wwPDB X-ray Structure Validation Summary Report (i)

Dec 2, 2023 – 05:00 pm GMT

PDB ID	:	2WIN
Title	:	C3 convertase (C3bBb) stabilized by SCIN
Authors	:	Wu, J.; Janssen, B.J.; Gros, P.
Deposited on	:	2009-05-13
Resolution	:	3.90 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:

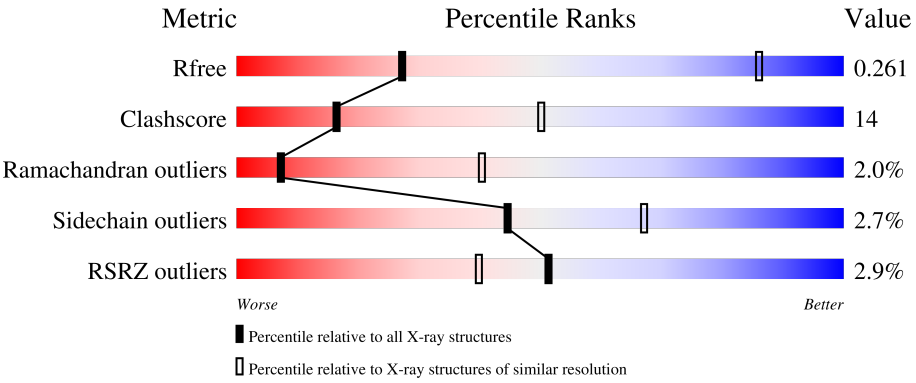
MolProbity	:	4.02b-467
Mogul	:	1.8.4, CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	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 3.90 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	1002 (4.14-3.66)
Clashscore	141614	1004 (4.12-3.68)
Ramachandran outliers	138981	1021 (4.14-3.66)
Sidechain outliers	138945	1014 (4.14-3.66)
RSRZ outliers	127900	1275 (4.20-3.60)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=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	645	2% 72% 25%
1	C	645	2% 72% 26%
1	E	645	2% 72% 26%
1	G	645	9% 71% 27%
2	B	915	% 69% 26%

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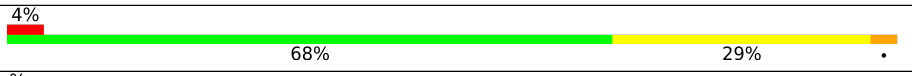
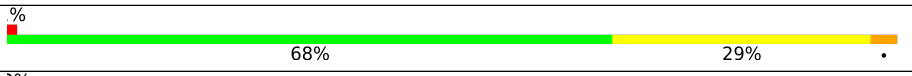
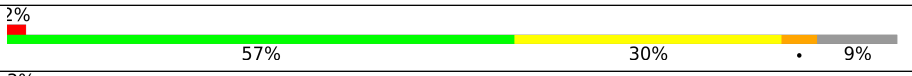
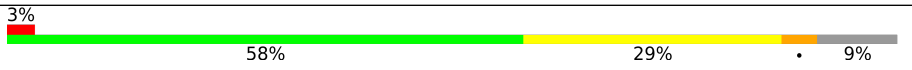
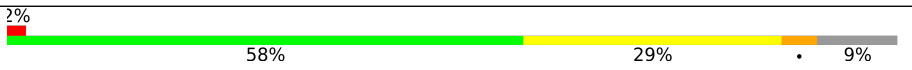
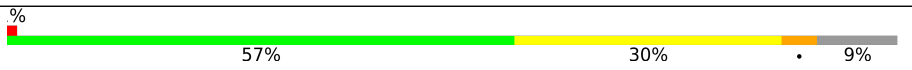
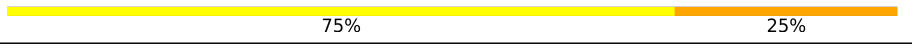
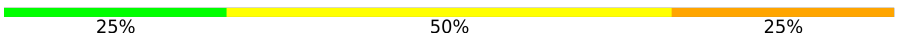
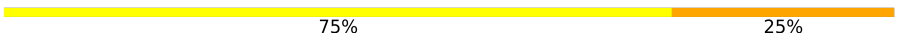
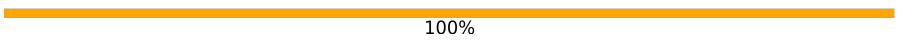
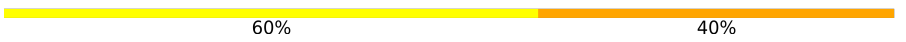
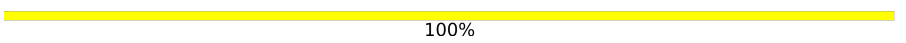
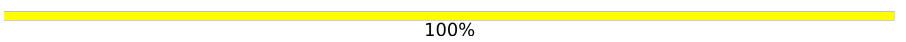
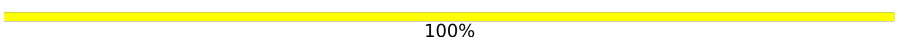
Mol	Chain	Length	Quality of chain
2	D	915	
2	F	915	
2	H	915	
3	I	507	
3	J	507	
3	K	507	
3	L	507	
4	M	92	
4	N	92	
4	P	92	
4	Q	92	
5	O	4	
5	R	4	
5	T	4	
5	U	4	
6	S	5	
6	W	5	
7	V	6	
8	X	4	
9	Y	3	
9	a	3	
10	Z	2	
11	b	5	
12	c	3	

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 crite-

ria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
10	NAG	Z	1	X	-	-	-
11	NAG	b	1	X	-	-	-
11	MAN	b	3	X	-	-	-
11	MAN	b	4	X	-	-	-
11	MAN	b	5	X	-	-	-
16	NAG	K	1749	X	-	-	-
16	NAG	L	1746	X	-	-	-
5	NAG	O	1	X	-	-	-
6	BMA	W	5	-	-	-	X
7	NAG	V	1	X	-	-	-
8	MAN	X	3	X	-	-	-
8	MAN	X	4	X	-	-	-
9	MAN	Y	3	X	-	-	-
9	MAN	a	3	X	-	-	-

2 Entry composition (i)

There are 17 unique types of molecules in this entry. The entry contains 67989 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 COMPLEMENT C3 BETA CHAIN.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	638	Total	C	N	O	S	0	0	0
			4958	3157	841	945	15			
1	C	638	Total	C	N	O	S	0	0	0
			4958	3157	841	945	15			
1	E	638	Total	C	N	O	S	0	0	0
			4958	3157	841	945	15			
1	G	638	Total	C	N	O	S	0	0	0
			4958	3157	841	945	15			

- Molecule 2 is a protein called COMPLEMENT C3B ALPHA' CHAIN.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	901	Total	C	N	O	S	0	0	0
			7177	4545	1209	1386	37			
2	D	901	Total	C	N	O	S	0	0	0
			7166	4537	1208	1384	37			
2	F	900	Total	C	N	O	S	0	0	0
			7172	4545	1206	1384	37			
2	H	900	Total	C	N	O	S	2313	0	0
			7175	4547	1209	1382	37			

- Molecule 3 is a protein called COMPLEMENT FACTOR B.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	I	507	Total	C	N	O	S	0	0	0
			4004	2543	685	756	20			
3	J	507	Total	C	N	O	S	0	0	0
			4004	2543	685	756	20			
3	K	507	Total	C	N	O	S	0	0	0
			4004	2543	685	756	20			
3	L	507	Total	C	N	O	S	0	0	0
			4004	2543	685	756	20			

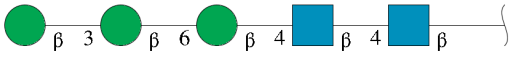
- Molecule 4 is a protein called STAPHYLOCOCCAL COMPLEMENT INHIBITOR.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	M	84	Total	C	N	O	S	0	0	0
			682	432	111	137	2			
4	N	84	Total	C	N	O	S	0	0	0
			682	432	111	137	2			
4	P	84	Total	C	N	O	S	0	0	0
			682	432	111	137	2			
4	Q	84	Total	C	N	O	S	0	0	0
			682	432	111	137	2			

- Molecule 5 is an oligosaccharide called beta-D-mannopyranose-(1-6)-beta-D-mannopyranose -(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucop yranose.

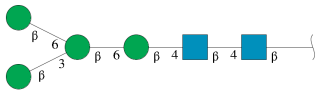
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
5	O	4	Total	C	N	O	0	0	0
			50	28	2	20			
5	R	4	Total	C	N	O	0	0	0
			50	28	2	20			
5	T	4	Total	C	N	O	0	0	0
			50	28	2	20			
5	U	4	Total	C	N	O	0	0	0
			50	28	2	20			

- Molecule 6 is an oligosaccharide called beta-D-mannopyranose-(1-3)-beta-D-mannopyranose -(1-6)-beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acet amido-2-deoxy-beta-D-glucopyranose.



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
6	S	5	Total	C	N	O	0	0	0
			61	34	2	25			
6	W	5	Total	C	N	O	0	0	0
			61	34	2	25			

- Molecule 7 is an oligosaccharide called beta-D-mannopyranose-(1-3)-[beta-D-mannopyranose-(1-6)]beta-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.

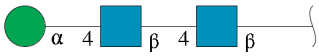


Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
7	V	6	Total	C	N	O	0	0	0
			72	40	2	30			

- Molecule 8 is an oligosaccharide called alpha-D-mannopyranose-(1-6)-alpha-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
8	X	4	Total	C	N	O	0	0	0
			50	28	2	20			

- Molecule 9 is an oligosaccharide called alpha-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose.

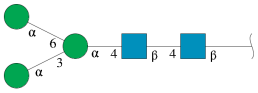


Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
9	Y	3	Total	C	N	O	0	0	0
			39	22	2	15			
9	a	3	Total	C	N	O	0	0	0
			39	22	2	15			

- Molecule 10 is an oligosaccharide called 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose.

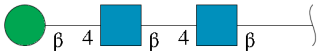
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
10	Z	2	Total	C	N	O	0	0	0
			28	16	2	10			

- Molecule 11 is an oligosaccharide called alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-6)]alpha-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose.



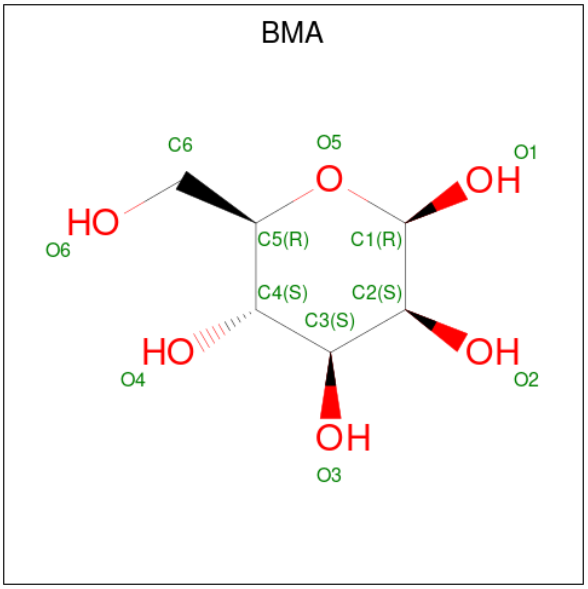
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
11	b	5	Total	C	N	O	0	0	0
			61	34	2	25			

- Molecule 12 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.



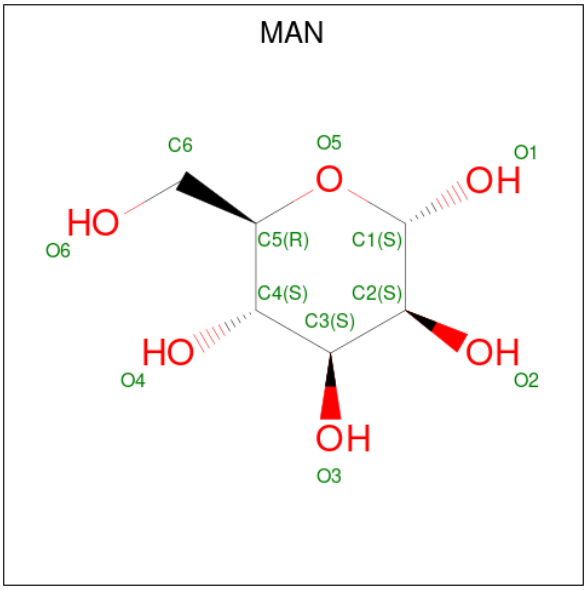
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
12	c	3	Total	C	N	O	0	0	0
			39	22	2	15			

- Molecule 13 is beta-D-mannopyranose (three-letter code: BMA) (formula: $C_6H_{12}O_6$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
13	B	1	Total C O 11 6 5	0	0
13	K	1	Total C O 11 6 5	0	0

- Molecule 14 is alpha-D-mannopyranose (three-letter code: MAN) (formula: $C_6H_{12}O_6$).

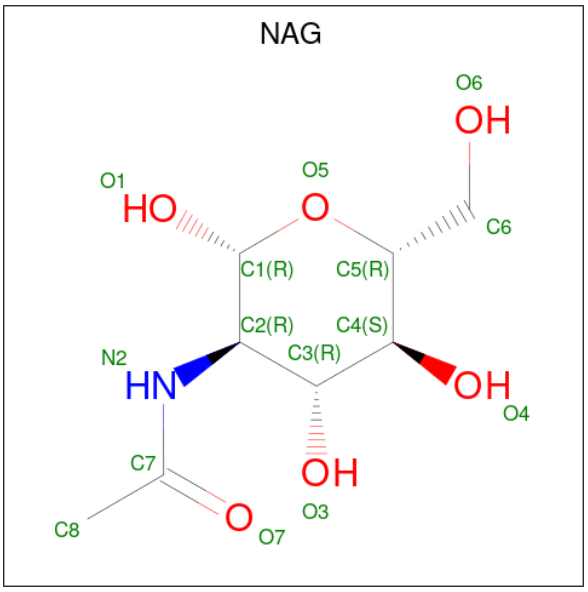


Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
14	G	1	Total C O 11 6 5	0	0

- Molecule 15 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
15	I	1	Total Mg 1 1	0	0
15	J	1	Total Mg 1 1	0	0
15	K	1	Total Mg 1 1	0	0
15	L	1	Total Mg 1 1	0	0

- Molecule 16 is 2-acetamido-2-deoxy-beta-D-glucopyranose (three-letter code: NAG) (formula: $C_8H_{15}NO_6$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
16	K	1	Total C N O 14 8 1 5	0	0
16	L	1	Total C N O 14 8 1 5	0	0

- Molecule 17 is water.

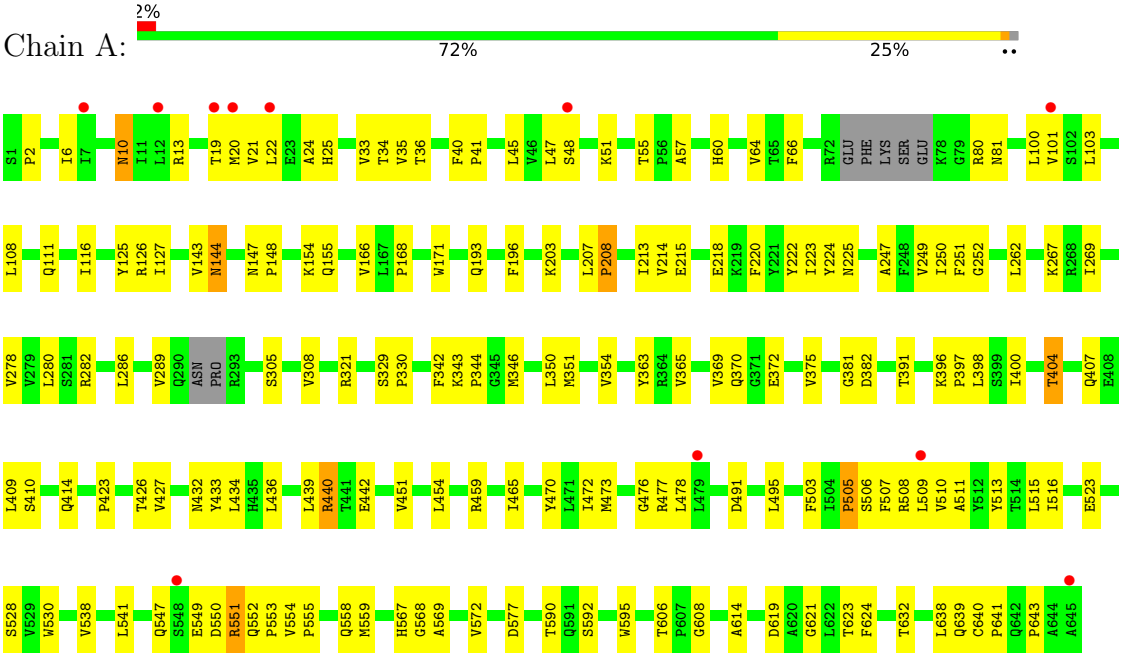
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
17	B	1	Total O 1 1	0	0
17	I	2	Total O 2 2	0	0
17	J	2	Total O 2 2	0	0
17	K	2	Total O 2 2	0	0
17	L	1	Total O 1 1	0	0

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.

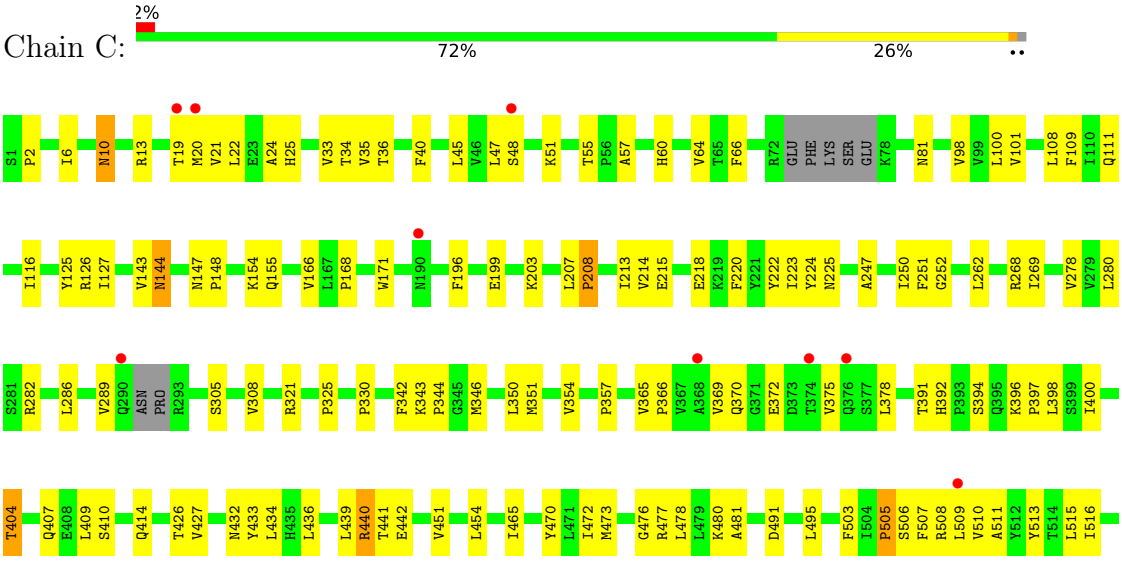
• Molecule 1: COMPLEMENT C3 BETA CHAIN

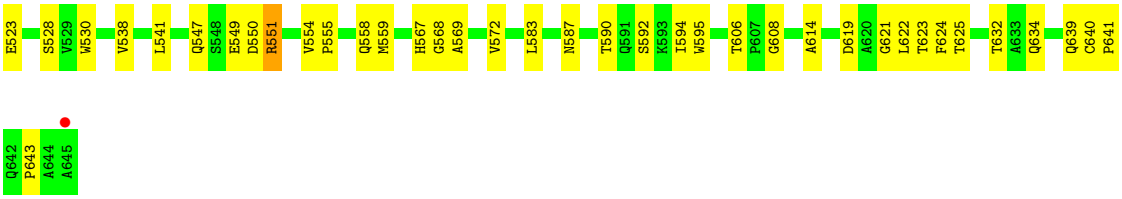
Chain A:



• Molecule 1: COMPLEMENT C3 BETA CHAIN

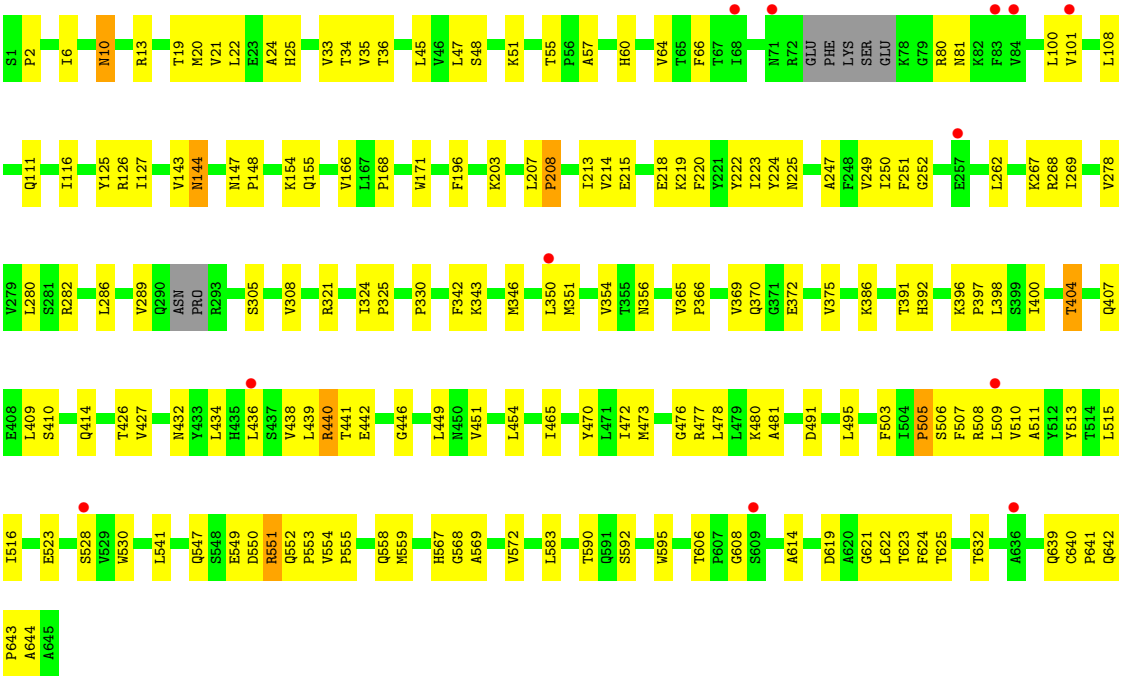
Chain C:





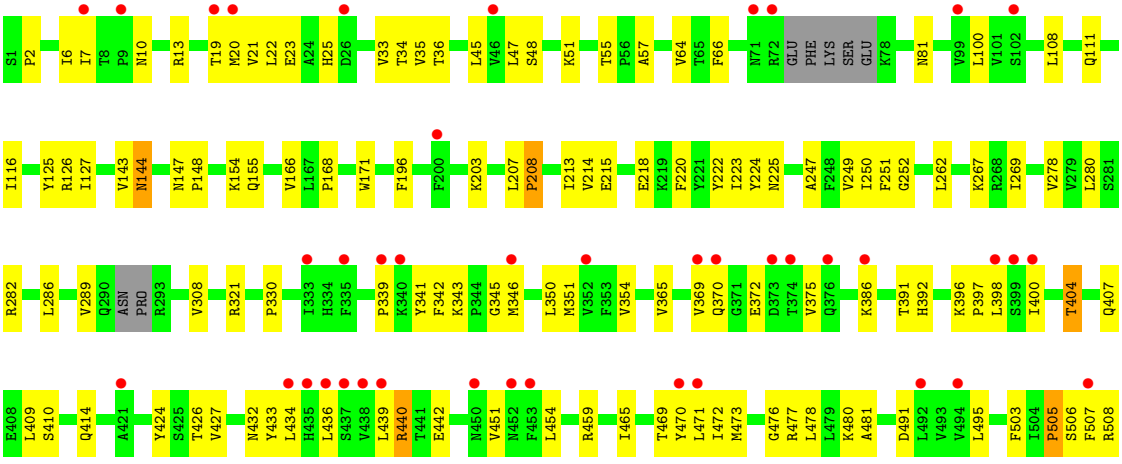
• Molecule 1: COMPLEMENT C3 BETA CHAIN

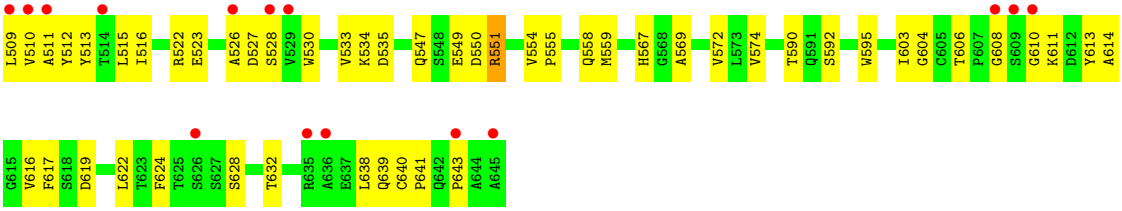
Chain E:



• Molecule 1: COMPLEMENT C3 BETA CHAIN

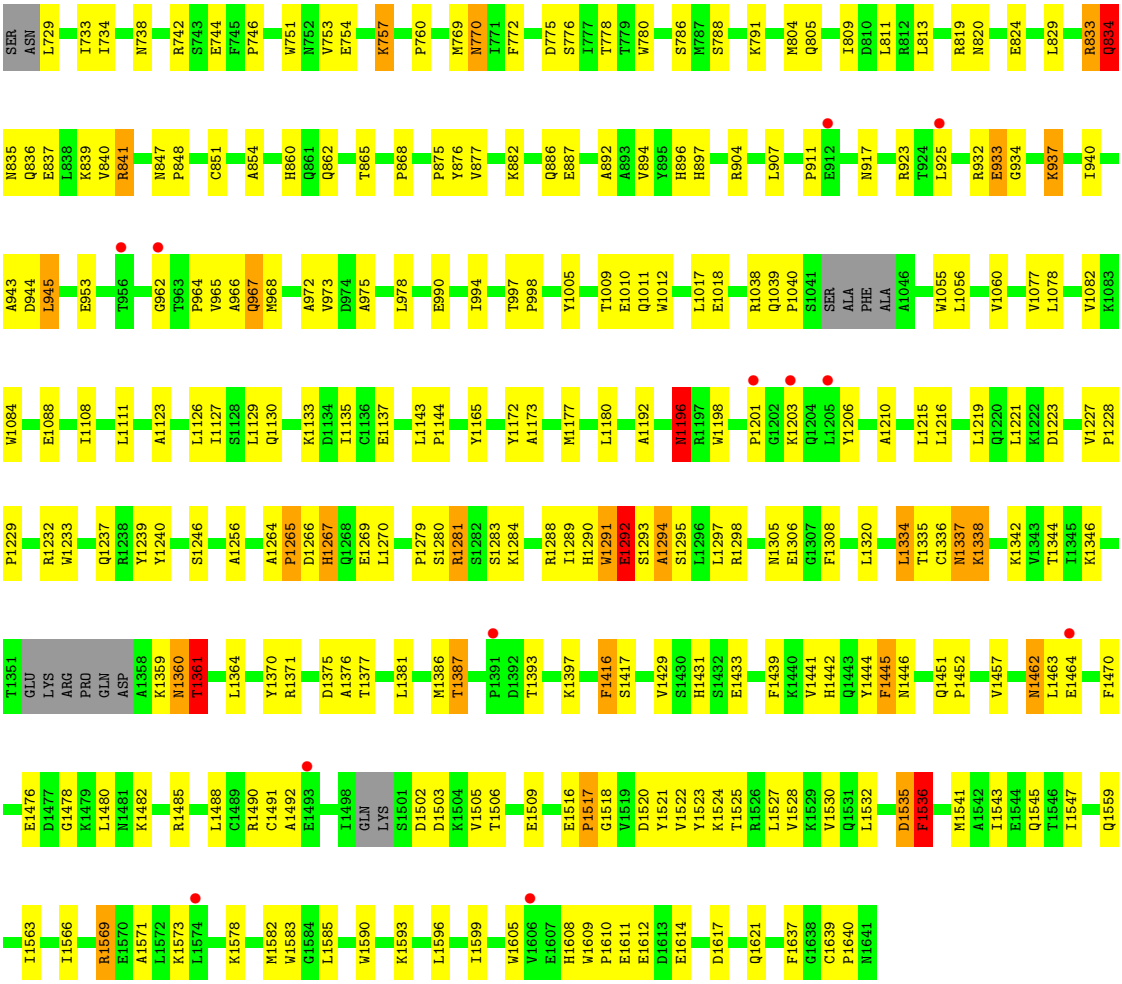
Chain G:





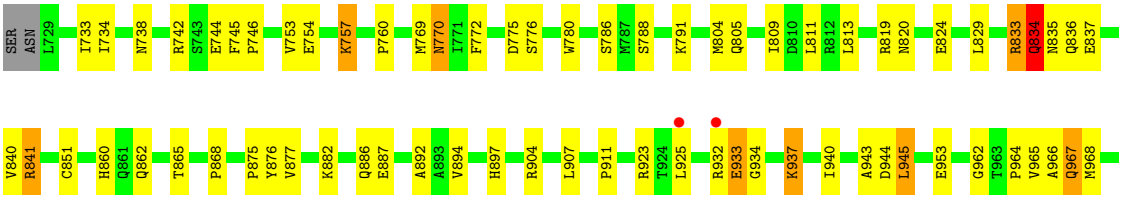
• Molecule 2: COMPLEMENT C3B ALPHA' CHAIN

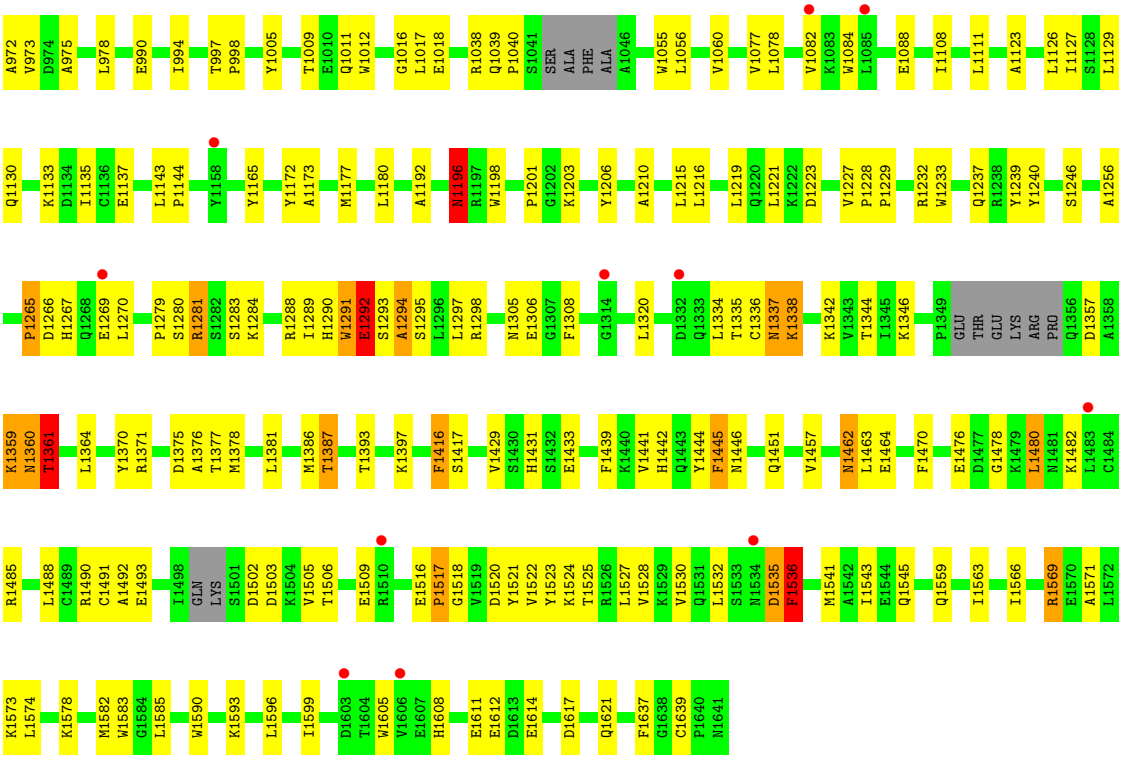
Chain B:



• Molecule 2: COMPLEMENT C3B ALPHA' CHAIN

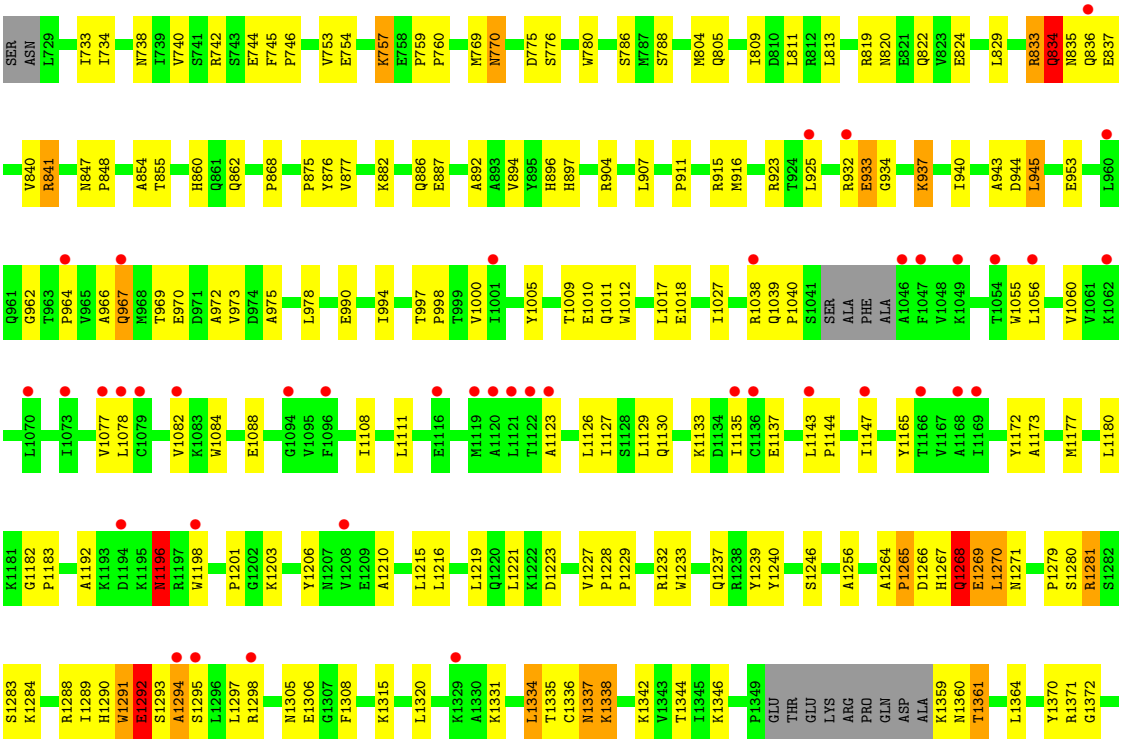
Chain D:

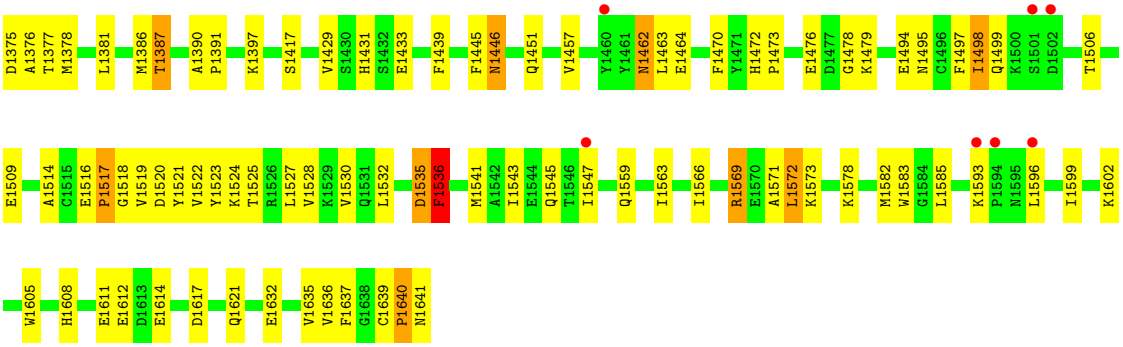




• Molecule 2: COMPLEMENT C3B ALPHA' CHAIN

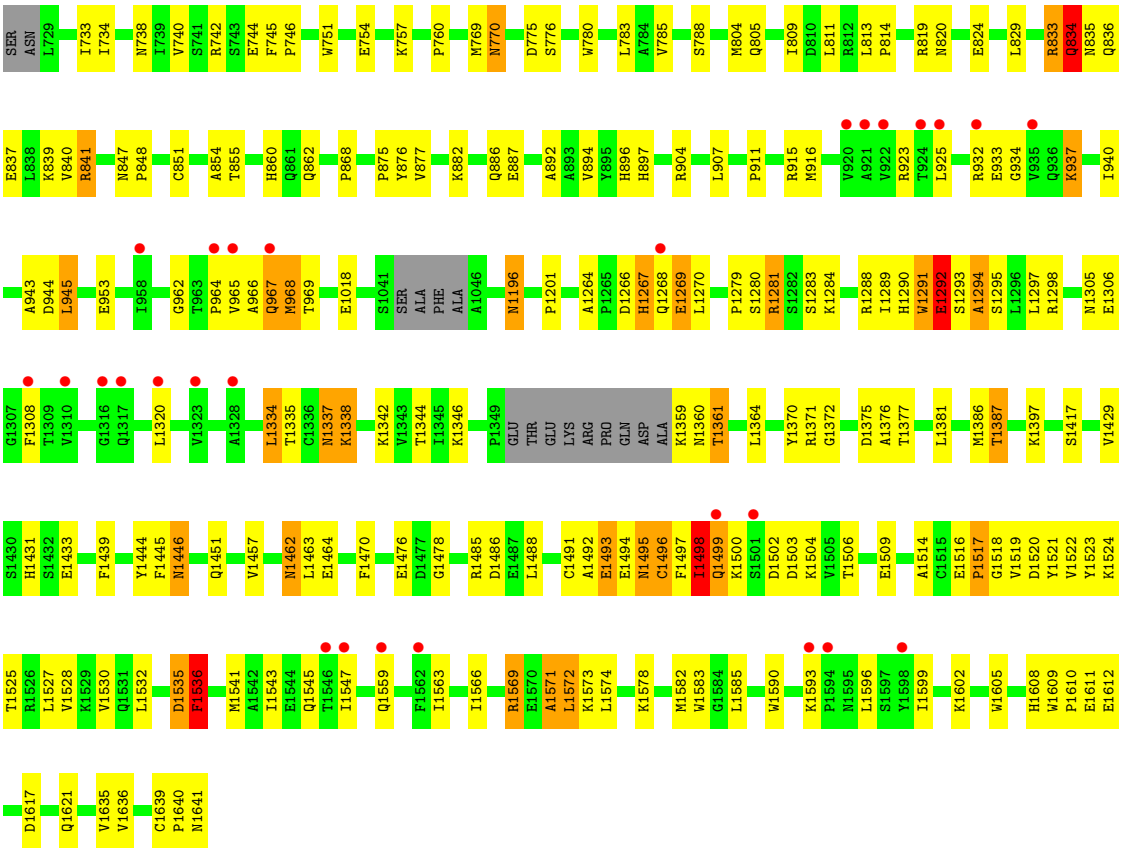
Chain F:





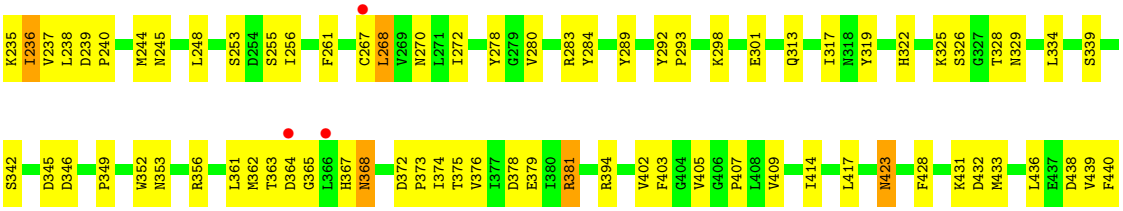
• Molecule 2: COMPLEMENT C3B ALPHA' CHAIN

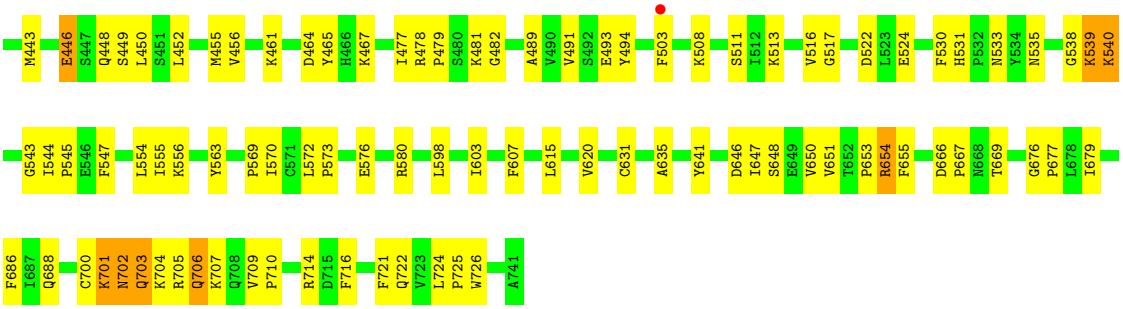
Chain H:



• Molecule 3: COMPLEMENT FACTOR B

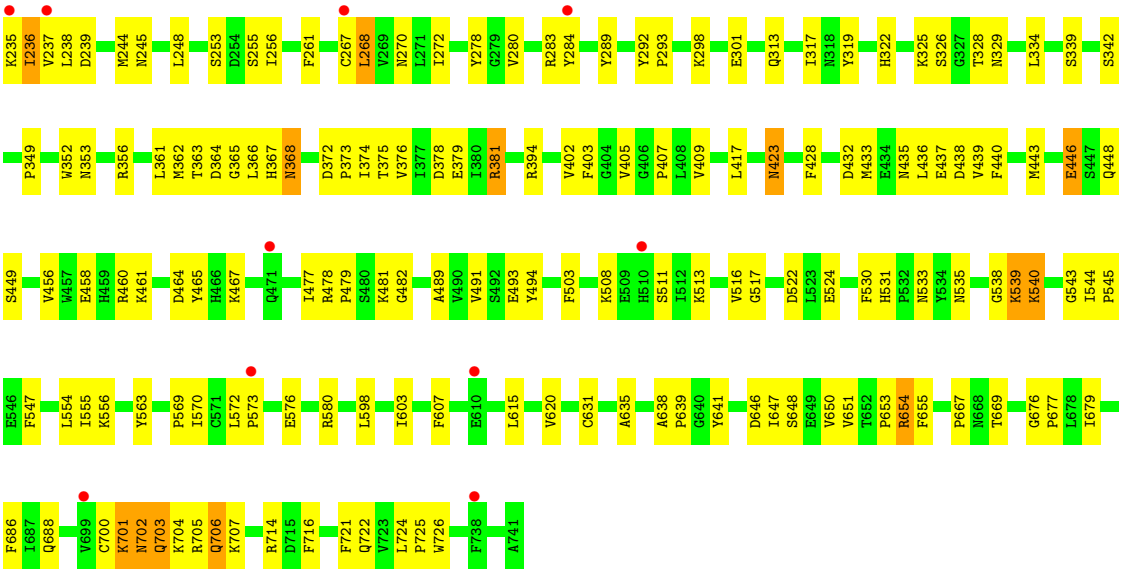
Chain I:





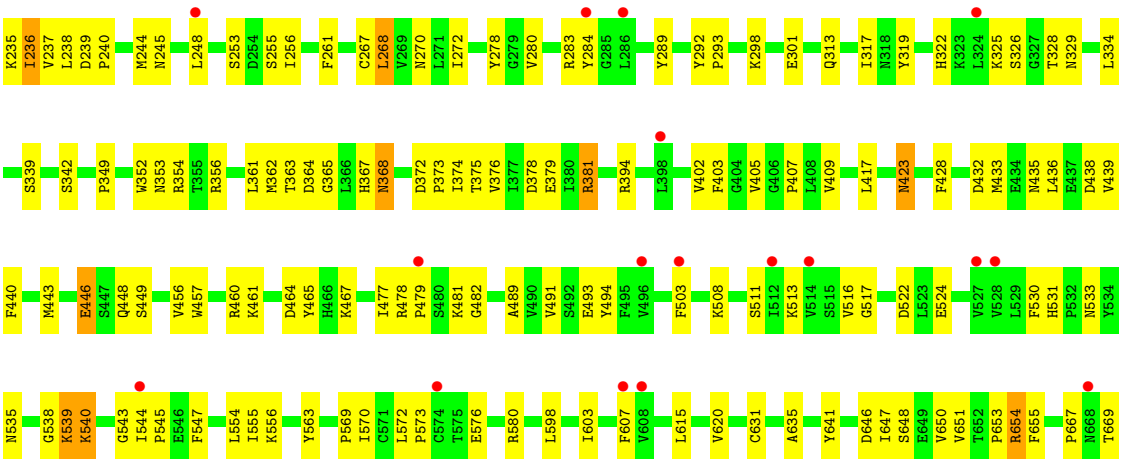
• Molecule 3: COMPLEMENT FACTOR B

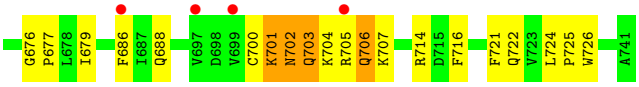
Chain J:



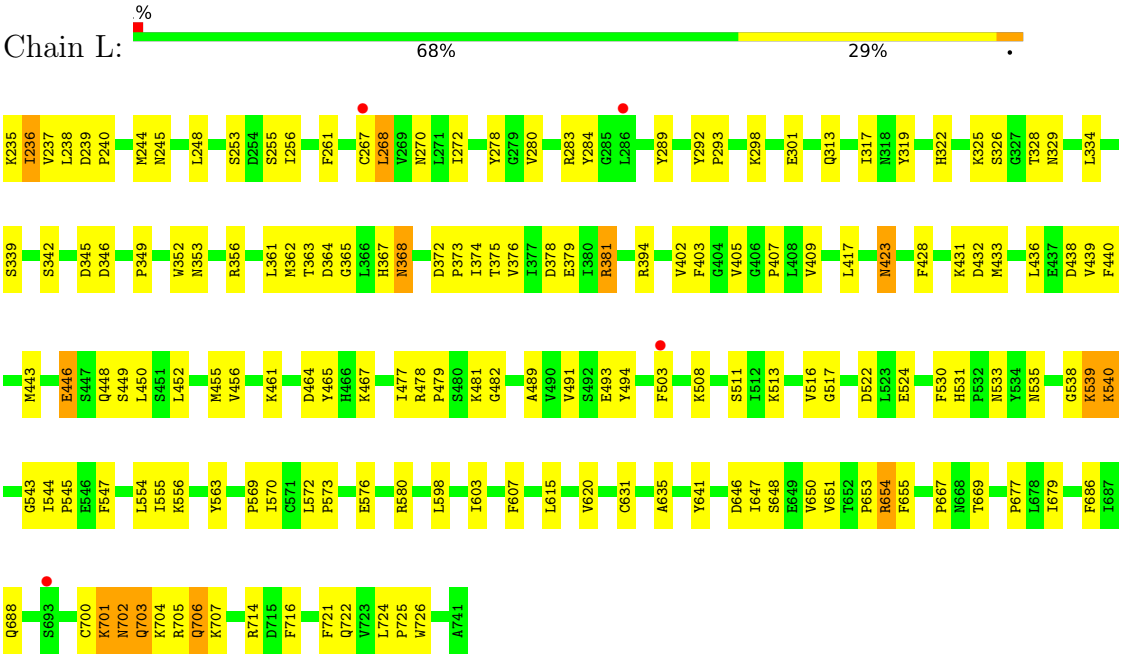
• Molecule 3: COMPLEMENT FACTOR B

Chain K:

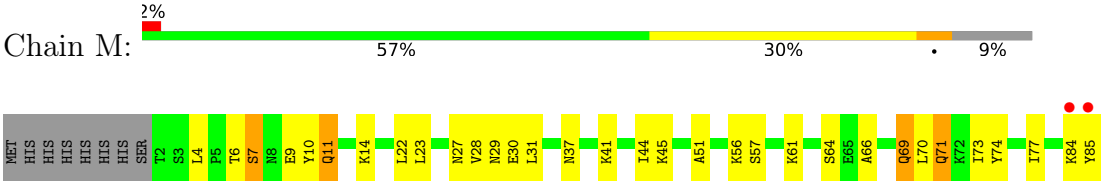




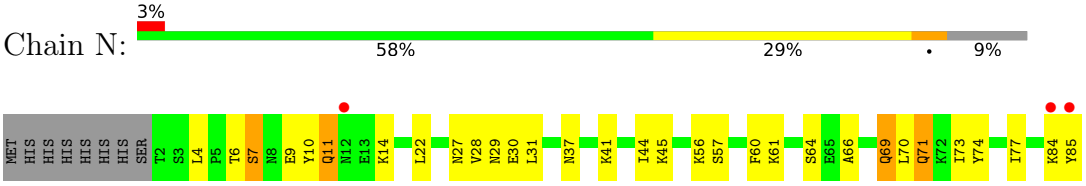
• Molecule 3: COMPLEMENT FACTOR B



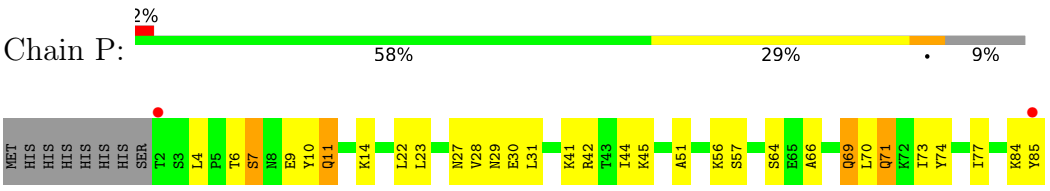
• Molecule 4: STAPHYLOCOCCAL COMPLEMENT INHIBITOR



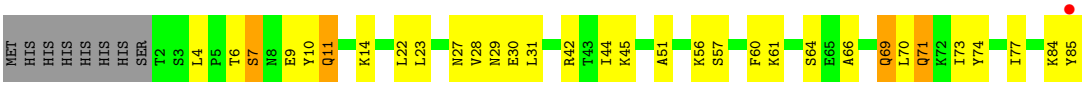
• Molecule 4: STAPHYLOCOCCAL COMPLEMENT INHIBITOR



• Molecule 4: STAPHYLOCOCCAL COMPLEMENT INHIBITOR

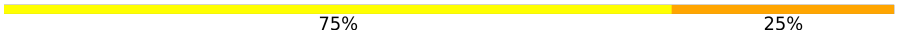


• Molecule 4: STAPHYLOCOCCAL COMPLEMENT INHIBITOR



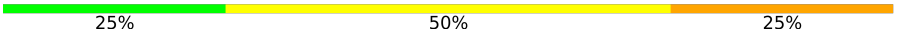
• Molecule 5: beta-D-mannopyranose-(1-6)-beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain O:



• Molecule 5: beta-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 R:



• Molecule 5: beta-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

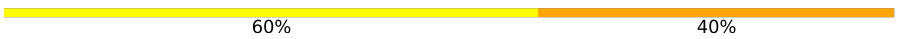
Chain T:

• Molecule 5: beta-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 U:

• Molecule 6: beta-D-mannopyranose-(1-3)-beta-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 S:



• Molecule 6: beta-D-mannopyranose-(1-3)-beta-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 W:

• Molecule 7: beta-D-mannopyranose-(1-3)-[beta-D-mannopyranose-(1-6)]beta-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 V: 

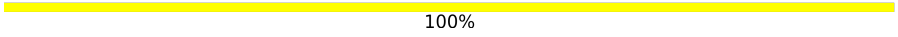
• Molecule 8: alpha-D-mannopyranose-(1-6)-alpha-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain X: 

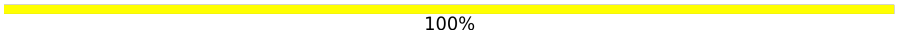
• Molecule 9: alpha-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain Y: 

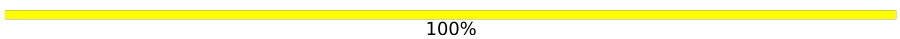
• Molecule 9: alpha-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain a: 

• Molecule 10: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain Z: 

• Molecule 11: alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-6)]alpha-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain b: 

• Molecule 12: beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain c:

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	228.63Å 121.49Å 280.78Å 90.00° 91.64° 90.00°	Depositor
Resolution (Å)	39.67 – 3.90 39.68 – 3.90	Depositor EDS
% Data completeness (in resolution range)	97.6 (39.67-3.90) 89.7 (39.68-3.90)	Depositor EDS
R_{merge}	0.13	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.95 (at 3.87Å)	Xtriage
Refinement program	PHENIX (PHENIX.REFINE)	Depositor
R, R_{free}	0.253 , 0.268 0.247 , 0.261	Depositor DCC
R_{free} test set	2089 reflections (1.52%)	wwPDB-VP
Wilson B-factor (Å^2)	125.3	Xtriage
Anisotropy	0.223	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.28 , 76.7	EDS
L-test for twinning[2]	$< \|L\| > = 0.41$, $< L^2 > = 0.23$	Xtriage
Estimated twinning fraction	0.128 for h,-k,-l	Xtriage
F_o,F_c correlation	0.89	EDS
Total number of atoms	67989	wwPDB-VP
Average B, all atoms (Å^2)	158.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.41% 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: MG, MAN, BMA, NAG

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	0.20	0/5056	0.37	0/6870
1	C	0.20	0/5056	0.37	0/6870
1	E	0.20	0/5056	0.37	0/6870
1	G	0.21	0/5056	0.38	0/6870
2	B	0.21	0/7317	0.36	0/9907
2	D	0.21	0/7306	0.36	0/9894
2	F	0.21	0/7314	0.36	0/9905
2	H	0.22	0/7315	0.36	0/9902
3	I	0.20	0/4092	0.37	0/5543
3	J	0.20	0/4092	0.37	0/5543
3	K	0.20	0/4092	0.37	0/5543
3	L	0.20	0/4092	0.37	0/5543
4	M	0.21	0/690	0.33	0/923
4	N	0.21	0/690	0.32	0/923
4	P	0.21	0/690	0.33	0/923
4	Q	0.21	0/690	0.33	0/923
All	All	0.21	0/68604	0.36	0/92952

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	4958	0	5017	127	0
1	C	4958	0	5017	128	0
1	E	4958	0	5017	130	0
1	G	4958	0	5016	144	0
2	B	7177	0	7085	201	0
2	D	7166	0	7062	193	0
2	F	7172	0	7080	220	0
2	H	7175	0	7087	195	0
3	I	4004	0	3966	128	0
3	J	4004	0	3967	129	0
3	K	4004	0	3965	125	0
3	L	4004	0	3966	126	0
4	M	682	0	697	35	0
4	N	682	0	697	38	0
4	P	682	0	697	33	0
4	Q	682	0	697	38	0
5	O	50	0	43	1	0
5	R	50	0	42	1	0
5	T	50	0	43	1	0
5	U	50	0	43	3	0
6	S	61	0	52	1	0
6	W	61	0	52	5	0
7	V	72	0	61	2	0
8	X	50	0	43	2	0
9	Y	39	0	34	2	0
9	a	39	0	34	0	0
10	Z	28	0	25	0	0
11	b	61	0	52	0	0
12	c	39	0	34	0	0
13	B	11	0	10	0	0
13	K	11	0	10	0	0
14	G	11	0	10	1	0
15	I	1	0	0	0	0
15	J	1	0	0	0	0
15	K	1	0	0	0	0
15	L	1	0	0	0	0
16	K	14	0	13	3	0
16	L	14	0	13	0	0
17	B	1	0	0	0	0
17	I	2	0	0	0	0
17	J	2	0	0	1	0
17	K	2	0	0	0	0
17	L	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
All	All	67989	0	67647	1863	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 14.

The worst 5 of 1863 close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:426:THR:HG21	1:G:432:ASN:H	1.20	1.07
2:H:1494:GLU:HB3	2:H:1602:LYS:HB3	1.36	1.04
2:D:1569:ARG:HB2	2:D:1569:ARG:HH11	1.32	0.94
2:F:1569:ARG:HB2	2:F:1569:ARG:HH11	1.32	0.94
2:H:1569:ARG:HB2	2:H:1569:ARG:HH11	1.32	0.94

There are no symmetry-related clashes.

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	632/645 (98%)	576 (91%)	52 (8%)	4 (1%)	25	63
1	C	632/645 (98%)	576 (91%)	52 (8%)	4 (1%)	25	63
1	E	632/645 (98%)	575 (91%)	53 (8%)	4 (1%)	25	63
1	G	632/645 (98%)	575 (91%)	53 (8%)	4 (1%)	25	63
2	B	893/915 (98%)	785 (88%)	80 (9%)	28 (3%)	4	32
2	D	893/915 (98%)	784 (88%)	82 (9%)	27 (3%)	4	33
2	F	894/915 (98%)	786 (88%)	78 (9%)	30 (3%)	3	31
2	H	890/915 (97%)	782 (88%)	75 (8%)	33 (4%)	3	29
3	I	505/507 (100%)	446 (88%)	51 (10%)	8 (2%)	9	44

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
3	J	505/507 (100%)	446 (88%)	51 (10%)	8 (2%)	9 44
3	K	505/507 (100%)	445 (88%)	52 (10%)	8 (2%)	9 44
3	L	505/507 (100%)	446 (88%)	51 (10%)	8 (2%)	9 44
4	M	82/92 (89%)	77 (94%)	4 (5%)	1 (1%)	13 49
4	N	82/92 (89%)	77 (94%)	4 (5%)	1 (1%)	13 49
4	P	82/92 (89%)	77 (94%)	4 (5%)	1 (1%)	13 49
4	Q	82/92 (89%)	77 (94%)	4 (5%)	1 (1%)	13 49
All	All	8446/8636 (98%)	7530 (89%)	746 (9%)	170 (2%)	7 40

5 of 170 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	B	933	GLU
2	B	967	GLN
2	B	1269	GLU
2	B	1281	ARG
2	B	1291	TRP

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	558/567 (98%)	549 (98%)	9 (2%)	62 79
1	C	558/567 (98%)	549 (98%)	9 (2%)	62 79
1	E	558/567 (98%)	549 (98%)	9 (2%)	62 79
1	G	558/567 (98%)	549 (98%)	9 (2%)	62 79
2	B	793/810 (98%)	769 (97%)	24 (3%)	41 64
2	D	790/810 (98%)	766 (97%)	24 (3%)	41 64
2	F	793/810 (98%)	769 (97%)	24 (3%)	41 64
2	H	793/810 (98%)	766 (97%)	27 (3%)	37 62
3	I	442/446 (99%)	429 (97%)	13 (3%)	42 65

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
3	J	442/446 (99%)	429 (97%)	13 (3%)	42	65
3	K	442/446 (99%)	429 (97%)	13 (3%)	42	65
3	L	442/446 (99%)	429 (97%)	13 (3%)	42	65
4	M	76/84 (90%)	73 (96%)	3 (4%)	32	59
4	N	76/84 (90%)	73 (96%)	3 (4%)	32	59
4	P	76/84 (90%)	73 (96%)	3 (4%)	32	59
4	Q	76/84 (90%)	73 (96%)	3 (4%)	32	59
All	All	7473/7628 (98%)	7274 (97%)	199 (3%)	44	67

5 of 199 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	H	953	GLU
3	I	539	LYS
2	H	1196	ASN
2	H	1520	ASP
3	J	322	HIS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 256 such sidechains are listed below:

Mol	Chain	Res	Type
3	L	466	HIS
4	M	49	GLN
2	D	1620	ASN
2	D	1559	GLN
4	N	49	GLN

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates (i)

52 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	$\#\|Z\| > 2$
5	NAG	O	1	1,5	14,14,15	0.46	0	17,19,21	0.79	0
5	NAG	O	2	5	14,14,15	0.65	0	17,19,21	1.80	4 (23%)
5	BMA	O	3	5	11,11,12	0.57	0	15,15,17	1.40	2 (13%)
5	BMA	O	4	5	11,11,12	0.67	0	15,15,17	1.38	2 (13%)
5	NAG	R	1	5,2	14,14,15	0.55	0	17,19,21	1.11	2 (11%)
5	NAG	R	2	5	14,14,15	0.54	0	17,19,21	2.19	3 (17%)
5	BMA	R	3	5	11,11,12	0.95	0	15,15,17	1.97	6 (40%)
5	BMA	R	4	5	11,11,12	0.73	0	15,15,17	0.81	0
6	NAG	S	1	1,6	14,14,15	0.62	0	17,19,21	1.17	2 (11%)
6	NAG	S	2	6	14,14,15	0.67	0	17,19,21	1.13	2 (11%)
6	BMA	S	3	6	11,11,12	0.68	0	15,15,17	1.14	1 (6%)
6	BMA	S	4	6	11,11,12	0.77	0	15,15,17	1.54	3 (20%)
6	BMA	S	5	6	11,11,12	0.67	0	15,15,17	1.76	4 (26%)
5	NAG	T	1	5,2	14,14,15	0.50	0	17,19,21	0.83	0
5	NAG	T	2	5	14,14,15	0.58	0	17,19,21	1.05	2 (11%)
5	BMA	T	3	5	11,11,12	0.64	0	15,15,17	1.37	2 (13%)
5	BMA	T	4	5	11,11,12	0.67	0	15,15,17	1.30	2 (13%)
5	NAG	U	1	1,5	14,14,15	0.56	0	17,19,21	0.87	1 (5%)
5	NAG	U	2	5	14,14,15	0.60	0	17,19,21	1.16	2 (11%)
5	BMA	U	3	5	11,11,12	0.70	0	15,15,17	1.07	1 (6%)
5	BMA	U	4	5	11,11,12	0.94	1 (9%)	15,15,17	1.70	3 (20%)
7	NAG	V	1	7,2	14,14,15	0.39	0	17,19,21	1.28	3 (17%)
7	NAG	V	2	7	14,14,15	0.44	0	17,19,21	1.66	4 (23%)
7	BMA	V	3	7	11,11,12	0.60	0	15,15,17	1.60	4 (26%)
7	BMA	V	4	7	11,11,12	1.00	1 (9%)	15,15,17	1.68	4 (26%)
7	BMA	V	5	7	11,11,12	0.67	0	15,15,17	1.86	4 (26%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
7	BMA	V	6	7	11,11,12	0.71	0	15,15,17	1.05	1 (6%)
6	NAG	W	1	1,6	14,14,15	0.45	0	17,19,21	1.17	1 (5%)
6	NAG	W	2	6	14,14,15	0.50	0	17,19,21	2.17	4 (23%)
6	BMA	W	3	6	11,11,12	0.52	0	15,15,17	2.97	6 (40%)
6	BMA	W	4	6	11,11,12	0.57	0	15,15,17	4.54	6 (40%)
6	BMA	W	5	6	11,11,12	0.65	0	15,15,17	1.41	2 (13%)
8	NAG	X	1	2,8	14,14,15	0.59	0	17,19,21	0.80	0
8	NAG	X	2	8	14,14,15	0.49	0	17,19,21	0.79	0
8	MAN	X	3	8	11,11,12	0.78	0	15,15,17	1.39	2 (13%)
8	MAN	X	4	8	11,11,12	0.77	0	15,15,17	1.06	2 (13%)
9	NAG	Y	1	9,3	14,14,15	0.57	0	17,19,21	1.00	2 (11%)
9	NAG	Y	2	9	14,14,15	0.63	0	17,19,21	1.03	1 (5%)
9	MAN	Y	3	9	11,11,12	0.65	0	15,15,17	1.05	1 (6%)
10	NAG	Z	1	3,10	14,14,15	0.55	0	17,19,21	1.12	2 (11%)
10	NAG	Z	2	10	14,14,15	0.55	0	17,19,21	0.93	1 (5%)
9	NAG	a	1	9,3	14,14,15	0.52	0	17,19,21	1.01	1 (5%)
9	NAG	a	2	9	14,14,15	0.61	0	17,19,21	1.05	1 (5%)
9	MAN	a	3	9	11,11,12	0.65	0	15,15,17	0.99	1 (6%)
11	NAG	b	1	11,3	14,14,15	0.63	0	17,19,21	1.04	2 (11%)
11	NAG	b	2	11	14,14,15	0.71	0	17,19,21	1.39	3 (17%)
11	MAN	b	3	11	11,11,12	0.57	0	15,15,17	1.91	5 (33%)
11	MAN	b	4	11	11,11,12	0.61	0	15,15,17	1.15	3 (20%)
11	MAN	b	5	11	11,11,12	0.76	0	15,15,17	1.64	3 (20%)
12	NAG	c	1	3,12	14,14,15	0.49	0	17,19,21	0.89	0
12	NAG	c	2	12	14,14,15	0.61	0	17,19,21	1.06	1 (5%)
12	BMA	c	3	12	11,11,12	0.65	0	15,15,17	0.90	1 (6%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	NAG	O	1	1,5	1/1/5/7	2/6/23/26	0/1/1/1
5	NAG	O	2	5	-	4/6/23/26	0/1/1/1
5	BMA	O	3	5	-	2/2/19/22	0/1/1/1
5	BMA	O	4	5	-	0/2/19/22	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	NAG	R	1	5,2	-	3/6/23/26	0/1/1/1
5	NAG	R	2	5	-	2/6/23/26	0/1/1/1
5	BMA	R	3	5	-	2/2/19/22	0/1/1/1
5	BMA	R	4	5	-	0/2/19/22	0/1/1/1
6	NAG	S	1	1,6	-	3/6/23/26	0/1/1/1
6	NAG	S	2	6	-	4/6/23/26	0/1/1/1
6	BMA	S	3	6	-	2/2/19/22	0/1/1/1
6	BMA	S	4	6	-	0/2/19/22	0/1/1/1
6	BMA	S	5	6	-	0/2/19/22	0/1/1/1
5	NAG	T	1	5,2	-	3/6/23/26	0/1/1/1
5	NAG	T	2	5	-	2/6/23/26	0/1/1/1
5	BMA	T	3	5	-	2/2/19/22	0/1/1/1
5	BMA	T	4	5	-	0/2/19/22	0/1/1/1
5	NAG	U	1	1,5	-	3/6/23/26	0/1/1/1
5	NAG	U	2	5	-	2/6/23/26	0/1/1/1
5	BMA	U	3	5	-	2/2/19/22	0/1/1/1
5	BMA	U	4	5	-	0/2/19/22	0/1/1/1
7	NAG	V	1	7,2	1/1/5/7	3/6/23/26	0/1/1/1
7	NAG	V	2	7	-	4/6/23/26	0/1/1/1
7	BMA	V	3	7	-	2/2/19/22	0/1/1/1
7	BMA	V	4	7	-	2/2/19/22	0/1/1/1
7	BMA	V	5	7	-	1/2/19/22	0/1/1/1
7	BMA	V	6	7	-	0/2/19/22	0/1/1/1
6	NAG	W	1	1,6	-	3/6/23/26	0/1/1/1
6	NAG	W	2	6	-	2/6/23/26	0/1/1/1
6	BMA	W	3	6	-	0/2/19/22	0/1/1/1
6	BMA	W	4	6	-	0/2/19/22	0/1/1/1
6	BMA	W	5	6	-	0/2/19/22	0/1/1/1
8	NAG	X	1	2,8	-	3/6/23/26	0/1/1/1
8	NAG	X	2	8	-	2/6/23/26	0/1/1/1
8	MAN	X	3	8	1/1/4/5	2/2/19/22	0/1/1/1
8	MAN	X	4	8	1/1/4/5	2/2/19/22	0/1/1/1
9	NAG	Y	1	9,3	-	3/6/23/26	0/1/1/1
9	NAG	Y	2	9	-	2/6/23/26	0/1/1/1
9	MAN	Y	3	9	1/1/4/5	0/2/19/22	0/1/1/1
10	NAG	Z	1	3,10	1/1/5/7	3/6/23/26	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
10	NAG	Z	2	10	-	2/6/23/26	0/1/1/1
9	NAG	a	1	9,3	-	3/6/23/26	0/1/1/1
9	NAG	a	2	9	-	2/6/23/26	0/1/1/1
9	MAN	a	3	9	1/1/4/5	0/2/19/22	0/1/1/1
11	NAG	b	1	11,3	1/1/5/7	4/6/23/26	0/1/1/1
11	NAG	b	2	11	-	4/6/23/26	0/1/1/1
11	MAN	b	3	11	1/1/4/5	0/2/19/22	0/1/1/1
11	MAN	b	4	11	1/1/4/5	0/2/19/22	0/1/1/1
11	MAN	b	5	11	1/1/4/5	2/2/19/22	0/1/1/1
12	NAG	c	1	3,12	-	3/6/23/26	0/1/1/1
12	NAG	c	2	12	-	2/6/23/26	0/1/1/1
12	BMA	c	3	12	-	0/2/19/22	0/1/1/1

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	U	4	BMA	O5-C1	-2.34	1.40	1.43
7	V	4	BMA	O5-C1	-2.22	1.40	1.43

The worst 5 of 115 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
6	W	4	BMA	C1-C2-C3	-10.68	96.54	109.67
6	W	4	BMA	C3-C4-C5	-7.10	97.58	110.24
5	R	2	NAG	C1-O5-C5	7.08	121.79	112.19
6	W	4	BMA	C1-O5-C5	-6.98	102.74	112.19
6	W	4	BMA	O5-C5-C6	6.86	117.96	107.20

5 of 11 chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
5	O	1	NAG	C1
7	V	1	NAG	C1
8	X	3	MAN	C1
8	X	4	MAN	C1
9	Y	3	MAN	C1

5 of 94 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	O	2	NAG	C8-C7-N2-C2
5	O	2	NAG	O7-C7-N2-C2
5	R	1	NAG	C8-C7-N2-C2
5	R	1	NAG	O7-C7-N2-C2
5	T	1	NAG	C8-C7-N2-C2

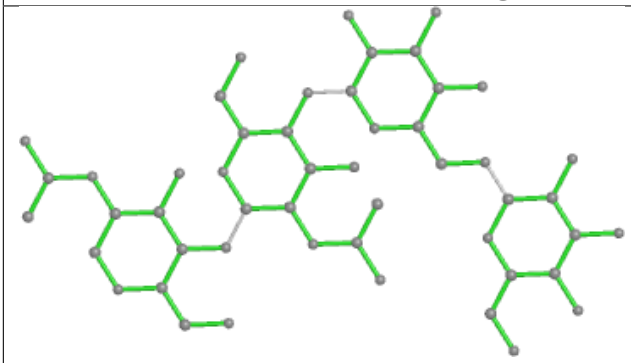
There are no ring outliers.

23 monomers are involved in 18 short contacts:

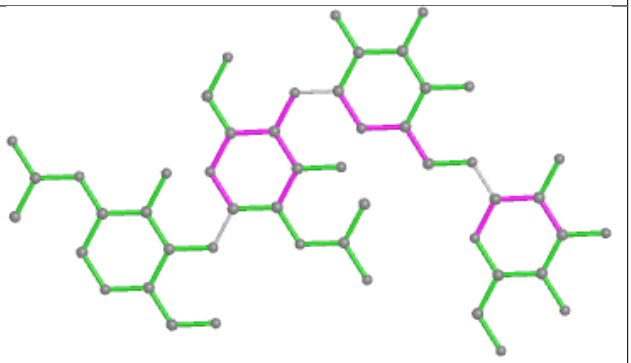
Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	O	1	NAG	1	0
7	V	6	BMA	1	0
6	S	2	NAG	1	0
6	W	4	BMA	2	0
8	X	4	MAN	1	0
8	X	3	MAN	1	0
6	W	1	NAG	1	0
6	W	2	NAG	3	0
9	Y	2	NAG	2	0
6	W	3	BMA	2	0
6	S	1	NAG	1	0
5	U	3	BMA	1	0
8	X	2	NAG	1	0
7	V	3	BMA	1	0
5	O	2	NAG	1	0
5	T	2	NAG	1	0
5	T	1	NAG	1	0
9	Y	1	NAG	1	0
5	U	1	NAG	2	0
5	U	4	BMA	1	0
5	U	2	NAG	1	0
7	V	4	BMA	2	0
5	R	1	NAG	1	0

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

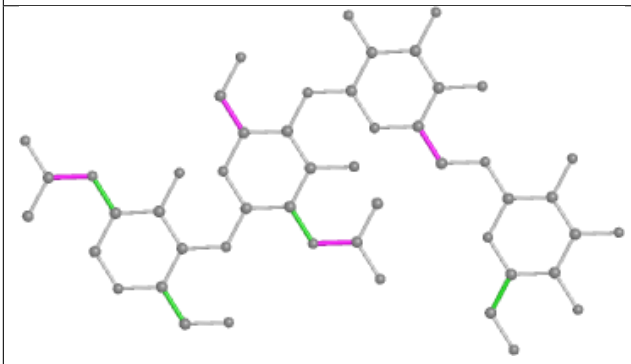
Oligosaccharide Chain O



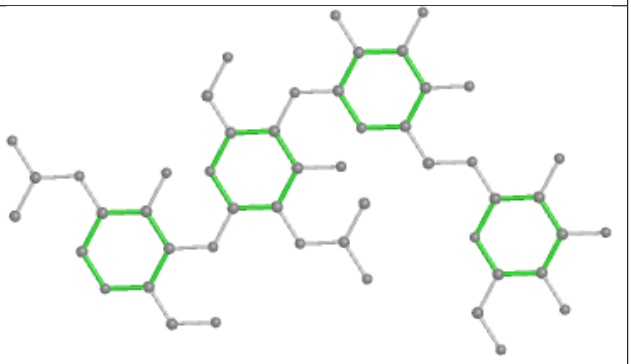
Bond lengths



Bond angles

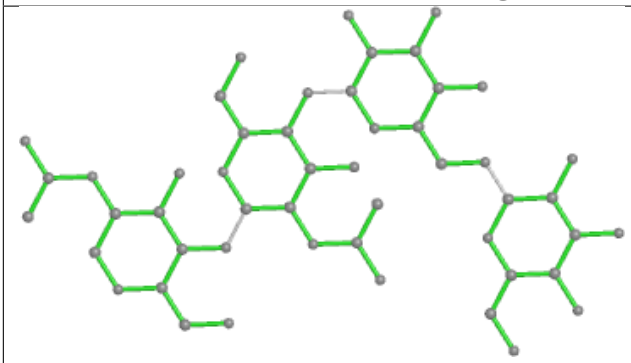


Torsions

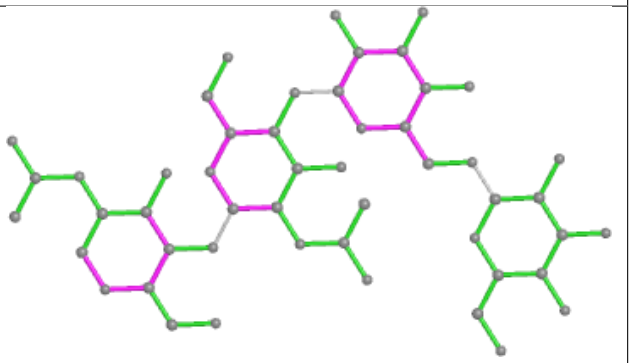


Rings

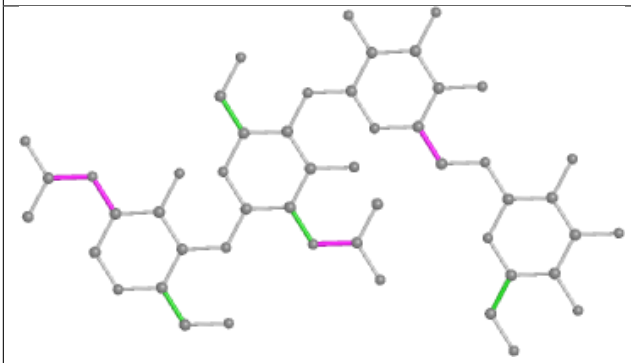
Oligosaccharide Chain R



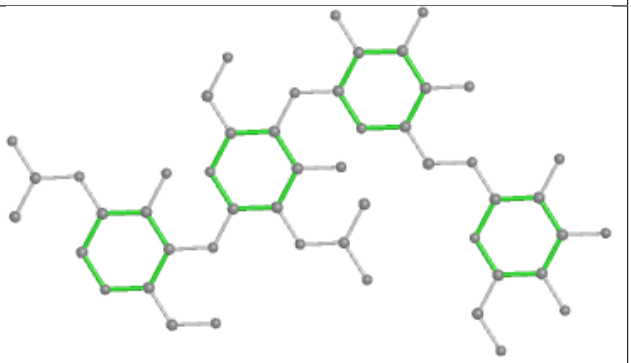
Bond lengths



Bond angles

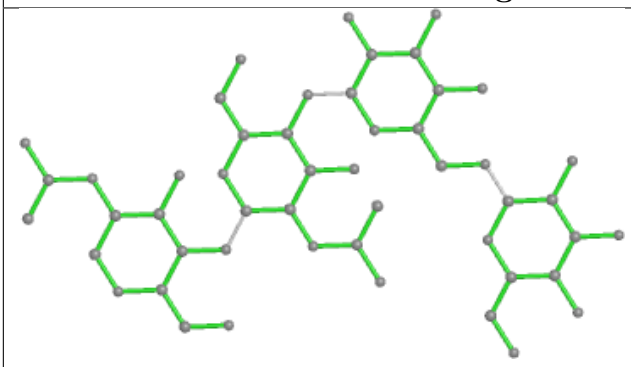


Torsions

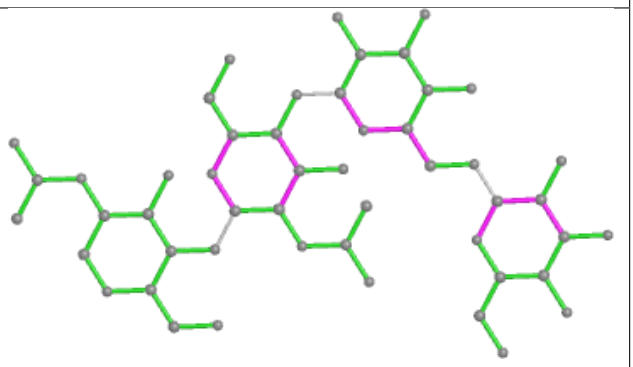


Rings

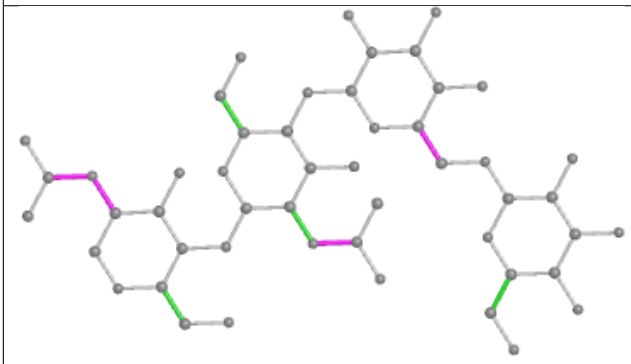
Oligosaccharide Chain T



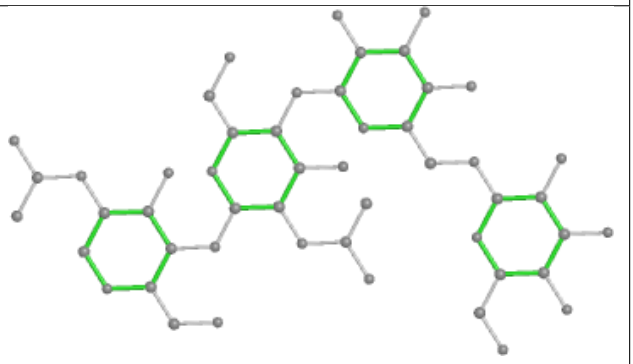
Bond lengths



Bond angles

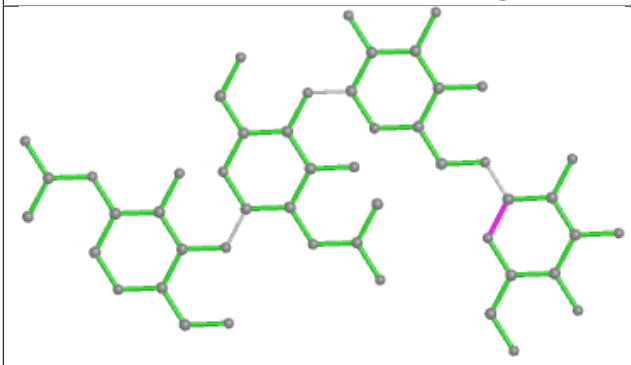


Torsions

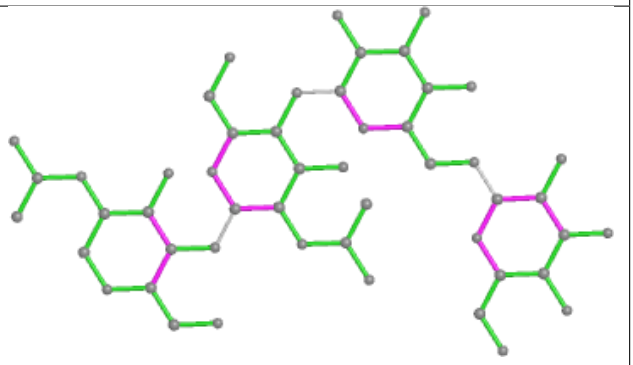


Rings

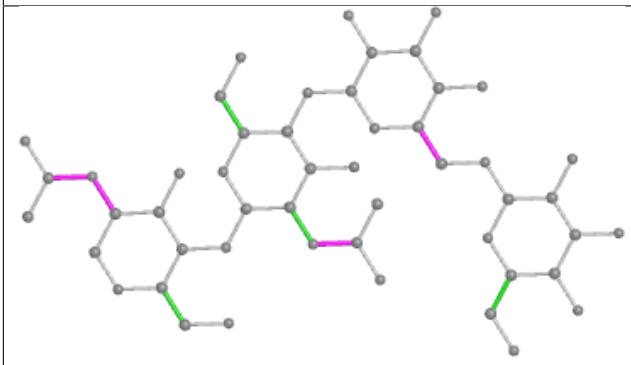
Oligosaccharide Chain U



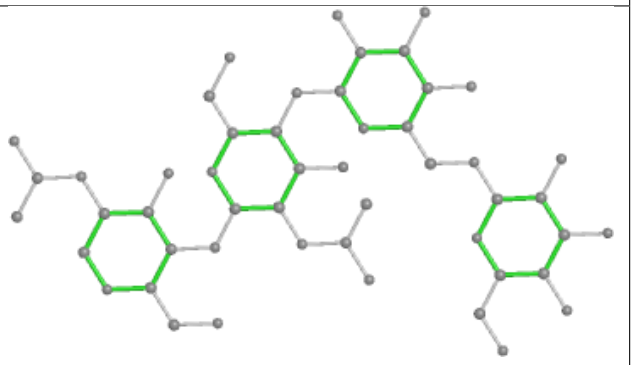
Bond lengths



Bond angles

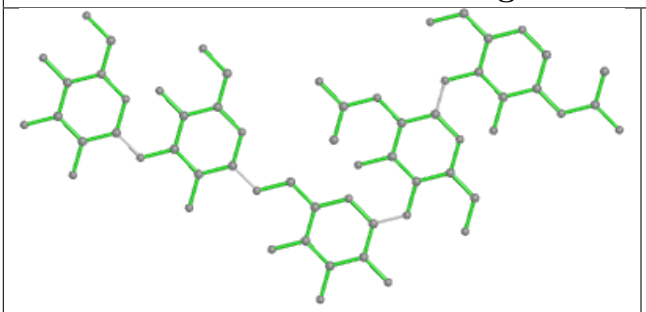


Torsions

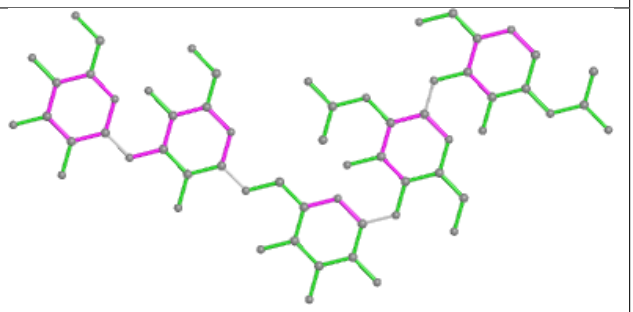


Rings

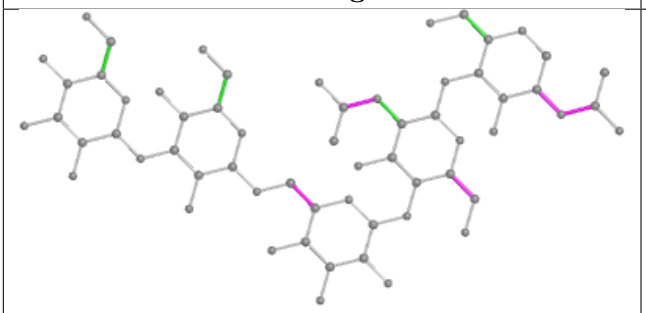
Oligosaccharide Chain S



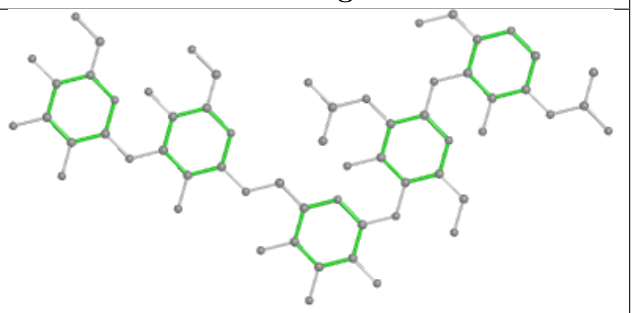
Bond lengths



Bond angles

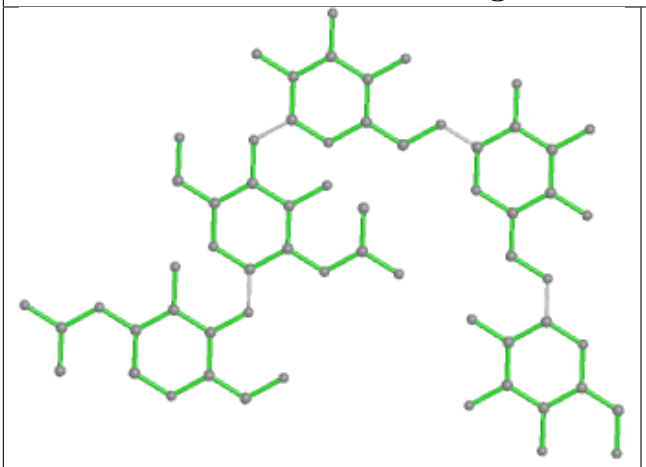


Torsions

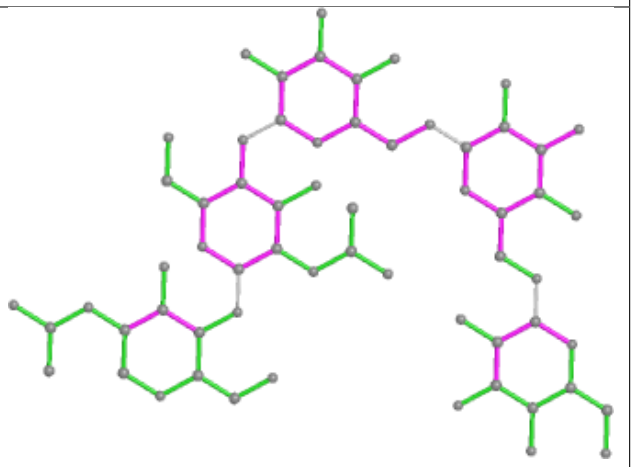


Rings

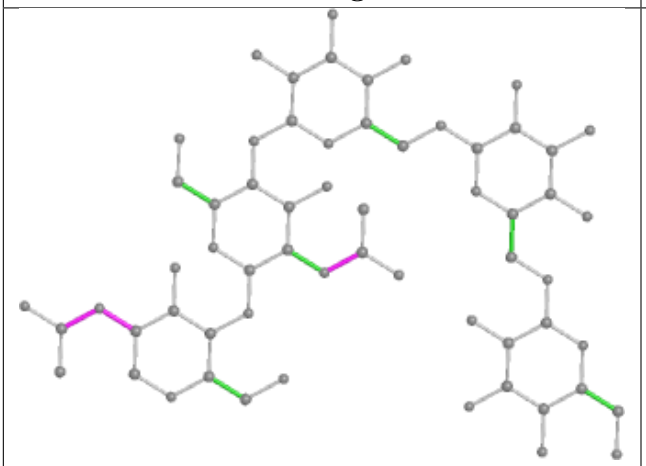
Oligosaccharide Chain W



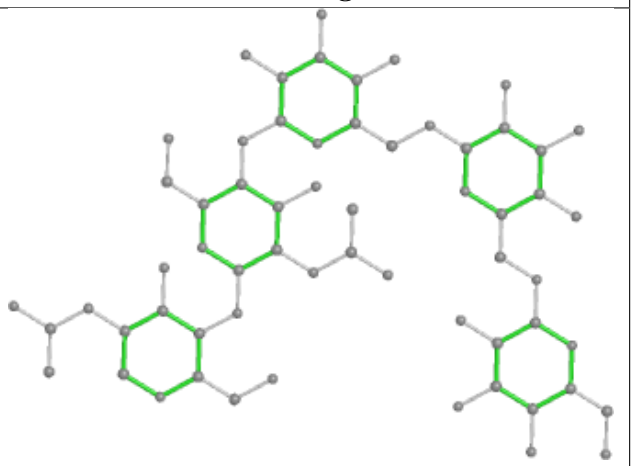
Bond lengths



Bond angles

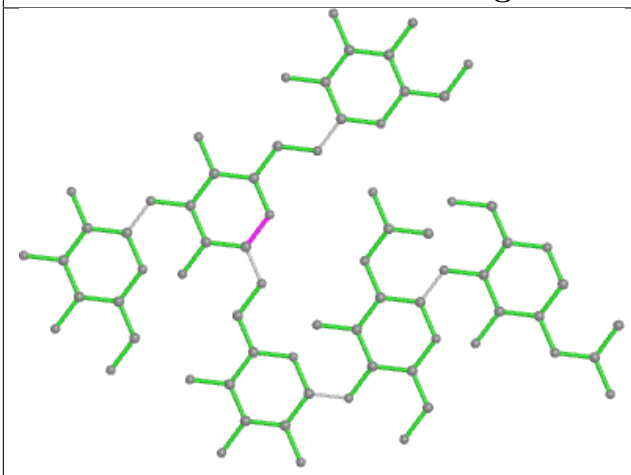


Torsions

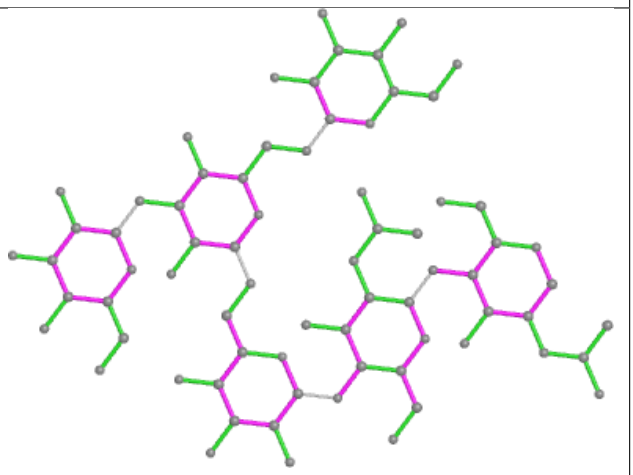


Rings

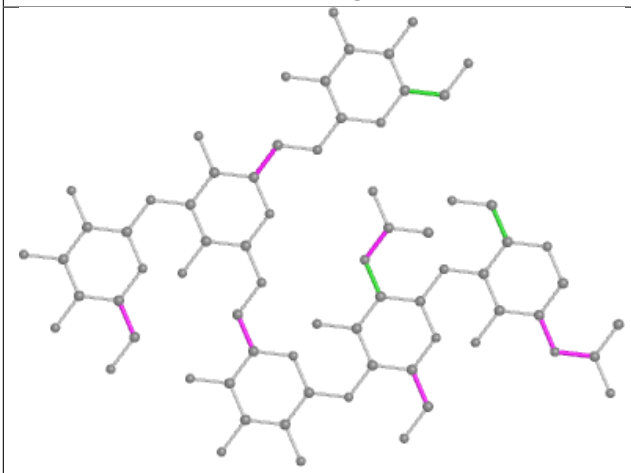
Oligosaccharide Chain V



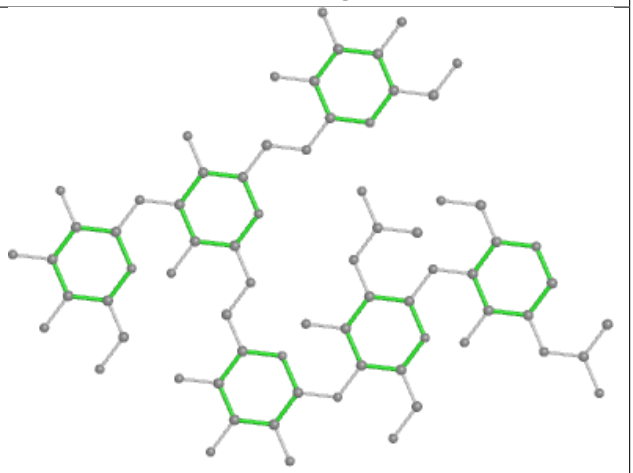
Bond lengths



Bond angles

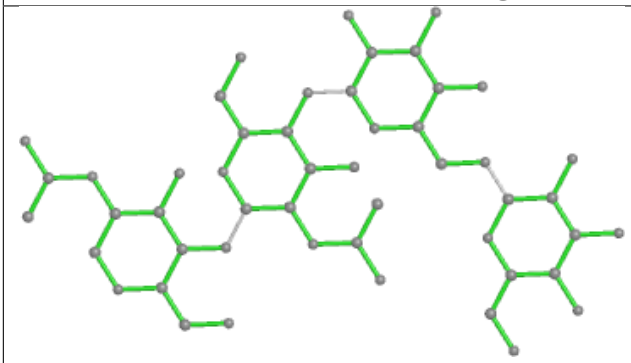


Torsions

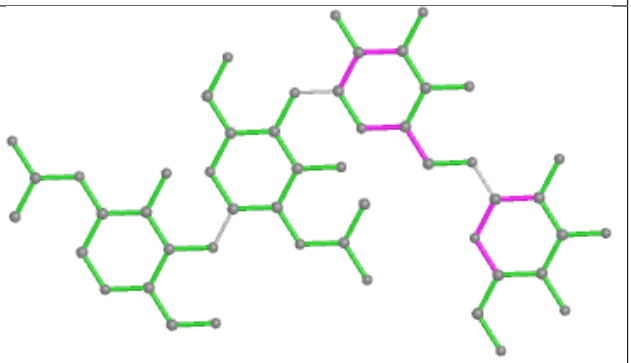


Rings

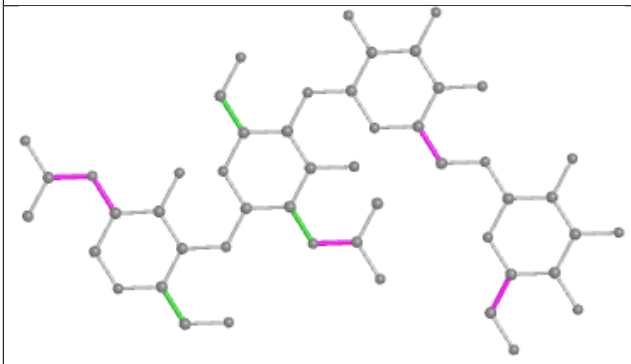
Oligosaccharide Chain X



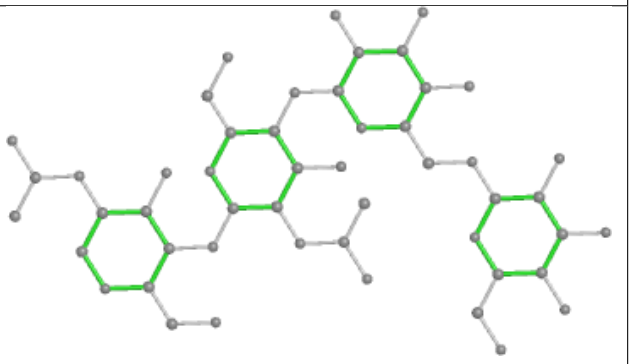
Bond lengths



Bond angles

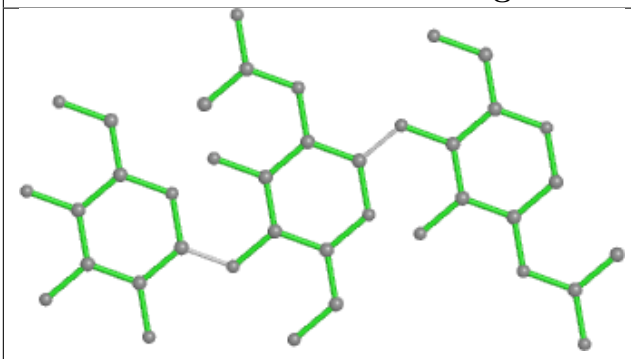


Torsions

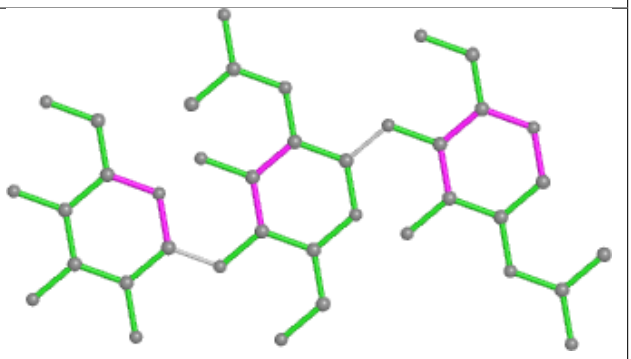


Rings

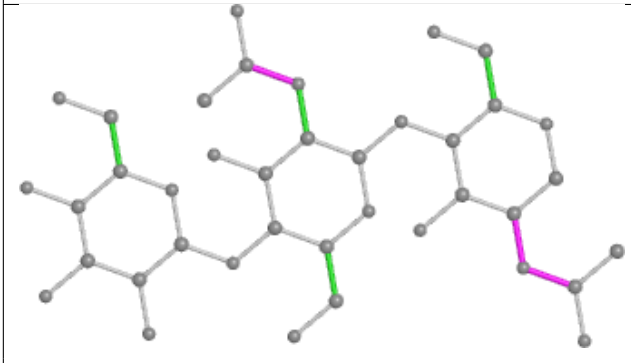
Oligosaccharide Chain Y



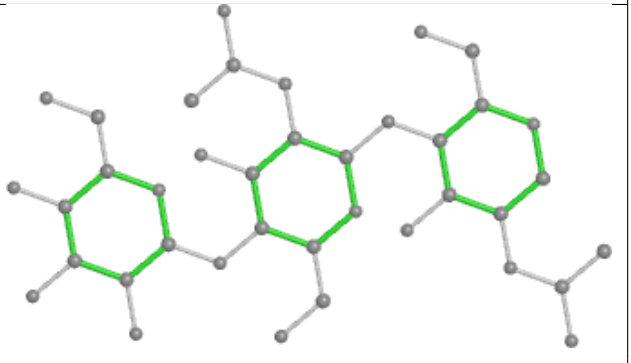
Bond lengths



Bond angles

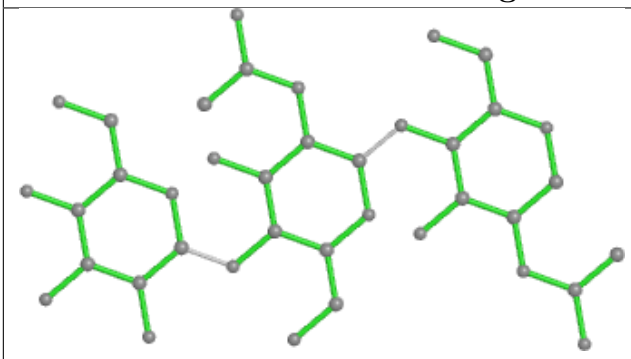


Torsions

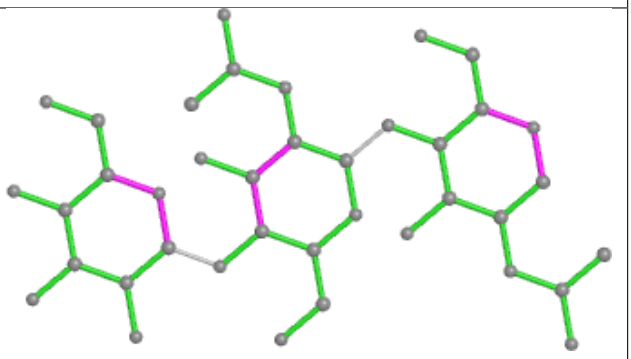


Rings

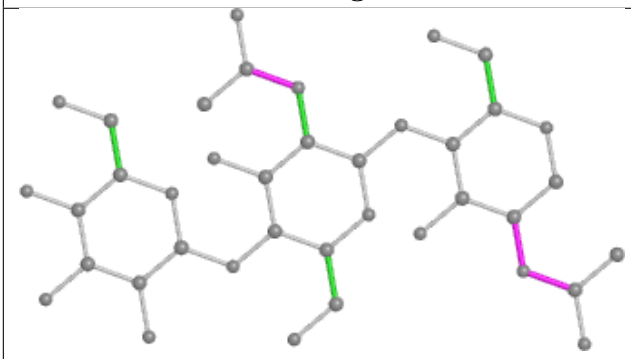
Oligosaccharide Chain a



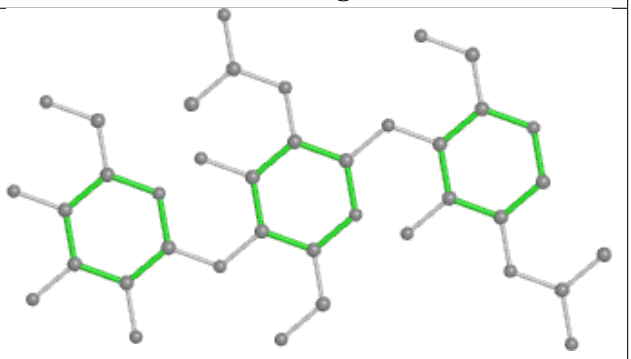
Bond lengths



Bond angles

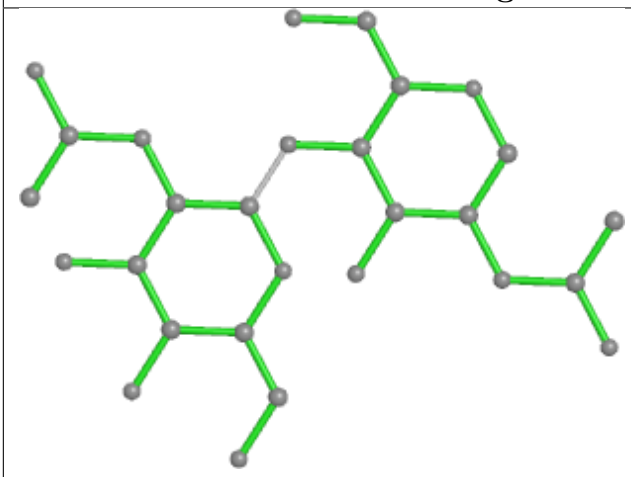


Torsions

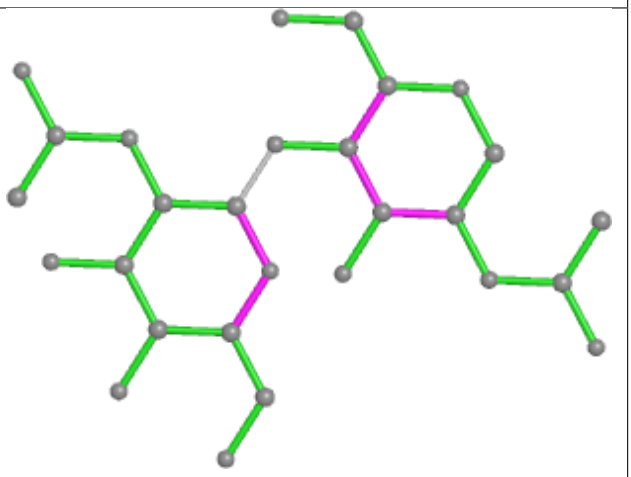


Rings

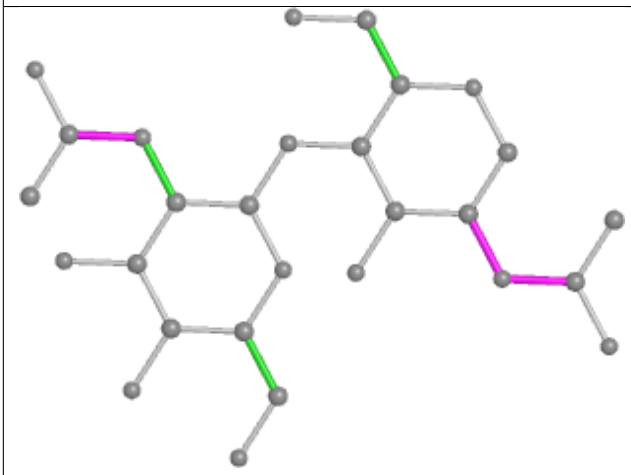
Oligosaccharide Chain Z



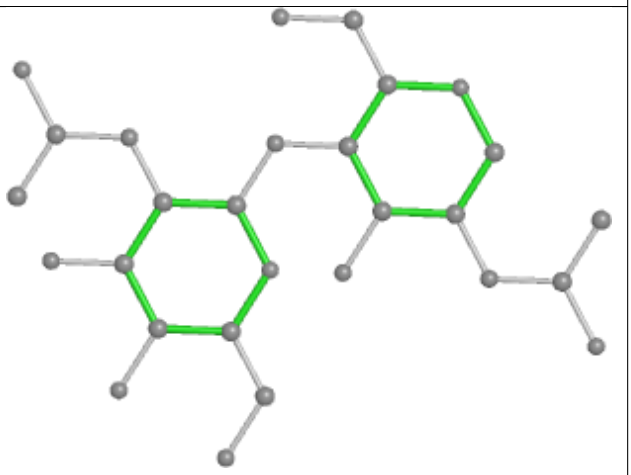
Bond lengths



Bond angles

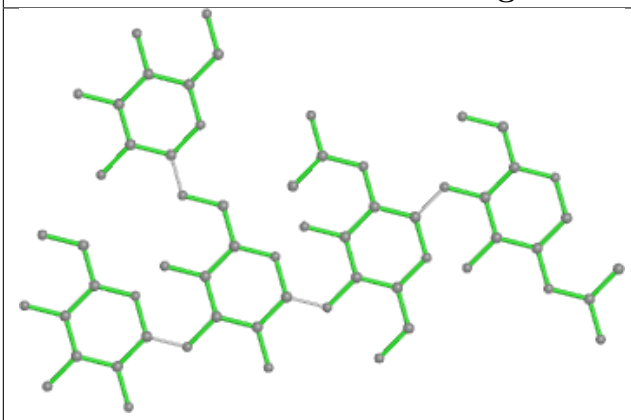


Torsions

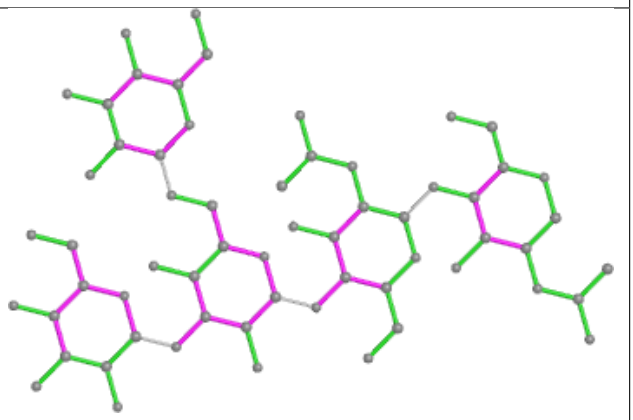


Rings

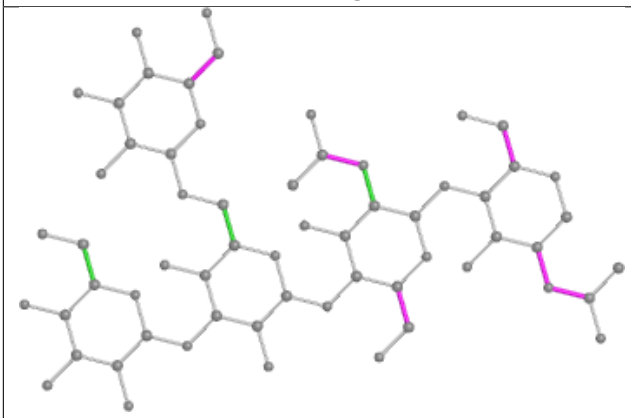
Oligosaccharide Chain b



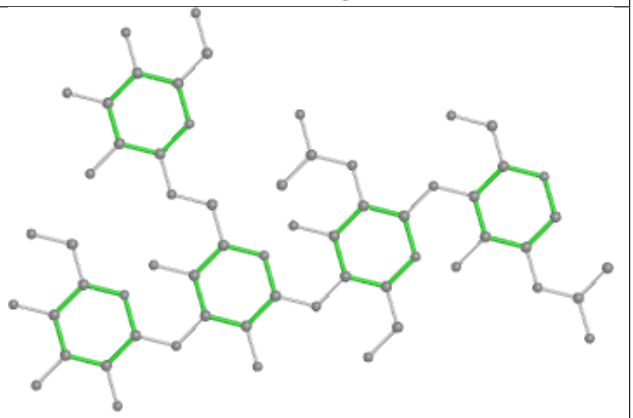
Bond lengths



Bond angles

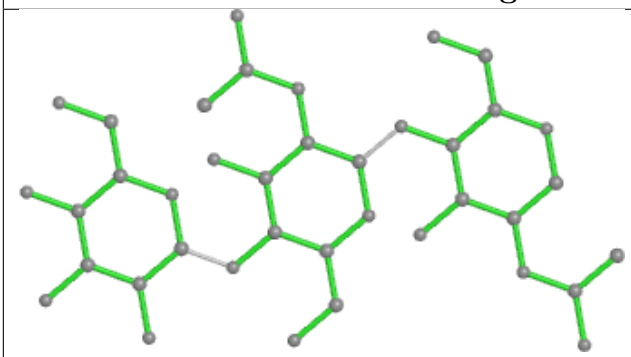


Torsions

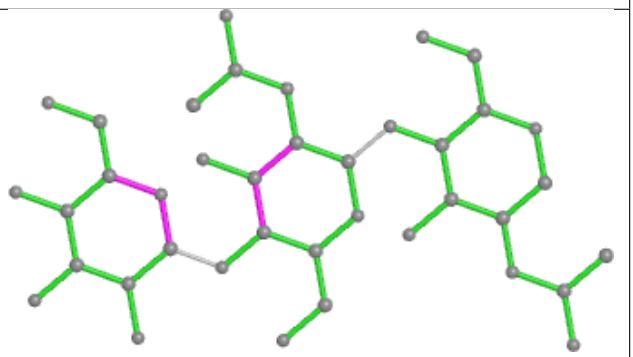


Rings

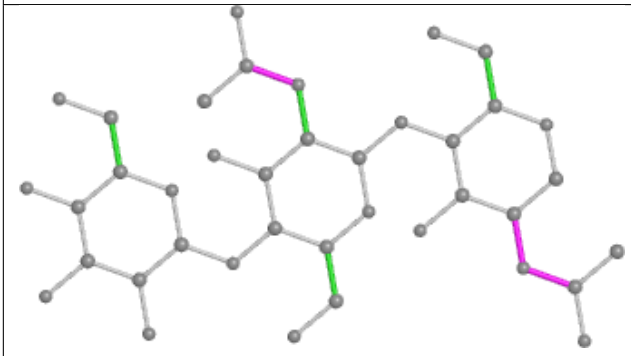
Oligosaccharide Chain c



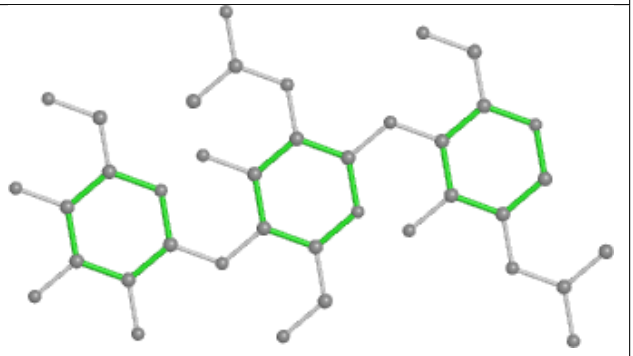
Bond lengths



Bond angles



Torsions



Rings

5.6 Ligand geometry (i)

Of 9 ligands modelled in this entry, 4 are monoatomic - leaving 5 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	$\#\|Z\| > 2$
14	MAN	G	1651	-	11,11,12	0.83	1 (9%)	15,15,17	1.71	4 (26%)
16	NAG	K	1749	3	14,14,15	0.52	0	17,19,21	1.79	2 (11%)
13	BMA	B	2646	-	11,11,12	0.74	0	15,15,17	1.42	3 (20%)
16	NAG	L	1746	3	14,14,15	0.52	0	17,19,21	0.69	0
13	BMA	K	1747	-	11,11,12	0.81	0	15,15,17	1.93	4 (26%)

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
14	MAN	G	1651	-	-	0/2/19/22	0/1/1/1
16	NAG	K	1749	3	1/1/5/7	3/6/23/26	0/1/1/1
13	BMA	B	2646	-	-	0/2/19/22	0/1/1/1
16	NAG	L	1746	3	1/1/5/7	3/6/23/26	0/1/1/1
13	BMA	K	1747	-	-	0/2/19/22	0/1/1/1

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
14	G	1651	MAN	O5-C1	-2.03	1.40	1.43

The worst 5 of 13 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
13	K	1747	BMA	C1-O5-C5	-5.03	105.37	112.19
16	K	1749	NAG	O5-C1-C2	-4.75	103.78	111.29
14	G	1651	MAN	C1-C2-C3	-4.04	104.70	109.67
16	K	1749	NAG	C1-C2-N2	3.83	117.04	110.49

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
13	K	1747	BMA	C1-C2-C3	-3.78	105.01	109.67

All (2) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
16	K	1749	NAG	C1
16	L	1746	NAG	C1

5 of 6 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
16	K	1749	NAG	C8-C7-N2-C2
16	K	1749	NAG	O7-C7-N2-C2
16	L	1746	NAG	C8-C7-N2-C2
16	L	1746	NAG	O7-C7-N2-C2
16	K	1749	NAG	C1-C2-N2-C7

There are no ring outliers.

2 monomers are involved in 4 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
14	G	1651	MAN	1	0
16	K	1749	NAG	3	0

5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
2	H	2

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	H	1500:LYS	C	1501:SER	N	3.64
1	H	988:CYS	C	989:GLY	N	2.97

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	638/645 (98%)	0.24	11 (1%)	70	60	87, 142, 190, 237	0
1	C	638/645 (98%)	0.27	10 (1%)	72	62	80, 127, 176, 228	0
1	E	638/645 (98%)	0.28	12 (1%)	66	57	84, 142, 196, 245	0
1	G	638/645 (98%)	0.53	56 (8%)	10	7	93, 180, 241, 267	0
2	B	901/915 (98%)	0.17	12 (1%)	77	68	91, 167, 229, 260	0
2	D	901/915 (98%)	0.23	13 (1%)	75	66	81, 155, 216, 266	0
2	F	900/915 (98%)	0.40	49 (5%)	25	21	96, 179, 284, 329	0
2	H	605/915 (66%)	0.38	28 (4%)	32	26	98, 162, 231, 294	0
3	I	507/507 (100%)	0.17	4 (0%)	86	79	93, 142, 197, 240	0
3	J	507/507 (100%)	0.15	10 (1%)	65	55	127, 170, 220, 261	0
3	K	507/507 (100%)	0.20	21 (4%)	37	29	132, 183, 230, 284	0
3	L	507/507 (100%)	0.15	4 (0%)	86	79	101, 144, 194, 239	0
4	M	84/92 (91%)	0.34	2 (2%)	59	48	87, 110, 186, 221	0
4	N	84/92 (91%)	0.33	3 (3%)	42	33	97, 116, 189, 227	0
4	P	84/92 (91%)	0.23	2 (2%)	59	48	100, 124, 176, 211	0
4	Q	84/92 (91%)	0.20	1 (1%)	79	70	100, 119, 186, 200	0
All	All	8223/8636 (95%)	0.27	238 (2%)	51	40	80, 154, 228, 329	0

The worst 5 of 238 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	G	421	ALA	8.9
1	G	529	VAL	7.9
1	G	509	LEU	7.7
1	G	437	SER	7.0
1	C	645	ALA	6.4

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
5	BMA	R	4	11/12	0.29	0.30	237,239,240,241	0
5	BMA	R	3	11/12	0.56	0.23	218,220,222,223	0
6	BMA	S	4	11/12	0.58	0.21	235,237,239,240	0
6	BMA	W	5	11/12	0.62	0.41	229,231,232,232	0
7	BMA	V	6	11/12	0.66	0.39	214,215,217,217	0
8	MAN	X	4	11/12	0.67	0.37	234,236,237,238	0
10	NAG	Z	2	14/15	0.70	0.37	222,223,224,224	0
6	BMA	S	3	11/12	0.72	0.19	219,220,222,223	0
9	MAN	a	3	11/12	0.73	0.21	206,210,211,212	0
9	MAN	Y	3	11/12	0.73	0.28	205,207,208,209	0
6	BMA	W	3	11/12	0.74	0.32	247,249,250,251	0
7	BMA	V	4	11/12	0.75	0.17	248,249,249,250	0
11	MAN	b	3	11/12	0.75	0.16	249,252,253,254	0
12	BMA	c	3	11/12	0.75	0.21	197,201,202,202	0
6	BMA	W	4	11/12	0.76	0.18	226,228,229,230	0
7	BMA	V	5	11/12	0.76	0.23	221,222,224,224	0
6	BMA	S	5	11/12	0.76	0.23	231,233,235,235	0
5	BMA	T	3	11/12	0.77	0.19	220,221,223,223	0
6	NAG	S	1	14/15	0.79	0.28	163,191,192,193	0
6	NAG	S	2	14/15	0.80	0.21	200,202,203,203	0
10	NAG	Z	1	14/15	0.81	0.33	198,225,227,227	0
5	BMA	U	4	11/12	0.81	0.17	209,212,214,215	0
7	BMA	V	3	11/12	0.83	0.18	232,233,234,234	0
5	NAG	O	2	14/15	0.84	0.19	199,200,201,203	0
5	NAG	U	1	14/15	0.84	0.17	174,204,206,206	0
8	MAN	X	3	11/12	0.84	0.19	229,230,231,232	0
6	NAG	W	1	14/15	0.84	0.14	198,201,208,215	0
11	MAN	b	4	11/12	0.84	0.22	230,232,235,235	0
5	BMA	O	3	11/12	0.84	0.17	212,214,215,216	0
11	NAG	b	2	14/15	0.85	0.16	196,199,201,202	0
9	NAG	a	2	14/15	0.85	0.18	177,179,180,180	0
5	BMA	T	4	11/12	0.85	0.13	229,232,233,234	0

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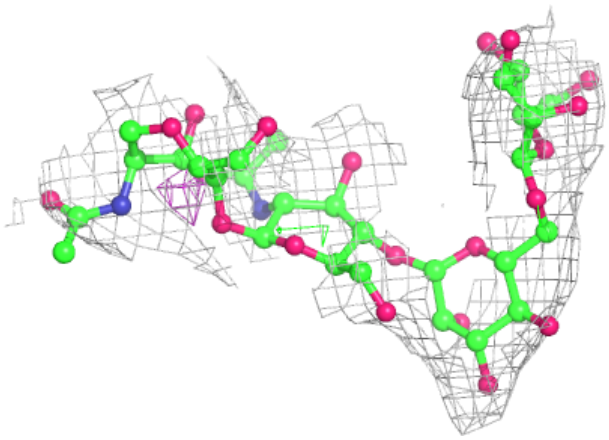
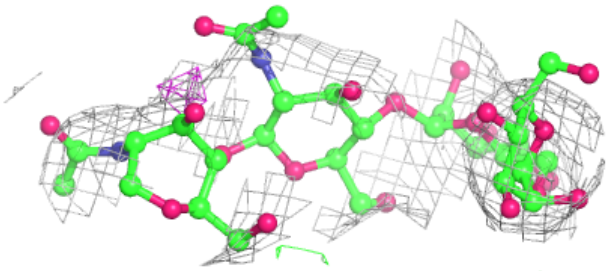
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
11	MAN	b	5	11/12	0.85	0.25	229,230,232,232	0
11	NAG	b	1	14/15	0.85	0.19	174,204,206,207	0
5	BMA	U	3	11/12	0.86	0.19	229,230,231,232	0
8	NAG	X	2	14/15	0.86	0.17	221,222,224,225	0
12	NAG	c	2	14/15	0.86	0.26	185,187,189,189	0
5	NAG	O	1	14/15	0.86	0.24	156,185,187,188	0
7	NAG	V	1	14/15	0.87	0.24	169,193,194,194	0
5	BMA	O	4	11/12	0.87	0.24	226,227,228,228	0
5	NAG	R	1	14/15	0.88	0.23	163,194,194,195	0
9	NAG	a	1	14/15	0.89	0.21	158,188,189,189	0
12	NAG	c	1	14/15	0.89	0.27	122,147,148,148	0
5	NAG	T	1	14/15	0.89	0.23	147,176,178,179	0
5	NAG	U	2	14/15	0.89	0.17	223,225,227,227	0
7	NAG	V	2	14/15	0.90	0.14	200,202,204,204	0
6	NAG	W	2	14/15	0.90	0.12	213,216,216,217	0
5	NAG	T	2	14/15	0.91	0.17	200,201,202,203	0
5	NAG	R	2	14/15	0.91	0.14	193,196,196,197	0
8	NAG	X	1	14/15	0.92	0.17	183,213,214,215	0
9	NAG	Y	1	14/15	0.93	0.26	122,149,151,152	0
9	NAG	Y	2	14/15	0.93	0.21	178,180,181,182	0

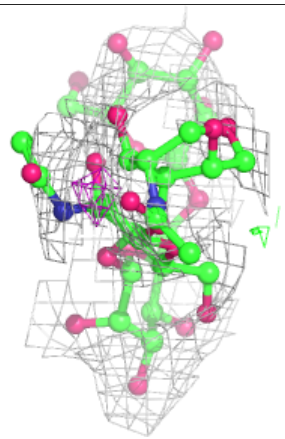
The following is a graphical depiction of the model fit to experimental electron density for oligosaccharide. Each fit is shown from different orientation to approximate a three-dimensional view.

Electron density around Chain O:

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

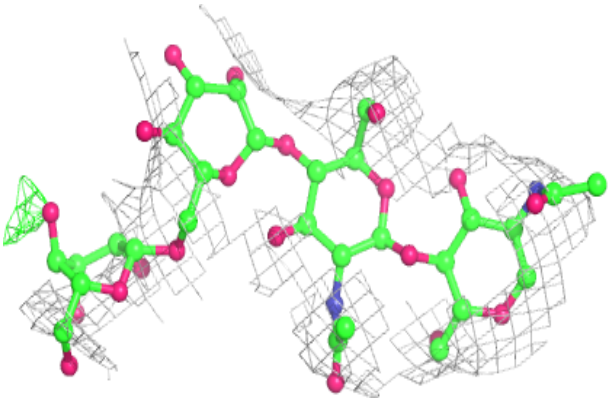


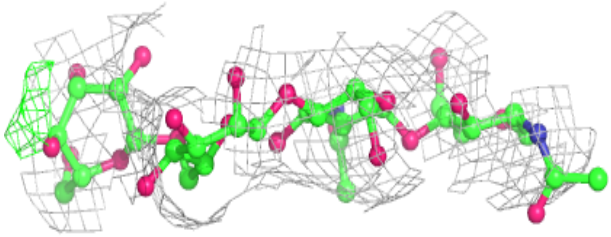


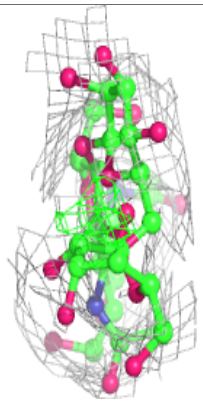


Electron density around Chain R:

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

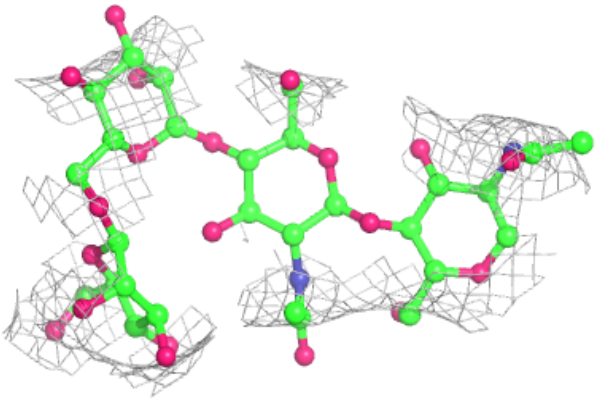


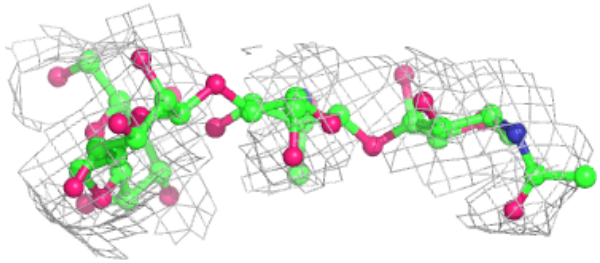


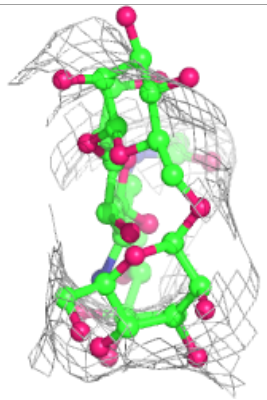


Electron density around Chain T:

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

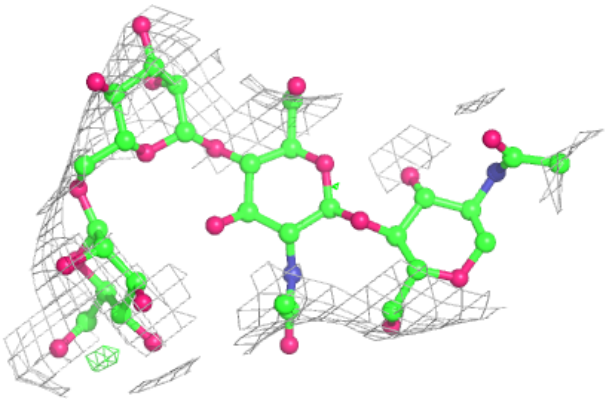


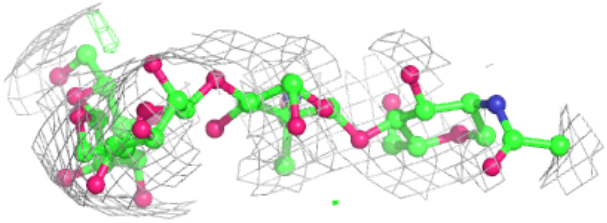


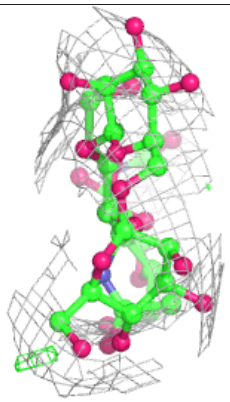


Electron density around Chain U:

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

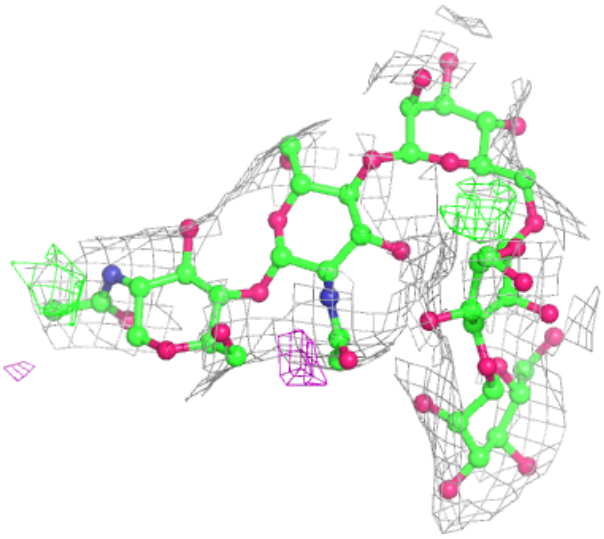


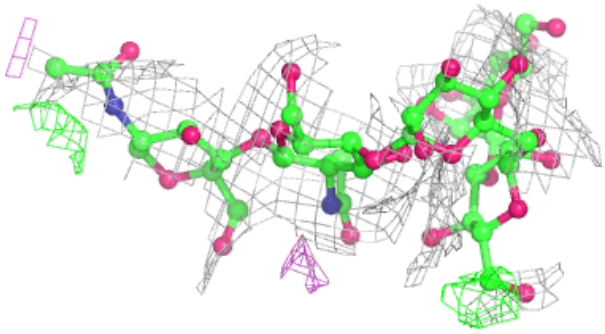


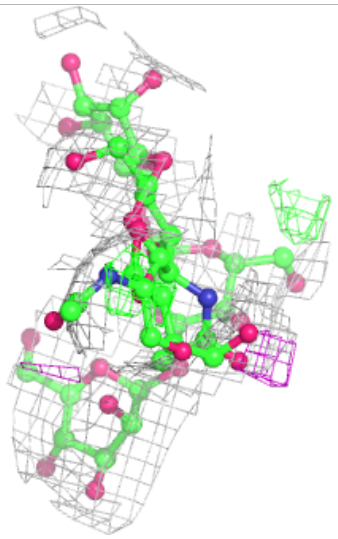


Electron density around Chain S:

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

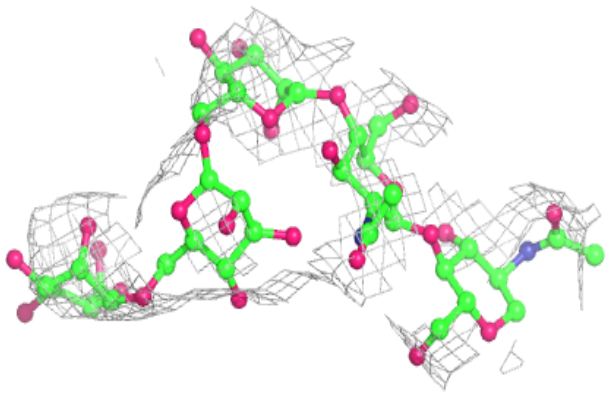


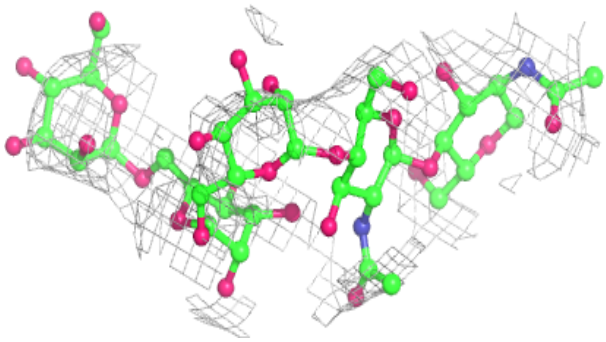


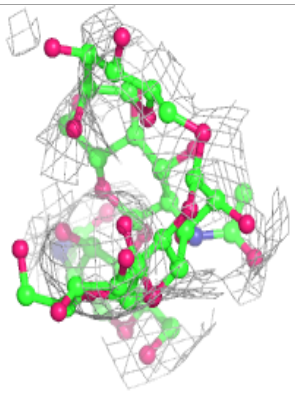


Electron density around Chain W:

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

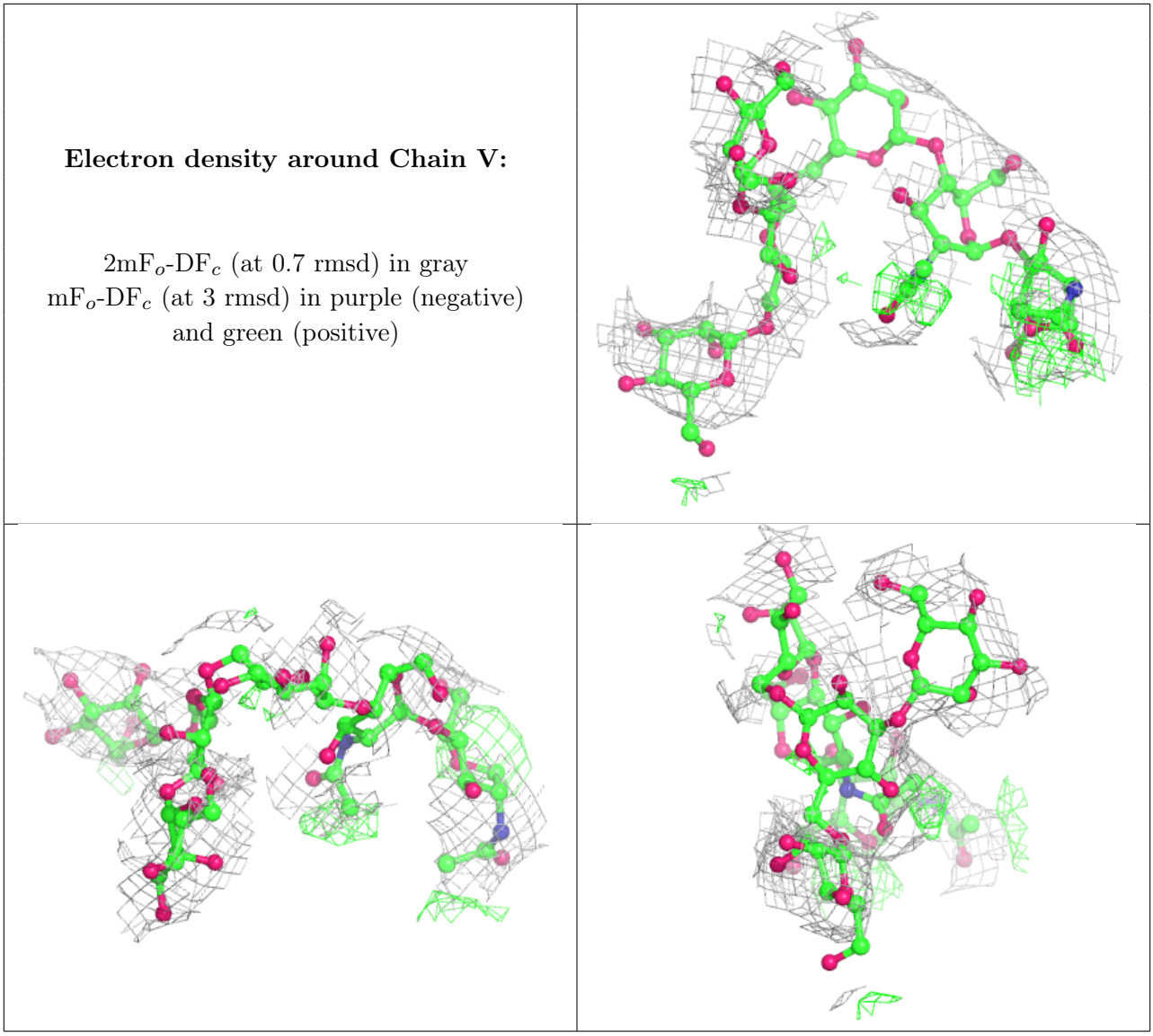






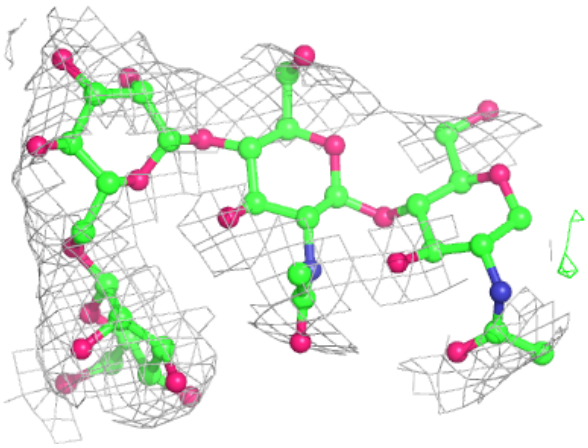
Electron density around Chain V:

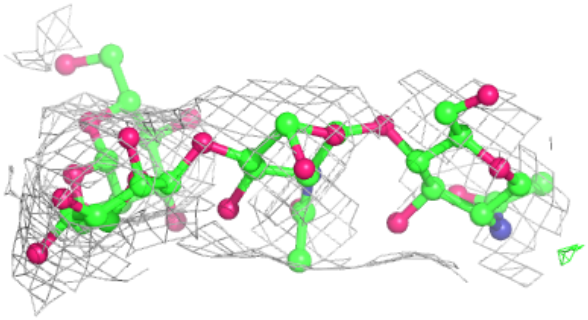
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

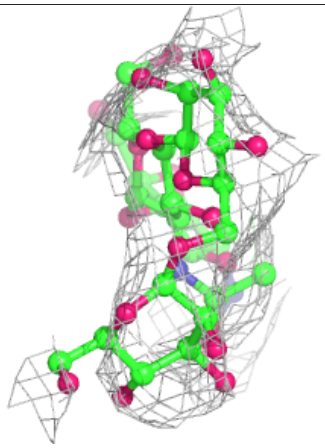


Electron density around Chain X:

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

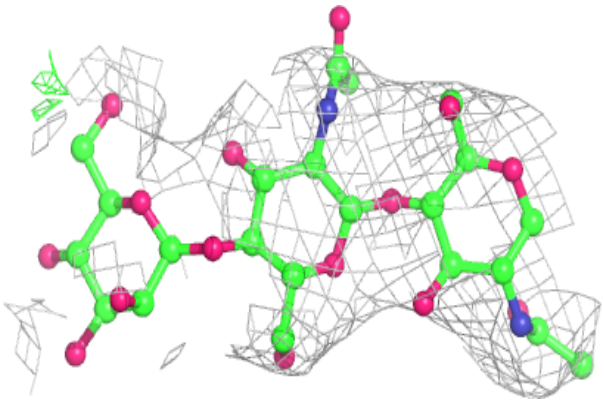


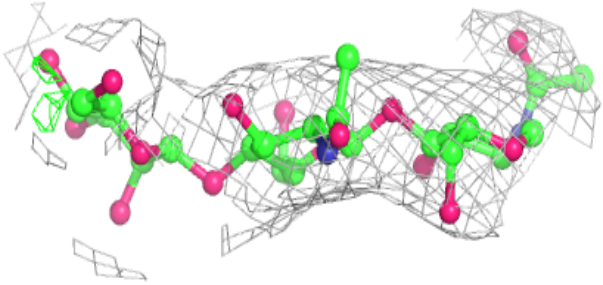


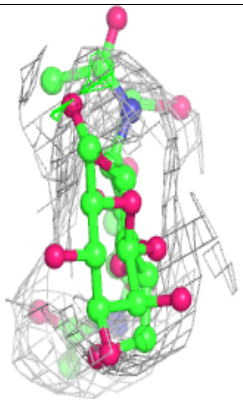


Electron density around Chain Y:

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

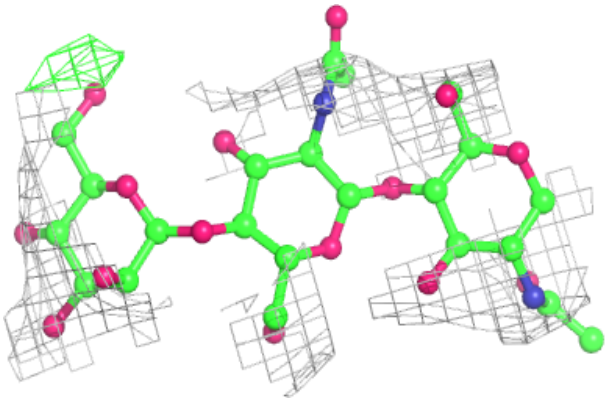


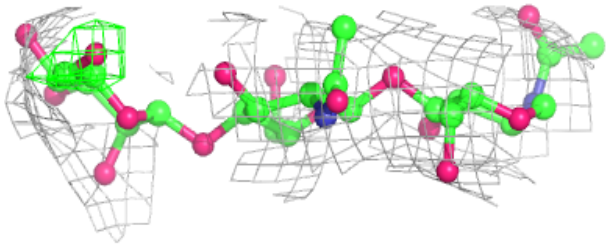


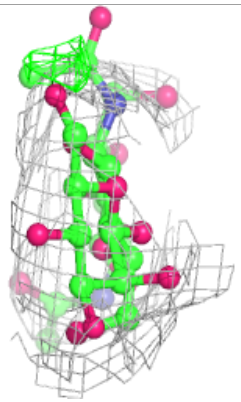


Electron density around Chain a:

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

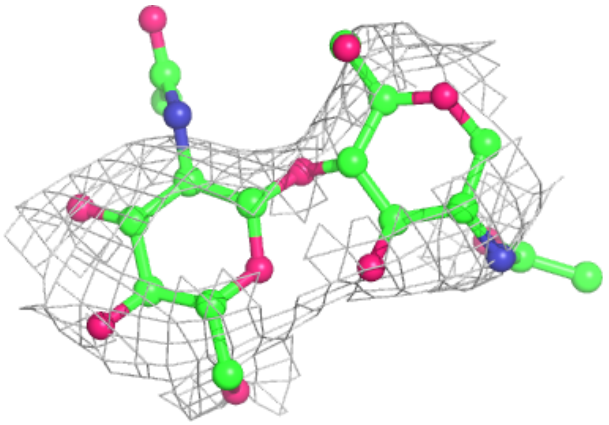


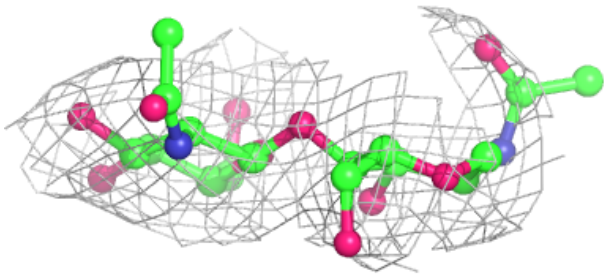


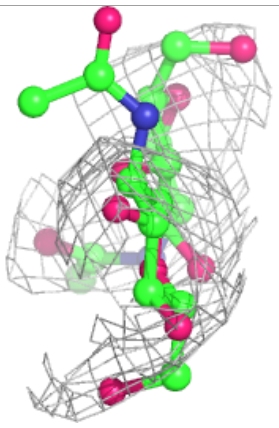


Electron density around Chain Z:

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

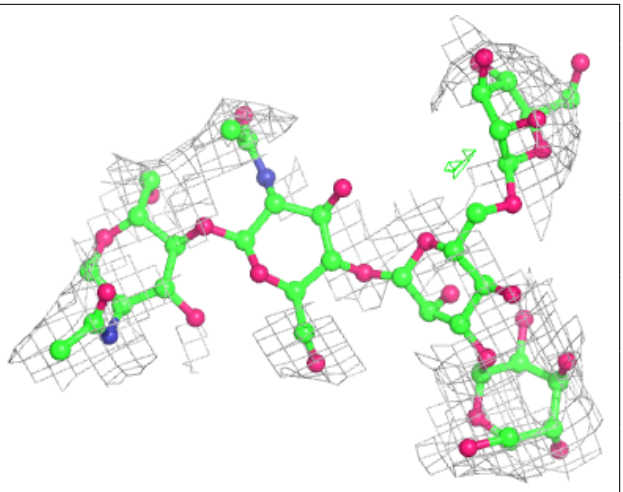


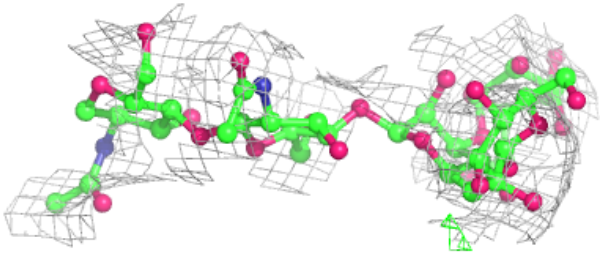


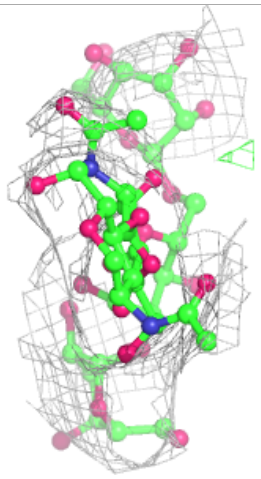


Electron density around Chain b:

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

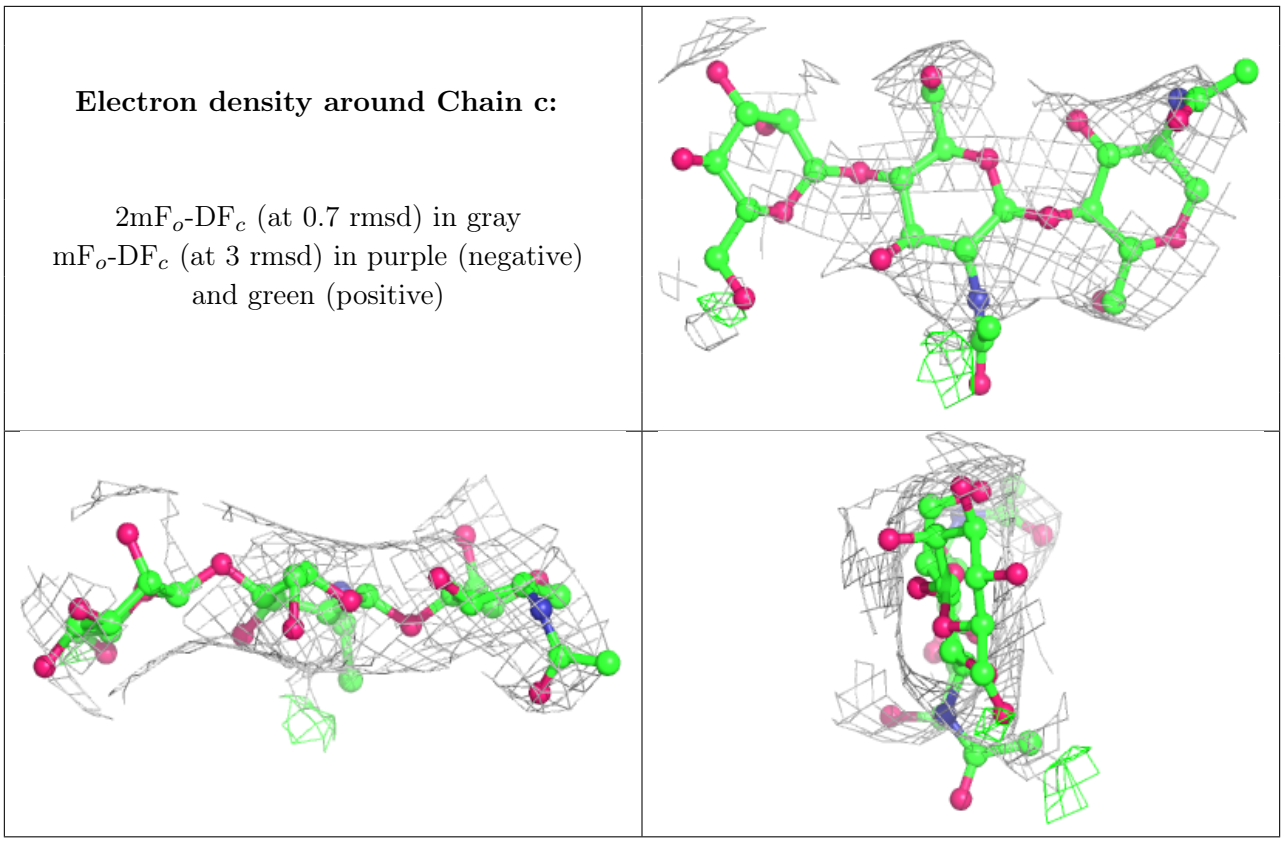






Electron density around Chain c:

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



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	MAN	G	1651	11/12	0.55	0.25	222,225,227,228	0
13	BMA	B	2646	11/12	0.65	0.29	198,200,200,201	0
15	MG	I	1742	1/1	0.71	0.20	120,120,120,120	0
16	NAG	K	1749	14/15	0.78	0.24	184,214,216,217	0
13	BMA	K	1747	11/12	0.79	0.35	194,195,196,196	0
15	MG	J	1742	1/1	0.80	0.14	148,148,148,148	0
15	MG	K	1742	1/1	0.87	0.14	138,138,138,138	0
16	NAG	L	1746	14/15	0.88	0.26	176,204,205,205	0
15	MG	L	1742	1/1	0.93	0.24	127,127,127,127	0

6.5 Other polymers

There are no such residues in this entry.