wwPDB X-ray Structure Validation Summary Report (i)

Aug 6, 2020 – 09:41 PM BST

PDB ID	:	5O32
Title	:	The structure of complement complex
Authors	:	Xue, X.; Wu, J.; Forneris, F.; Gros, P.
Deposited on	:	2017-05-23
Resolution	:	4.21 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 following versions of software and data (see references (1)) were used in the production of this report:

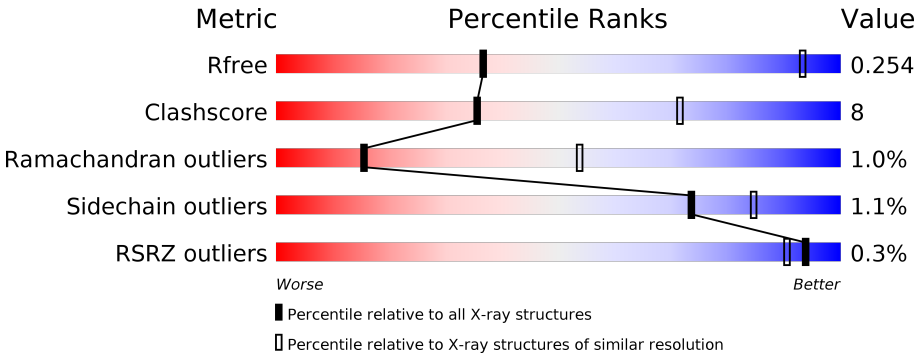
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.13.1
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.13.1

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 4.21 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	1005 (4.62-3.78)
Clashscore	141614	1044 (4.60-3.80)
Ramachandran outliers	138981	1000 (4.60-3.80)
Sidechain outliers	138945	1007 (4.62-3.78)
RSRZ outliers	127900	1063 (4.70-3.70)

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 on 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	80% 19%
1	E	645	82% 17%
2	B	915	78% 20%
2	F	915	78% 20%
3	C	383	% 78% 18%
3	G	383	% 81% 14%

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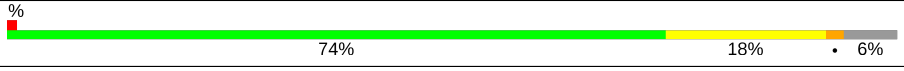
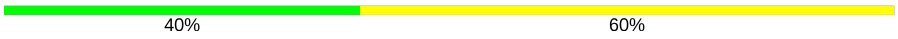
Mol	Chain	Length	Quality of chain
4	D	321	
4	H	321	
5	I	244	
5	J	244	
6	K	5	
6	M	5	
7	L	2	
7	N	2	

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
6	BMA	M	5	-	-	-	X
7	NAG	L	2	-	-	-	X
9	NAG	D	404	-	-	-	X
9	NAG	H	404	-	-	-	X

2 Entry composition

There are 10 unique types of molecules in this entry. The entry contains 39091 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.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	640	Total	C	N	O	S	0	0	0
			4992	3179	846	952	15			
1	E	640	Total	C	N	O	S	0	0	0
			4992	3179	846	952	15			

- Molecule 2 is a protein called Complement C3.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	903	Total	C	N	O	S	0	0	0
			7203	4565	1211	1389	38			
2	F	903	Total	C	N	O	S	0	0	0
			7203	4565	1211	1389	38			

- Molecule 3 is a protein called Complement factor H,Complement factor H.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	C	371	Total	C	N	O	S	0	0	0
			2940	1836	510	565	29			
3	G	371	Total	C	N	O	S	0	0	0
			2940	1836	510	565	29			

There are 26 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
C	265	LYS	-	linker	UNP P08603
C	1095	GLY	-	linker	UNP P08603
C	1096	GLY	-	linker	UNP P08603
C	1097	GLY	-	linker	UNP P08603
C	1098	GLY	-	linker	UNP P08603
C	1099	GLY	-	linker	UNP P08603
C	1100	GLY	-	linker	UNP P08603
C	1101	GLY	-	linker	UNP P08603

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Chain	Residue	Modelled	Actual	Comment	Reference
C	1102	GLY	-	linker	UNP P08603
C	1103	GLY	-	linker	UNP P08603
C	1104	GLY	-	linker	UNP P08603
C	1105	GLY	-	linker	UNP P08603
C	1106	GLY	-	linker	UNP P08603
G	265	LYS	-	linker	UNP P08603
G	1095	GLY	-	linker	UNP P08603
G	1096	GLY	-	linker	UNP P08603
G	1097	GLY	-	linker	UNP P08603
G	1098	GLY	-	linker	UNP P08603
G	1099	GLY	-	linker	UNP P08603
G	1100	GLY	-	linker	UNP P08603
G	1101	GLY	-	linker	UNP P08603
G	1102	GLY	-	linker	UNP P08603
G	1103	GLY	-	linker	UNP P08603
G	1104	GLY	-	linker	UNP P08603
G	1105	GLY	-	linker	UNP P08603
G	1106	GLY	-	linker	UNP P08603

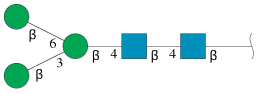
- Molecule 4 is a protein called Complement factor I.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	D	301	Total	C	N	O	S	0	0	0
			2320	1422	407	456	35			
4	H	301	Total	C	N	O	S	0	0	0
			2320	1422	407	456	35			

- Molecule 5 is a protein called Complement factor I.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
5	I	241	Total	C	N	O	S	0	0	0
			1911	1224	324	349	14			
5	J	241	Total	C	N	O	S	0	0	0
			1911	1224	324	349	14			

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



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

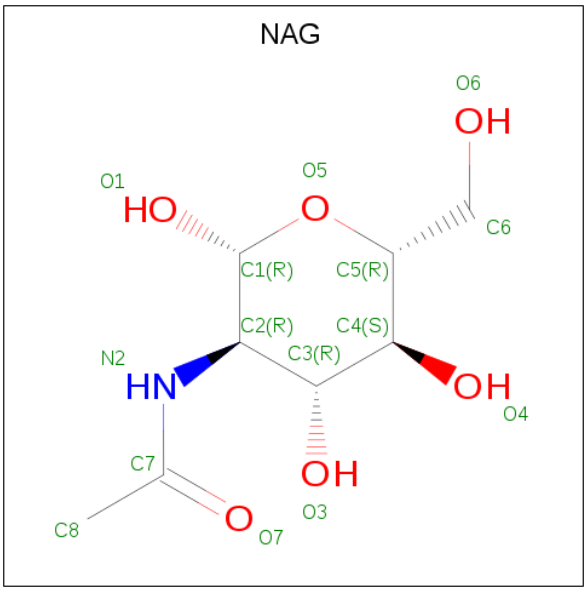
- Molecule 7 is an oligosaccharide called 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose.

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

- Molecule 8 is CALCIUM ION (three-letter code: CA) (formula: Ca).

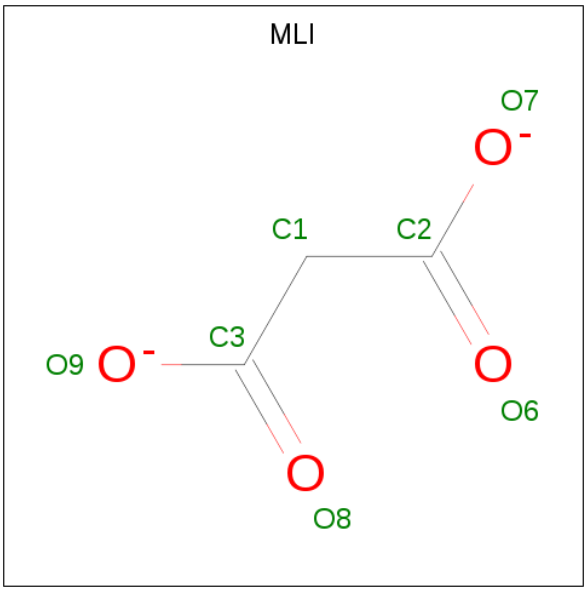
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
8	H	2	Total Ca 2 2	0	0
8	A	1	Total Ca 1 1	0	0
8	D	2	Total Ca 2 2	0	0
8	E	1	Total Ca 1 1	0	0

- Molecule 9 is 2-acetamido-2-deoxy-beta-D-glucopyranose (three-letter code: NAG) (formula: $C_8H_{15}NO_6$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
9	D	1	Total C N O 14 8 1 5	0	0
9	D	1	Total C N O 14 8 1 5	0	0
9	D	1	Total C N O 14 8 1 5	0	0
9	I	1	Total C N O 14 8 1 5	0	0
9	I	1	Total C N O 14 8 1 5	0	0
9	I	1	Total C N O 14 8 1 5	0	0
9	H	1	Total C N O 14 8 1 5	0	0
9	H	1	Total C N O 14 8 1 5	0	0
9	H	1	Total C N O 14 8 1 5	0	0
9	J	1	Total C N O 14 8 1 5	0	0
9	J	1	Total C N O 14 8 1 5	0	0
9	J	1	Total C N O 14 8 1 5	0	0

- Molecule 10 is MALONATE ION (three-letter code: MLI) (formula: $C_3H_2O_4$).



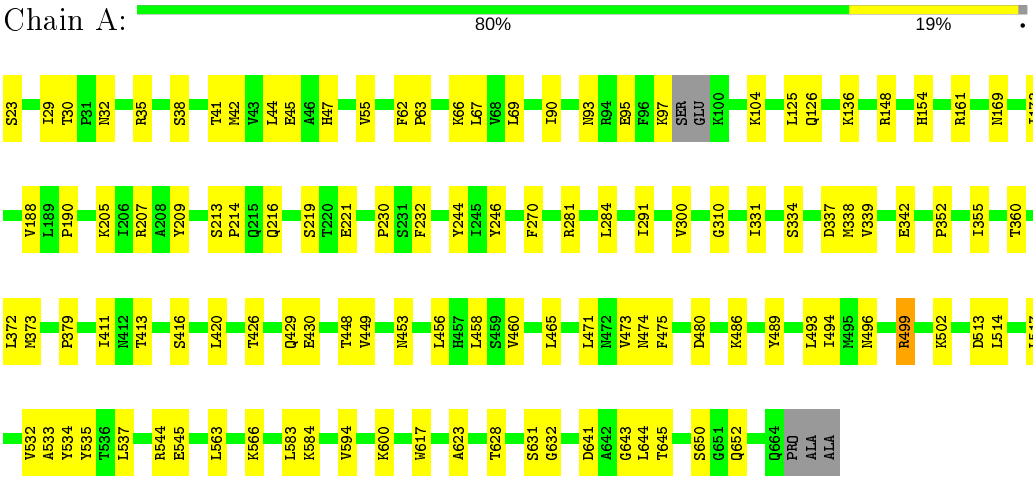
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	C	O		
10	J	1	7	3	4	0	0

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.

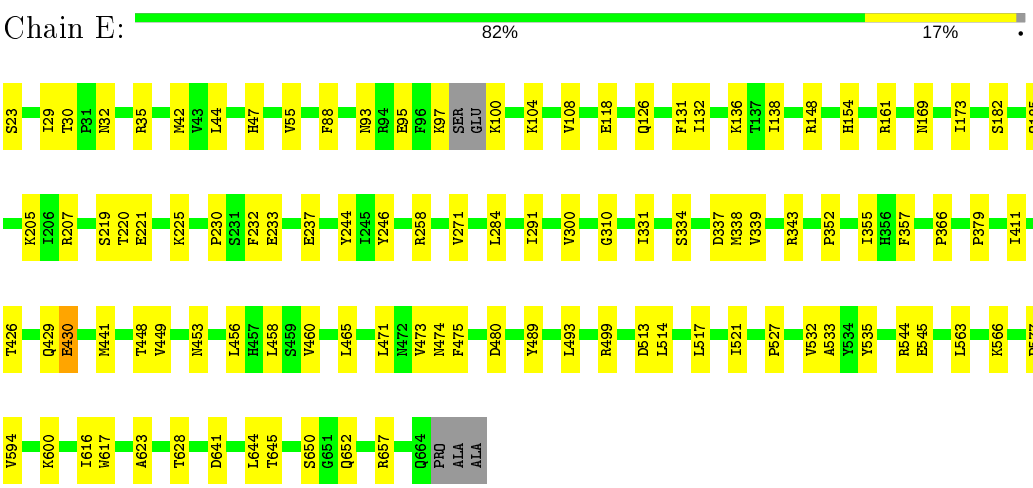
- Molecule 1: Complement C3

Chain A:



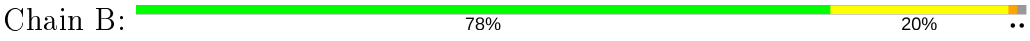
- Molecule 1: Complement C3

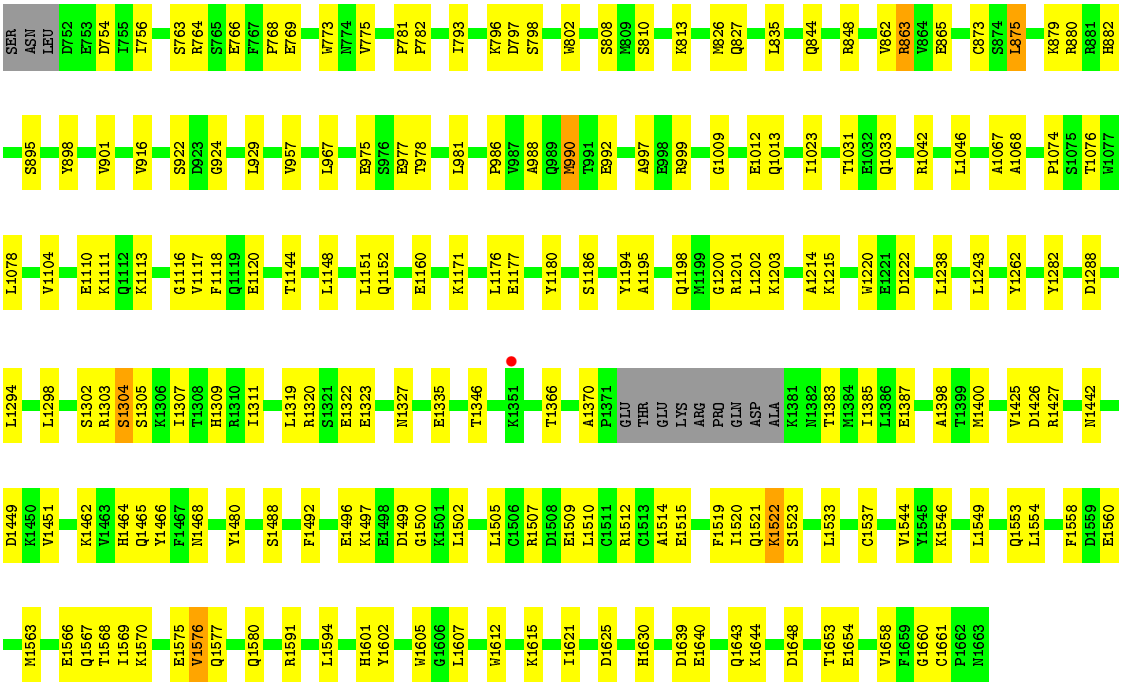
Chain E:



- Molecule 2: Complement C3

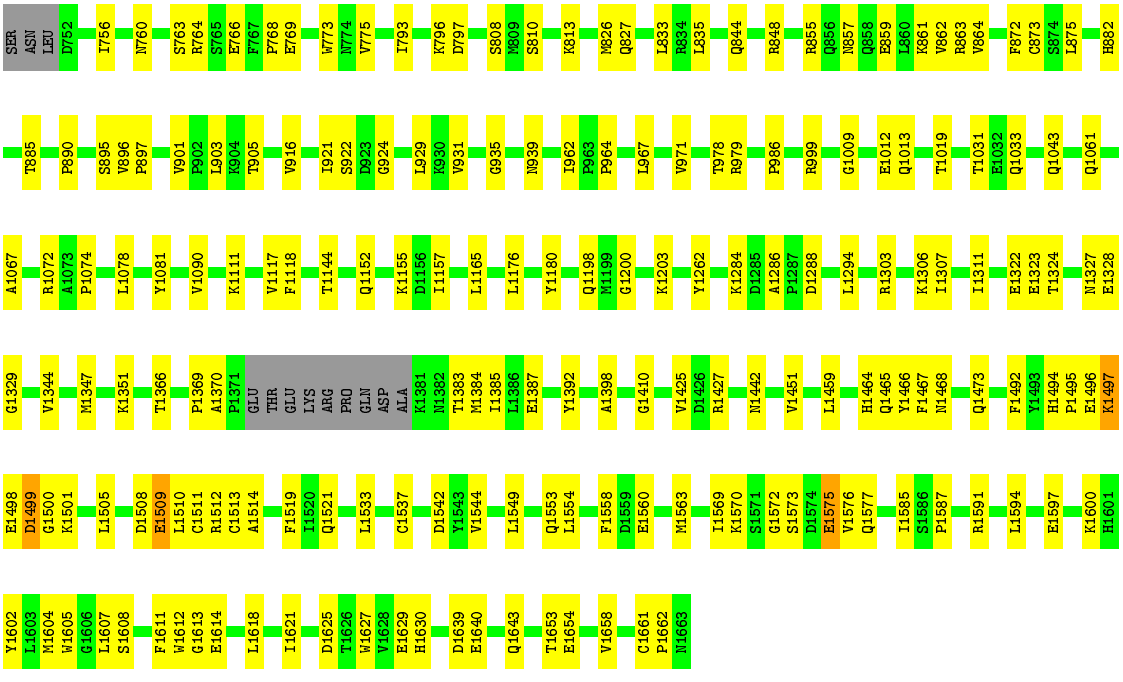
Chain B:





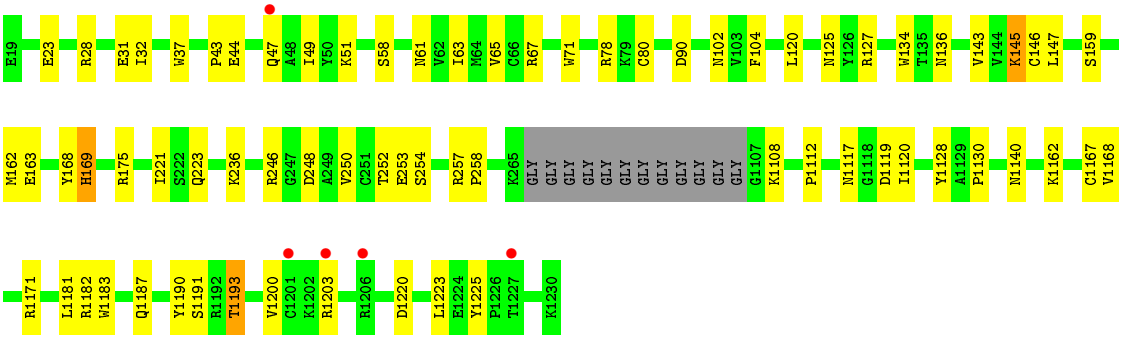
• Molecule 2: Complement C3

Chain F:

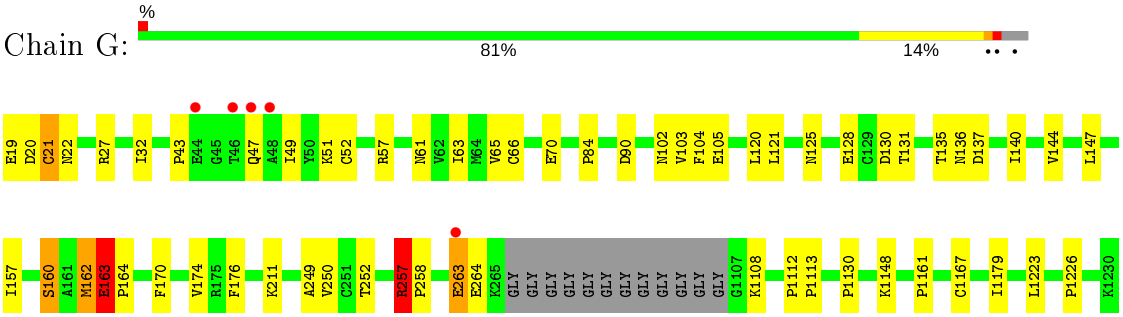


• Molecule 3: Complement factor H,Complement factor H

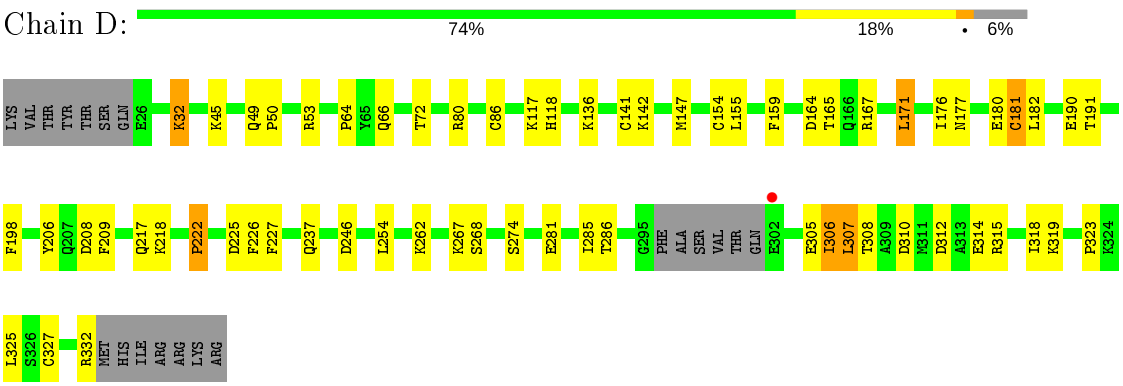
Chain C:



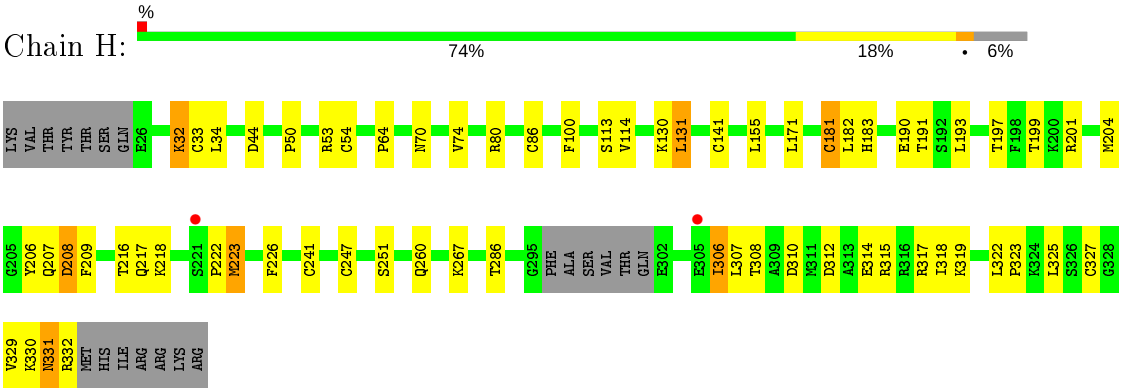
- Molecule 3: Complement factor H,Complement factor H



- Molecule 4: Complement factor I

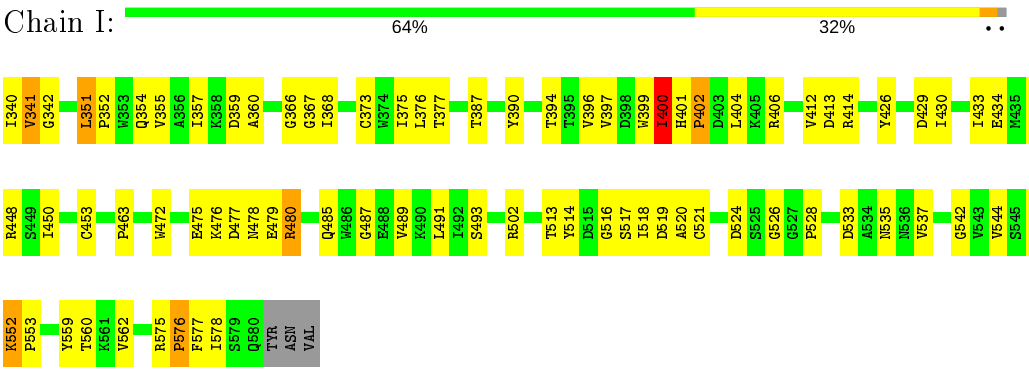


- Molecule 4: Complement factor I



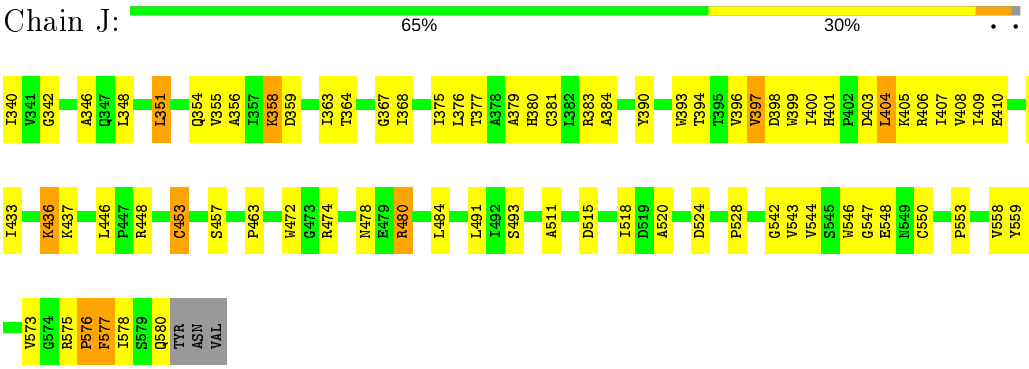
- Molecule 5: Complement factor I

Chain I:



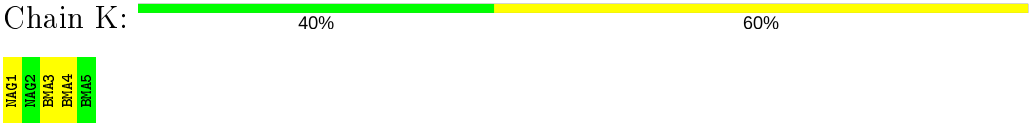
• Molecule 5: Complement factor I

Chain J:



• 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 K:

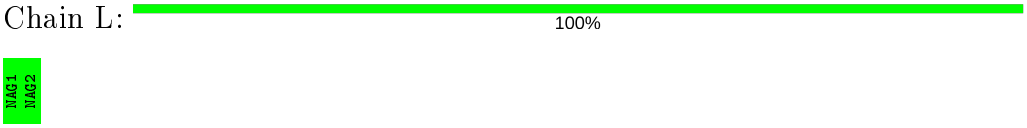


• Molecule 6: beta-D-mannopyranose-(1-3)-[beta-D-mannopyranose-(1-6)]beta-D-mannopyranose -(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain M:

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

Chain L:



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

Chain N:

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α, β, γ	116.37Å 122.79Å 157.20Å 69.76° 76.10° 70.13°	Depositor
Resolution (Å)	49.13 – 4.21 49.13 – 4.21	Depositor EDS
% Data completeness (in resolution range)	93.4 (49.13-4.21) 93.5 (49.13-4.21)	Depositor EDS
R_{merge}	0.17	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.24 (at 4.14Å)	Xtriage
Refinement program	PHENIX 1.10.1_2155	Depositor
R, R_{free}	0.229 , 0.254 0.229 , 0.254	Depositor DCC
R_{free} test set	2625 reflections (5.09%)	wwPDB-VP
Wilson B-factor (Å^2)	83.4	Xtriage
Anisotropy	0.010	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.26 , 44.6	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	0.82	EDS
Total number of atoms	39091	wwPDB-VP
Average B, all atoms (Å^2)	108.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.74% 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: CA, MLI, NAG, BMA

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#$\|Z\|>5$	RMSZ	#$\|Z\|>5$
1	A	0.27	0/5092	0.49	0/6917
1	E	0.29	1/5092 (0.0%)	0.50	1/6917 (0.0%)
2	B	0.27	0/7347	0.55	1/9949 (0.0%)
2	F	0.27	0/7347	0.55	1/9949 (0.0%)
3	C	0.25	0/3015	0.46	0/4084
3	G	0.29	1/3015 (0.0%)	0.47	0/4084
4	D	0.24	0/2355	0.47	0/3163
4	H	0.28	0/2355	0.48	1/3163 (0.0%)
5	I	0.28	0/1967	0.51	0/2675
5	J	0.27	0/1967	0.48	0/2675
All	All	0.27	2/39552 (0.0%)	0.51	4/53576 (0.0%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand.A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
2	B	0	2
2	F	0	2
3	C	0	1
3	G	0	3
4	D	0	1
4	H	0	2
5	I	0	1
All	All	0	12

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	G	257	ARG	C-N	8.16	1.49	1.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	E	430	GLU	CD-OE1	-6.51	1.18	1.25

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	B	1660	GLY	C-N-CA	8.81	143.73	121.70
4	H	131	LEU	CA-CB-CG	-5.86	101.83	115.30
2	F	1497	LYS	N-CA-C	-5.58	95.92	111.00
1	E	198	LEU	CA-CB-CG	5.28	127.43	115.30

There are no chirality outliers.

5 of 12 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	B	1509	GLU	Peptide
2	B	1576	VAL	Peptide
3	C	1190	TYR	Peptide
4	D	222	PRO	Peptide
5	I	400	ILE	Peptide

5.2 Too-close contacts (i)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	4992	0	5052	72	0
1	E	4992	0	5052	70	0
2	B	7203	0	7119	133	0
2	F	7203	0	7119	130	0
3	C	2940	0	2798	41	0
3	G	2940	0	2798	37	0
4	D	2320	0	2223	39	0
4	H	2320	0	2222	38	0
5	I	1911	0	1813	59	0
5	J	1911	0	1811	60	0
6	K	61	0	52	1	0
6	M	61	0	52	0	0
7	L	28	0	25	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
7	N	28	0	25	1	0
8	A	1	0	0	0	0
8	D	2	0	0	0	0
8	E	1	0	0	0	0
8	H	2	0	0	0	0
9	D	42	0	39	1	0
9	H	42	0	39	0	0
9	I	42	0	39	0	0
9	J	42	0	39	0	0
10	J	7	0	2	0	0
All	All	39091	0	38319	624	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 8.

The worst 5 of 624 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:E:30:THR:HG22	1:E:42:MET:HG2	1.49	0.94
1:A:30:THR:HG22	1:A:42:MET:HG2	1.50	0.92
2:B:1303:ARG:NH1	5:I:520:ALA:O	2.09	0.86
4:D:225:ASP:HB3	4:D:237:GLN:HG3	1.59	0.83
2:F:1654:GLU:OE2	4:H:80:ARG:NH2	2.12	0.83

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	636/645 (99%)	612 (96%)	24 (4%)	0	100	100
1	E	636/645 (99%)	612 (96%)	24 (4%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
2	B	899/915 (98%)	848 (94%)	44 (5%)	7 (1%)	19 60
2	F	899/915 (98%)	846 (94%)	49 (6%)	4 (0%)	34 72
3	C	367/383 (96%)	341 (93%)	21 (6%)	5 (1%)	11 47
3	G	367/383 (96%)	339 (92%)	22 (6%)	6 (2%)	9 45
4	D	297/321 (92%)	266 (90%)	25 (8%)	6 (2%)	7 40
4	H	297/321 (92%)	270 (91%)	21 (7%)	6 (2%)	7 40
5	I	239/244 (98%)	201 (84%)	30 (13%)	8 (3%)	4 30
5	J	239/244 (98%)	207 (87%)	26 (11%)	6 (2%)	5 35
All	All	4876/5016 (97%)	4542 (93%)	286 (6%)	48 (1%)	15 54

5 of 48 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	B	975	GLU
2	B	1522	LYS
2	B	1615	LYS
3	C	71	TRP
5	I	402	PRO

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	564/567 (100%)	561 (100%)	3 (0%)	88 93
1	E	564/567 (100%)	562 (100%)	2 (0%)	91 94
2	B	797/810 (98%)	791 (99%)	6 (1%)	81 89
2	F	797/810 (98%)	792 (99%)	5 (1%)	86 92
3	C	328/328 (100%)	320 (98%)	8 (2%)	49 69
3	G	328/328 (100%)	324 (99%)	4 (1%)	71 83
4	D	264/283 (93%)	258 (98%)	6 (2%)	50 70
4	H	264/283 (93%)	258 (98%)	6 (2%)	50 70

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
5	I	202/207 (98%)	200 (99%)	2 (1%)	76 86
5	J	202/207 (98%)	195 (96%)	7 (4%)	36 60
All	All	4310/4390 (98%)	4261 (99%)	49 (1%)	73 84

5 of 49 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
4	D	332	ARG
2	F	857	ASN
5	J	383	ARG
5	I	550	CYS
2	F	986	PRO

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (4) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	154	HIS
2	B	1465	GLN
2	F	844	GLN
3	G	22	ASN

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)

14 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	$\#\|Z\| > 2$
6	NAG	K	1	1,6	14,14,15	0.20	0	17,19,21	0.42	0
6	NAG	K	2	6	14,14,15	0.46	0	17,19,21	0.38	0
6	BMA	K	3	6	11,11,12	1.20	1 (9%)	15,15,17	1.42	3 (20%)
6	BMA	K	4	6	11,11,12	0.69	0	15,15,17	1.05	1 (6%)
6	BMA	K	5	6	11,11,12	0.61	0	15,15,17	0.80	0
7	NAG	L	1	2,7	14,14,15	0.30	0	17,19,21	0.41	0
7	NAG	L	2	7	14,14,15	0.48	0	17,19,21	0.36	0
6	NAG	M	1	1,6	14,14,15	0.22	0	17,19,21	0.43	0
6	NAG	M	2	6	14,14,15	0.46	0	17,19,21	0.38	0
6	BMA	M	3	6	11,11,12	1.19	1 (9%)	15,15,17	1.43	3 (20%)
6	BMA	M	4	6	11,11,12	0.65	0	15,15,17	1.06	1 (6%)
6	BMA	M	5	6	11,11,12	0.65	0	15,15,17	0.80	0
7	NAG	N	1	2,7	14,14,15	0.48	0	17,19,21	0.44	0
7	NAG	N	2	7	14,14,15	0.27	0	17,19,21	0.41	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
6	NAG	K	1	1,6	-	1/6/23/26	0/1/1/1
6	NAG	K	2	6	-	2/6/23/26	0/1/1/1
6	BMA	K	3	6	-	1/2/19/22	0/1/1/1
6	BMA	K	4	6	-	1/2/19/22	1/1/1/1
6	BMA	K	5	6	-	2/2/19/22	0/1/1/1
7	NAG	L	1	2,7	-	2/6/23/26	0/1/1/1
7	NAG	L	2	7	-	0/6/23/26	0/1/1/1
6	NAG	M	1	1,6	-	0/6/23/26	0/1/1/1
6	NAG	M	2	6	-	0/6/23/26	0/1/1/1
6	BMA	M	3	6	-	1/2/19/22	0/1/1/1
6	BMA	M	4	6	-	1/2/19/22	1/1/1/1
6	BMA	M	5	6	-	2/2/19/22	0/1/1/1
7	NAG	N	1	2,7	-	2/6/23/26	0/1/1/1
7	NAG	N	2	7	-	2/6/23/26	0/1/1/1

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	K	3	BMA	C2-C3	2.69	1.56	1.52
6	M	3	BMA	C2-C3	2.67	1.56	1.52

The worst 5 of 8 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
6	M	3	BMA	C1-C2-C3	3.10	113.48	109.67
6	K	3	BMA	C1-C2-C3	3.05	113.41	109.67
6	M	4	BMA	C1-O5-C5	2.94	116.18	112.19
6	K	4	BMA	C1-O5-C5	2.91	116.13	112.19
6	K	3	BMA	C2-C3-C4	2.55	115.31	110.89

There are no chirality outliers.

5 of 17 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
6	K	5	BMA	O5-C5-C6-O6
6	M	5	BMA	O5-C5-C6-O6
7	N	2	NAG	O5-C5-C6-O6
6	K	5	BMA	C4-C5-C6-O6
6	K	2	NAG	O5-C5-C6-O6

All (2) ring outliers are listed below:

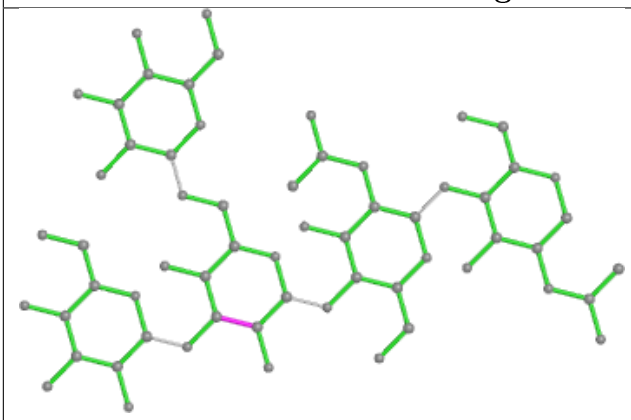
Mol	Chain	Res	Type	Atoms
6	K	4	BMA	C1-C2-C3-C4-C5-O5
6	M	4	BMA	C1-C2-C3-C4-C5-O5

2 monomers are involved in 2 short contacts:

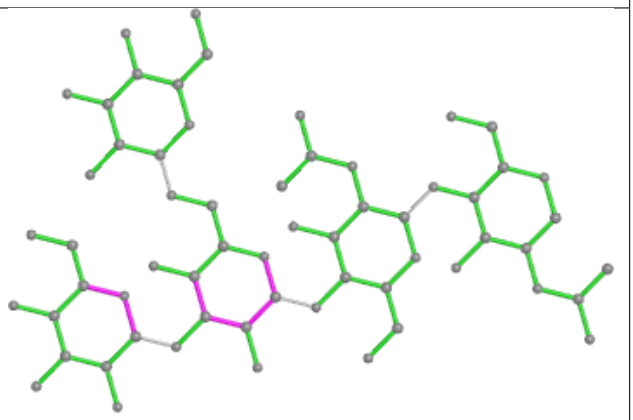
Mol	Chain	Res	Type	Clashes	Symm-Clashes
7	N	1	NAG	1	0
6	K	1	NAG	1	0

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

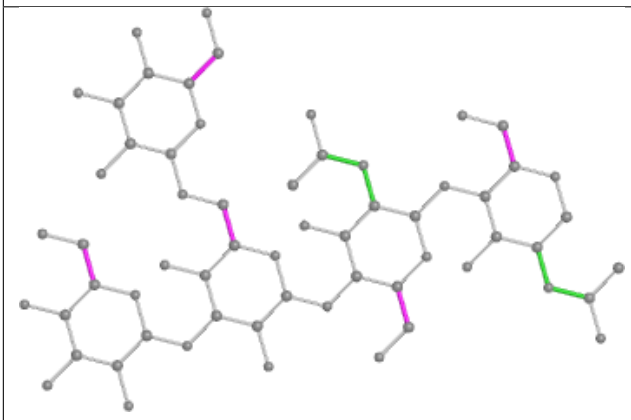
Oligosaccharide Chain K



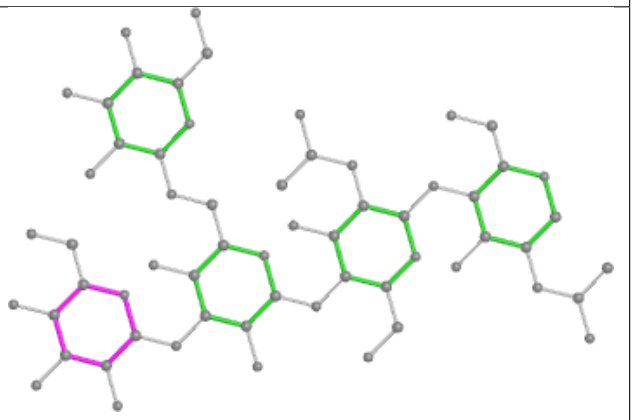
Bond lengths



Bond angles

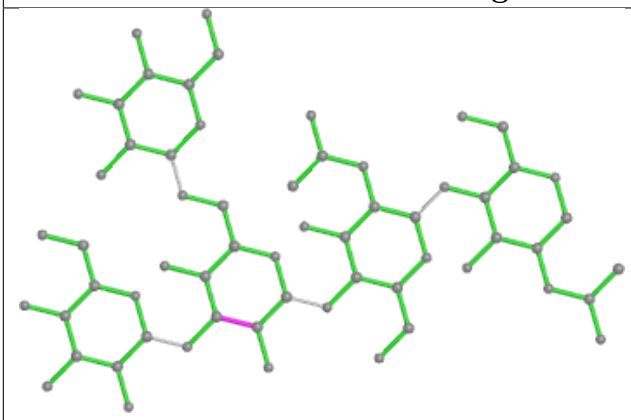


Torsions

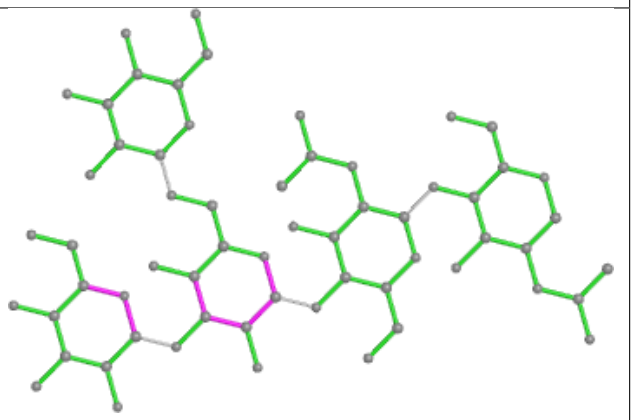


Rings

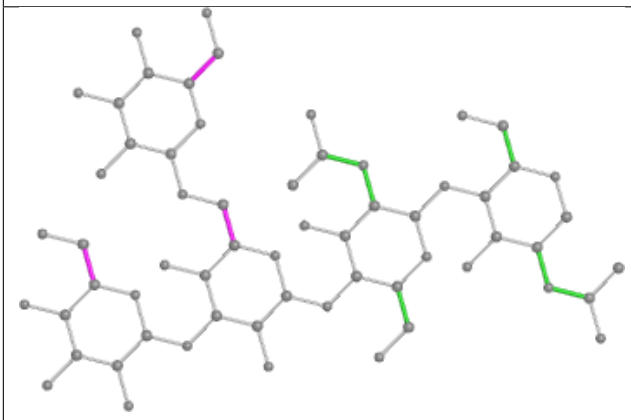
Oligosaccharide Chain M



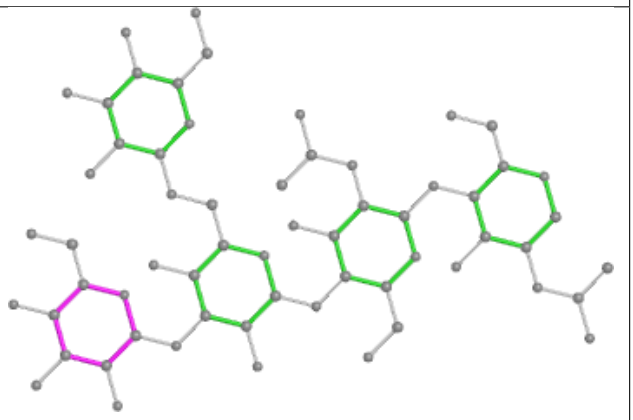
Bond lengths



Bond angles

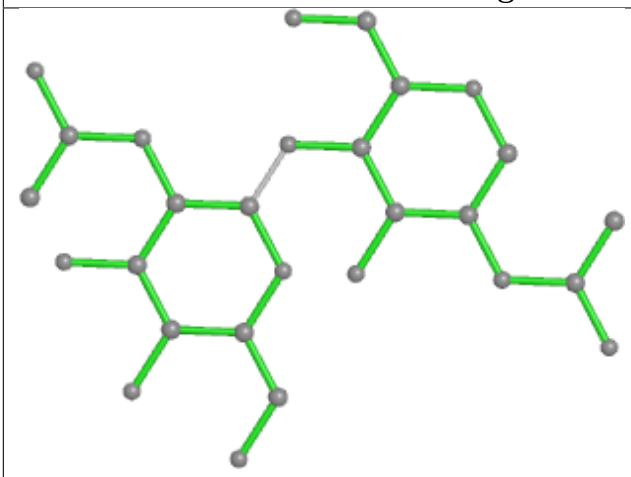


Torsions

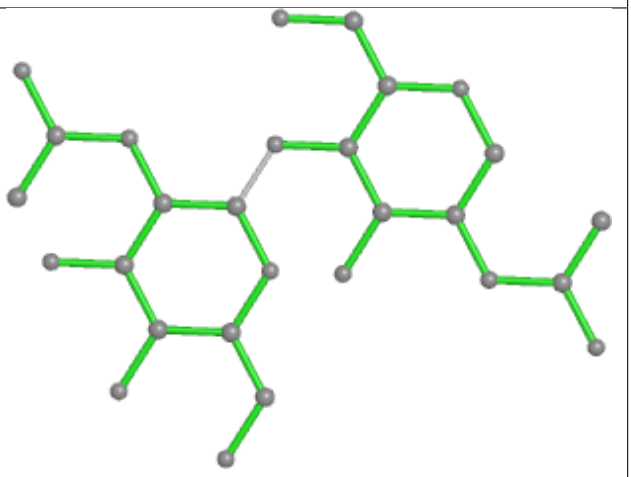


Rings

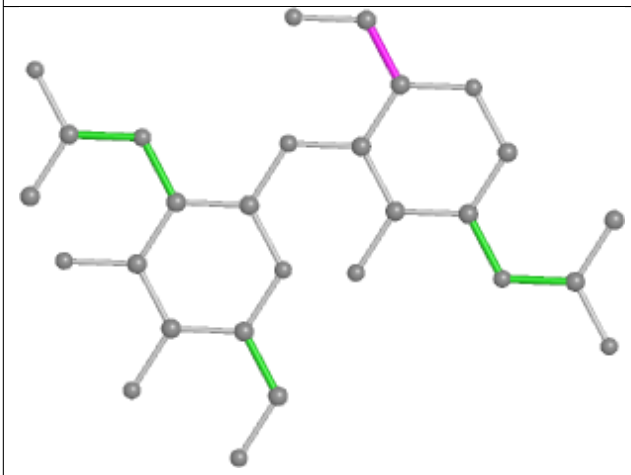
Oligosaccharide Chain L



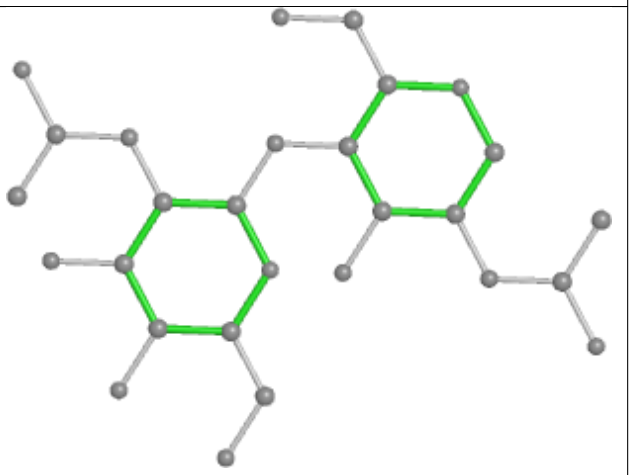
Bond lengths



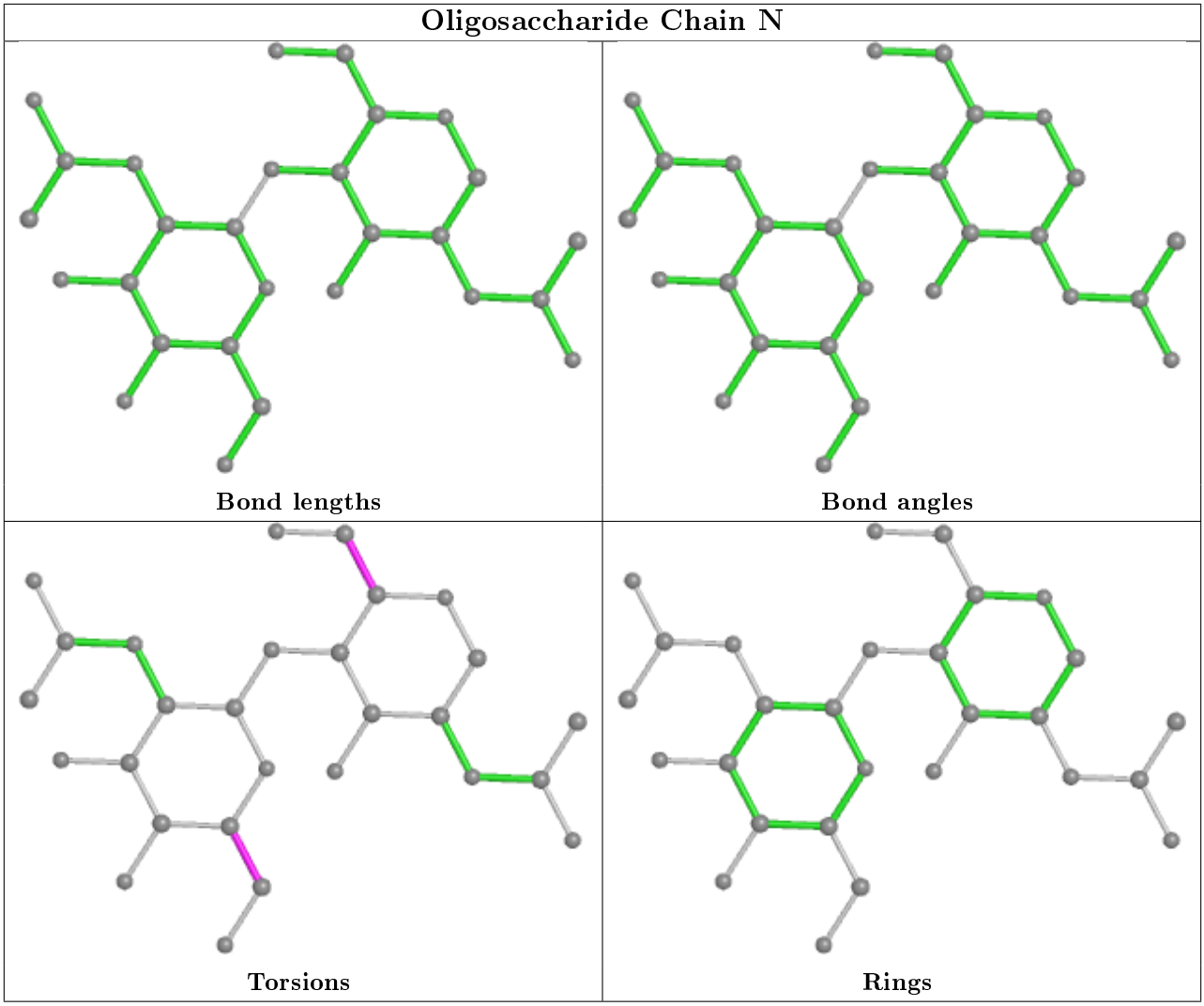
Bond angles



Torsions



Rings



5.6 Ligand geometry

Of 19 ligands modelled in this entry, 6 are monoatomic - leaving 13 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	$\#\|Z\| > 2$
9	NAG	I	601	5	14,14,15	0.48	0	17,19,21	0.45	0
9	NAG	J	601	5	14,14,15	0.19	0	17,19,21	0.59	0
9	NAG	H	403	4	14,14,15	0.31	0	17,19,21	0.76	1 (5%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
9	NAG	H	405	4	14,14,15	0.22	0	17,19,21	0.40	0
9	NAG	D	403	4	14,14,15	0.71	0	17,19,21	1.19	1 (5%)
9	NAG	J	602	5	14,14,15	0.23	0	17,19,21	0.49	0
9	NAG	D	404	4	14,14,15	0.21	0	17,19,21	0.43	0
9	NAG	I	603	5	14,14,15	0.26	0	17,19,21	0.37	0
9	NAG	I	602	5	14,14,15	0.21	0	17,19,21	0.42	0
9	NAG	D	405	4	14,14,15	0.21	0	17,19,21	0.40	0
9	NAG	H	404	4	14,14,15	0.25	0	17,19,21	0.40	0
9	NAG	J	603	5	14,14,15	0.47	0	17,19,21	0.77	1 (5%)
10	MLI	J	604	-	0,6,6	0.00	-	0,7,7	0.00	-

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
9	NAG	I	601	5	-	2/6/23/26	0/1/1/1
9	NAG	J	601	5	-	3/6/23/26	0/1/1/1
9	NAG	H	403	4	-	3/6/23/26	0/1/1/1
9	NAG	H	405	4	-	2/6/23/26	0/1/1/1
9	NAG	D	403	4	-	1/6/23/26	0/1/1/1
9	NAG	J	602	5	-	2/6/23/26	0/1/1/1
9	NAG	D	404	4	-	0/6/23/26	0/1/1/1
9	NAG	I	603	5	-	2/6/23/26	0/1/1/1
9	NAG	I	602	5	-	1/6/23/26	0/1/1/1
9	NAG	D	405	4	-	2/6/23/26	0/1/1/1
9	NAG	H	404	4	-	2/6/23/26	0/1/1/1
9	NAG	J	603	5	-	2/6/23/26	0/1/1/1
10	MLI	J	604	-	-	0/0/4/4	-

There are no bond length outliers.

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
9	D	403	NAG	C1-O5-C5	4.49	118.28	112.19
9	J	603	NAG	C1-O5-C5	2.93	116.17	112.19
9	H	403	NAG	C1-O5-C5	2.47	115.54	112.19

There are no chirality outliers.

5 of 22 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
9	J	603	NAG	O5-C5-C6-O6
9	J	603	NAG	C4-C5-C6-O6
9	H	403	NAG	O5-C5-C6-O6
9	J	601	NAG	O5-C5-C6-O6
9	I	601	NAG	C4-C5-C6-O6

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
9	D	405	NAG	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	640/645 (99%)	-0.42	0 100 100	40, 87, 131, 170	0
1	E	640/645 (99%)	-0.36	0 100 100	41, 91, 132, 156	0
2	B	903/915 (98%)	-0.25	1 (0%) 95 95	48, 115, 159, 180	0
2	F	903/915 (98%)	-0.27	0 100 100	47, 110, 152, 182	0
3	C	371/383 (96%)	-0.11	5 (1%) 77 68	65, 124, 192, 207	0
3	G	371/383 (96%)	-0.05	5 (1%) 77 68	60, 126, 197, 217	0
4	D	301/321 (93%)	-0.21	1 (0%) 94 90	96, 123, 157, 187	0
4	H	301/321 (93%)	-0.33	2 (0%) 87 82	77, 102, 140, 170	0
5	I	241/244 (98%)	-0.33	0 100 100	71, 111, 148, 164	0
5	J	241/244 (98%)	-0.33	0 100 100	64, 96, 126, 145	0
All	All	4912/5016 (97%)	-0.27	14 (0%) 94 90	40, 107, 159, 217	0

The worst 5 of 14 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
3	C	1227	THR	4.6
4	H	305	GLU	3.7
3	G	48	ALA	3.0
3	C	1201	CYS	2.8
3	G	46	THR	2.7

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

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

6.3 Carbohydrates (i)

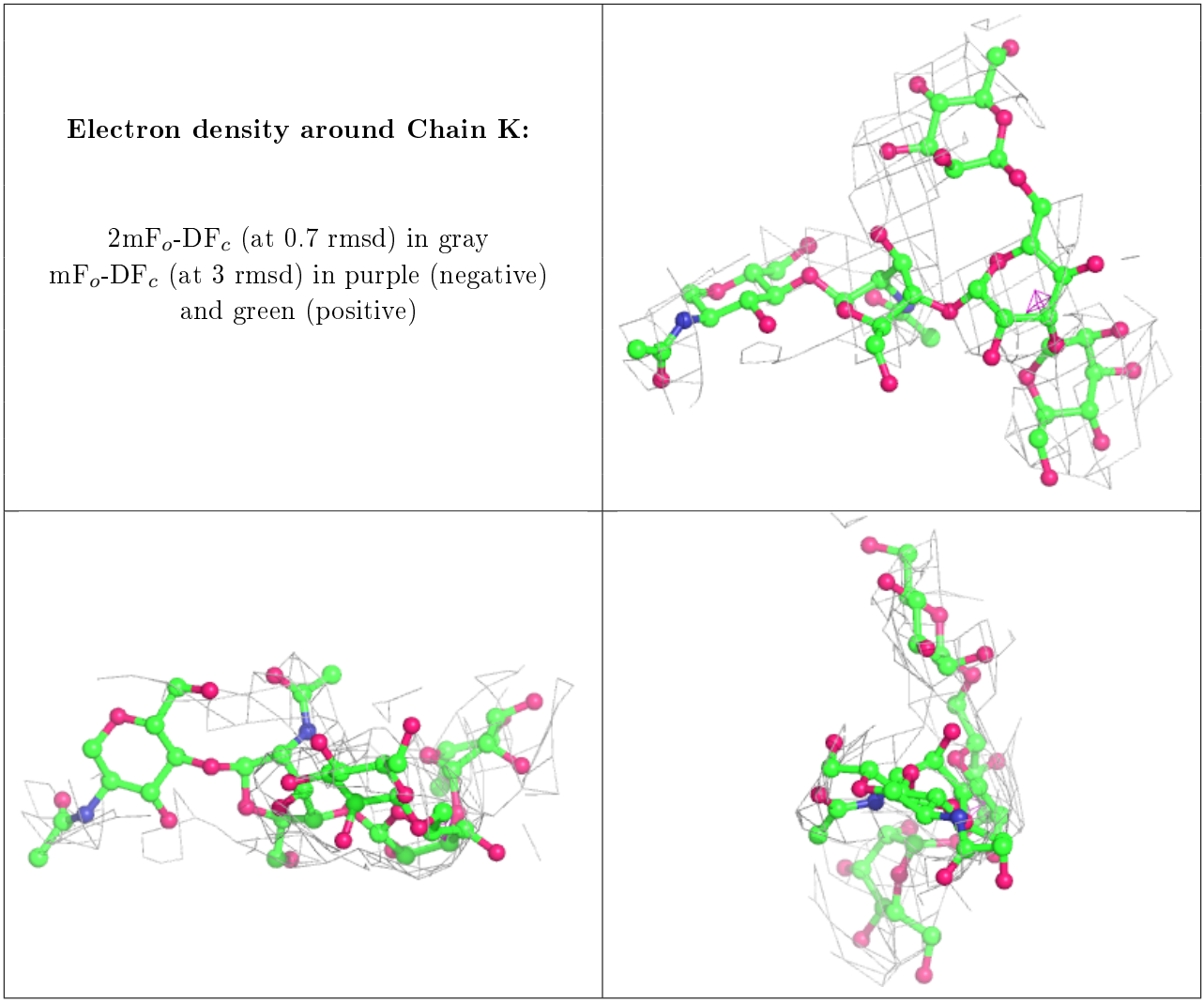
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' 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
6	BMA	M	5	11/12	0.56	0.52	175,182,188,191	0
7	NAG	L	2	14/15	0.73	0.55	158,160,163,166	0
6	BMA	M	4	11/12	0.75	0.37	164,170,183,188	0
6	BMA	K	3	11/12	0.76	0.33	141,151,155,161	0
6	BMA	K	5	11/12	0.78	0.39	142,150,163,167	0
6	BMA	K	4	11/12	0.78	0.34	147,152,164,167	0
7	NAG	N	2	14/15	0.79	0.36	139,145,158,162	0
6	BMA	M	3	11/12	0.79	0.25	160,170,176,183	0
6	NAG	M	2	14/15	0.83	0.28	136,142,152,154	0
7	NAG	N	1	14/15	0.86	0.31	133,139,145,145	0
7	NAG	L	1	14/15	0.90	0.27	143,146,150,152	0
6	NAG	M	1	14/15	0.90	0.22	86,100,111,112	0
6	NAG	K	2	14/15	0.91	0.23	116,124,130,132	0
6	NAG	K	1	14/15	0.92	0.22	77,90,98,102	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.

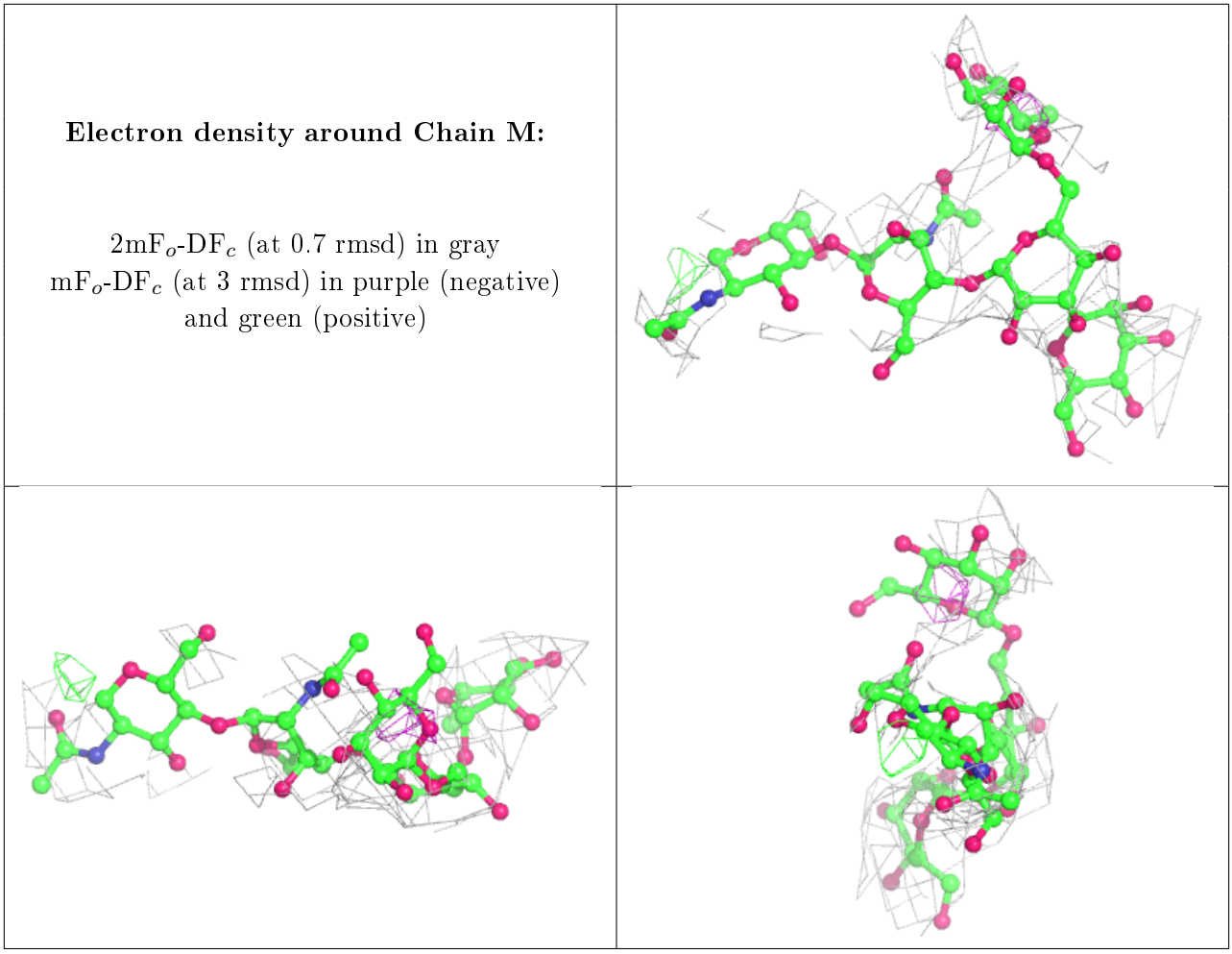
Electron density around Chain K:

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



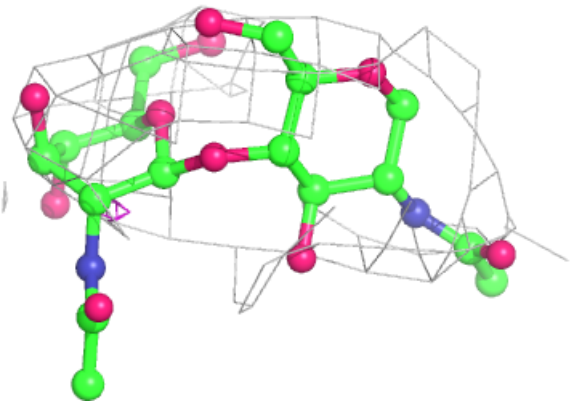
Electron density around Chain M:

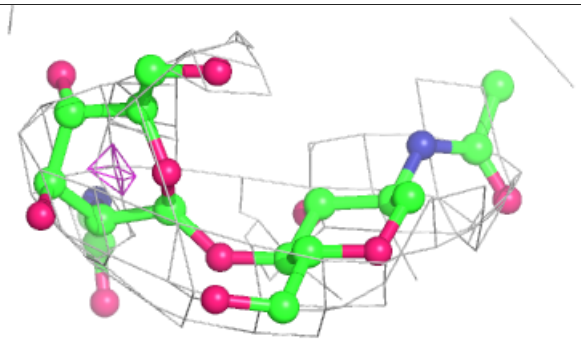
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

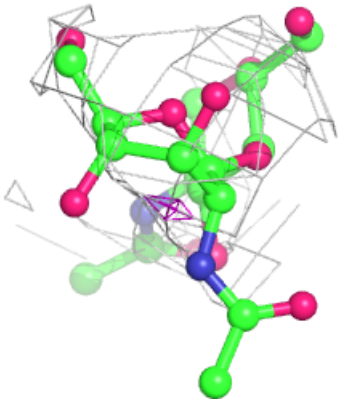


Electron density around Chain L:

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

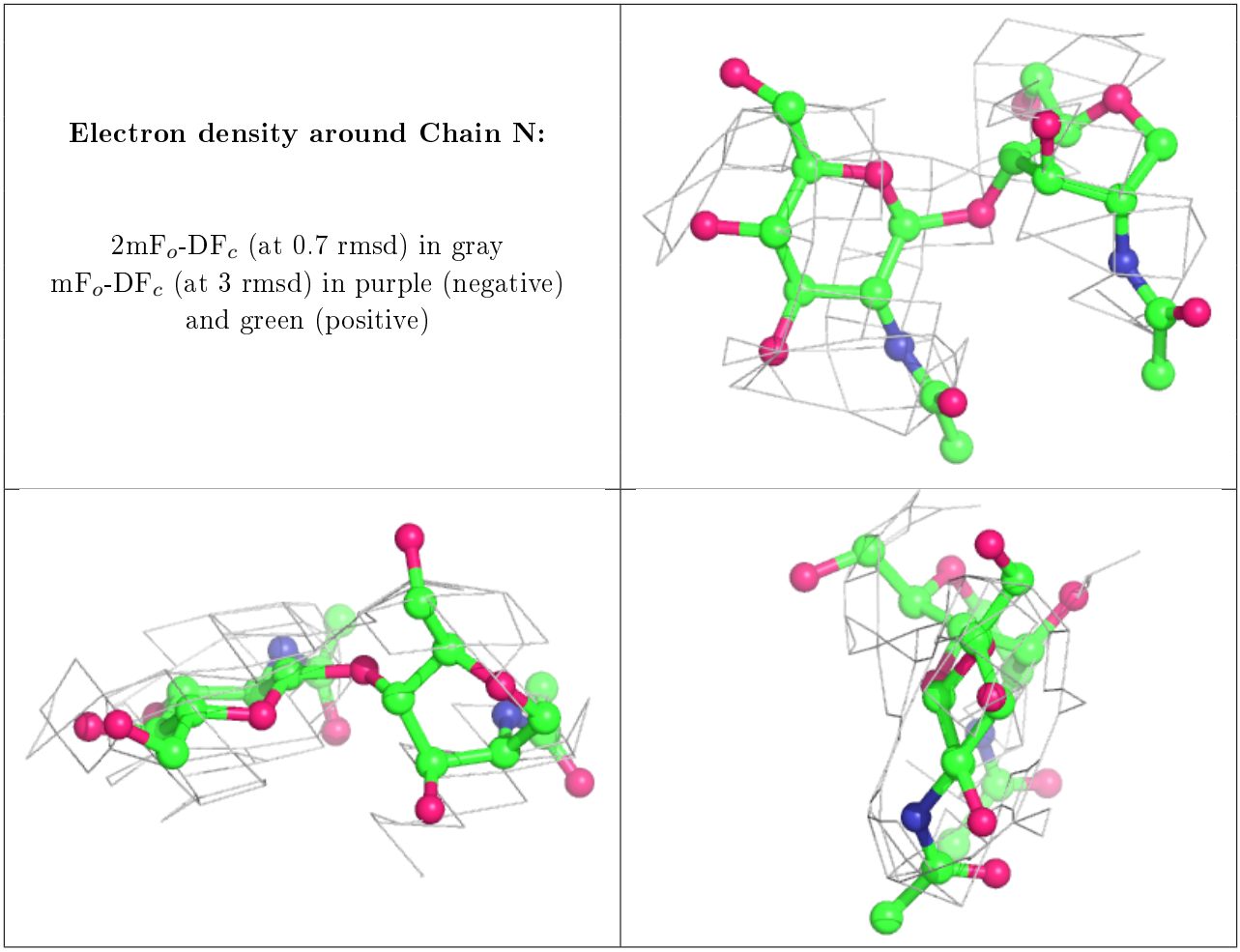






Electron density around Chain N:

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



6.4 Ligands

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
9	NAG	H	404	14/15	0.57	0.54	129,134,140,141	0
9	NAG	D	404	14/15	0.78	0.42	159,162,167,169	0
9	NAG	H	405	14/15	0.80	0.34	119,129,144,149	0
9	NAG	I	601	14/15	0.81	0.44	153,155,161,162	0
9	NAG	I	603	14/15	0.81	0.34	171,178,187,187	0
9	NAG	J	602	14/15	0.81	0.49	139,143,147,149	0
8	CA	D	402	1/1	0.81	0.11	124,124,124,124	0
9	NAG	I	602	14/15	0.82	0.37	156,158,165,170	0
8	CA	D	401	1/1	0.84	0.07	123,123,123,123	0
8	CA	H	402	1/1	0.84	0.12	102,102,102,102	0
9	NAG	J	603	14/15	0.84	0.20	144,151,157,159	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
9	NAG	D	403	14/15	0.86	0.35	128,138,147,147	0
9	NAG	H	403	14/15	0.87	0.60	118,125,131,134	0
9	NAG	J	601	14/15	0.88	0.37	122,128,137,140	0
9	NAG	D	405	14/15	0.89	0.34	122,133,143,148	0
10	MLI	J	604	7/7	0.90	0.17	91,94,99,103	0
8	CA	H	401	1/1	0.93	0.11	93,93,93,93	0
8	CA	A	701	1/1	0.96	0.07	61,61,61,61	0
8	CA	E	701	1/1	0.96	0.19	51,51,51,51	0

6.5 Other polymers (i)

There are no such residues in this entry.