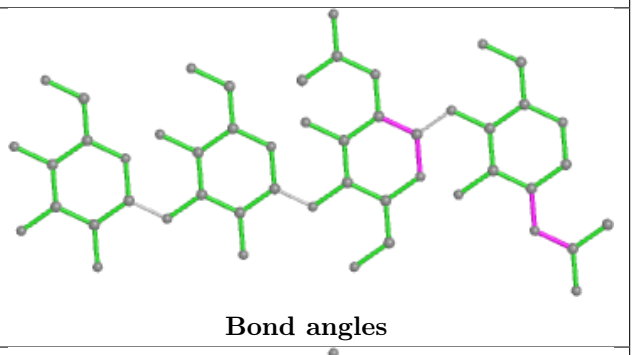


Rings

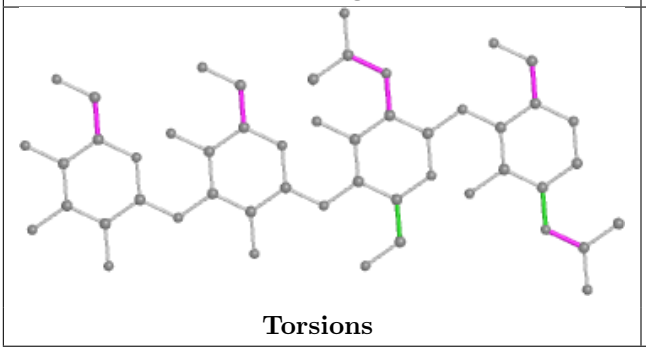
Oligosaccharide Chain M



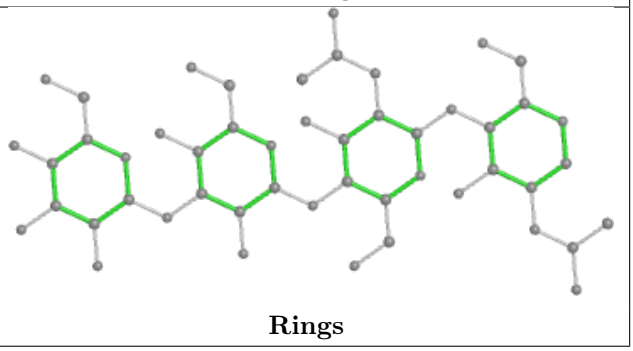
Bond lengths



Bond angles

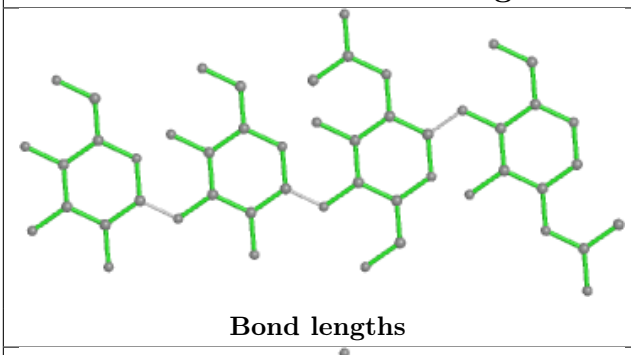


Torsions

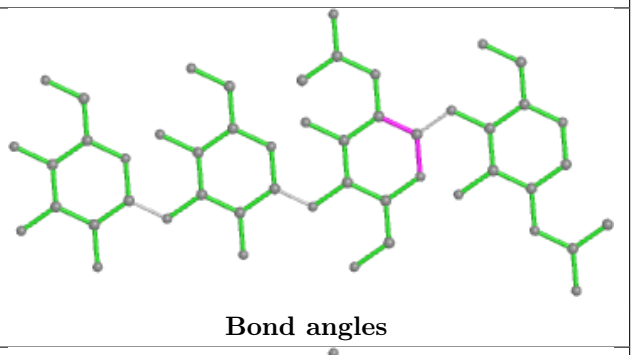


Rings

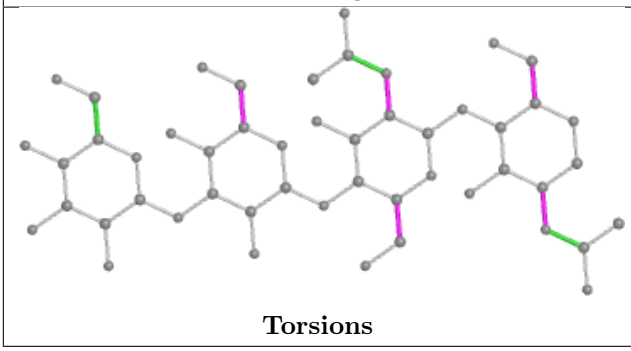
Oligosaccharide Chain O



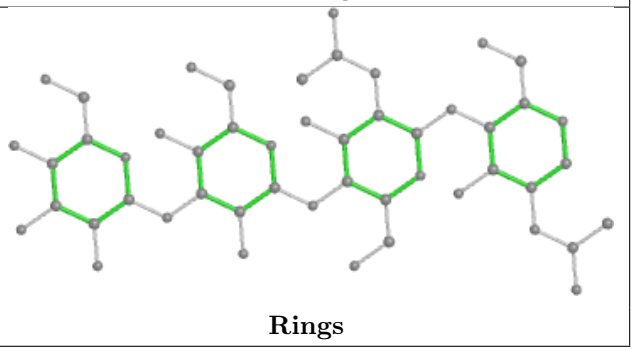
Bond lengths



Bond angles

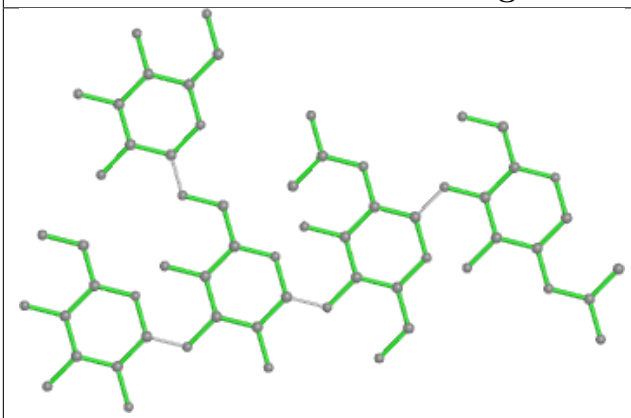


Torsions

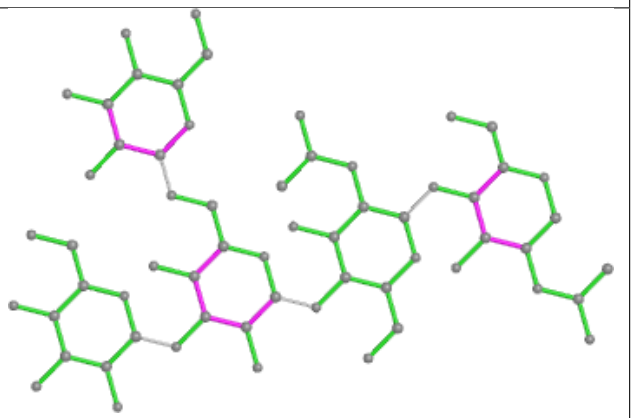


Rings

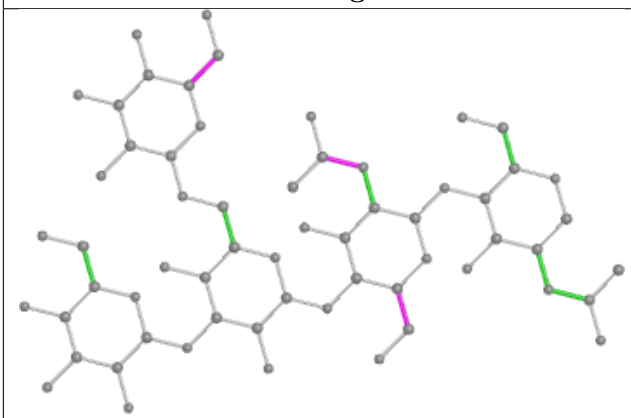
Oligosaccharide Chain J



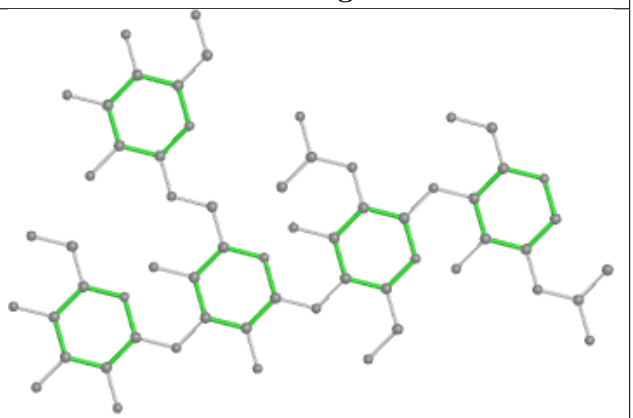
Bond lengths



Bond angles

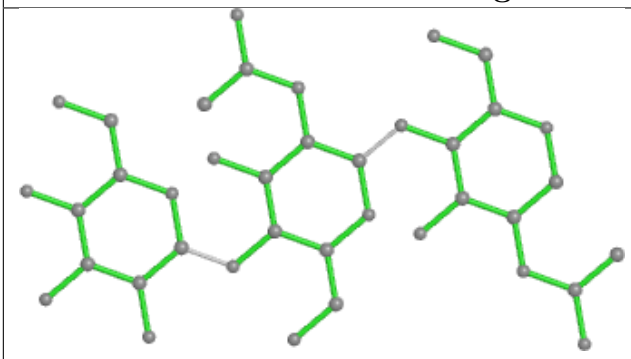


Torsions

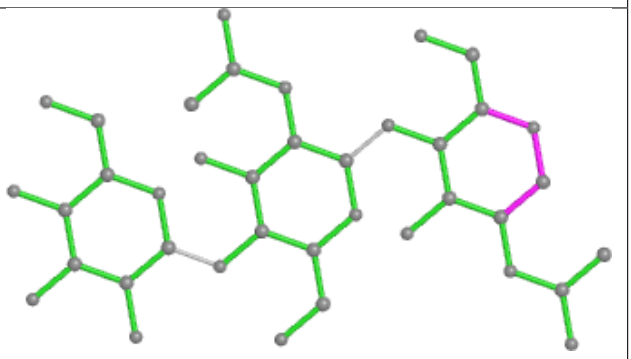


Rings

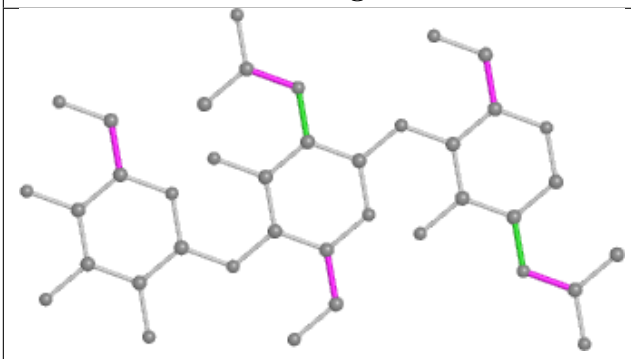
Oligosaccharide Chain K



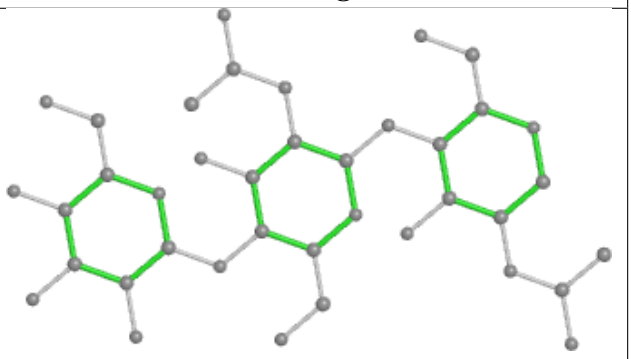
Bond lengths



Bond angles

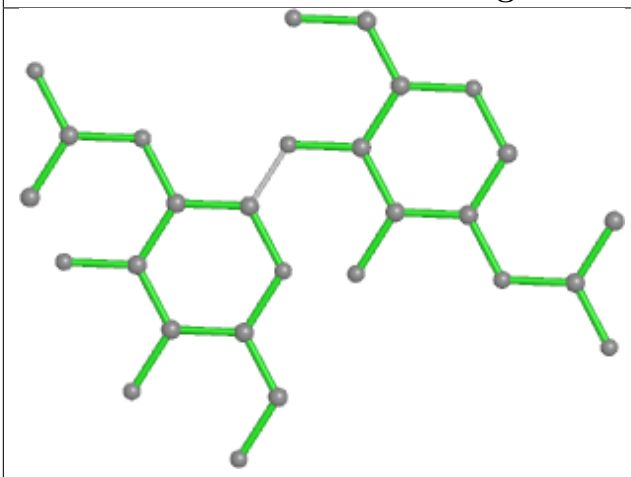


Torsions

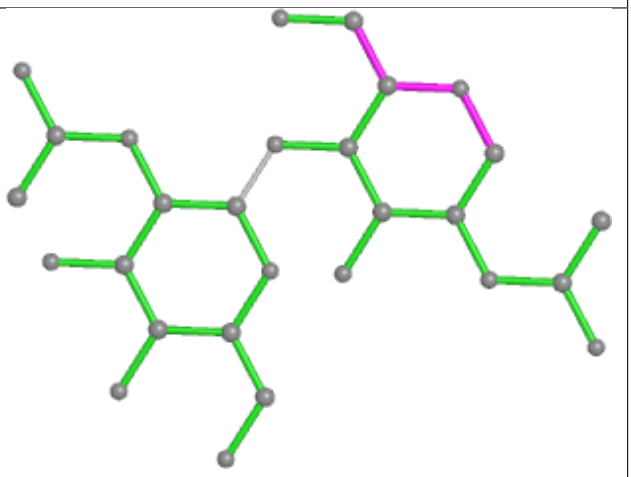


Rings

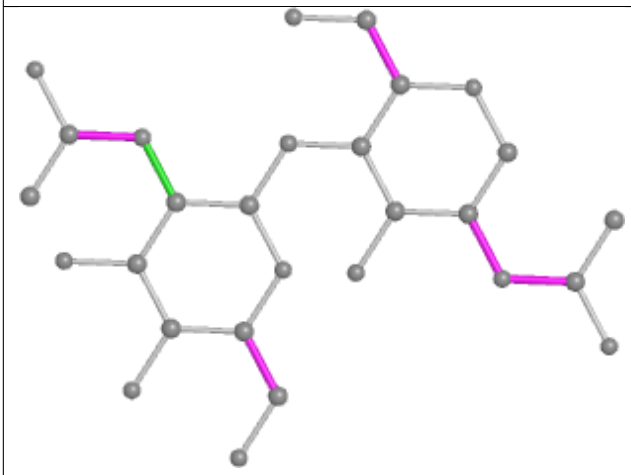
Oligosaccharide Chain L



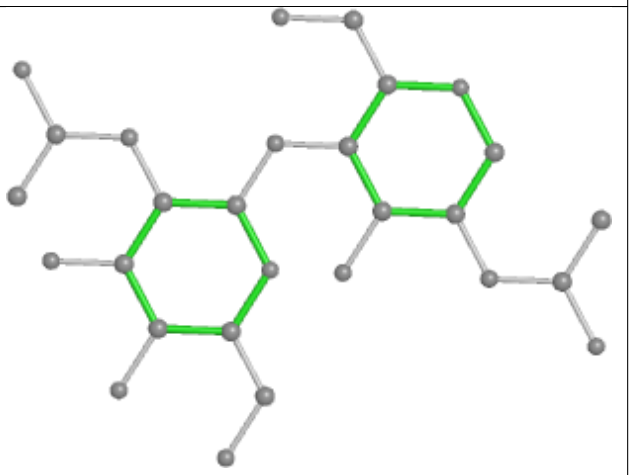
Bond lengths



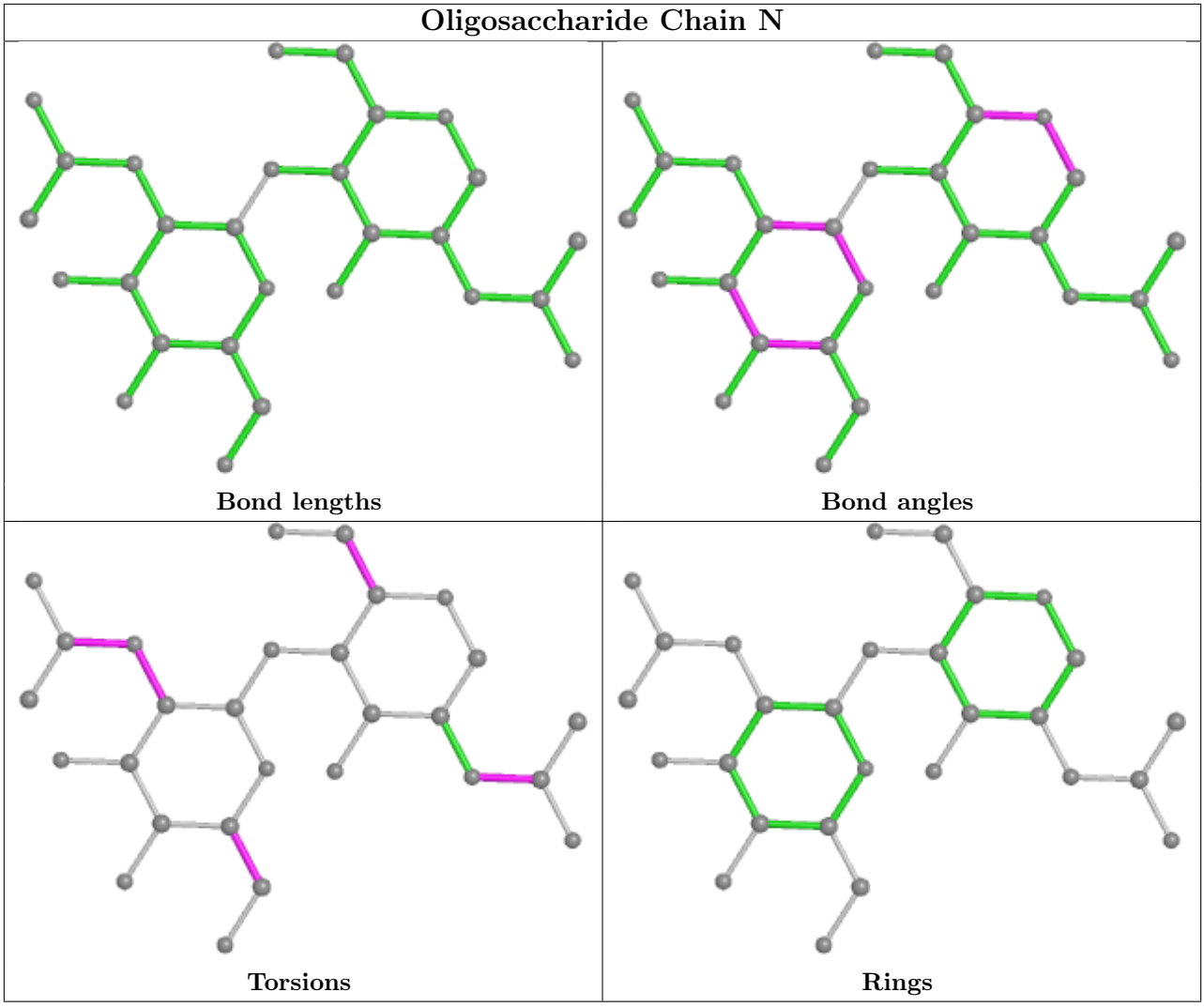
Bond angles



Torsions



Rings



5.6 Ligand geometry (i)

7 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	$\#\|Z\| > 2$
7	NAG	D	601	1	14,14,15	0.61	1 (7%)	17,19,21	0.67	1 (5%)
7	NAG	A	3201	1	14,14,15	0.33	0	17,19,21	1.09	2 (11%)
7	NAG	A	3206	1	14,14,15	0.28	0	17,19,21	0.72	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
7	NAG	A	3207	1	14,14,15	0.28	0	17,19,21	1.20	2 (11%)
7	NAG	B	601	1	14,14,15	0.28	0	17,19,21	0.60	0
7	NAG	C	603	1	14,14,15	0.18	0	17,19,21	0.62	0
7	NAG	B	602	1	14,14,15	0.29	0	17,19,21	0.44	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
7	NAG	D	601	1	-	2/6/23/26	0/1/1/1
7	NAG	A	3201	1	-	4/6/23/26	0/1/1/1
7	NAG	A	3206	1	-	1/6/23/26	0/1/1/1
7	NAG	A	3207	1	-	2/6/23/26	0/1/1/1
7	NAG	B	601	1	-	2/6/23/26	0/1/1/1
7	NAG	C	603	1	-	2/6/23/26	0/1/1/1
7	NAG	B	602	1	-	1/6/23/26	0/1/1/1

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	D	601	NAG	C1-C2	2.17	1.55	1.52

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
7	A	3207	NAG	C1-O5-C5	3.35	116.73	112.19
7	A	3207	NAG	O5-C1-C2	2.68	115.51	111.29
7	A	3201	NAG	O5-C5-C6	2.43	111.01	107.20
7	A	3201	NAG	O5-C1-C2	-2.40	107.50	111.29
7	D	601	NAG	C1-O5-C5	2.03	114.94	112.19

There are no chirality outliers.

5 of 14 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
7	B	601	NAG	C8-C7-N2-C2
7	B	601	NAG	O7-C7-N2-C2
7	A	3207	NAG	C4-C5-C6-O6

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Mol	Chain	Res	Type	Atoms
7	A	3201	NAG	C8-C7-N2-C2
7	D	601	NAG	O5-C5-C6-O6

There are no ring outliers.

No monomer is involved in short contacts.

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

6.1 Protein, DNA and RNA chains

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, 95^{th} 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	A	500/507 (98%)	-0.20	8 (1%) 72 73	44, 72, 121, 181	0
1	B	504/507 (99%)	-0.25	6 (1%) 79 80	34, 65, 129, 178	0
1	C	500/507 (98%)	0.06	23 (4%) 32 32	36, 88, 167, 266	0
1	D	499/507 (98%)	0.42	55 (11%) 5 5	60, 120, 188, 253	0
2	E	47/62 (75%)	-0.01	1 (2%) 63 64	54, 74, 118, 132	0
2	F	45/62 (72%)	-0.19	1 (2%) 62 63	49, 70, 120, 166	0
2	G	47/62 (75%)	0.17	3 (6%) 19 17	74, 110, 154, 188	0
2	H	44/62 (70%)	0.69	5 (11%) 5 4	111, 131, 168, 184	0
All	All	2186/2276 (96%)	0.02	102 (4%) 31 31	34, 82, 166, 266	0

The worst 5 of 102 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	448	ALA	8.1
1	C	451	ILE	8.0
1	D	415	ALA	7.2
1	D	374	VAL	6.3
1	D	399	LEU	6.0

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

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,

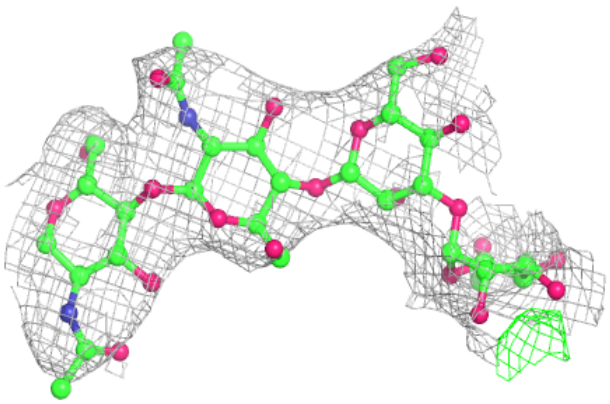
median, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

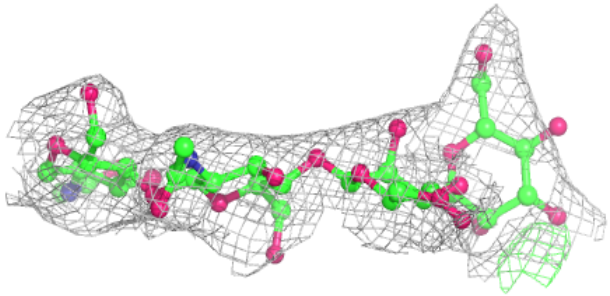
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
5	BMA	K	3	11/12	0.51	0.41	149,174,191,195	0
3	NAG	O	2	14/15	0.70	0.34	134,151,170,185	0
3	MAN	I	4	11/12	0.71	0.23	116,148,154,161	0
4	BMA	J	3	11/12	0.75	0.27	124,141,152,158	0
4	MAN	J	4	11/12	0.78	0.36	146,165,171,173	0
6	NAG	L	2	14/15	0.78	0.31	106,150,160,161	0
6	NAG	N	2	14/15	0.78	0.24	126,157,164,164	0
6	NAG	N	1	14/15	0.79	0.24	92,117,137,151	0
3	NAG	O	1	14/15	0.84	0.27	109,145,180,189	0
3	BMA	M	3	11/12	0.84	0.16	142,156,167,173	0
3	MAN	O	4	11/12	0.84	0.57	114,133,147,148	0
3	MAN	M	4	11/12	0.85	0.18	139,142,152,153	0
5	NAG	K	1	14/15	0.86	0.21	120,145,161,163	0
4	MAN	J	5	11/12	0.86	0.20	138,153,161,163	0
6	NAG	L	1	14/15	0.86	0.16	122,138,156,159	0
5	NAG	K	2	14/15	0.88	0.43	140,161,175,190	0
3	BMA	O	3	11/12	0.90	0.39	135,141,145,149	0
3	BMA	I	3	11/12	0.90	0.12	123,132,136,141	0
3	NAG	M	2	14/15	0.92	0.16	114,122,144,156	0
3	NAG	M	1	14/15	0.93	0.17	81,108,124,128	0
4	NAG	J	1	14/15	0.93	0.25	62,85,93,99	0
3	NAG	I	2	14/15	0.94	0.15	91,111,124,126	0
4	NAG	J	2	14/15	0.94	0.17	42,72,112,114	0
3	NAG	I	1	14/15	0.95	0.17	62,77,92,115	0

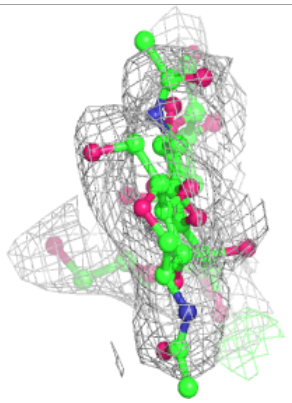
The following is a graphical depiction of the model fit to experimental electron density for oligosaccharide. Each fit is shown from different orientation to approximate a three-dimensional view.

Electron density around Chain I:

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

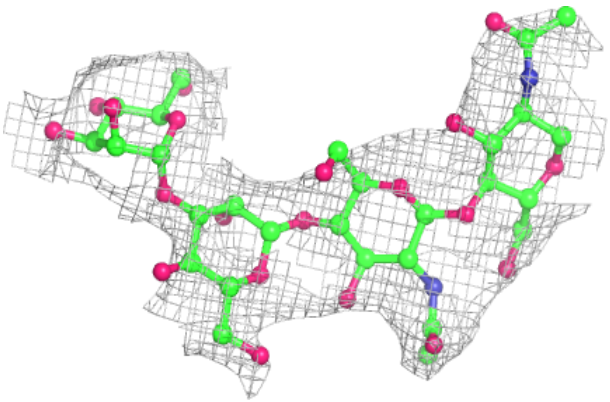


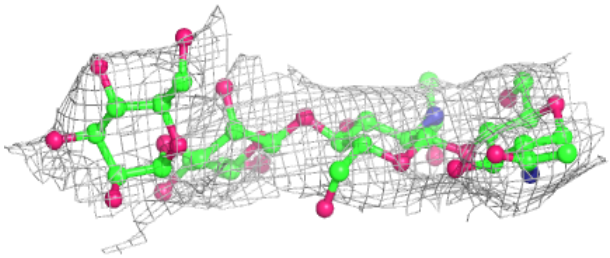


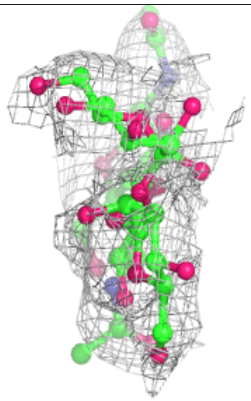


Electron density around Chain M:

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

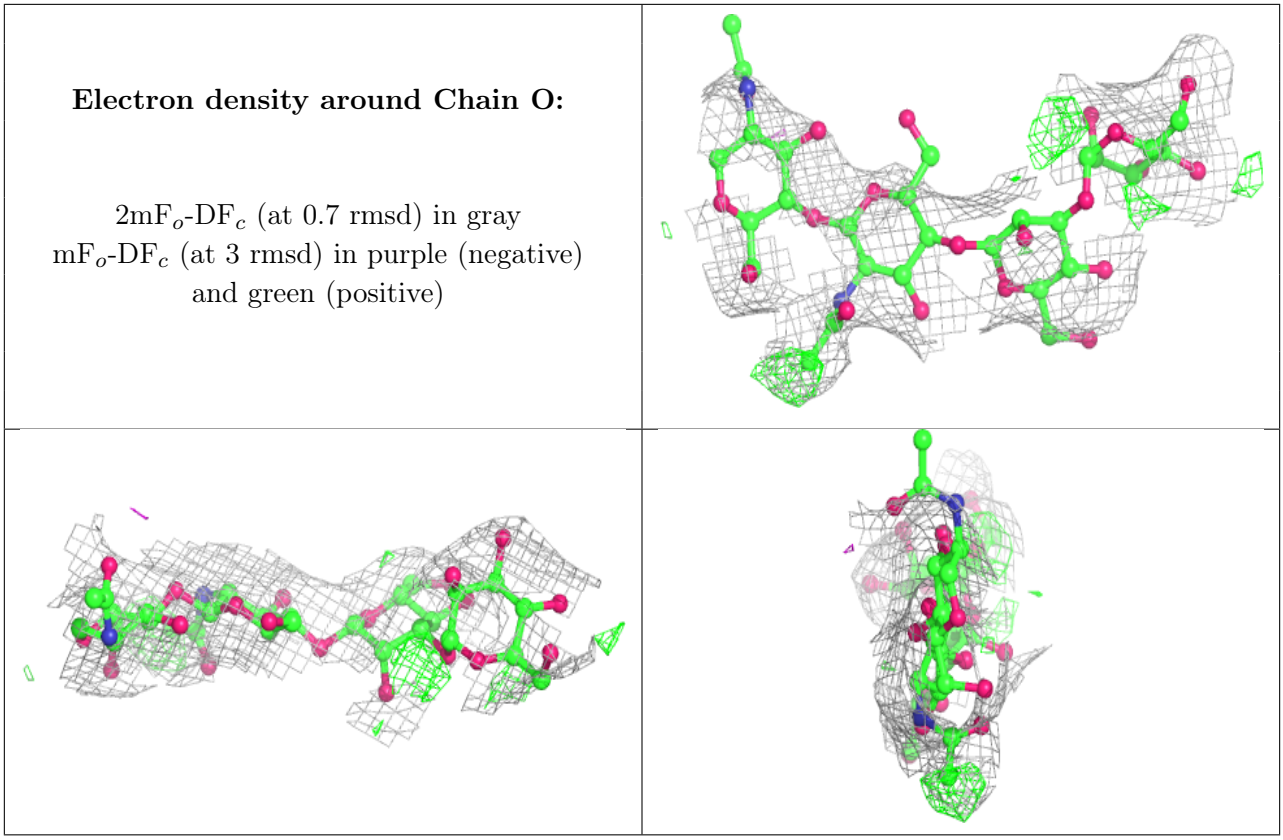






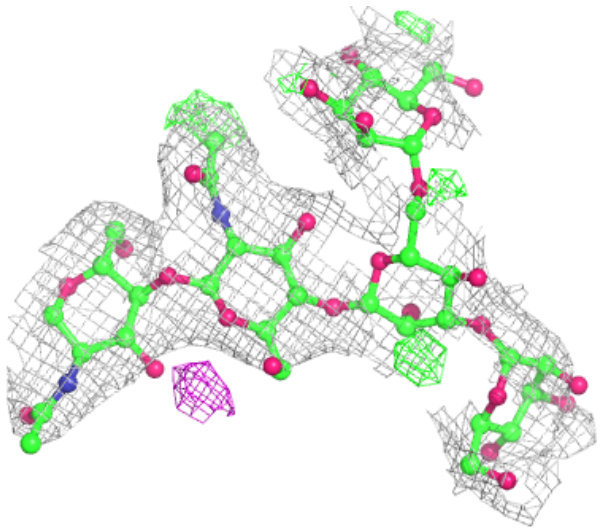
Electron density around Chain O:

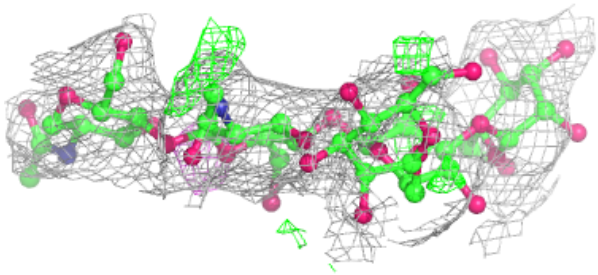
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

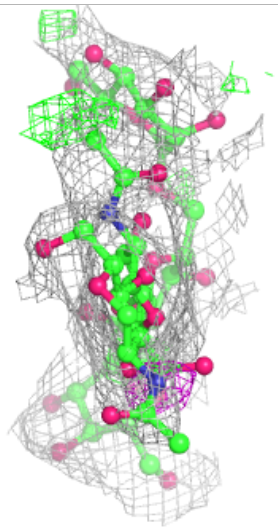


Electron density around Chain J:

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

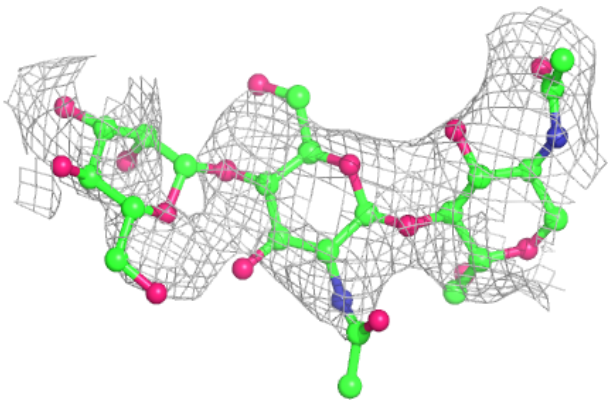


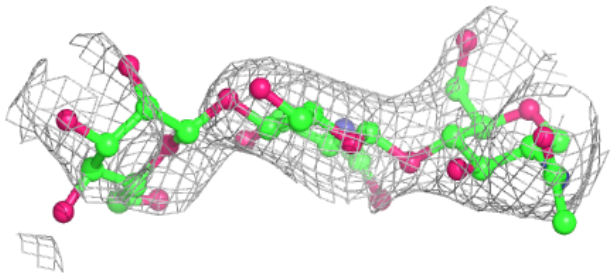


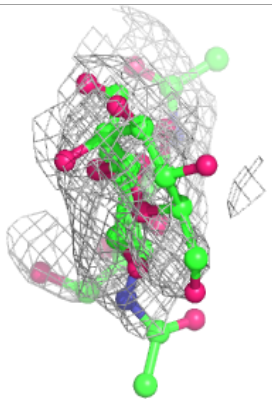


Electron density around Chain K:

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

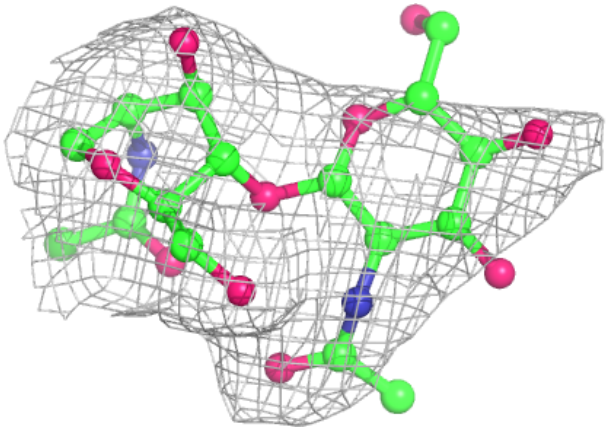


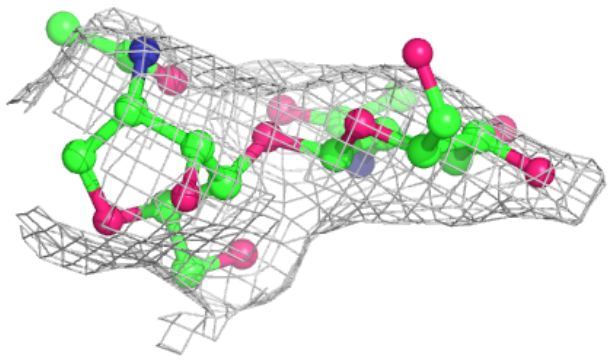


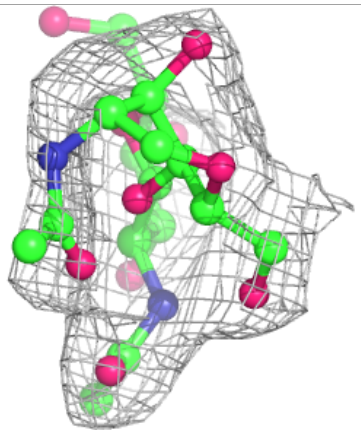


Electron density around Chain L:

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

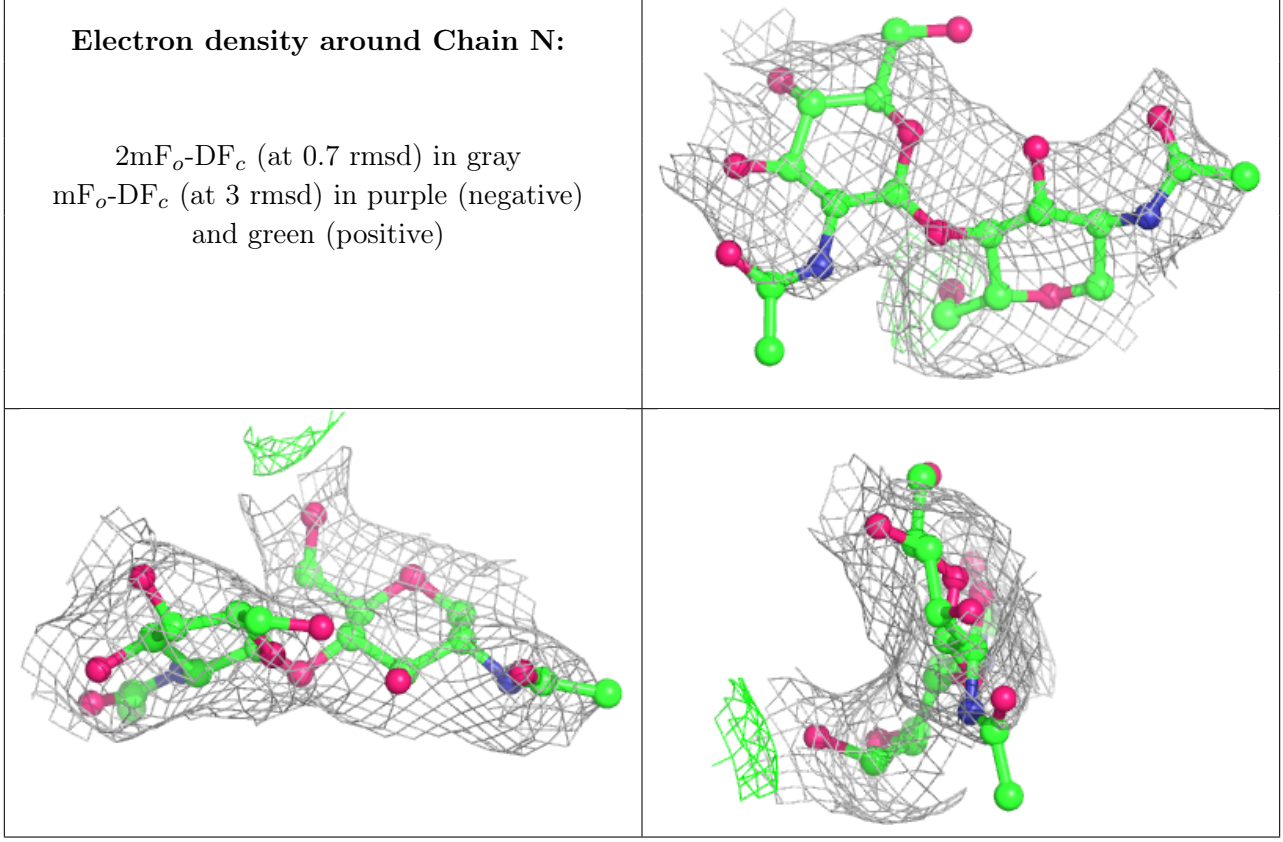






Electron density around Chain N:

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



6.4 Ligands

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, 95^{th} 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
7	NAG	A	3207	14/15	0.40	0.25	124,142,162,164	0
7	NAG	A	3201	14/15	0.72	0.25	113,136,143,154	0
7	NAG	D	601	14/15	0.72	0.28	127,144,158,166	0
7	NAG	A	3206	14/15	0.76	0.19	124,140,169,193	0
7	NAG	B	601	14/15	0.79	0.25	127,150,161,161	0
7	NAG	B	602	14/15	0.80	0.19	92,114,128,133	0
7	NAG	C	603	14/15	0.89	0.18	74,89,112,123	0

6.5 Other polymers

There are no such residues in this entry.