Full wwPDB X-ray Structure Validation Report (i)

Jan 4, 2024 – 02:18 am GMT

PDB ID	:	4UM8
Title	:	Crystal structure of alpha V beta 6
Authors	:	Dong, X.; Springer, T.A.
Deposited on	:	2014-05-15
Resolution	:	2.85 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at *validation@mail.wwpdb.org*
A user guide is available at
https://www.wwpdb.org/validation/2017/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:

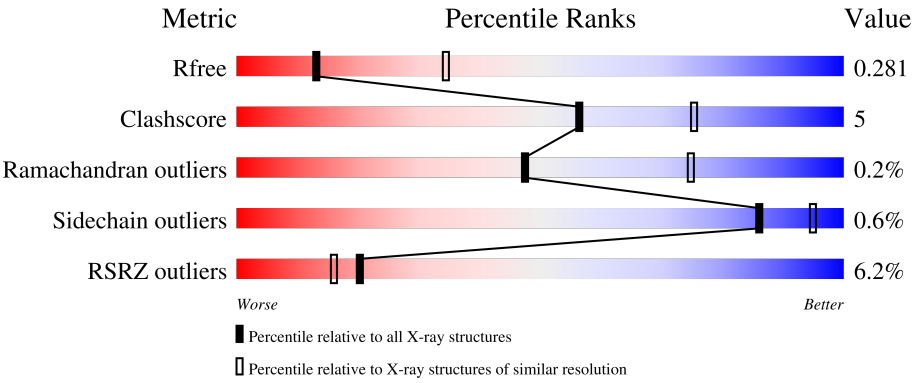
MolProbity	:	4.02b-467
Mogul	:	1.8.4, CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

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 2.85 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	3168 (2.90-2.82)
Clashscore	141614	3438 (2.90-2.82)
Ramachandran outliers	138981	3348 (2.90-2.82)
Sidechain outliers	138945	3351 (2.90-2.82)
RSRZ outliers	127900	3103 (2.90-2.82)

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	681	77% 10% 13%
1	C	681	7% 73% 13% 14%
2	B	788	5% 47% 6% 46%
2	D	788	3% 45% 7% 47%
3	E	4	50% 25% 25%

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Mol	Chain	Length	Quality of chain
3	Q	4	25% 25% 50%
4	F	5	60% 40%
5	G	6	17% 50% 33%
5	M	6	17% 50% 33%
6	H	3	33% 33% 33%
6	K	3	33% 67%
7	I	5	40% 20% 40%
8	J	2	100%
8	L	2	100%
8	P	2	100%
9	N	4	25% 50% 25%
10	O	7	43% 57%

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
10	NAG	O	2	-	-	-	X
14	CA	A	2002	-	-	-	X
3	NAG	Q	1	-	-	-	X
3	BMA	Q	3	-	-	-	X
4	MAN	F	5	-	-	-	X
5	NAG	M	1	X	-	-	-
7	MAN	I	5	-	-	-	X
8	NAG	P	2	-	-	-	X

2 Entry composition (i)

There are 18 unique types of molecules in this entry. The entry contains 16497 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 INTEGRIN ALPHA-V.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	591	Total	C	N	O	S	0	0	0
			4579	2904	776	878	21			
1	C	588	Total	C	N	O	S	0	0	0
			4559	2893	773	872	21			

There are 174 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	596	THR	-	expression tag	UNP P06756
A	597	GLY	-	expression tag	UNP P06756
A	598	GLY	-	expression tag	UNP P06756
A	599	LEU	-	expression tag	UNP P06756
A	600	GLU	-	expression tag	UNP P06756
A	601	VAL	-	expression tag	UNP P06756
A	602	LEU	-	expression tag	UNP P06756
A	603	PHE	-	expression tag	UNP P06756
A	604	GLN	-	expression tag	UNP P06756
A	605	GLY	-	expression tag	UNP P06756
A	606	PRO	-	expression tag	UNP P06756
A	607	GLY	-	expression tag	UNP P06756
A	608	GLU	-	expression tag	UNP P06756
A	609	ASN	-	expression tag	UNP P06756
A	610	ALA	-	expression tag	UNP P06756
A	611	GLN	-	expression tag	UNP P06756
A	612	LEU	-	expression tag	UNP P06756
A	613	GLU	-	expression tag	UNP P06756
A	614	LYS	-	expression tag	UNP P06756
A	615	GLU	-	expression tag	UNP P06756
A	616	LEU	-	expression tag	UNP P06756
A	617	GLN	-	expression tag	UNP P06756
A	618	ALA	-	expression tag	UNP P06756
A	619	LEU	-	expression tag	UNP P06756
A	620	GLU	-	expression tag	UNP P06756

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Chain	Residue	Modelled	Actual	Comment	Reference
A	621	LYS	-	expression tag	UNP P06756
A	622	GLU	-	expression tag	UNP P06756
A	623	ASN	-	expression tag	UNP P06756
A	624	ALA	-	expression tag	UNP P06756
A	625	GLN	-	expression tag	UNP P06756
A	626	LEU	-	expression tag	UNP P06756
A	627	GLU	-	expression tag	UNP P06756
A	628	TRP	-	expression tag	UNP P06756
A	629	GLU	-	expression tag	UNP P06756
A	630	LEU	-	expression tag	UNP P06756
A	631	GLN	-	expression tag	UNP P06756
A	632	ALA	-	expression tag	UNP P06756
A	633	LEU	-	expression tag	UNP P06756
A	634	GLU	-	expression tag	UNP P06756
A	635	LYS	-	expression tag	UNP P06756
A	636	GLU	-	expression tag	UNP P06756
A	637	LEU	-	expression tag	UNP P06756
A	638	ALA	-	expression tag	UNP P06756
A	639	GLN	-	expression tag	UNP P06756
A	640	THR	-	expression tag	UNP P06756
A	641	THR	-	expression tag	UNP P06756
A	642	GLY	-	expression tag	UNP P06756
A	643	TRP	-	expression tag	UNP P06756
A	644	ARG	-	expression tag	UNP P06756
A	645	GLY	-	expression tag	UNP P06756
A	646	GLY	-	expression tag	UNP P06756
A	647	HIS	-	expression tag	UNP P06756
A	648	VAL	-	expression tag	UNP P06756
A	649	VAL	-	expression tag	UNP P06756
A	650	GLU	-	expression tag	UNP P06756
A	651	GLY	-	expression tag	UNP P06756
A	652	LEU	-	expression tag	UNP P06756
A	653	ALA	-	expression tag	UNP P06756
A	654	GLY	-	expression tag	UNP P06756
A	655	GLU	-	expression tag	UNP P06756
A	656	LEU	-	expression tag	UNP P06756
A	657	GLU	-	expression tag	UNP P06756
A	658	GLN	-	expression tag	UNP P06756
A	659	LEU	-	expression tag	UNP P06756
A	660	ARG	-	expression tag	UNP P06756
A	661	ALA	-	expression tag	UNP P06756
A	662	ARG	-	expression tag	UNP P06756

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Chain	Residue	Modelled	Actual	Comment	Reference
A	663	LEU	-	expression tag	UNP P06756
A	664	GLU	-	expression tag	UNP P06756
A	665	HIS	-	expression tag	UNP P06756
A	666	HIS	-	expression tag	UNP P06756
A	667	PRO	-	expression tag	UNP P06756
A	668	GLN	-	expression tag	UNP P06756
A	669	GLY	-	expression tag	UNP P06756
A	670	GLN	-	expression tag	UNP P06756
A	671	ARG	-	expression tag	UNP P06756
A	672	GLU	-	expression tag	UNP P06756
A	673	PRO	-	expression tag	UNP P06756
A	674	ALA	-	expression tag	UNP P06756
A	675	GLY	-	expression tag	UNP P06756
A	676	HIS	-	expression tag	UNP P06756
A	677	HIS	-	expression tag	UNP P06756
A	678	HIS	-	expression tag	UNP P06756
A	679	HIS	-	expression tag	UNP P06756
A	680	HIS	-	expression tag	UNP P06756
A	681	HIS	-	expression tag	UNP P06756
A	400	CYS	MET	engineered mutation	UNP P06756
C	596	THR	-	expression tag	UNP P06756
C	597	GLY	-	expression tag	UNP P06756
C	598	GLY	-	expression tag	UNP P06756
C	599	LEU	-	expression tag	UNP P06756
C	600	GLU	-	expression tag	UNP P06756
C	601	VAL	-	expression tag	UNP P06756
C	602	LEU	-	expression tag	UNP P06756
C	603	PHE	-	expression tag	UNP P06756
C	604	GLN	-	expression tag	UNP P06756
C	605	GLY	-	expression tag	UNP P06756
C	606	PRO	-	expression tag	UNP P06756
C	607	GLY	-	expression tag	UNP P06756
C	608	GLU	-	expression tag	UNP P06756
C	609	ASN	-	expression tag	UNP P06756
C	610	ALA	-	expression tag	UNP P06756
C	611	GLN	-	expression tag	UNP P06756
C	612	LEU	-	expression tag	UNP P06756
C	613	GLU	-	expression tag	UNP P06756
C	614	LYS	-	expression tag	UNP P06756
C	615	GLU	-	expression tag	UNP P06756
C	616	LEU	-	expression tag	UNP P06756
C	617	GLN	-	expression tag	UNP P06756

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Chain	Residue	Modelled	Actual	Comment	Reference
C	618	ALA	-	expression tag	UNP P06756
C	619	LEU	-	expression tag	UNP P06756
C	620	GLU	-	expression tag	UNP P06756
C	621	LYS	-	expression tag	UNP P06756
C	622	GLU	-	expression tag	UNP P06756
C	623	ASN	-	expression tag	UNP P06756
C	624	ALA	-	expression tag	UNP P06756
C	625	GLN	-	expression tag	UNP P06756
C	626	LEU	-	expression tag	UNP P06756
C	627	GLU	-	expression tag	UNP P06756
C	628	TRP	-	expression tag	UNP P06756
C	629	GLU	-	expression tag	UNP P06756
C	630	LEU	-	expression tag	UNP P06756
C	631	GLN	-	expression tag	UNP P06756
C	632	ALA	-	expression tag	UNP P06756
C	633	LEU	-	expression tag	UNP P06756
C	634	GLU	-	expression tag	UNP P06756
C	635	LYS	-	expression tag	UNP P06756
C	636	GLU	-	expression tag	UNP P06756
C	637	LEU	-	expression tag	UNP P06756
C	638	ALA	-	expression tag	UNP P06756
C	639	GLN	-	expression tag	UNP P06756
C	640	THR	-	expression tag	UNP P06756
C	641	THR	-	expression tag	UNP P06756
C	642	GLY	-	expression tag	UNP P06756
C	643	TRP	-	expression tag	UNP P06756
C	644	ARG	-	expression tag	UNP P06756
C	645	GLY	-	expression tag	UNP P06756
C	646	GLY	-	expression tag	UNP P06756
C	647	HIS	-	expression tag	UNP P06756
C	648	VAL	-	expression tag	UNP P06756
C	649	VAL	-	expression tag	UNP P06756
C	650	GLU	-	expression tag	UNP P06756
C	651	GLY	-	expression tag	UNP P06756
C	652	LEU	-	expression tag	UNP P06756
C	653	ALA	-	expression tag	UNP P06756
C	654	GLY	-	expression tag	UNP P06756
C	655	GLU	-	expression tag	UNP P06756
C	656	LEU	-	expression tag	UNP P06756
C	657	GLU	-	expression tag	UNP P06756
C	658	GLN	-	expression tag	UNP P06756
C	659	LEU	-	expression tag	UNP P06756

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Chain	Residue	Modelled	Actual	Comment	Reference
C	660	ARG	-	expression tag	UNP P06756
C	661	ALA	-	expression tag	UNP P06756
C	662	ARG	-	expression tag	UNP P06756
C	663	LEU	-	expression tag	UNP P06756
C	664	GLU	-	expression tag	UNP P06756
C	665	HIS	-	expression tag	UNP P06756
C	666	HIS	-	expression tag	UNP P06756
C	667	PRO	-	expression tag	UNP P06756
C	668	GLN	-	expression tag	UNP P06756
C	669	GLY	-	expression tag	UNP P06756
C	670	GLN	-	expression tag	UNP P06756
C	671	ARG	-	expression tag	UNP P06756
C	672	GLU	-	expression tag	UNP P06756
C	673	PRO	-	expression tag	UNP P06756
C	674	ALA	-	expression tag	UNP P06756
C	675	GLY	-	expression tag	UNP P06756
C	676	HIS	-	expression tag	UNP P06756
C	677	HIS	-	expression tag	UNP P06756
C	678	HIS	-	expression tag	UNP P06756
C	679	HIS	-	expression tag	UNP P06756
C	680	HIS	-	expression tag	UNP P06756
C	681	HIS	-	expression tag	UNP P06756
C	400	CYS	MET	engineered mutation	UNP P06756

- Molecule 2 is a protein called INTEGRIN BETA-6.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	423	Total	C	N	O	S	0	0	0
			3252	2051	548	628	25			
2	D	414	Total	C	N	O	S	0	0	0
			3202	2020	539	618	25			

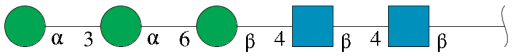
There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	270	CYS	ILE	engineered mutation	UNP P18564
D	270	CYS	ILE	engineered mutation	UNP P18564

- Molecule 3 is an oligosaccharide called 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.

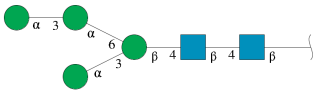
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
3	E	4	Total	C	N	O	0	0	0
			50	28	2	20			
3	Q	4	Total	C	N	O	0	0	0
			50	28	2	20			

- 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-acetamido-2-deoxy-beta-D-glucopyranose.



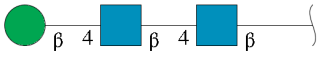
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
4	F	5	Total	C	N	O	0	0	0
			61	34	2	25			

- Molecule 5 is an oligosaccharide called alpha-D-mannopyranose-(1-3)-alpha-D-mannopyranose-(1-6)-[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.



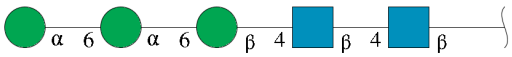
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
5	G	6	Total	C	N	O	0	0	0
			72	40	2	30			
5	M	6	Total	C	N	O	0	0	0
			72	40	2	30			

- Molecule 6 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
6	H	3	Total C N O 39 22 2 15	0	0	0
6	K	3	Total C N O 39 22 2 15	0	0	0

- Molecule 7 is an oligosaccharide called alpha-D-mannopyranose-(1-6)-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.



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

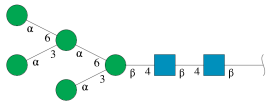
- Molecule 8 is an oligosaccharide called 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose.

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

- Molecule 9 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
9	N	4	Total	C	N	O	0	0	0
			50	28	2	20			

- Molecule 10 is an oligosaccharide called alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-6)]alpha-D-mannopyranose-(1-6)-[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.

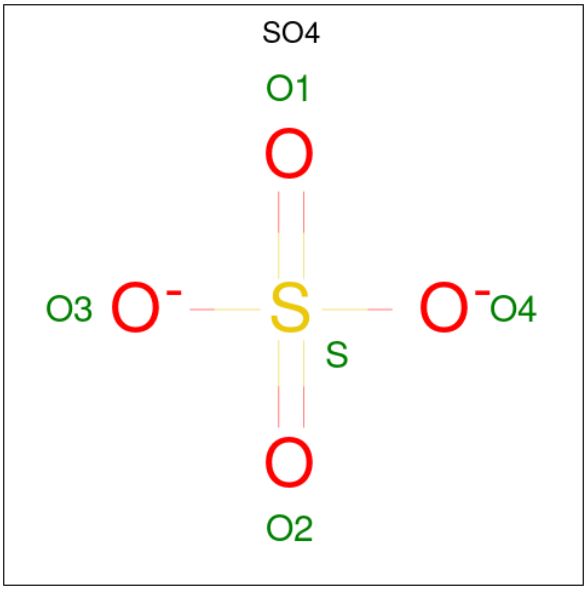


Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
10	O	7	Total	C	N	O	0	0	0
			83	46	2	35			

- Molecule 11 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
11	A	1	Total	Cl	0	0
			1	1		
11	C	2	Total	Cl	0	0
			2	2		

- Molecule 12 is SULFATE ION (three-letter code: SO4) (formula: O_4S).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
12	A	1	Total O S 5 4 1	0	0
12	A	1	Total O S 5 4 1	0	0
12	A	1	Total O S 5 4 1	0	0

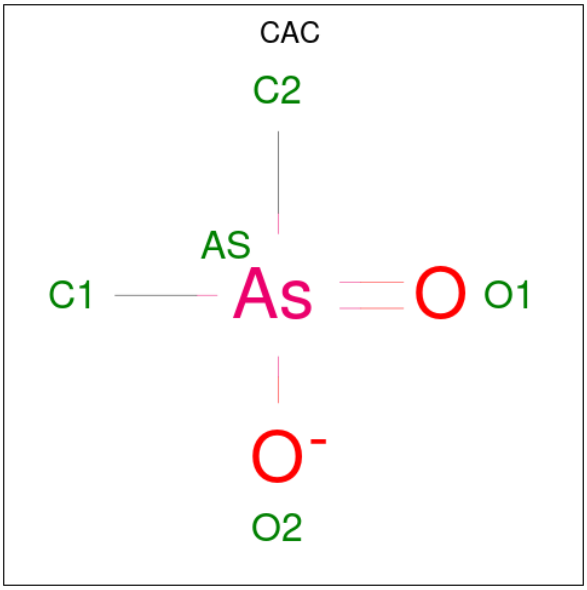
- Molecule 13 is NICKEL (II) ION (three-letter code: NI) (formula: Ni).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
13	A	1	Total Ni 1 1	0	0

- Molecule 14 is CALCIUM ION (three-letter code: CA) (formula: Ca).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
14	A	4	Total Ca 4 4	0	0
14	B	1	Total Ca 1 1	0	0
14	C	4	Total Ca 4 4	0	0
14	D	1	Total Ca 1 1	0	0

- Molecule 15 is CACODYLATE ION (three-letter code: CAC) (formula: $C_2H_6AsO_2$).

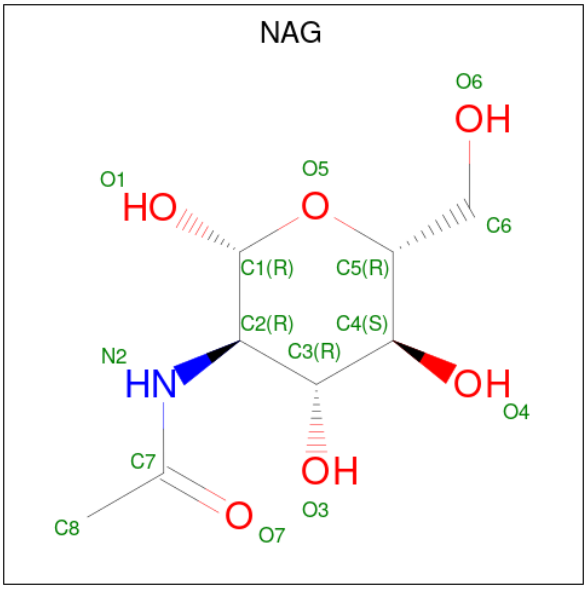


Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
15	B	1	Total As C O 5 1 2 2	0	0
15	D	1	Total As C O 5 1 2 2	0	0

- Molecule 16 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
16	B	1	Total Mg 1 1	0	0
16	D	1	Total Mg 1 1	0	0

- Molecule 17 is 2-acetamido-2-deoxy-beta-D-glucopyranose (three-letter code: NAG) (formula: $C_8H_{15}NO_6$).



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

- Molecule 18 is water.

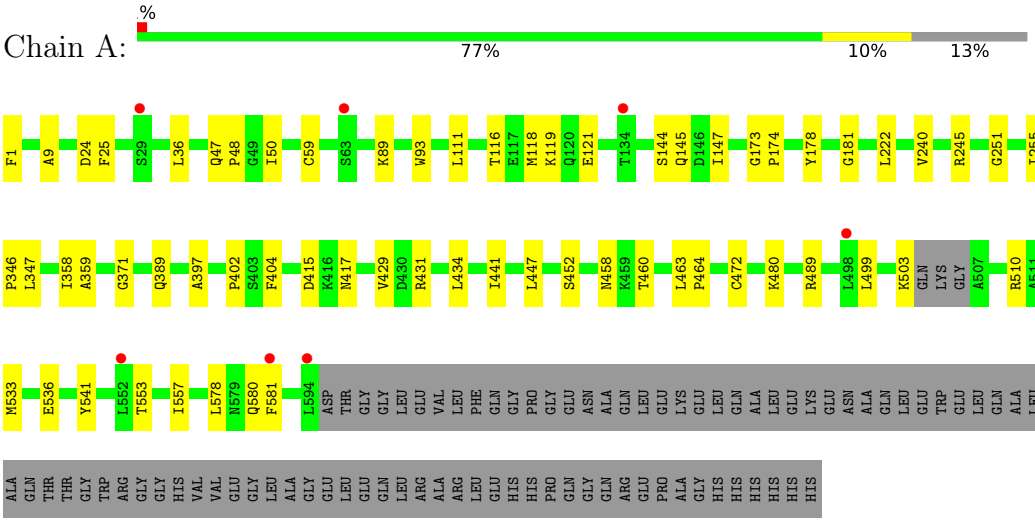
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
18	A	65	Total O 65 65	0	0
18	B	32	Total O 32 32	0	0
18	C	38	Total O 38 38	0	0
18	D	26	Total O 26 26	0	0

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.

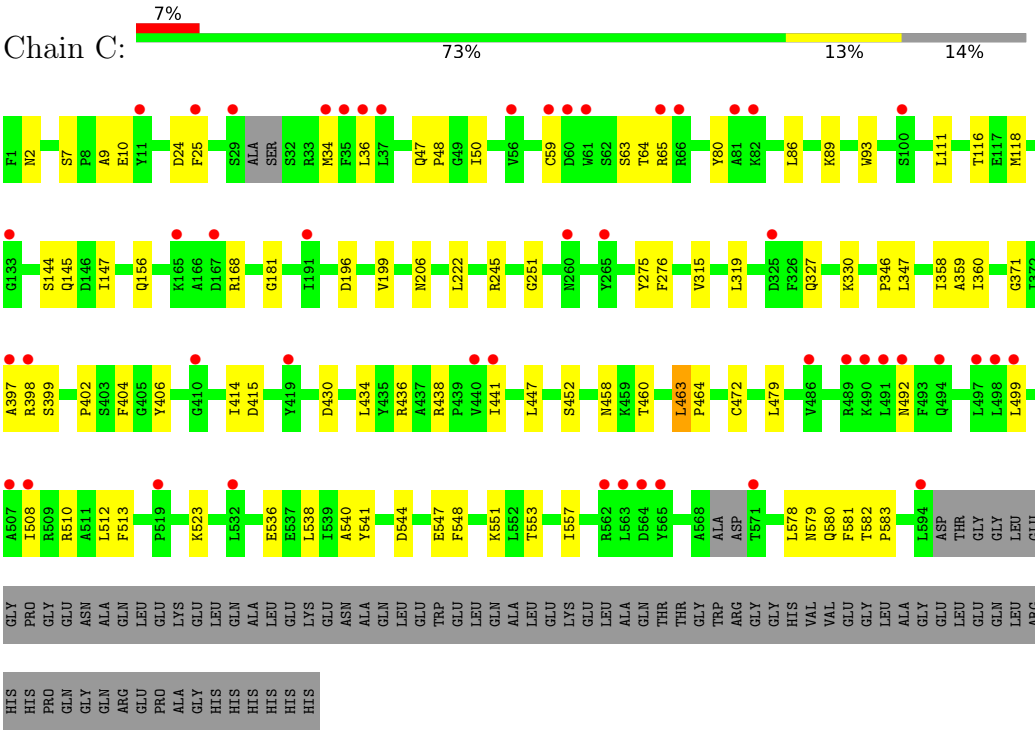
• Molecule 1: INTEGRIN ALPHA-V

Chain A:



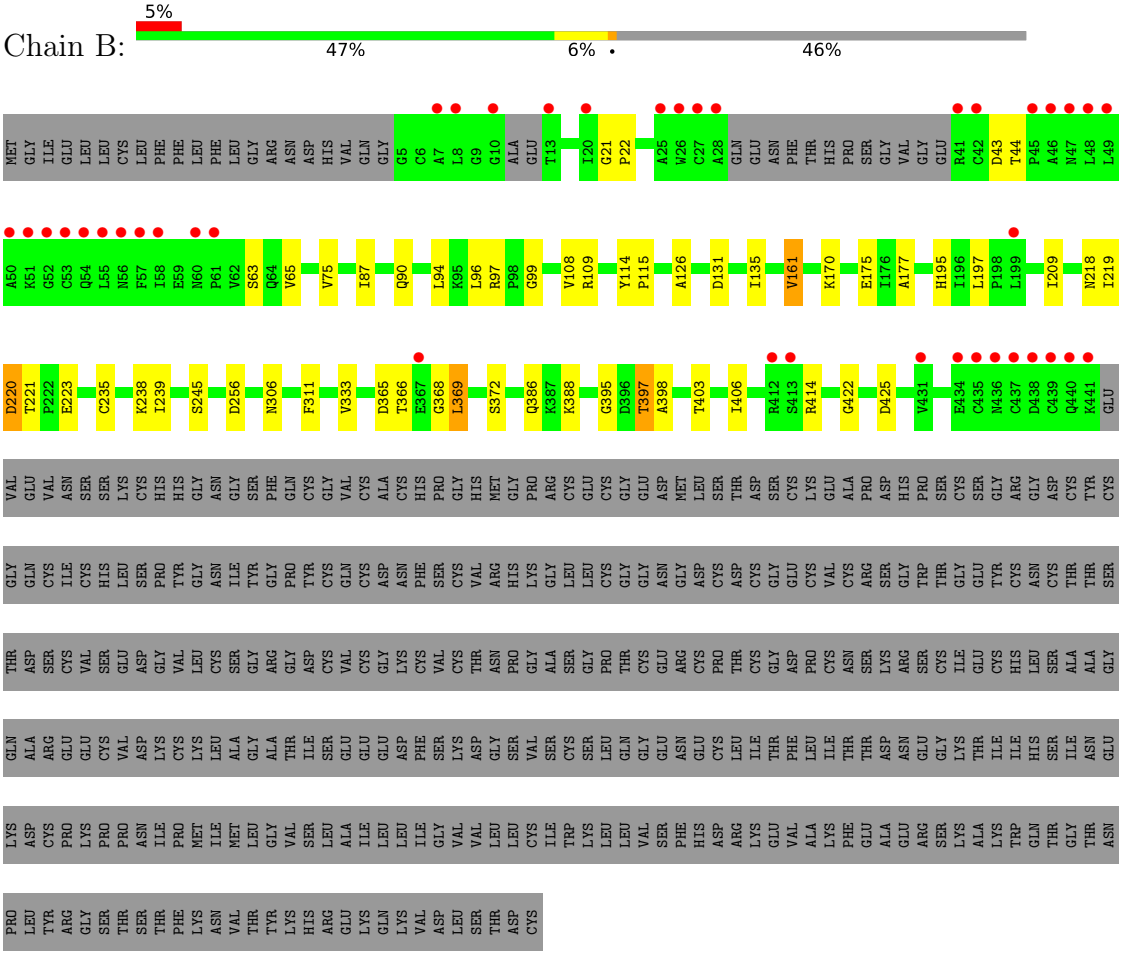
• Molecule 1: INTEGRIN ALPHA-V

Chain C:



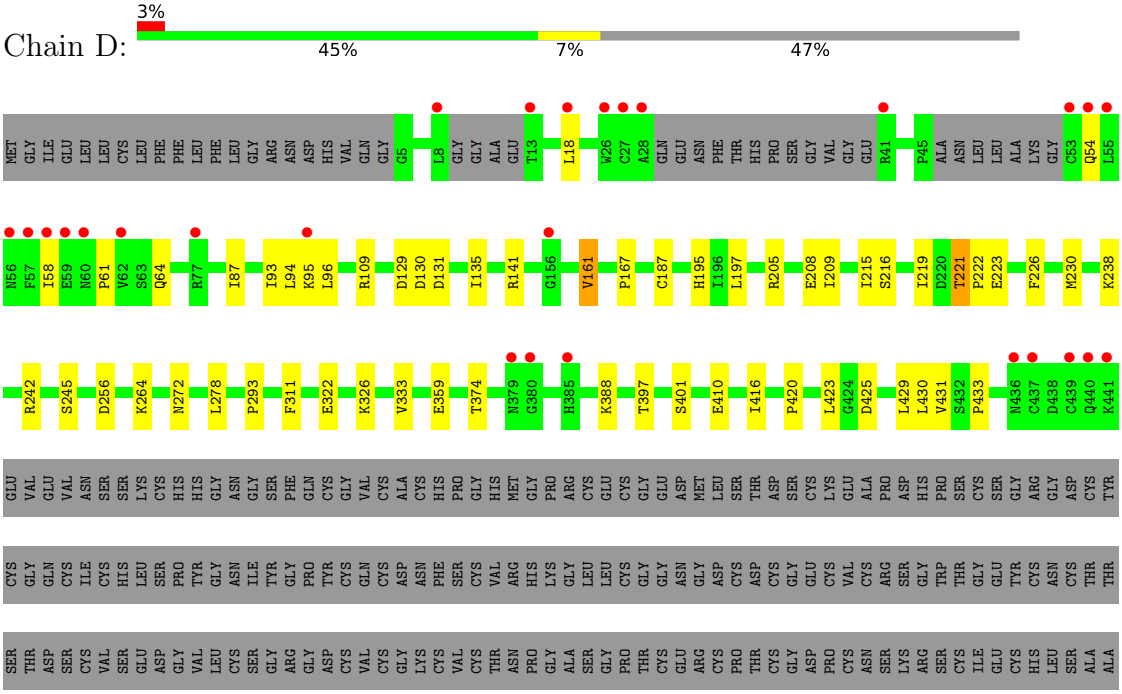
• Molecule 2: INTEGRIN BETA-6

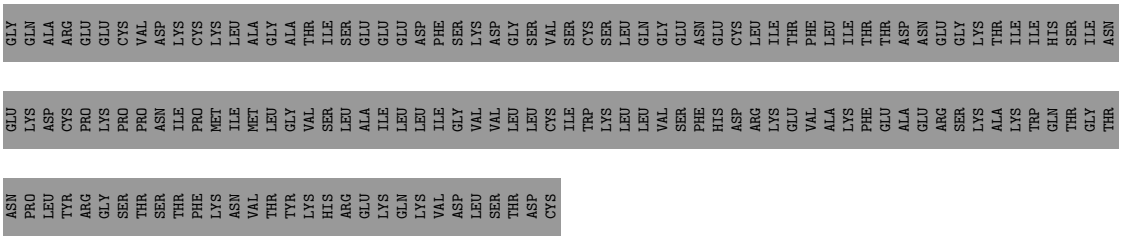
Chain B:



• Molecule 2: INTEGRIN BETA-6

Chain D:





• Molecule 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 E:

• Molecule 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 Q:

• 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

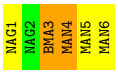
Chain F:

• Molecule 5: alpha-D-mannopyranose-(1-3)-alpha-D-mannopyranose-(1-6)-[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 G:

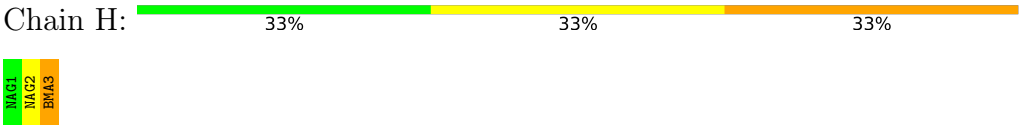
• Molecule 5: alpha-D-mannopyranose-(1-3)-alpha-D-mannopyranose-(1-6)-[alpha-D-mannopyranose-(1-3)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain M:



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

Chain H:

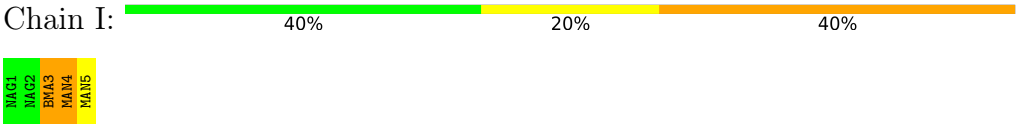


• Molecule 6: beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain K:

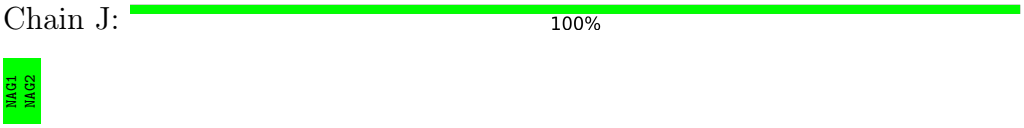
• Molecule 7: alpha-D-mannopyranose-(1-6)-alpha-D-mannopyranose-(1-6)-beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain I:



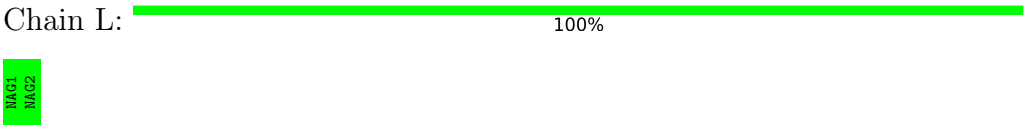
• Molecule 8: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain J:



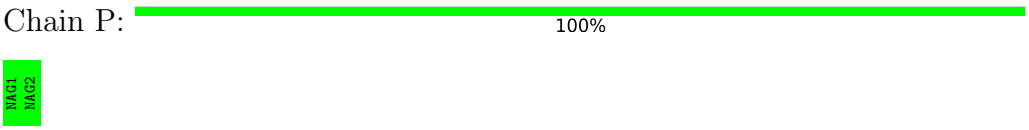
• Molecule 8: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain L:



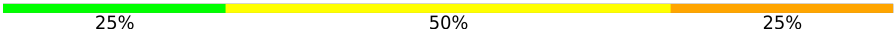
• Molecule 8: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain P:



• Molecule 9: 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 N:



• Molecule 10: alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-6)]alpha-D-mannopyranose-(1-6)-[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:

4 Data and refinement statistics (i)

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α, β, γ	184.45Å 170.01Å 102.39Å 90.00° 98.68° 90.00°	Depositor
Resolution (Å)	48.66 – 2.85 48.66 – 2.85	Depositor EDS
% Data completeness (in resolution range)	96.4 (48.66-2.85) 96.4 (48.66-2.85)	Depositor EDS
R_{merge}	0.18	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.34 (at 2.86Å)	Xtriage
Refinement program	PHENIX (PHENIX.REFINE)	Depositor
R, R_{free}	0.238 , 0.281 0.239 , 0.281	Depositor DCC
R_{free} test set	1799 reflections (2.57%)	wwPDB-VP
Wilson B-factor (Å^2)	61.1	Xtriage
Anisotropy	0.384	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.29 , 75.6	EDS
L-test for twinning[2]	$< \|L\| > = 0.45$, $< L^2 > = 0.28$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.92	EDS
Total number of atoms	16497	wwPDB-VP
Average B, all atoms (Å^2)	86.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.31% 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: NAG, BMA, CL, SO4, NI, CAC, CA, MAN, MG

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	0.21	0/4682	0.39	0/6339
1	C	0.21	0/4660	0.37	0/6305
2	B	0.21	0/3308	0.40	0/4481
2	D	0.21	0/3258	0.39	0/4413
All	All	0.21	0/15908	0.39	0/21538

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	4579	0	4426	34	1
1	C	4559	0	4408	51	1
2	B	3252	0	3234	35	0
2	D	3202	0	3176	36	0
3	E	50	0	43	1	0
3	Q	50	0	43	2	0
4	F	61	0	52	0	0
5	G	72	0	61	1	0
5	M	72	0	61	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
6	H	39	0	34	1	0
6	K	39	0	34	0	0
7	I	61	0	52	1	0
8	J	28	0	25	0	0
8	L	28	0	25	0	0
8	P	28	0	25	0	0
9	N	50	0	43	1	0
10	O	83	0	70	2	0
11	A	1	0	0	0	0
11	C	2	0	0	0	0
12	A	15	0	0	1	0
13	A	1	0	0	0	0
14	A	4	0	0	0	0
14	B	1	0	0	0	0
14	C	4	0	0	0	0
14	D	1	0	0	0	0
15	B	5	0	0	0	0
15	D	5	0	0	0	0
16	B	1	0	0	0	0
16	D	1	0	0	0	0
17	B	14	0	13	0	0
17	D	28	0	26	0	0
18	A	65	0	0	0	0
18	B	32	0	0	0	0
18	C	38	0	0	0	0
18	D	26	0	0	1	0
All	All	16497	0	15851	160	1

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 5.

All (160) 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:B:109:ARG:NH2	2:B:397:THR:OG1	2.19	0.76
2:B:220:ASP:N	2:B:220:ASP:OD1	2.24	0.70
1:C:116:THR:HG22	1:C:118:MET:H	1.55	0.70
1:A:116:THR:HG22	1:A:118:MET:H	1.57	0.70
1:A:480:LYS:HB2	1:A:533:MET:HB3	1.74	0.70
1:C:245:ARG:NH2	2:D:256:ASP:OD2	2.26	0.69
1:C:406:TYR:OH	2:D:264:LYS:NZ	2.25	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:230:MET:HG2	2:D:272:ASN:HD21	1.58	0.67
1:C:548:PHE:O	1:C:551:LYS:NZ	2.29	0.65
2:D:420:PRO:HG2	2:D:423:LEU:HB2	1.77	0.64
1:C:371:GLY:HA3	1:C:404:PHE:HB3	1.78	0.64
2:B:366:THR:HG22	2:B:368:GLY:H	1.63	0.63
1:A:24:ASP:OD1	1:A:25:PHE:N	2.33	0.61
1:A:245:ARG:NH2	2:B:256:ASP:OD2	2.33	0.61
1:A:1:PHE:HA	1:A:389:GLN:HB2	1.82	0.60
1:C:24:ASP:OD1	1:C:25:PHE:N	2.34	0.60
2:B:369:LEU:HD11	2:B:406:ILE:HG12	1.84	0.60
2:B:170:LYS:HB2	2:B:175:GLU:HG2	1.84	0.60
1:C:347:LEU:HD11	1:C:359:ALA:HB2	1.83	0.59
1:C:510:ARG:NH1	1:C:553:THR:O	2.33	0.59
1:C:398:ARG:NH1	1:C:430:ASP:OD2	2.36	0.59
10:O:1:NAG:O3	10:O:2:NAG:N2	2.37	0.58
2:D:187:CYS:HB3	2:D:216:SER:O	2.04	0.58
1:C:319:LEU:HB2	1:C:327:GLN:HB3	1.85	0.57
1:A:489:ARG:NH1	12:A:1596:SO4:O2	2.37	0.57
2:D:359:GLU:HB2	2:D:388:LYS:HD3	1.85	0.57
1:A:50:ILE:HD13	1:A:89:LYS:HB2	1.86	0.57
2:D:221:THR:HG22	2:D:222:PRO:HD2	1.86	0.56
2:D:322:GLU:HG3	2:D:333:VAL:HG21	1.86	0.56
2:D:141:ARG:NH1	18:D:4005:HOH:O	2.39	0.55
1:A:181:GLY:HA3	1:A:222:LEU:HB3	1.88	0.55
1:A:415:ASP:OD2	1:A:417:ASN:ND2	2.39	0.55
1:C:34:MET:HE2	1:C:414:ILE:HA	1.89	0.55
2:D:18:LEU:HD13	2:D:61:PRO:HG3	1.88	0.55
1:C:93:TRP:CD1	1:C:111:LEU:HD12	2.42	0.55
1:A:503:LYS:HD3	1:A:553:THR:HG21	1.88	0.54
2:B:115:PRO:HB2	2:B:245:SER:HB3	1.90	0.54
1:A:371:GLY:HA3	1:A:404:PHE:HB3	1.88	0.54
1:C:346:PRO:HA	1:C:358:ILE:HG13	1.89	0.54
2:B:366:THR:HB	2:B:369:LEU:H	1.72	0.54
1:A:251:GLY:HA3	1:A:276:PHE:HB3	1.91	0.53
1:C:330:LYS:O	3:Q:4:MAN:O3	2.25	0.53
1:A:472:CYS:HA	1:A:541:TYR:HA	1.90	0.53
2:B:366:THR:HB	2:B:369:LEU:HB2	1.90	0.53
1:A:347:LEU:HD11	1:A:359:ALA:HB2	1.91	0.53
2:B:87:ILE:HG22	2:B:425:ASP:HB3	1.91	0.53
1:C:116:THR:HG23	1:C:147:ILE:HG21	1.90	0.52
1:C:7:SER:O	1:C:436:ARG:NH2	2.41	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:22:PRO:HG3	2:B:99:GLY:HA3	1.91	0.52
2:B:75:VAL:HG21	2:B:109:ARG:HH11	1.75	0.51
2:D:226:PHE:HB3	2:D:293:PRO:HG2	1.91	0.51
1:C:544:ASP:HB3	1:C:547:GLU:HG3	1.93	0.51
2:D:129:ASP:HA	2:D:215:ILE:HD11	1.93	0.51
2:B:126:ALA:HB3	2:B:218:ASN:HB3	1.93	0.51
1:C:397:ALA:HB2	1:C:402:PRO:HD3	1.92	0.51
1:A:36:LEU:HB2	1:A:59:CYS:HB2	1.93	0.51
1:A:144:SER:OG	1:A:145:GLN:N	2.44	0.51
1:C:315:VAL:HG21	1:C:360:ILE:HD13	1.93	0.50
1:C:508:ILE:HD13	1:C:548:PHE:HB3	1.93	0.50
1:A:441:ILE:HB	1:A:578:LEU:HD23	1.92	0.50
1:C:2:ASN:O	1:C:438:ARG:N	2.37	0.49
2:B:87:ILE:O	2:B:90:GLN:NE2	2.43	0.49
2:B:311:PHE:HB2	2:B:333:VAL:HG12	1.94	0.49
1:A:397:ALA:HB2	1:A:402:PRO:HD3	1.95	0.49
2:D:410:GLU:HB2	2:D:433:PRO:HG3	1.94	0.49
1:C:499:LEU:HD12	1:C:512:LEU:HA	1.95	0.48
1:C:50:ILE:HD13	1:C:89:LYS:HB2	1.94	0.48
1:C:373:VAL:HB	1:C:391:LEU:HB2	1.95	0.48
1:C:513:PHE:HA	1:C:540:ALA:HA	1.95	0.48
2:D:238:LYS:NZ	2:D:278:LEU:O	2.46	0.48
1:A:499:LEU:HD12	1:A:512:LEU:HA	1.95	0.48
1:C:36:LEU:HB2	1:C:59:CYS:HB2	1.94	0.47
2:D:93:ILE:HG12	2:D:430:LEU:HB3	1.95	0.47
2:D:131:ASP:O	2:D:135:ILE:HG13	2.14	0.47
2:D:195:HIS:NE2	2:D:238:LYS:O	2.35	0.47
1:A:523:LYS:HG2	1:A:536:GLU:OE1	2.14	0.47
2:B:195:HIS:NE2	2:B:238:LYS:O	2.43	0.47
1:C:181:GLY:HA3	1:C:222:LEU:HB3	1.96	0.47
1:C:441:ILE:HB	1:C:578:LEU:HD23	1.96	0.47
1:C:523:LYS:HG2	1:C:536:GLU:OE1	2.15	0.47
2:D:242:ARG:HB2	2:D:245:SER:OG	2.14	0.47
2:D:311:PHE:HB2	2:D:333:VAL:HG12	1.96	0.47
1:A:116:THR:HG23	1:A:147:ILE:HG21	1.96	0.47
1:C:10:GLU:H	1:C:65:ARG:NH1	2.12	0.47
1:C:63:SER:OG	1:C:64:THR:N	2.47	0.47
3:E:3:BMA:H62	3:E:4:MAN:H2	1.59	0.47
1:A:346:PRO:HA	1:A:358:ILE:HG13	1.97	0.47
1:A:93:TRP:CD1	1:A:111:LEU:HD12	2.50	0.46
1:A:458:ASN:OD1	1:A:460:THR:OG1	2.18	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:472:CYS:HA	1:C:541:TYR:HA	1.97	0.46
2:B:108:VAL:HG23	2:B:398:ALA:HB3	1.98	0.46
2:D:109:ARG:HH21	2:D:397:THR:HB	1.80	0.46
2:D:94:LEU:HD21	2:D:96:LEU:HD12	1.98	0.46
2:B:386:GLN:NE2	2:B:388:LYS:O	2.46	0.46
10:O:3:BMA:H61	10:O:4:MAN:H2	1.30	0.45
3:Q:3:BMA:H61	3:Q:4:MAN:H2	1.55	0.45
2:D:64:GLN:HG2	2:D:95:LYS:HD2	1.99	0.45
2:B:43:ASP:OD1	2:B:44:THR:N	2.47	0.45
2:B:22:PRO:HA	2:B:97:ARG:NH1	2.32	0.45
1:C:251:GLY:HA3	1:C:276:PHE:HB3	1.98	0.45
2:B:372:SER:HG	2:B:403:THR:HG1	1.50	0.44
2:D:205:ARG:NH1	2:D:208:GLU:OE1	2.49	0.44
2:B:75:VAL:HG21	2:B:109:ARG:NH1	2.33	0.44
1:C:144:SER:OG	1:C:145:GLN:N	2.48	0.44
2:B:21:GLY:HA2	2:B:22:PRO:HD3	1.86	0.44
2:B:235:CYS:HB2	2:B:239:ILE:HD13	2.00	0.44
2:D:109:ARG:NH2	2:D:397:THR:HB	2.33	0.44
2:B:109:ARG:NE	2:B:395:GLY:O	2.51	0.44
2:B:22:PRO:HA	2:B:97:ARG:HH11	1.83	0.43
1:C:582:THR:HA	1:C:583:PRO:HD3	1.88	0.43
1:C:463:LEU:HD23	1:C:464:PRO:HD2	2.00	0.43
1:C:580:GLN:HG3	1:C:581:PHE:H	1.84	0.43
1:A:9:ALA:HB3	1:A:434:LEU:HB3	2.01	0.43
1:C:80:TYR:HB2	1:C:86:LEU:HD13	2.01	0.43
2:D:416:ILE:HB	2:D:429:LEU:HB2	2.00	0.43
6:H:2:NAG:H4	6:H:3:BMA:O2	2.14	0.43
1:A:47:GLN:HA	1:A:48:PRO:HD3	1.90	0.43
2:B:114:TYR:HA	2:B:115:PRO:HD3	1.91	0.42
2:B:197:LEU:HD22	2:B:209:ILE:HD12	2.01	0.42
1:C:579:ASN:OD1	1:C:580:GLN:N	2.52	0.42
1:A:429:VAL:HG23	1:A:431:ARG:HG2	2.01	0.42
1:A:463:LEU:HD23	1:A:464:PRO:HD2	2.02	0.42
5:M:3:BMA:H62	5:M:4:MAN:H2	1.76	0.42
1:C:479:LEU:HD23	1:C:479:LEU:HA	1.91	0.42
5:G:3:BMA:H62	5:G:4:MAN:H2	1.74	0.42
2:D:94:LEU:HD22	2:D:431:VAL:HG22	2.00	0.42
2:D:374:THR:OG1	2:D:401:SER:HB2	2.20	0.42
2:D:161:VAL:O	2:D:223:GLU:HB3	2.20	0.42
1:A:510:ARG:NH1	1:A:553:THR:O	2.52	0.42
2:B:161:VAL:O	2:B:223:GLU:HB3	2.20	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:398:ARG:HG3	1:C:399:SER:H	1.84	0.42
2:B:131:ASP:O	2:B:135:ILE:HG13	2.20	0.42
1:A:119:LYS:HG3	1:A:121:GLU:HG2	2.02	0.42
1:A:447:LEU:HD21	1:A:557:ILE:HG22	2.02	0.42
1:A:580:GLN:HG3	1:A:581:PHE:H	1.85	0.42
2:D:87:ILE:HG22	2:D:425:ASP:HB3	2.02	0.42
2:B:219:ILE:HG22	2:B:221:THR:H	1.85	0.41
1:C:492:ASN:OD1	1:C:492:ASN:N	2.47	0.41
1:A:240:VAL:HG22	1:A:255:ILE:HG12	2.01	0.41
1:C:47:GLN:HA	1:C:48:PRO:HD3	1.89	0.41
2:D:130:ASP:OD1	2:D:130:ASP:N	2.53	0.41
1:C:9:ALA:HB3	1:C:434:LEU:HB3	2.03	0.41
1:C:147:ILE:H	1:C:147:ILE:HG13	1.67	0.41
2:D:322:GLU:O	2:D:326:LYS:HG3	2.20	0.41
2:B:63:SER:HB3	2:B:96:LEU:HD23	2.02	0.41
2:D:197:LEU:HD22	2:D:209:ILE:HD12	2.01	0.41
1:C:196:ASP:HB3	1:C:199:VAL:HB	2.03	0.41
2:D:54:GLN:O	2:D:58:ILE:HG13	2.21	0.41
2:D:219:ILE:HG22	2:D:221:THR:H	1.84	0.41
9:N:2:NAG:H61	9:N:3:BMA:O2	2.21	0.41
1:A:173:GLY:HA2	1:A:174:PRO:HD3	1.90	0.41
1:C:458:ASN:OD1	1:C:460:THR:OG1	2.33	0.41
2:B:65:VAL:HG12	2:B:94:LEU:HD13	2.02	0.41
1:C:156:GLN:OE1	2:D:167:PRO:HG3	2.21	0.41
2:B:306:ASN:HD21	2:B:422:GLY:C	2.24	0.40
2:B:177:ALA:HA	2:D:374:THR:HG21	2.03	0.40
1:C:415:ASP:OD1	1:C:415:ASP:N	2.51	0.40
1:C:447:LEU:HD21	1:C:557:ILE:HG22	2.03	0.40
1:C:168:ARG:NH2	1:C:206:ASN:O	2.54	0.40
7:I:3:BMA:H61	7:I:4:MAN:H2	1.85	0.40

All (1) 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:452:SER:OG	1:C:452:SER:OG[4_555]	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	587/681 (86%)	562 (96%)	25 (4%)	0	100	100
1	C	580/681 (85%)	557 (96%)	23 (4%)	0	100	100
2	B	417/788 (53%)	397 (95%)	18 (4%)	2 (0%)	29	57
2	D	406/788 (52%)	389 (96%)	16 (4%)	1 (0%)	47	75
All	All	1990/2938 (68%)	1905 (96%)	82 (4%)	3 (0%)	47	75

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	B	365	ASP
2	B	161	VAL
2	D	161	VAL

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	485/555 (87%)	483 (100%)	2 (0%)	91	96
1	C	483/555 (87%)	480 (99%)	3 (1%)	86	95
2	B	371/685 (54%)	367 (99%)	4 (1%)	73	90
2	D	368/685 (54%)	367 (100%)	1 (0%)	92	97
All	All	1707/2480 (69%)	1697 (99%)	10 (1%)	86	95

All (10) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	178	TYR
1	A	275	TYR
2	B	220	ASP
2	B	369	LEU
2	B	397	THR
2	B	414	ARG
1	C	275	TYR
1	C	463	LEU
1	C	538	LEU
2	D	221	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (5) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	352	GLN
1	A	474	ASN
1	C	152	GLN
1	C	207	GLN
2	D	304	GLN

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

53 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	0.32	0	17,19,21	0.55	0
3	NAG	E	2	3	14,14,15	0.32	0	17,19,21	0.57	0
3	BMA	E	3	3	11,11,12	0.60	0	15,15,17	0.87	0
3	MAN	E	4	3	11,11,12	0.77	0	15,15,17	1.01	1 (6%)
4	NAG	F	1	4,1	14,14,15	0.19	0	17,19,21	0.36	0
4	NAG	F	2	4	14,14,15	0.22	0	17,19,21	0.38	0
4	BMA	F	3	4	11,11,12	0.80	0	15,15,17	0.88	0
4	MAN	F	4	4	11,11,12	0.89	1 (9%)	15,15,17	1.08	1 (6%)
4	MAN	F	5	4	11,11,12	0.74	0	15,15,17	0.96	2 (13%)
5	NAG	G	1	5,1	14,14,15	1.19	1 (7%)	17,19,21	1.00	1 (5%)
5	NAG	G	2	5	14,14,15	0.48	0	17,19,21	0.37	0
5	BMA	G	3	5	11,11,12	0.83	1 (9%)	15,15,17	0.87	0
5	MAN	G	4	5	11,11,12	0.81	1 (9%)	15,15,17	0.92	1 (6%)
5	MAN	G	5	5	11,11,12	0.79	1 (9%)	15,15,17	0.94	1 (6%)
5	MAN	G	6	5	11,11,12	0.77	1 (9%)	15,15,17	0.91	1 (6%)
6	NAG	H	1	6,1	14,14,15	0.30	0	17,19,21	0.51	0
6	NAG	H	2	6	14,14,15	0.29	0	17,19,21	0.55	0
6	BMA	H	3	6	11,11,12	0.84	0	15,15,17	1.08	2 (13%)
7	NAG	I	1	1,7	14,14,15	0.36	0	17,19,21	0.53	0
7	NAG	I	2	7	14,14,15	0.29	0	17,19,21	0.44	0
7	BMA	I	3	7	11,11,12	0.64	0	15,15,17	1.06	2 (13%)
7	MAN	I	4	7	11,11,12	0.76	0	15,15,17	1.24	2 (13%)
7	MAN	I	5	7	11,11,12	0.64	0	15,15,17	1.09	2 (13%)
8	NAG	J	1	8,1	14,14,15	0.34	0	17,19,21	0.45	0
8	NAG	J	2	8	14,14,15	0.29	0	17,19,21	0.45	0
6	NAG	K	1	6,1	14,14,15	0.53	0	17,19,21	0.57	0
6	NAG	K	2	6	14,14,15	0.41	0	17,19,21	0.72	1 (5%)
6	BMA	K	3	6	11,11,12	0.57	0	15,15,17	0.99	1 (6%)
8	NAG	L	1	8,1	14,14,15	0.27	0	17,19,21	0.41	0
8	NAG	L	2	8	14,14,15	0.22	0	17,19,21	0.43	0
5	NAG	M	1	5,1	14,14,15	1.76	2 (14%)	17,19,21	1.30	2 (11%)
5	NAG	M	2	5	14,14,15	0.43	0	17,19,21	0.37	0
5	BMA	M	3	5	11,11,12	0.74	1 (9%)	15,15,17	0.83	0
5	MAN	M	4	5	11,11,12	0.72	0	15,15,17	1.02	2 (13%)
5	MAN	M	5	5	11,11,12	0.70	0	15,15,17	0.98	2 (13%)
5	MAN	M	6	5	11,11,12	0.80	1 (9%)	15,15,17	0.88	1 (6%)
9	NAG	N	1	9,1	14,14,15	0.34	0	17,19,21	0.62	0
9	NAG	N	2	9	14,14,15	0.37	0	17,19,21	0.52	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
9	BMA	N	3	9	11,11,12	1.01	1 (9%)	15,15,17	1.35	2 (13%)
9	MAN	N	4	9	11,11,12	1.16	2 (18%)	15,15,17	1.21	3 (20%)
10	NAG	O	1	1,10	14,14,15	1.04	1 (7%)	17,19,21	0.88	1 (5%)
10	NAG	O	2	10	14,14,15	0.57	1 (7%)	17,19,21	0.73	1 (5%)
10	BMA	O	3	10	11,11,12	1.05	1 (9%)	15,15,17	1.55	4 (26%)
10	MAN	O	4	10	11,11,12	0.81	0	15,15,17	1.38	2 (13%)
10	MAN	O	5	10	11,11,12	0.61	0	15,15,17	1.12	2 (13%)
10	MAN	O	6	10	11,11,12	0.75	0	15,15,17	0.95	1 (6%)
10	MAN	O	7	10	11,11,12	1.03	1 (9%)	15,15,17	0.84	1 (6%)
8	NAG	P	1	8,1	14,14,15	0.39	0	17,19,21	0.37	0
8	NAG	P	2	8	14,14,15	0.29	0	17,19,21	0.43	0
3	NAG	Q	1	3,2	14,14,15	0.62	1 (7%)	17,19,21	0.50	0
3	NAG	Q	2	3	14,14,15	0.34	0	17,19,21	0.67	0
3	BMA	Q	3	3	11,11,12	0.60	0	15,15,17	1.12	1 (6%)
3	MAN	Q	4	3	11,11,12	0.76	0	15,15,17	1.00	2 (13%)

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	-	2/6/23/26	0/1/1/1
3	NAG	E	2	3	-	0/6/23/26	0/1/1/1
3	BMA	E	3	3	-	1/2/19/22	0/1/1/1
3	MAN	E	4	3	-	0/2/19/22	0/1/1/1
4	NAG	F	1	4,1	-	2/6/23/26	0/1/1/1
4	NAG	F	2	4	-	3/6/23/26	0/1/1/1
4	BMA	F	3	4	-	1/2/19/22	0/1/1/1
4	MAN	F	4	4	-	0/2/19/22	0/1/1/1
4	MAN	F	5	4	-	0/2/19/22	0/1/1/1
5	NAG	G	1	5,1	-	2/6/23/26	0/1/1/1
5	NAG	G	2	5	-	0/6/23/26	0/1/1/1
5	BMA	G	3	5	-	1/2/19/22	0/1/1/1
5	MAN	G	4	5	-	0/2/19/22	0/1/1/1
5	MAN	G	5	5	-	2/2/19/22	0/1/1/1
5	MAN	G	6	5	-	1/2/19/22	0/1/1/1
6	NAG	H	1	6,1	-	0/6/23/26	0/1/1/1
6	NAG	H	2	6	-	0/6/23/26	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
6	BMA	H	3	6	-	1/2/19/22	0/1/1/1
7	NAG	I	1	1,7	-	0/6/23/26	0/1/1/1
7	NAG	I	2	7	-	0/6/23/26	0/1/1/1
7	BMA	I	3	7	-	2/2/19/22	0/1/1/1
7	MAN	I	4	7	-	0/2/19/22	1/1/1/1
7	MAN	I	5	7	-	0/2/19/22	0/1/1/1
8	NAG	J	1	8,1	-	0/6/23/26	0/1/1/1
8	NAG	J	2	8	-	1/6/23/26	0/1/1/1
6	NAG	K	1	6,1	-	2/6/23/26	0/1/1/1
6	NAG	K	2	6	-	0/6/23/26	0/1/1/1
6	BMA	K	3	6	-	0/2/19/22	0/1/1/1
8	NAG	L	1	8,1	-	0/6/23/26	0/1/1/1
8	NAG	L	2	8	-	0/6/23/26	0/1/1/1
5	NAG	M	1	5,1	1/1/5/7	3/6/23/26	0/1/1/1
5	NAG	M	2	5	-	0/6/23/26	0/1/1/1
5	BMA	M	3	5	-	1/2/19/22	0/1/1/1
5	MAN	M	4	5	-	0/2/19/22	0/1/1/1
5	MAN	M	5	5	-	2/2/19/22	0/1/1/1
5	MAN	M	6	5	-	1/2/19/22	0/1/1/1
9	NAG	N	1	9,1	-	0/6/23/26	0/1/1/1
9	NAG	N	2	9	-	0/6/23/26	0/1/1/1
9	BMA	N	3	9	-	1/2/19/22	0/1/1/1
9	MAN	N	4	9	-	1/2/19/22	0/1/1/1
10	NAG	O	1	1,10	-	1/6/23/26	0/1/1/1
10	NAG	O	2	10	-	2/6/23/26	0/1/1/1
10	BMA	O	3	10	-	0/2/19/22	0/1/1/1
10	MAN	O	4	10	-	2/2/19/22	0/1/1/1
10	MAN	O	5	10	-	2/2/19/22	0/1/1/1
10	MAN	O	6	10	-	0/2/19/22	0/1/1/1
10	MAN	O	7	10	-	0/2/19/22	0/1/1/1
8	NAG	P	1	8,1	-	0/6/23/26	0/1/1/1
8	NAG	P	2	8	-	1/6/23/26	0/1/1/1
3	NAG	Q	1	3,2	-	2/6/23/26	0/1/1/1
3	NAG	Q	2	3	-	0/6/23/26	0/1/1/1
3	BMA	Q	3	3	-	2/2/19/22	0/1/1/1
3	MAN	Q	4	3	-	0/2/19/22	0/1/1/1

All (18) bond length outliers are listed below:

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	M	1	NAG	O5-C1	-6.16	1.33	1.43
5	G	1	NAG	O5-C1	-4.30	1.36	1.43
10	O	1	NAG	O5-C1	-3.23	1.38	1.43
10	O	7	MAN	O5-C1	-2.68	1.39	1.43
9	N	4	MAN	O5-C1	-2.34	1.40	1.43
5	G	3	BMA	O5-C1	-2.33	1.40	1.43
10	O	3	BMA	O3-C3	2.24	1.48	1.43
5	M	6	MAN	O5-C1	-2.21	1.40	1.43
5	G	4	MAN	O5-C1	-2.18	1.40	1.43
3	Q	1	NAG	O5-C1	-2.14	1.40	1.43
9	N	3	BMA	C2-C3	2.12	1.55	1.52
5	G	6	MAN	O5-C1	-2.12	1.40	1.43
5	G	5	MAN	O5-C1	-2.10	1.40	1.43
9	N	4	MAN	C4-C5	2.08	1.57	1.53
5	M	3	BMA	O5-C1	-2.06	1.40	1.43
4	F	4	MAN	O5-C1	-2.06	1.40	1.43
5	M	1	NAG	C1-C2	-2.04	1.49	1.52
10	O	2	NAG	C1-C2	2.03	1.55	1.52

All (45) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
10	O	3	BMA	O3-C3-C2	3.69	117.05	109.99
10	O	4	MAN	C1-O5-C5	3.66	117.15	112.19
7	I	4	MAN	C1-O5-C5	3.43	116.84	112.19
3	Q	3	BMA	C1-O5-C5	3.23	116.58	112.19
5	M	1	NAG	C3-C4-C5	3.23	116.00	110.24
7	I	5	MAN	C1-O5-C5	2.89	116.11	112.19
5	M	1	NAG	C1-O5-C5	-2.88	108.29	112.19
6	H	3	BMA	O2-C2-C3	-2.84	104.45	110.14
9	N	3	BMA	O5-C1-C2	2.74	115.01	110.77
6	K	3	BMA	C1-O5-C5	2.69	115.84	112.19
9	N	3	BMA	C1-C2-C3	2.65	112.92	109.67
9	N	4	MAN	C1-O5-C5	2.57	115.67	112.19
5	G	1	NAG	C3-C4-C5	2.49	114.68	110.24
10	O	3	BMA	C1-C2-C3	-2.43	106.69	109.67
10	O	5	MAN	C1-O5-C5	2.39	115.43	112.19
10	O	3	BMA	C3-C4-C5	-2.37	106.02	110.24
5	M	5	MAN	O2-C2-C3	-2.31	105.52	110.14
10	O	1	NAG	C3-C4-C5	2.29	114.32	110.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
7	I	3	BMA	O2-C2-C3	-2.29	105.56	110.14
3	E	4	MAN	O2-C2-C3	-2.29	105.56	110.14
10	O	2	NAG	C1-O5-C5	2.28	115.28	112.19
5	G	5	MAN	O2-C2-C3	-2.28	105.58	110.14
3	Q	4	MAN	O2-C2-C3	-2.27	105.59	110.14
4	F	4	MAN	O2-C2-C3	-2.25	105.63	110.14
4	F	5	MAN	O2-C2-C3	-2.24	105.64	110.14
10	O	3	BMA	O3-C3-C4	2.24	115.52	110.35
5	M	4	MAN	O2-C2-C3	-2.24	105.66	110.14
5	M	4	MAN	C1-O5-C5	2.23	115.22	112.19
5	M	5	MAN	C1-O5-C5	2.23	115.22	112.19
10	O	5	MAN	O2-C2-C3	-2.22	105.68	110.14
5	G	4	MAN	O2-C2-C3	-2.22	105.70	110.14
7	I	4	MAN	O2-C2-C3	-2.19	105.74	110.14
5	M	6	MAN	O2-C2-C3	-2.19	105.76	110.14
4	F	5	MAN	C1-O5-C5	2.18	115.15	112.19
10	O	6	MAN	O2-C2-C3	-2.17	105.78	110.14
5	G	6	MAN	O2-C2-C3	-2.17	105.78	110.14
6	H	3	BMA	C1-C2-C3	-2.17	107.00	109.67
10	O	4	MAN	O2-C2-C3	-2.16	105.80	110.14
7	I	5	MAN	O2-C2-C3	-2.16	105.81	110.14
9	N	4	MAN	C3-C4-C5	2.13	114.04	110.24
9	N	4	MAN	O2-C2-C3	-2.11	105.91	110.14
7	I	3	BMA	C1-O5-C5	2.07	115.00	112.19
10	O	7	MAN	O2-C2-C3	-2.07	106.00	110.14
6	K	2	NAG	C1-O5-C5	2.02	114.92	112.19
3	Q	4	MAN	C1-O5-C5	2.00	114.90	112.19

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
5	M	1	NAG	C1

All (42) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	M	1	NAG	C4-C5-C6-O6
3	Q	3	BMA	O5-C5-C6-O6
10	O	4	MAN	O5-C5-C6-O6
4	F	1	NAG	O5-C5-C6-O6
5	M	1	NAG	O5-C5-C6-O6
10	O	4	MAN	C4-C5-C6-O6

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Mol	Chain	Res	Type	Atoms
3	E	1	NAG	O5-C5-C6-O6
7	I	3	BMA	O5-C5-C6-O6
3	Q	3	BMA	C4-C5-C6-O6
6	K	1	NAG	O5-C5-C6-O6
10	O	5	MAN	O5-C5-C6-O6
3	Q	1	NAG	C4-C5-C6-O6
10	O	2	NAG	O5-C5-C6-O6
4	F	1	NAG	C4-C5-C6-O6
4	F	2	NAG	C8-C7-N2-C2
4	F	2	NAG	O7-C7-N2-C2
3	E	1	NAG	C4-C5-C6-O6
10	O	5	MAN	C4-C5-C6-O6
3	Q	1	NAG	O5-C5-C6-O6
5	G	5	MAN	O5-C5-C6-O6
5	M	5	MAN	O5-C5-C6-O6
6	H	3	BMA	O5-C5-C6-O6
10	O	2	NAG	C4-C5-C6-O6
4	F	3	BMA	O5-C5-C6-O6
5	M	3	BMA	O5-C5-C6-O6
8	J	2	NAG	O5-C5-C6-O6
9	N	3	BMA	O5-C5-C6-O6
5	G	5	MAN	C4-C5-C6-O6
5	M	6	MAN	O5-C5-C6-O6
5	G	6	MAN	O5-C5-C6-O6
5	G	3	BMA	O5-C5-C6-O6
9	N	4	MAN	O5-C5-C6-O6
8	P	2	NAG	O5-C5-C6-O6
5	M	5	MAN	C4-C5-C6-O6
6	K	1	NAG	C4-C5-C6-O6
5	G	1	NAG	C4-C5-C6-O6
10	O	1	NAG	C4-C5-C6-O6
5	G	1	NAG	O5-C5-C6-O6
7	I	3	BMA	C4-C5-C6-O6
4	F	2	NAG	O5-C5-C6-O6
5	M	1	NAG	C1-C2-N2-C7
3	E	3	BMA	C4-C5-C6-O6

All (1) ring outliers are listed below:

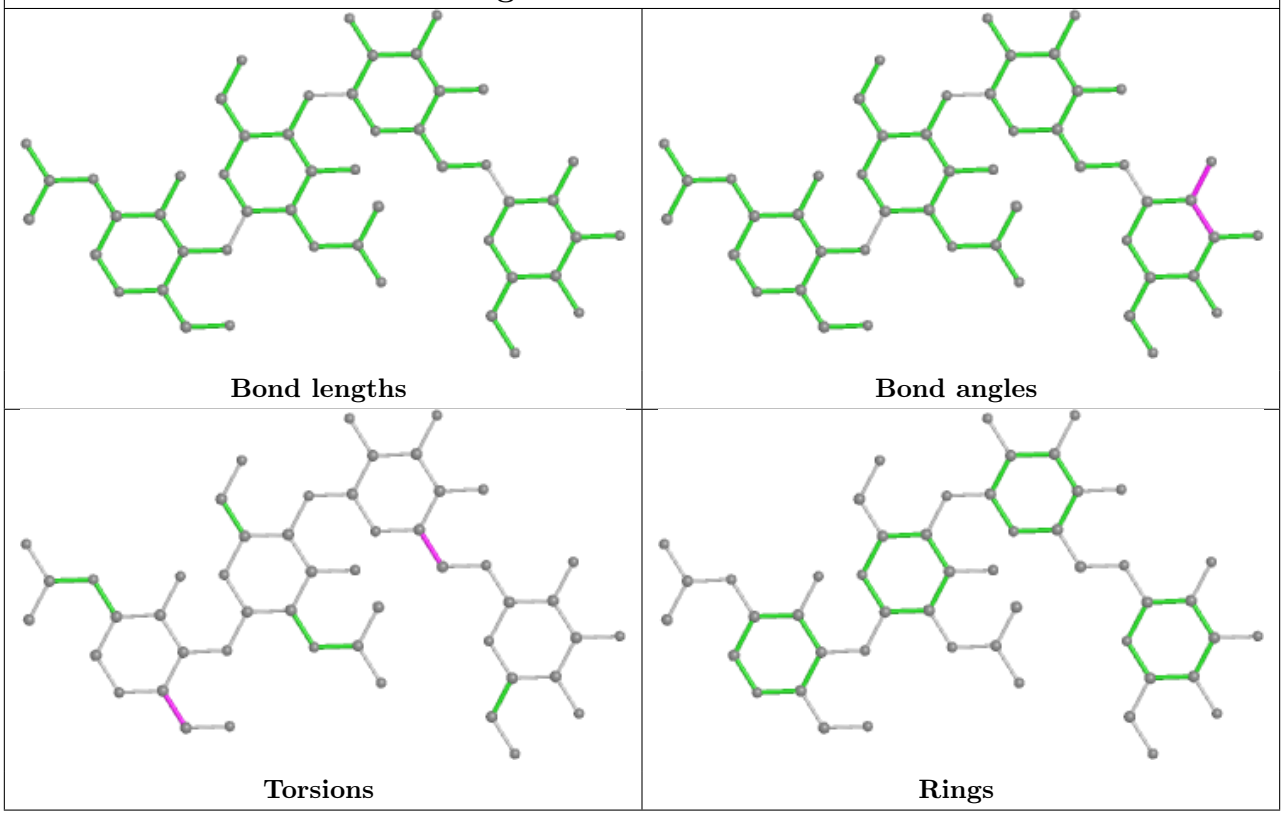
Mol	Chain	Res	Type	Atoms
7	I	4	MAN	C1-C2-C3-C4-C5-O5

18 monomers are involved in 10 short contacts:

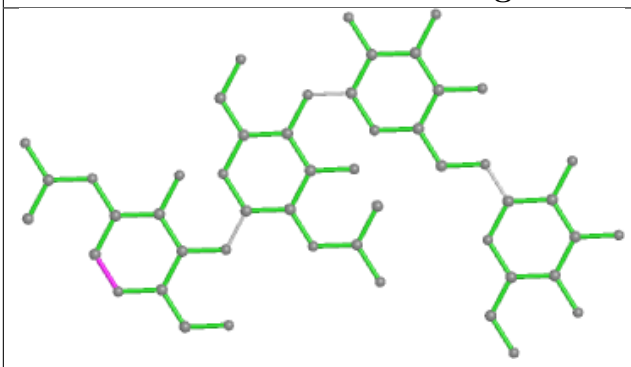
Mol	Chain	Res	Type	Clashes	Symm-Clashes
10	O	2	NAG	1	0
5	G	4	MAN	1	0
10	O	1	NAG	1	0
5	G	3	BMA	1	0
7	I	4	MAN	1	0
3	Q	3	BMA	1	0
7	I	3	BMA	1	0
6	H	3	BMA	1	0
9	N	2	NAG	1	0
3	E	4	MAN	1	0
10	O	4	MAN	1	0
10	O	3	BMA	1	0
3	E	3	BMA	1	0
3	Q	4	MAN	2	0
5	M	4	MAN	1	0
9	N	3	BMA	1	0
6	H	2	NAG	1	0
5	M	3	BMA	1	0

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

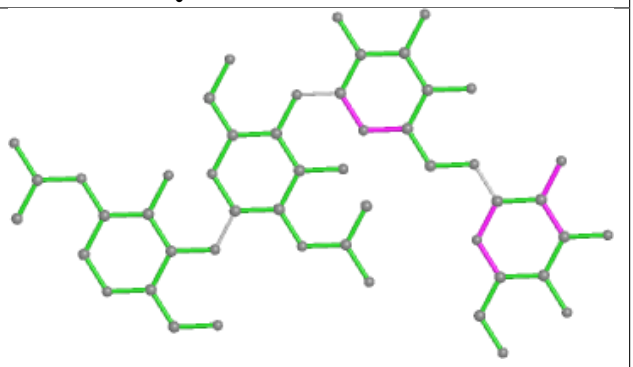
Oligosaccharide Chain E



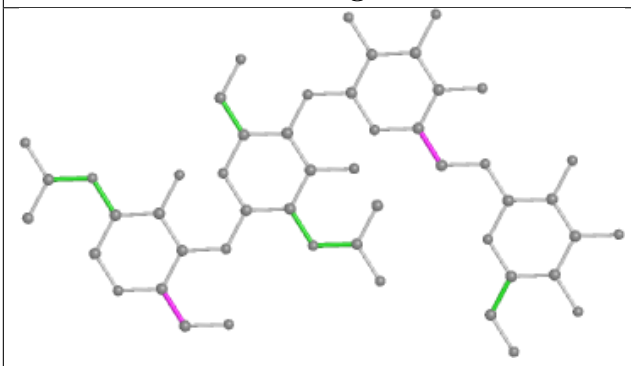
Oligosaccharide Chain Q



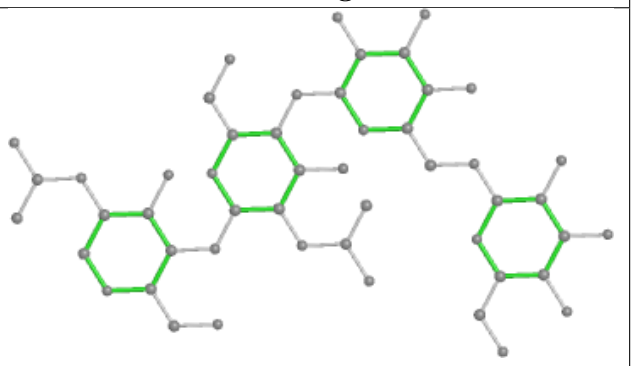
Bond lengths



Bond angles

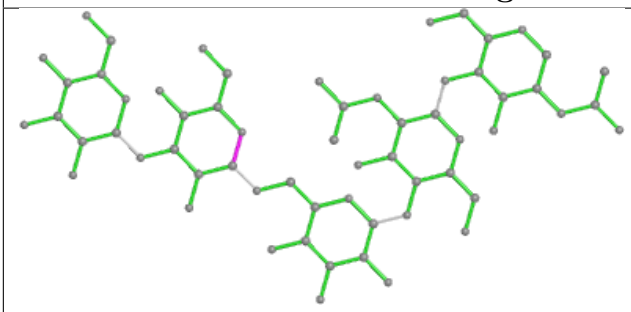


Torsions

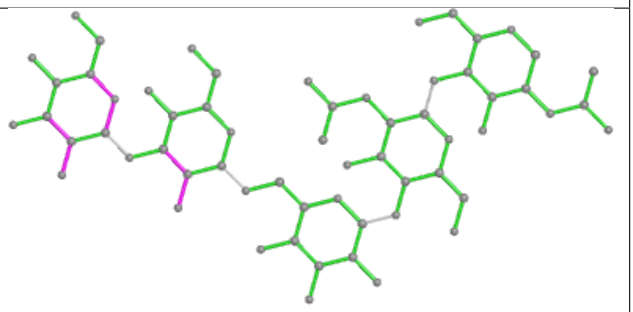


Rings

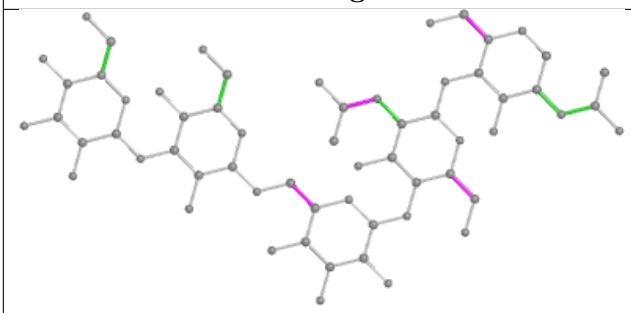
Oligosaccharide Chain F



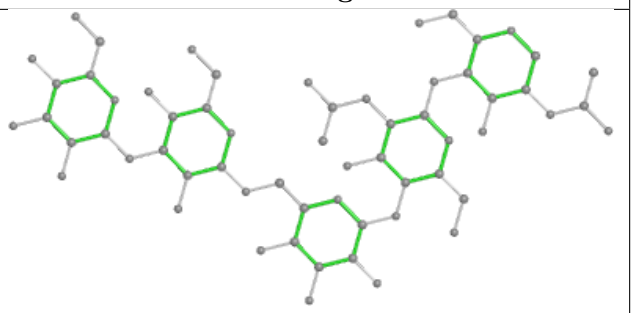
Bond lengths



Bond angles

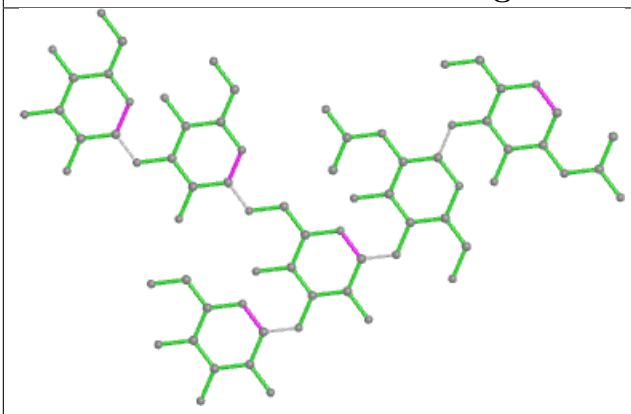


Torsions

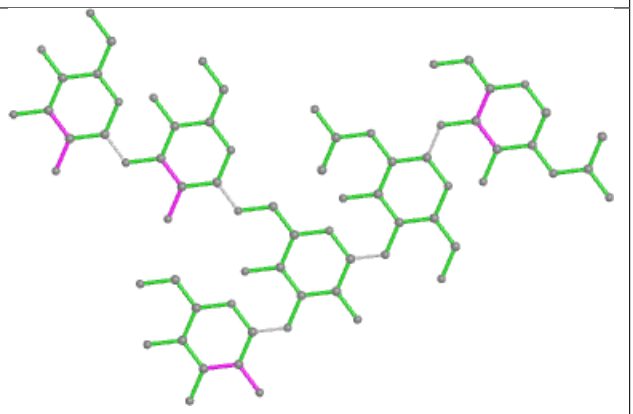


Rings

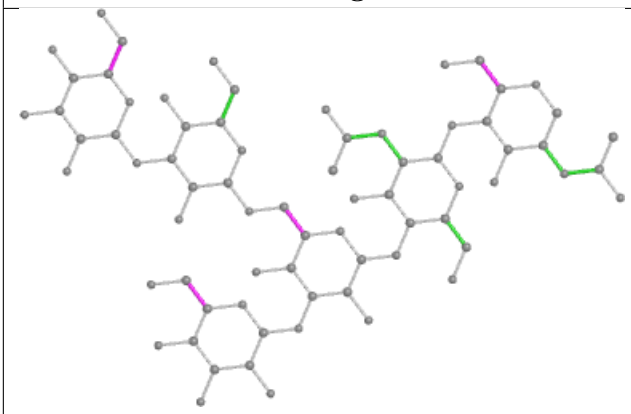
Oligosaccharide Chain G



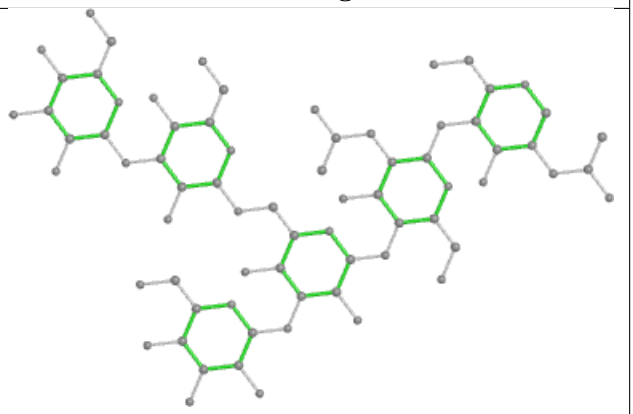
Bond lengths



Bond angles

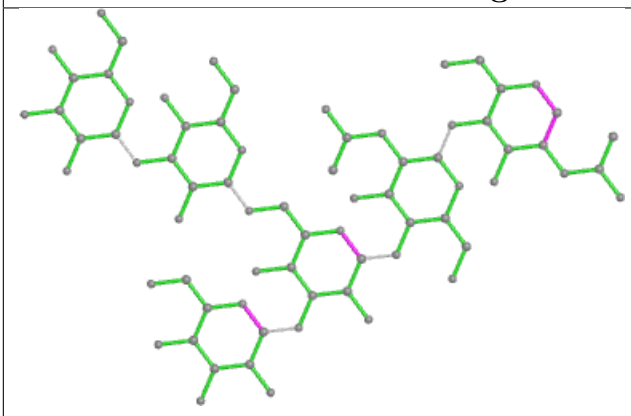


Torsions

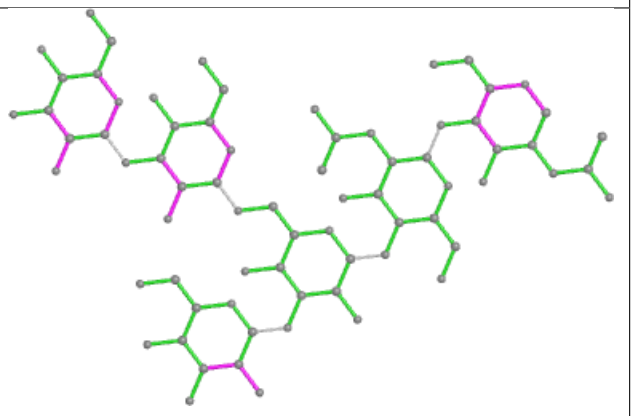


Rings

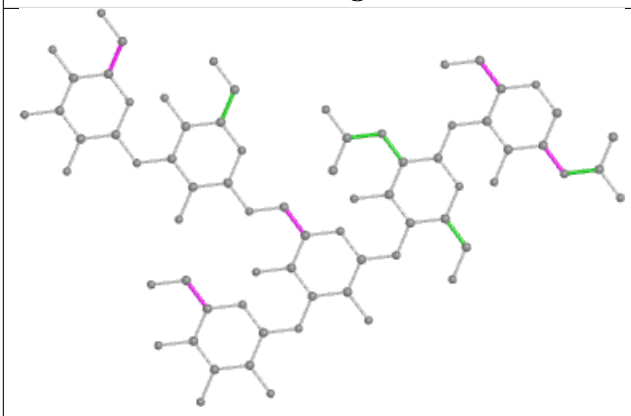
Oligosaccharide Chain M



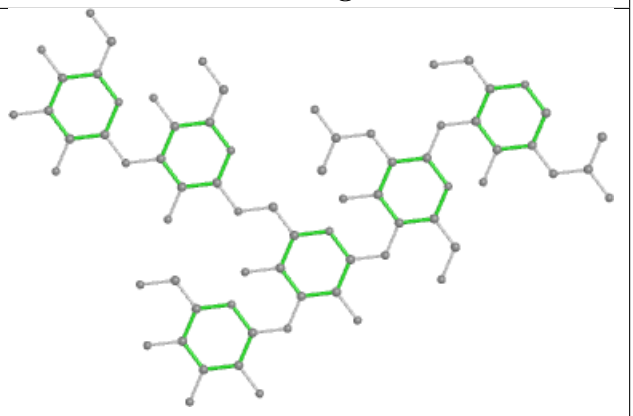
Bond lengths



Bond angles

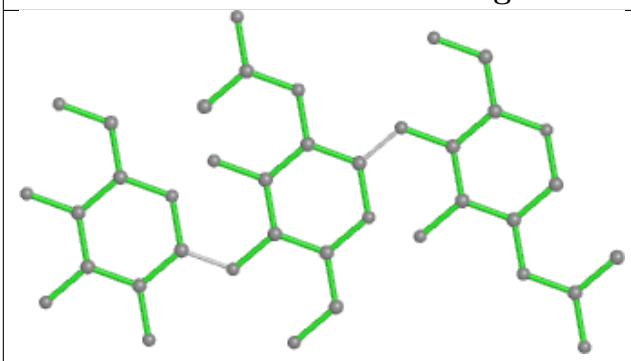


Torsions

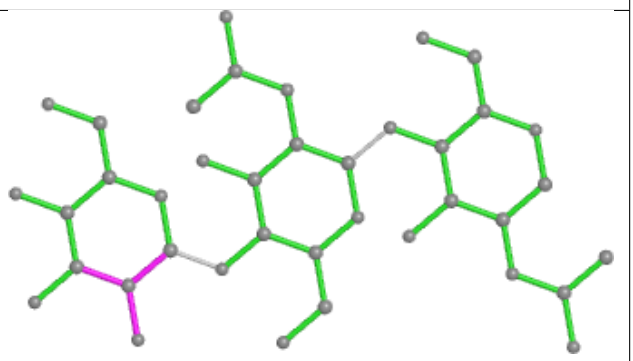


Rings

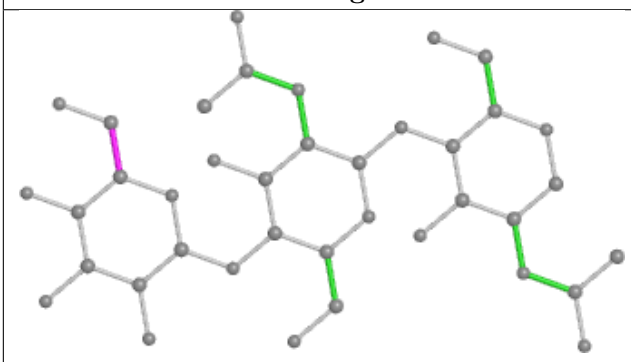
Oligosaccharide Chain H



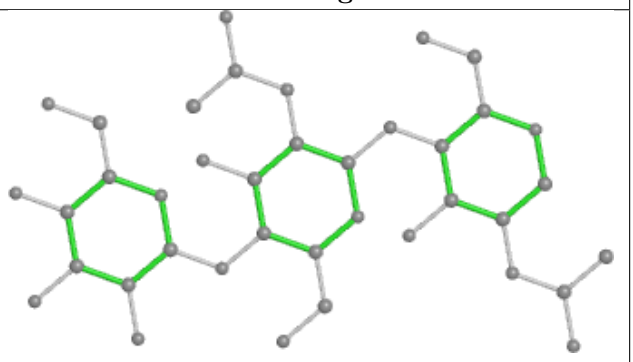
Bond lengths



Bond angles

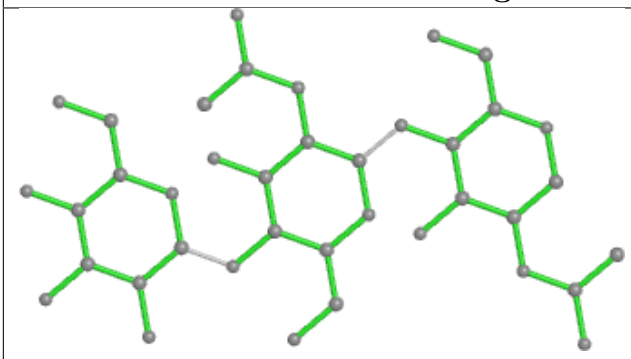


Torsions

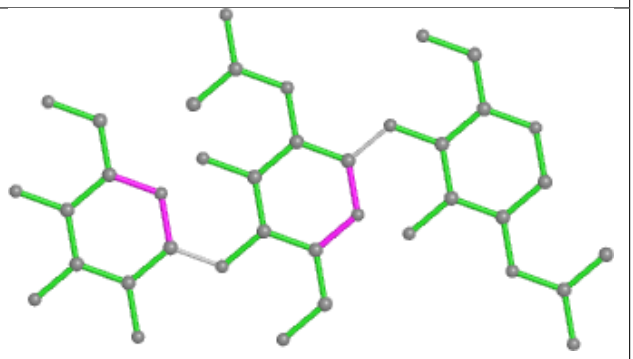


Rings

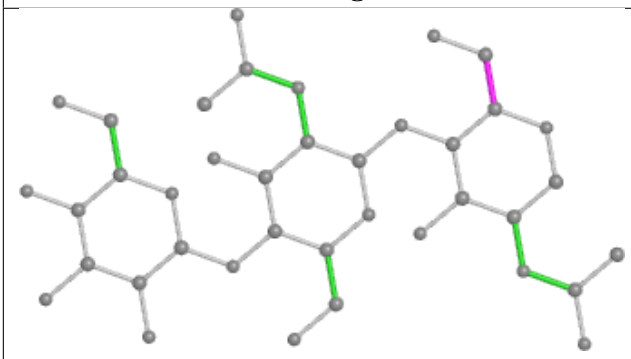
Oligosaccharide Chain K



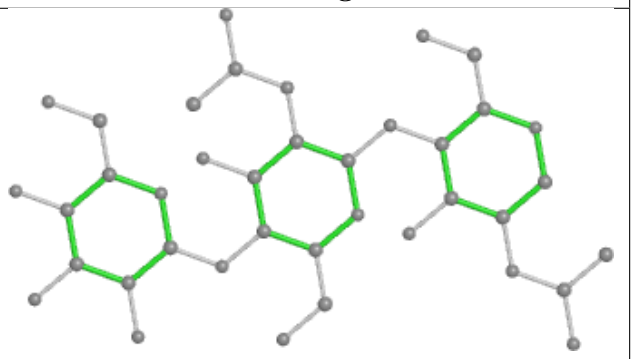
Bond lengths



Bond angles

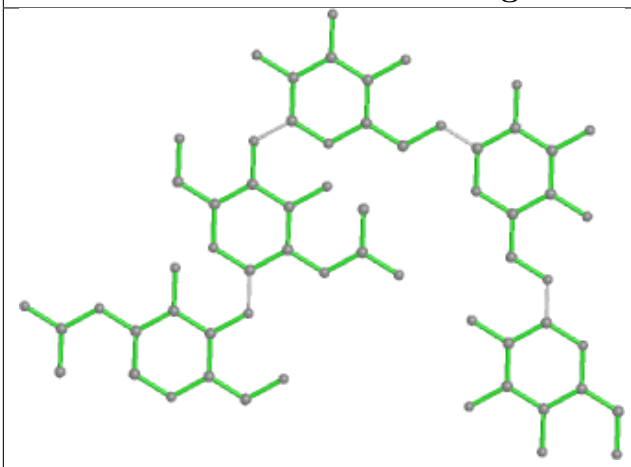


Torsions

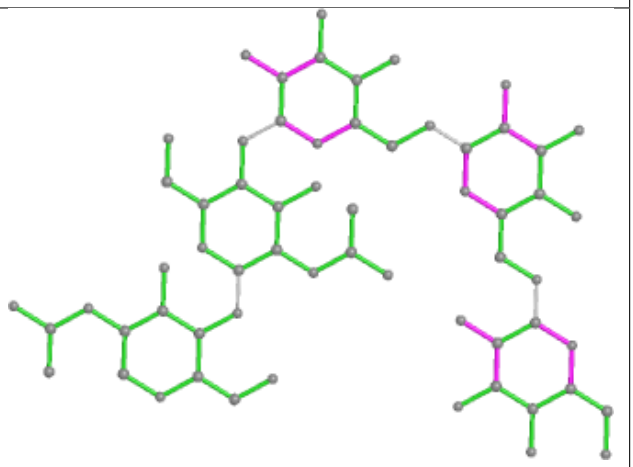


Rings

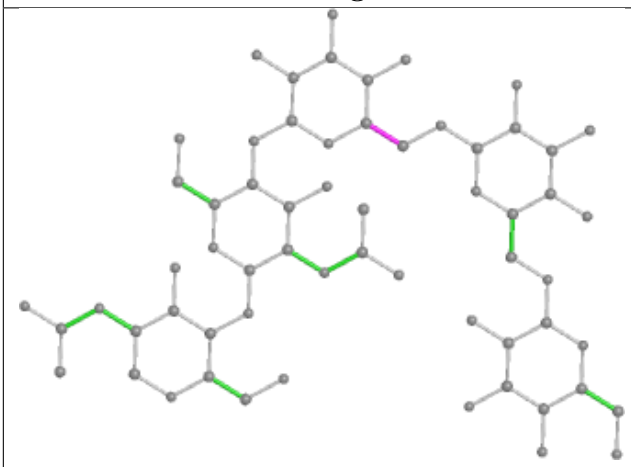
Oligosaccharide Chain I



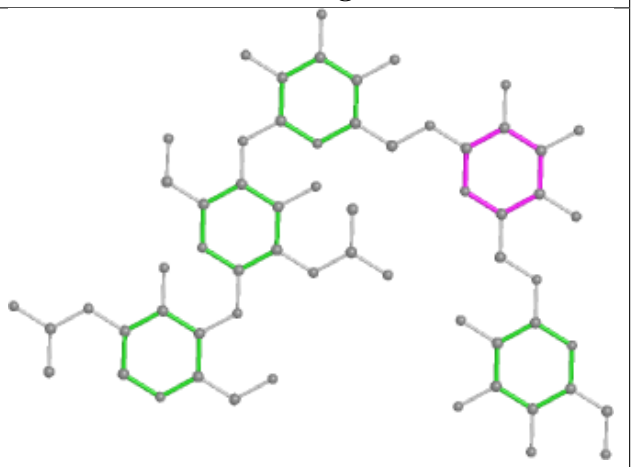
Bond lengths



Bond angles

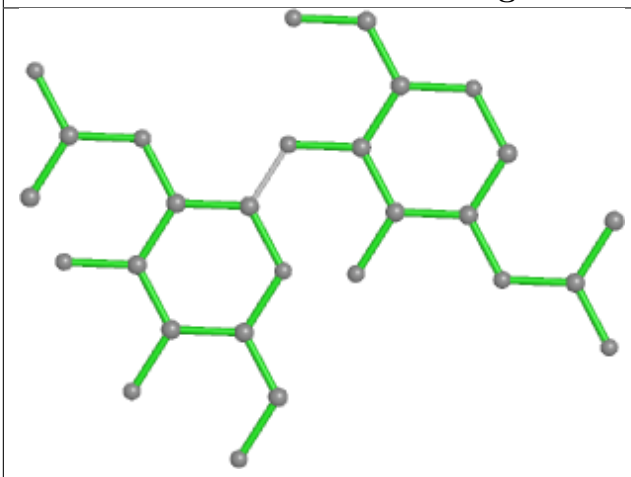


Torsions

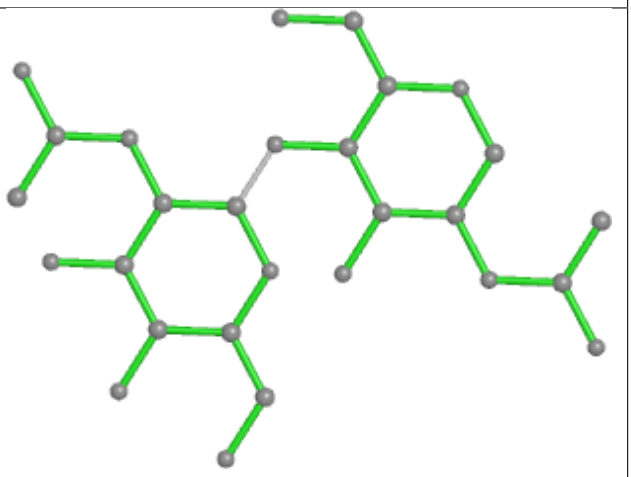


Rings

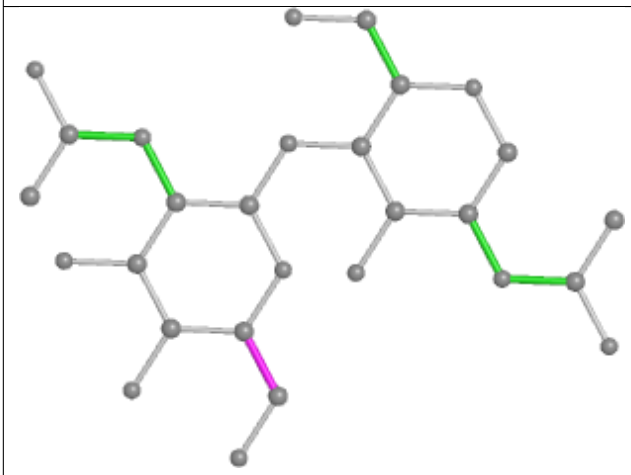
Oligosaccharide Chain J



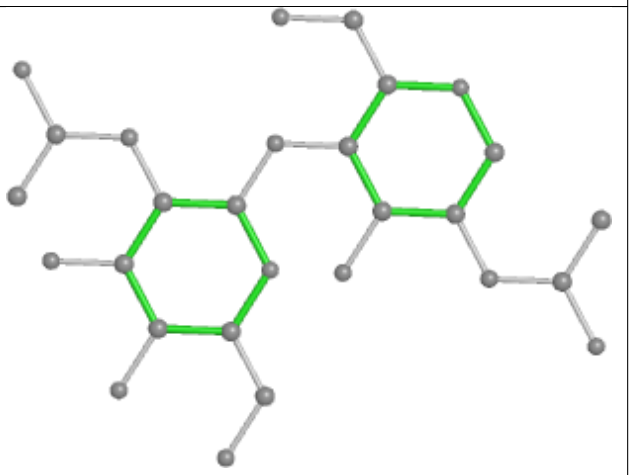
Bond lengths



Bond angles

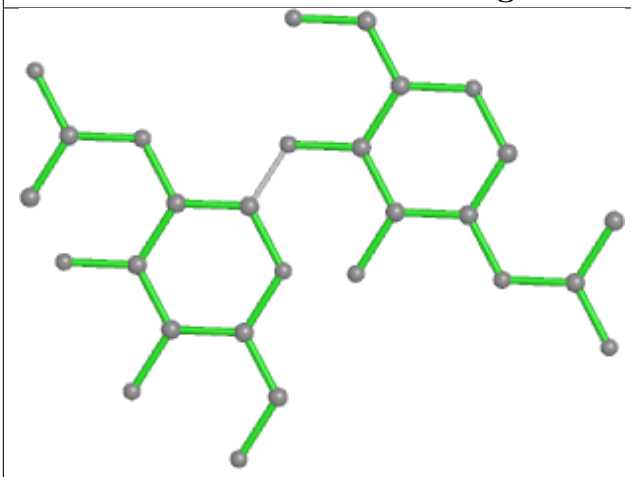


Torsions

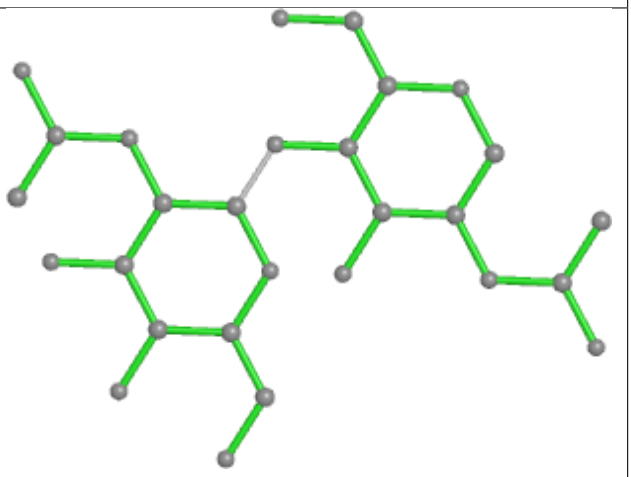


Rings

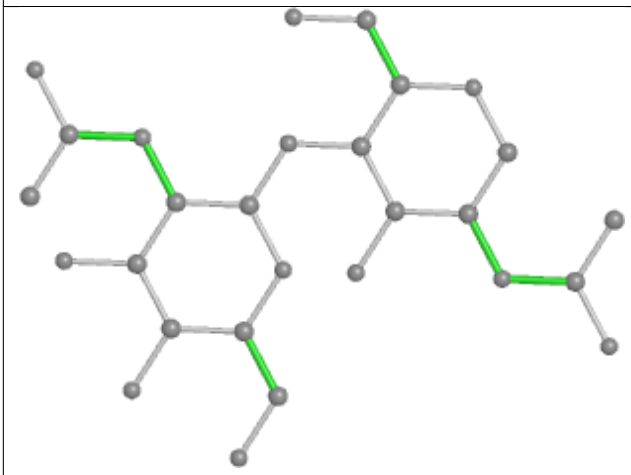
Oligosaccharide Chain L



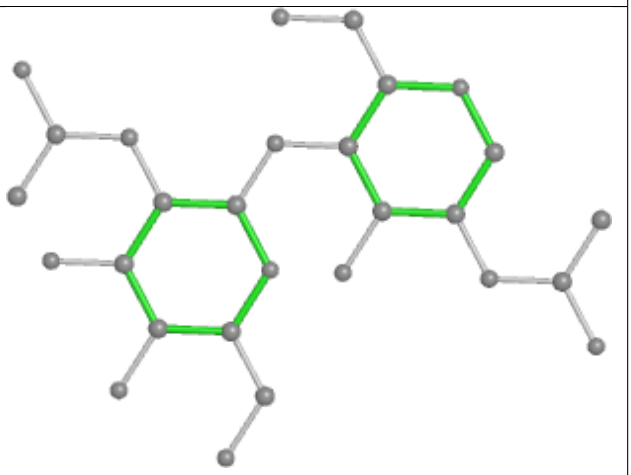
Bond lengths



Bond angles

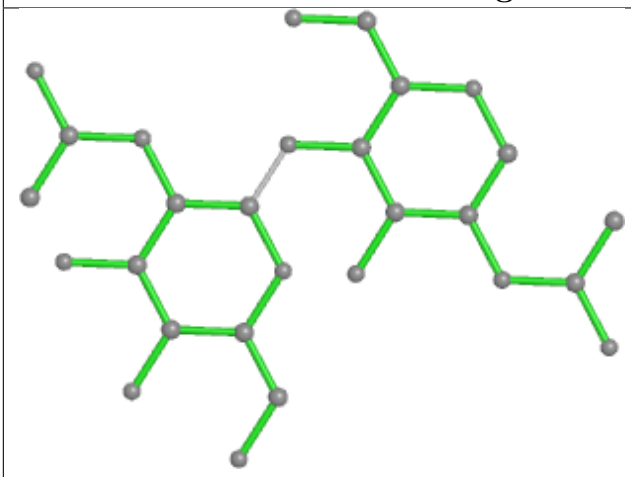


Torsions

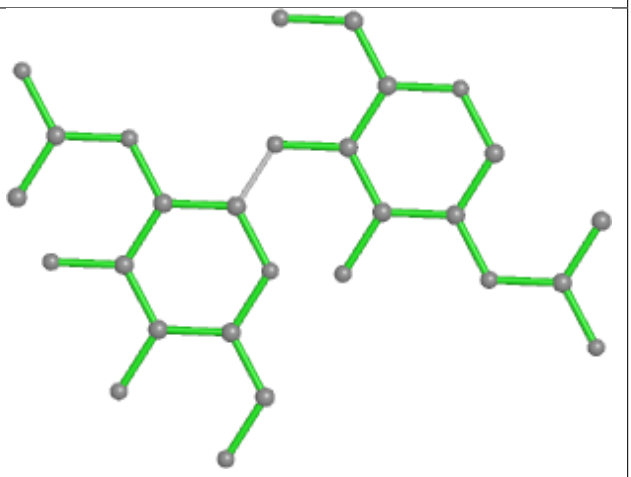


Rings

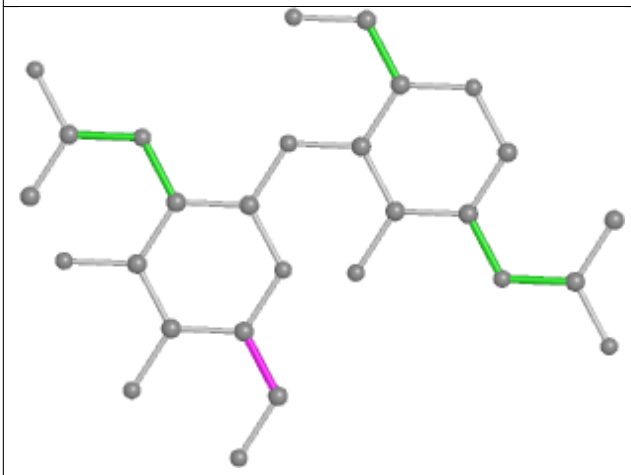
Oligosaccharide Chain P



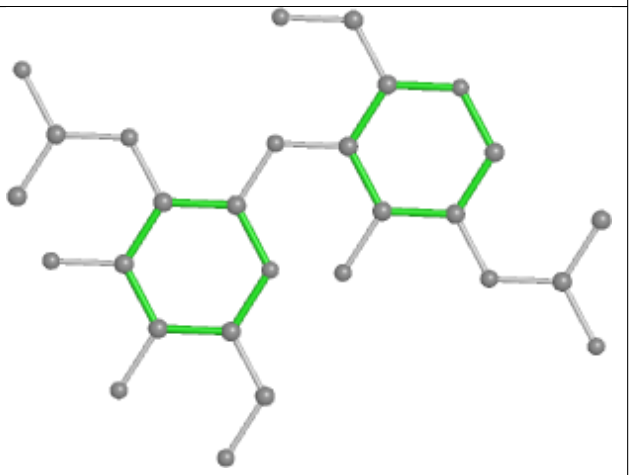
Bond lengths



Bond angles

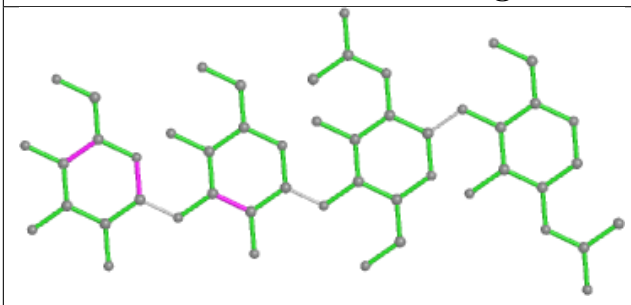


Torsions

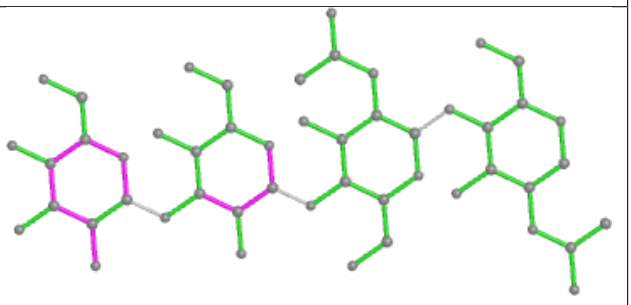


Rings

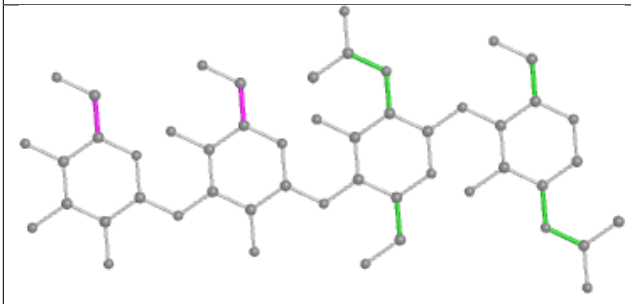
Oligosaccharide Chain N



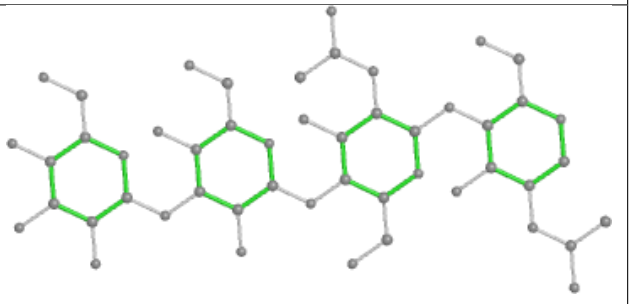
Bond lengths



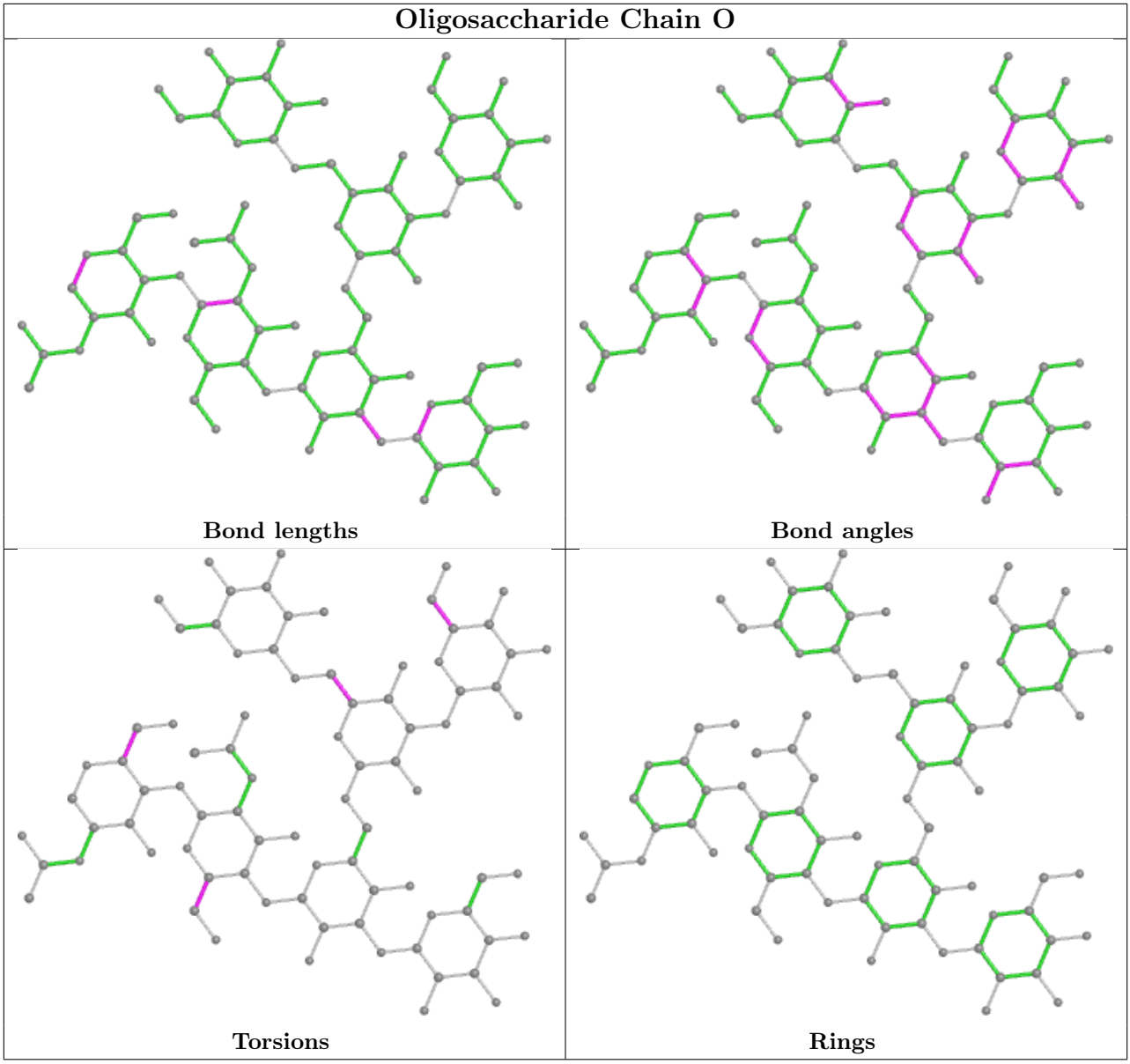
Bond angles



Torsions



Rings



5.6 Ligand geometry (i)

Of 24 ligands modelled in this entry, 16 are monoatomic - leaving 8 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	$\#\|Z\|>2$

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
15	CAC	B	1442	-	0,4,4	-	-	0,6,6	-	-
12	SO4	A	1597	-	4,4,4	0.15	0	6,6,6	0.05	0
17	NAG	B	3243	2	14,14,15	0.32	0	17,19,21	0.36	0
17	NAG	D	3080	2	14,14,15	0.39	0	17,19,21	0.58	0
17	NAG	D	3243	2	14,14,15	0.30	0	17,19,21	0.42	0
15	CAC	D	1442	-	0,4,4	-	-	0,6,6	-	-
12	SO4	A	1596	-	4,4,4	0.14	0	6,6,6	0.05	0
12	SO4	A	1598	-	4,4,4	0.14	0	6,6,6	0.05	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
17	NAG	D	3080	2	-	1/6/23/26	0/1/1/1
17	NAG	D	3243	2	-	1/6/23/26	0/1/1/1
17	NAG	B	3243	2	-	2/6/23/26	0/1/1/1

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (4) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
17	B	3243	NAG	C4-C5-C6-O6
17	B	3243	NAG	O5-C5-C6-O6
17	D	3243	NAG	O5-C5-C6-O6
17	D	3080	NAG	O5-C5-C6-O6

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
12	A	1596	SO4	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

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	591/681 (86%)	-0.01	7 (1%) 79 78	34, 64, 109, 185	0
1	C	588/681 (86%)	0.55	51 (8%) 10 7	52, 100, 155, 201	0
2	B	423/788 (53%)	0.41	40 (9%) 8 5	25, 70, 166, 245	0
2	D	414/788 (52%)	0.31	27 (6%) 18 14	33, 77, 150, 205	0
All	All	2016/2938 (68%)	0.31	125 (6%) 20 16	25, 78, 150, 245	0

All (125) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	B	58	ILE	8.0
2	B	50	ALA	7.6
2	B	55	LEU	7.1
2	D	8	LEU	7.0
2	B	53	CYS	7.0
1	C	129	PHE	6.8
2	B	49	LEU	5.6
1	C	532	LEU	5.6
2	B	56	ASN	5.4
2	D	27	CYS	5.4
2	B	54	GLN	5.3
2	D	55	LEU	5.2
1	C	61	TRP	5.1
2	B	57	PHE	4.9
1	C	265	TYR	4.9
2	B	26	TRP	4.9
1	C	60	ASP	4.8
2	B	52	GLY	4.8
2	D	58	ILE	4.7
2	B	46	ALA	4.6
1	C	82	LYS	4.5

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Mol	Chain	Res	Type	RSRZ
1	C	562	ARG	4.5
2	B	28	ALA	4.3
2	D	26	TRP	4.2
2	D	60	ASN	4.1
2	D	28	ALA	4.1
2	B	41	ARG	4.0
1	C	167	ASP	3.9
2	B	51	LYS	3.9
1	C	133	GLY	3.9
2	B	8	LEU	3.9
2	B	27	CYS	3.9
2	B	439	CYS	3.8
1	C	100	SER	3.8
1	C	131	GLN	3.7
2	D	59	GLU	3.7
2	D	379	ASN	3.6
2	B	436	ASN	3.6
2	B	435	CYS	3.5
2	B	10	GLY	3.5
2	B	441	LYS	3.5
2	B	45	PRO	3.4
1	C	494	GLN	3.4
2	B	367	GLU	3.4
1	C	563	LEU	3.3
1	C	11	TYR	3.3
1	C	503	LYS	3.2
1	C	594	LEU	3.2
1	C	507	ALA	3.2
2	D	41	ARG	3.1
2	D	440	GLN	3.1
2	D	57	PHE	3.1
2	D	18	LEU	3.1
2	D	441	LYS	3.1
1	C	36	LEU	3.1
1	A	552	LEU	3.0
1	C	325	ASP	3.0
2	B	47	ASN	3.0
2	D	439	CYS	3.0
1	A	594	LEU	3.0
1	C	497	LEU	3.0
1	C	191	ILE	3.0
1	C	498	LEU	3.0

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Mol	Chain	Res	Type	RSRZ
1	C	165	LYS	2.9
1	C	65	ARG	2.9
1	C	519	PRO	2.9
1	C	59	CYS	2.8
2	B	434	GLU	2.8
2	D	13	THR	2.8
2	B	440	GLN	2.8
1	C	260	ASN	2.7
1	C	490	LYS	2.7
1	C	35	PHE	2.6
1	C	489	ARG	2.6
1	C	25	PHE	2.6
2	D	380	GLY	2.6
1	C	37	LEU	2.6
1	C	565	TYR	2.5
1	C	81	ALA	2.5
2	D	95	LYS	2.5
2	B	20	ILE	2.5
1	A	134	THR	2.5
2	B	60	ASN	2.4
1	C	499	LEU	2.4
1	A	29	SER	2.4
1	C	66	ARG	2.4
1	C	397	ALA	2.4
1	C	29	SER	2.3
1	A	498	LEU	2.3
2	B	437	CYS	2.3
2	D	53	CYS	2.3
2	B	48	LEU	2.3
1	A	63	SER	2.3
2	D	54	GLN	2.3
2	D	62	VAL	2.3
1	C	571	THR	2.3
1	C	34	MET	2.3
1	C	410	GLY	2.2
1	C	419	TYR	2.2
1	C	564	ASP	2.2
2	B	61	PRO	2.2
2	D	77	ARG	2.2
2	B	431	VAL	2.2
1	C	441	ILE	2.2
2	D	385	HIS	2.2

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Mol	Chain	Res	Type	RSRZ
2	B	413	SER	2.2
1	C	491	LEU	2.1
2	B	412	ARG	2.1
2	B	42	CYS	2.1
1	C	440	VAL	2.1
1	C	492	ASN	2.1
2	D	56	ASN	2.1
2	D	156	GLY	2.1
2	D	436	ASN	2.1
1	C	486	VAL	2.1
2	B	199	LEU	2.1
1	C	508	ILE	2.1
2	B	438	ASP	2.1
2	D	437	CYS	2.1
2	B	13	THR	2.1
2	B	25	ALA	2.1
1	C	398	ARG	2.1
1	A	581	PHE	2.0
2	B	7	ALA	2.0
1	C	56	VAL	2.0

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 (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, 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	MAN	I	4	11/12	0.52	0.34	144,157,163,168	0
3	NAG	Q	1	14/15	0.60	0.48	120,139,148,162	0
10	NAG	O	2	14/15	0.60	0.40	134,143,150,152	0
3	MAN	E	4	11/12	0.61	0.23	138,152,165,166	0
6	BMA	K	3	11/12	0.62	0.17	125,146,155,161	0
4	MAN	F	5	11/12	0.63	0.57	169,187,191,194	0
8	NAG	P	2	14/15	0.64	0.41	149,155,163,168	0
9	BMA	N	3	11/12	0.66	0.31	149,163,235,236	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
6	BMA	H	3	11/12	0.66	0.39	175,182,191,192	0
4	BMA	F	3	11/12	0.67	0.28	149,158,166,171	0
3	MAN	Q	4	11/12	0.67	0.38	153,162,169,169	0
4	MAN	F	4	11/12	0.68	0.28	161,170,185,192	0
3	BMA	E	3	11/12	0.68	0.27	137,148,165,170	0
10	MAN	O	5	11/12	0.71	0.30	128,136,161,170	0
3	BMA	Q	3	11/12	0.72	0.49	168,186,195,202	0
10	MAN	O	6	11/12	0.73	0.27	118,135,150,152	0
6	NAG	H	2	14/15	0.74	0.24	132,155,172,174	0
9	NAG	N	2	14/15	0.74	0.22	117,137,149,149	0
10	MAN	O	7	11/12	0.74	0.36	131,142,151,152	0
7	MAN	I	5	11/12	0.77	0.43	152,163,169,172	0
3	NAG	E	2	14/15	0.78	0.24	103,130,141,149	0
8	NAG	L	2	14/15	0.78	0.33	111,124,129,133	0
10	MAN	O	4	11/12	0.78	0.26	130,139,148,152	0
9	MAN	N	4	11/12	0.79	0.28	95,155,172,173	0
5	MAN	M	4	11/12	0.80	0.38	166,172,177,180	0
7	BMA	I	3	11/12	0.80	0.27	135,141,150,154	0
8	NAG	J	2	14/15	0.80	0.37	124,147,157,161	0
10	BMA	O	3	11/12	0.80	0.20	120,130,140,143	0
5	MAN	G	6	11/12	0.81	0.29	104,115,137,152	0
3	NAG	Q	2	14/15	0.81	0.22	153,165,173,182	0
6	NAG	H	1	14/15	0.81	0.26	105,125,137,138	0
5	MAN	M	5	11/12	0.82	0.50	178,185,187,188	0
5	BMA	G	3	11/12	0.82	0.16	93,117,134,137	0
5	BMA	M	3	11/12	0.85	0.20	112,117,158,163	0
4	NAG	F	2	14/15	0.86	0.25	99,123,133,148	0
6	NAG	K	1	14/15	0.86	0.22	88,102,119,139	0
10	NAG	O	1	14/15	0.86	0.29	103,121,128,139	0
5	MAN	G	4	11/12	0.87	0.20	119,137,139,139	0
6	NAG	K	2	14/15	0.87	0.35	119,136,147,154	0
5	NAG	M	1	14/15	0.87	0.19	73,84,104,108	0
7	NAG	I	2	14/15	0.87	0.23	100,119,131,142	0
8	NAG	L	1	14/15	0.88	0.23	83,105,113,120	0
5	MAN	G	5	11/12	0.89	0.20	110,121,130,130	0
5	MAN	M	6	11/12	0.89	0.28	103,111,115,117	0
5	NAG	M	2	14/15	0.90	0.23	69,88,101,105	0
7	NAG	I	1	14/15	0.90	0.18	78,105,117,118	0
8	NAG	P	1	14/15	0.91	0.20	89,106,134,139	0
9	NAG	N	1	14/15	0.92	0.21	81,104,118,130	0
3	NAG	E	1	14/15	0.93	0.15	40,72,97,108	0
8	NAG	J	1	14/15	0.93	0.19	89,112,120,132	0

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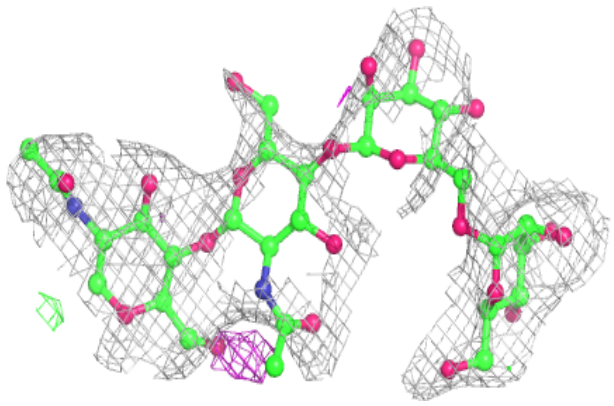
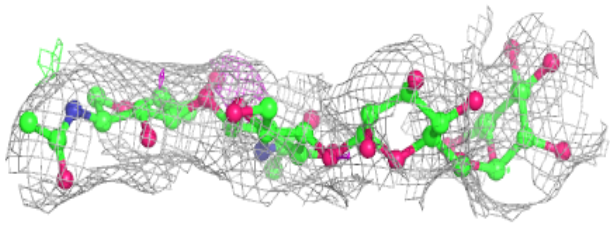
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
5	NAG	G	2	14/15	0.93	0.18	59,69,92,107	0
4	NAG	F	1	14/15	0.95	0.14	60,82,102,102	0
5	NAG	G	1	14/15	0.96	0.17	50,64,81,97	0

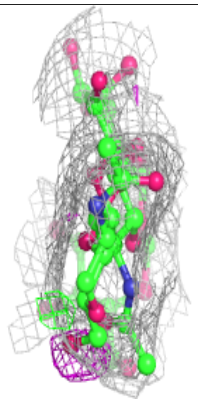
The following is a graphical depiction of the model fit to experimental electron density for oligosaccharide. Each fit is shown from different orientation to approximate a three-dimensional view.

Electron density around Chain E:

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

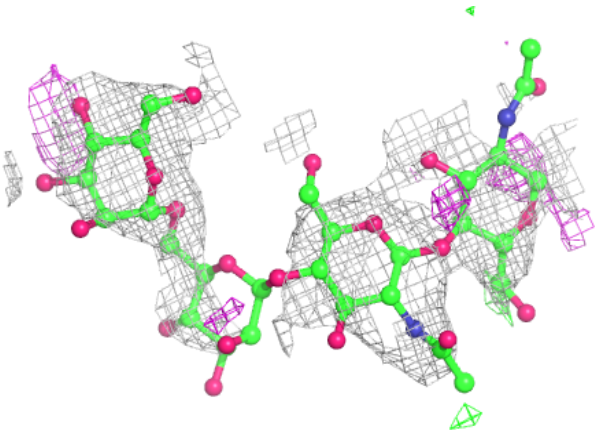


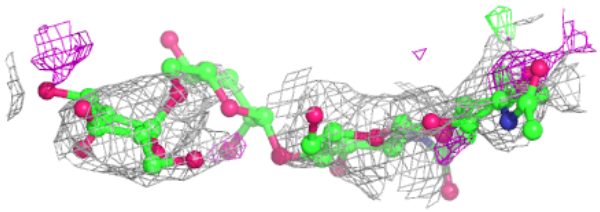


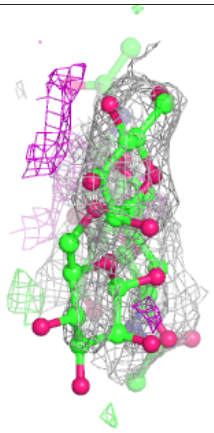


Electron density around Chain Q:

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

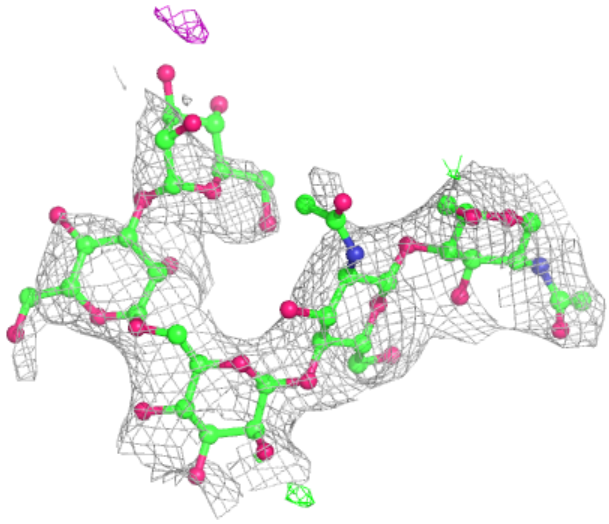


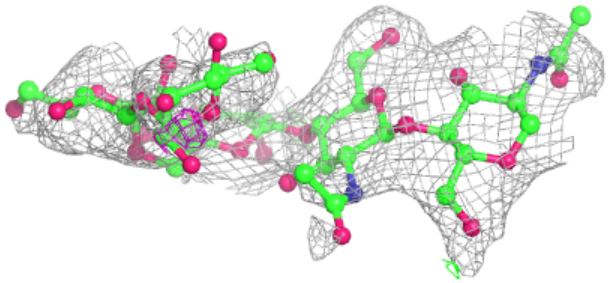


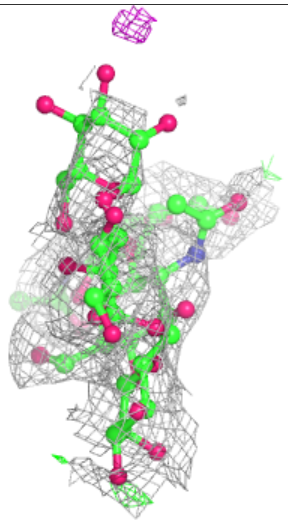


Electron density around Chain F:

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

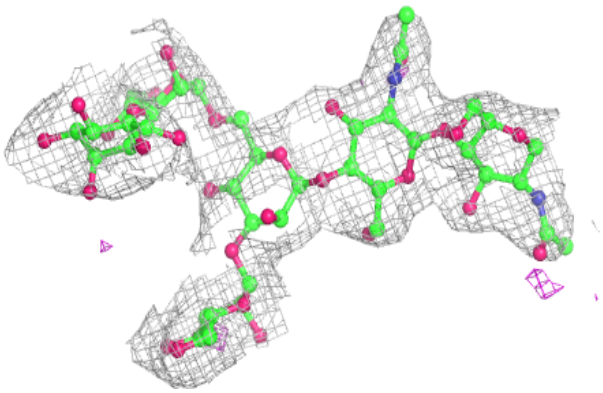


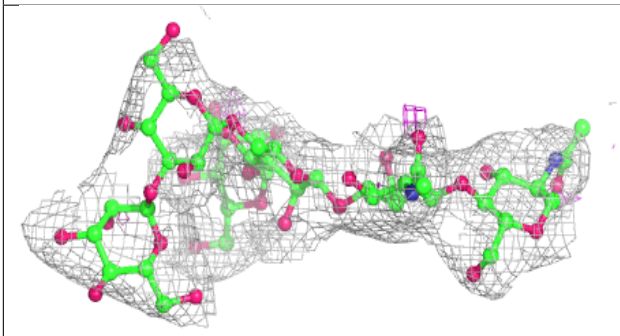


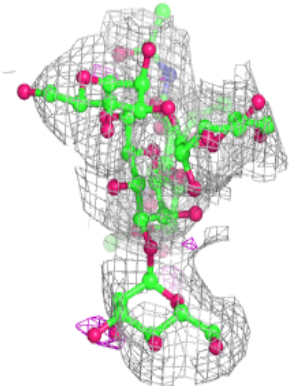


Electron density around Chain G:

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

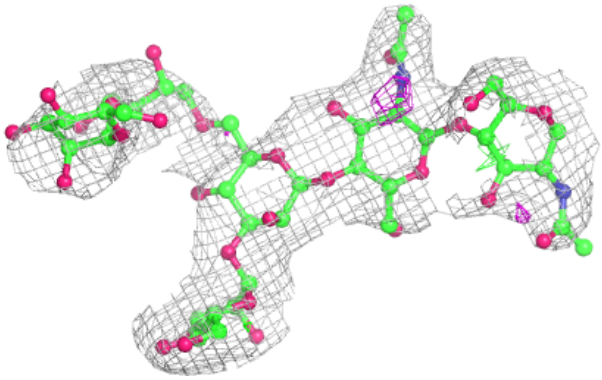


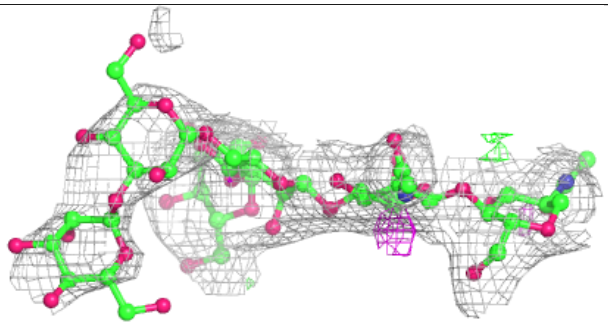


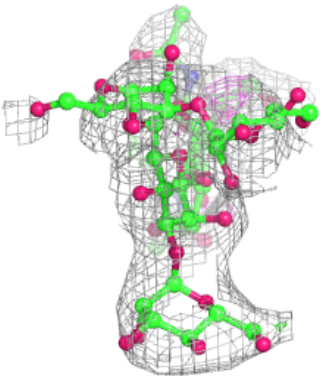


Electron density around Chain M:

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

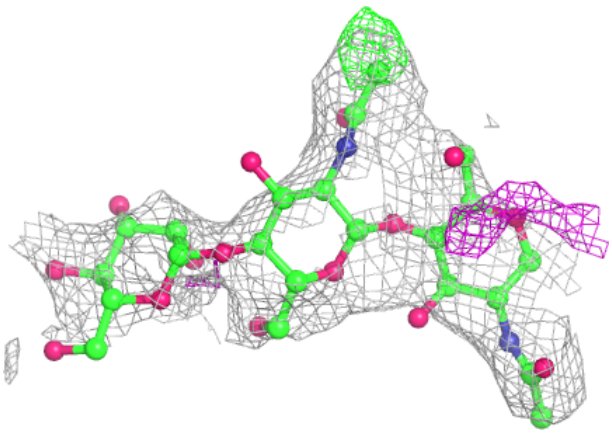


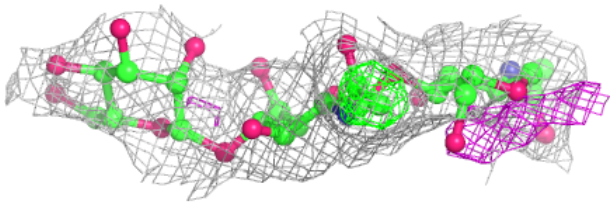


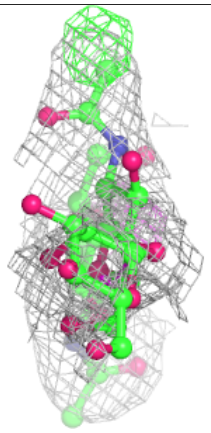


Electron density around Chain H:

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

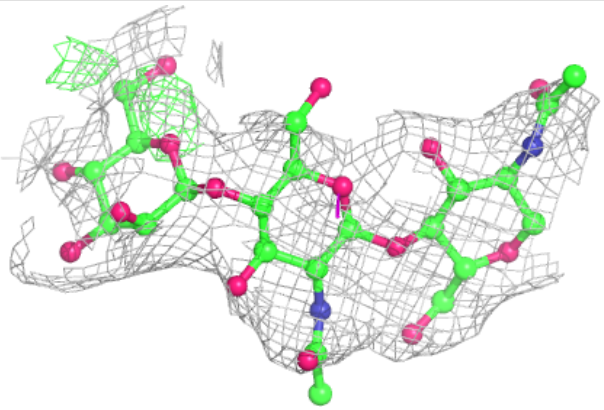


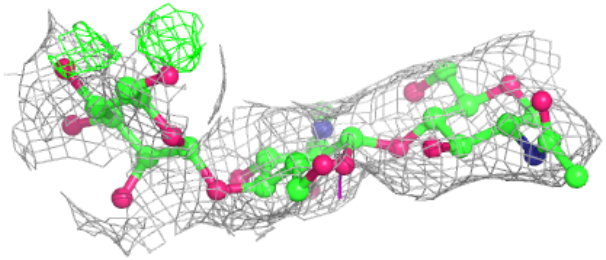


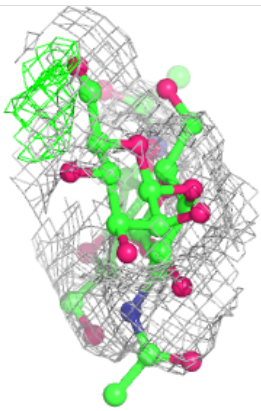


Electron density around Chain K:

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

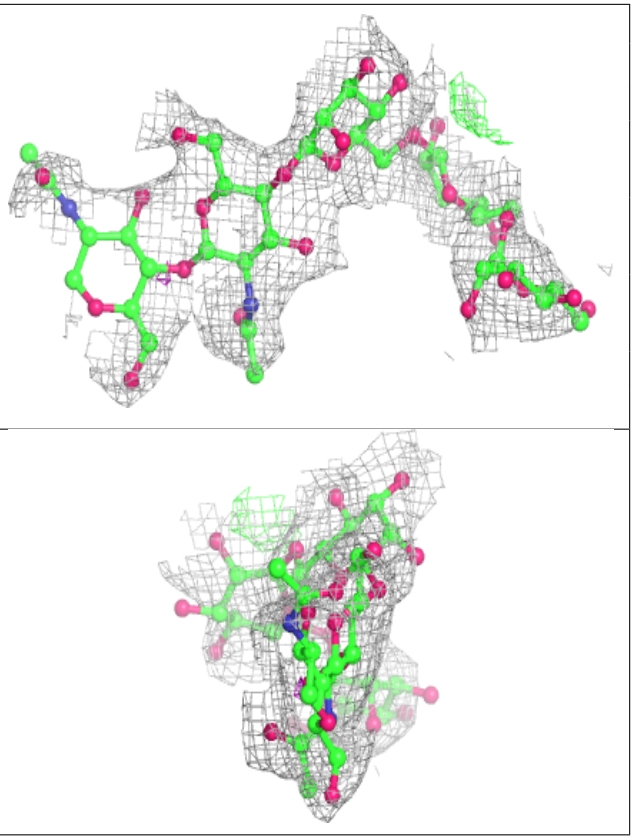


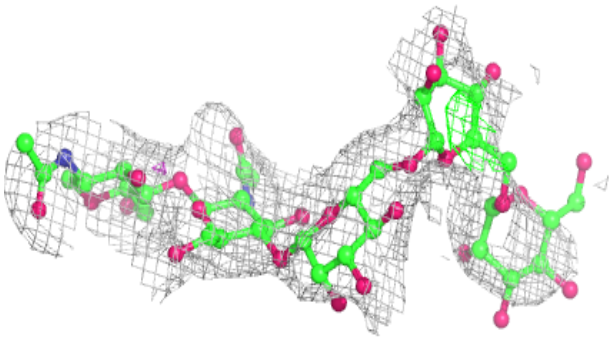




Electron density around Chain I:

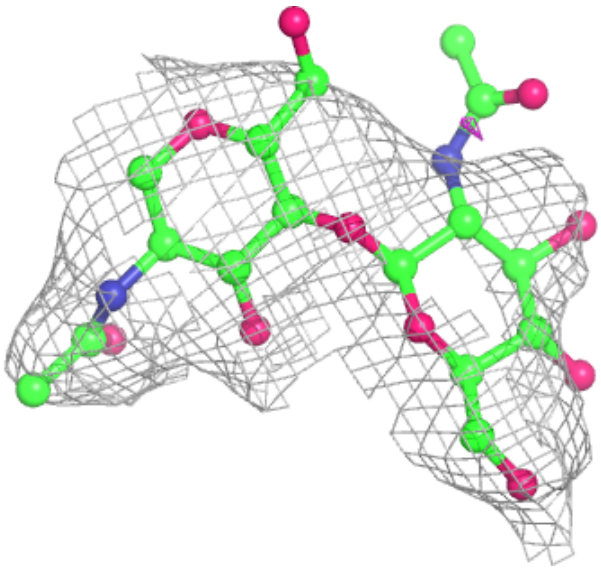
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

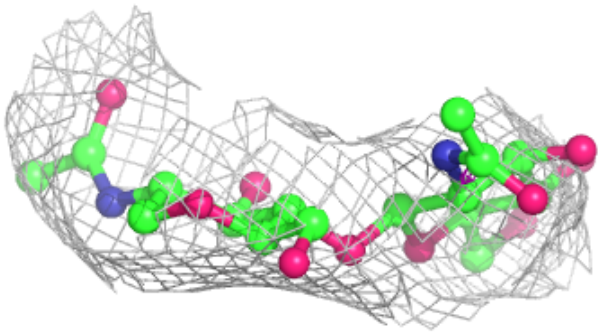


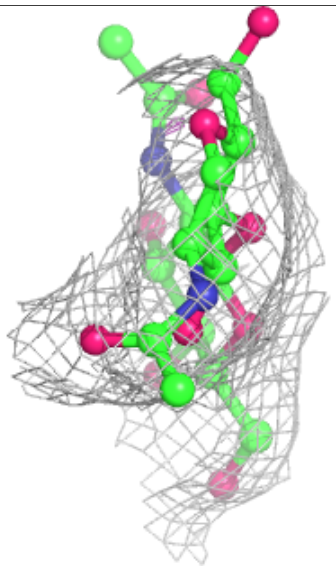


Electron density around Chain J:

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

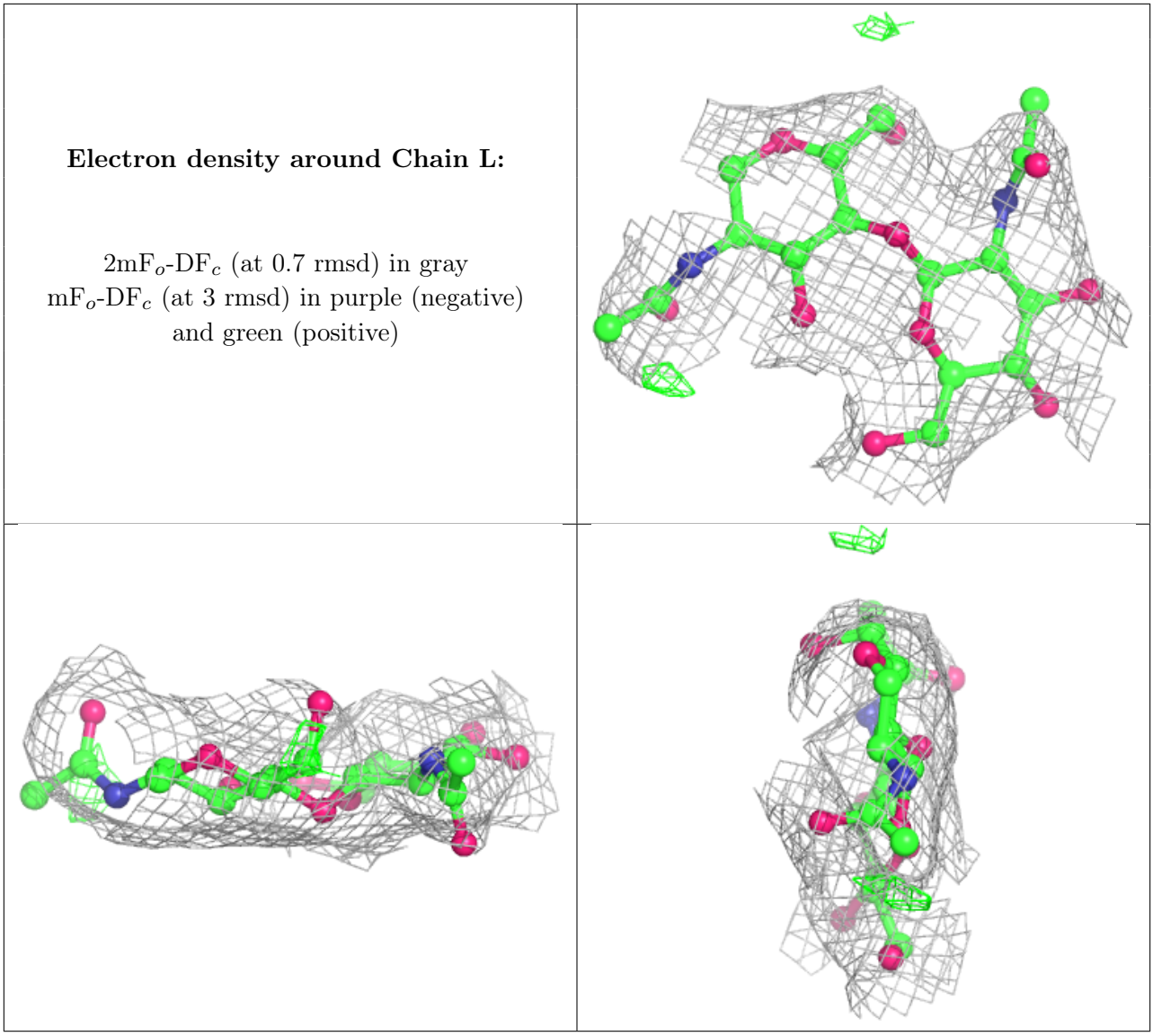






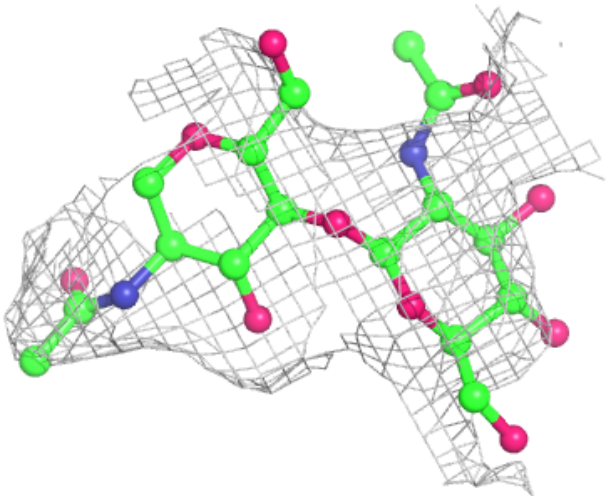
Electron density around Chain L:

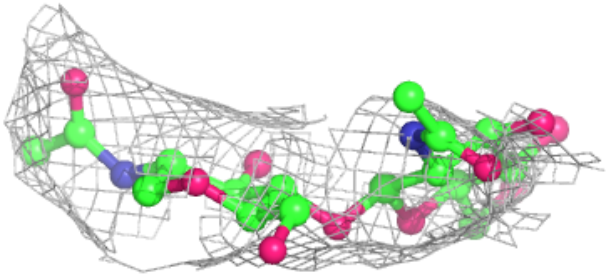
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

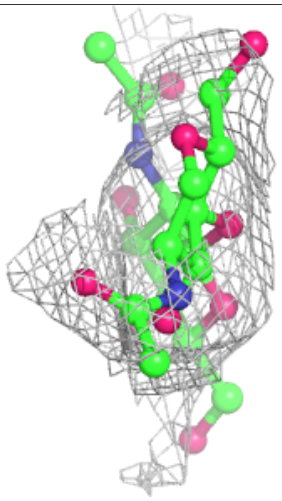


Electron density around Chain P:

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

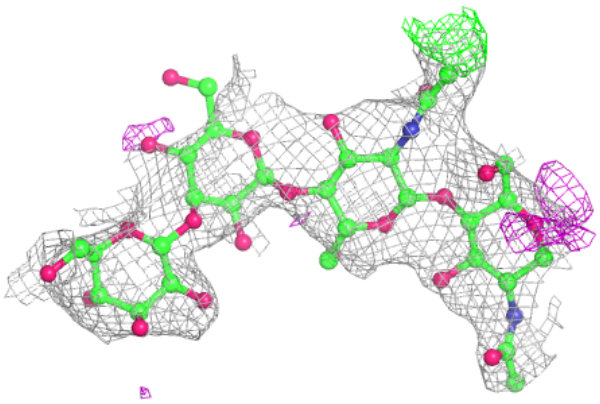


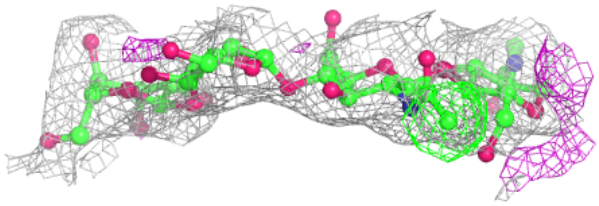


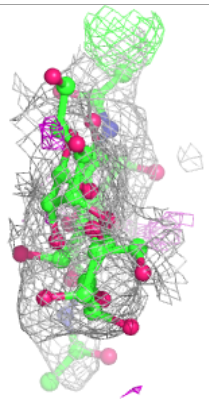


Electron density around Chain N:

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

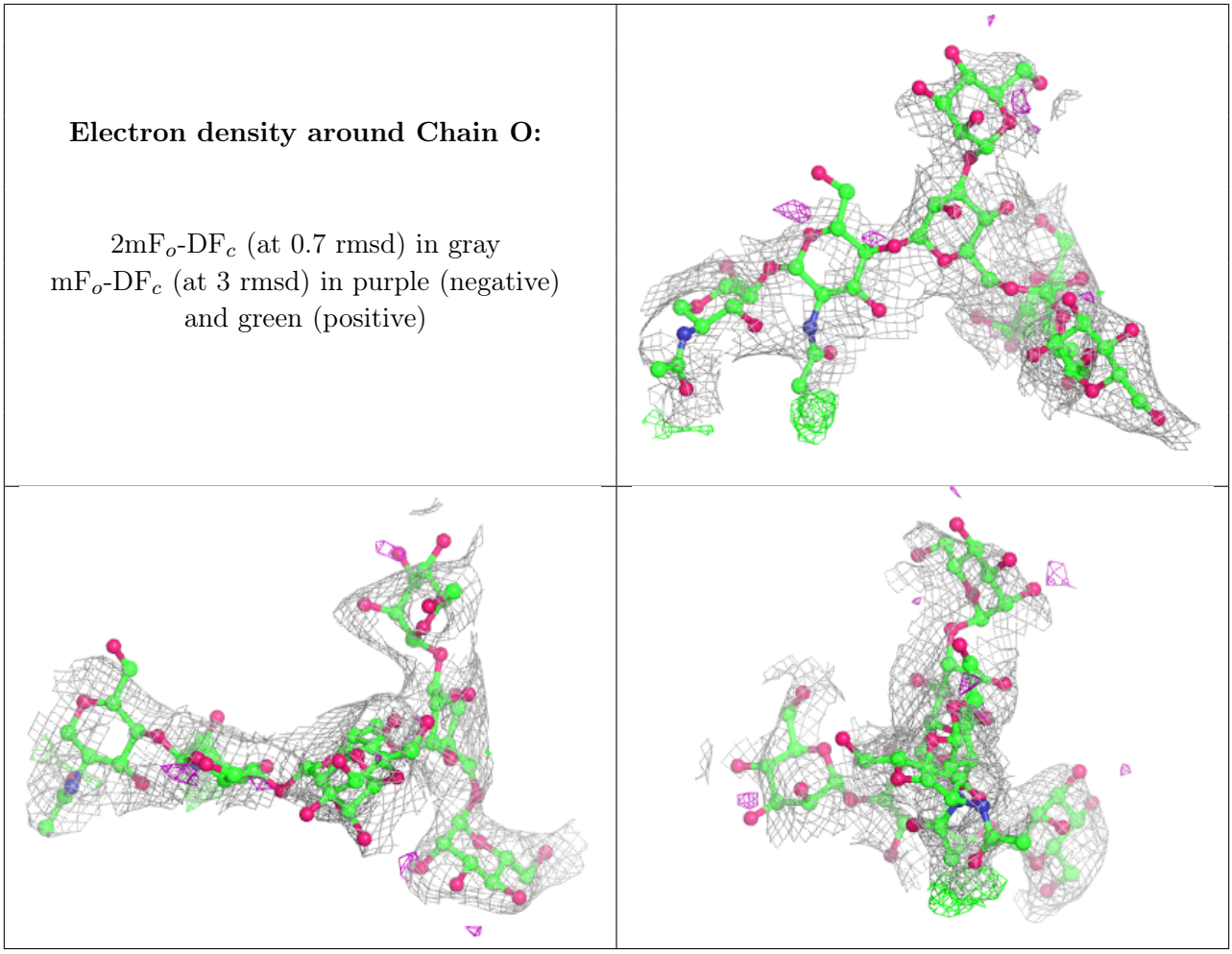






Electron density around Chain O:

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



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
14	CA	A	2002	1/1	0.45	0.53	219,219,219,219	0
14	CA	C	2004	1/1	0.68	0.06	151,151,151,151	0
14	CA	C	2003	1/1	0.74	0.05	115,115,115,115	0
11	CL	C	1595	1/1	0.76	0.14	111,111,111,111	1
14	CA	C	2001	1/1	0.77	0.07	104,104,104,104	0
17	NAG	D	3080	14/15	0.79	0.30	94,127,134,139	0
12	SO4	A	1598	5/5	0.80	0.52	155,156,156,157	5
14	CA	C	2002	1/1	0.84	0.10	106,106,106,106	0
17	NAG	B	3243	14/15	0.87	0.28	100,112,118,118	0
16	MG	B	2001	1/1	0.87	0.12	63,63,63,63	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
15	CAC	D	1442	5/5	0.89	0.24	28,51,133,223	0
16	MG	D	2001	1/1	0.89	0.15	117,117,117,117	0
17	NAG	D	3243	14/15	0.90	0.34	104,128,144,152	0
11	CL	C	1596	1/1	0.91	0.13	96,96,96,96	0
11	CL	A	1595	1/1	0.92	0.08	75,75,75,75	0
12	SO4	A	1597	5/5	0.94	0.27	133,133,136,140	0
14	CA	A	2003	1/1	0.95	0.18	71,71,71,71	0
15	CAC	B	1442	5/5	0.95	0.16	37,68,85,295	0
14	CA	A	2004	1/1	0.96	0.12	58,58,58,58	0
13	NI	A	1599	1/1	0.96	0.04	97,97,97,97	0
14	CA	D	2003	1/1	0.98	0.20	90,90,90,90	0
14	CA	B	2003	1/1	0.98	0.11	64,64,64,64	0
12	SO4	A	1596	5/5	0.99	0.10	64,65,71,72	5
14	CA	A	2001	1/1	0.99	0.14	76,76,76,76	0

6.5 Other polymers (i)

There are no such residues in this entry.