Full wwPDB X-ray Structure Validation Report ⓘ

Aug 9, 2020 – 02:11 PM BST

PDB ID	:	4HJ1
Title	:	Crystal structure of glycoprotein C from Rift Valley Fever Virus (glycosylated)
Authors	:	Dessau, M.; Modis, Y.
Deposited on	:	2012-10-12
Resolution	:	1.90 Å(reported)

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

We welcome your comments at *validation@mail.wwpdb.org*
A user guide is available at
https://www.wwpdb.org/validation/2017/XrayValidationReportHelp
with specific help available everywhere you see the ⓘ symbol.

The following versions of software and data (see references ⓘ) were used in the production of this report:

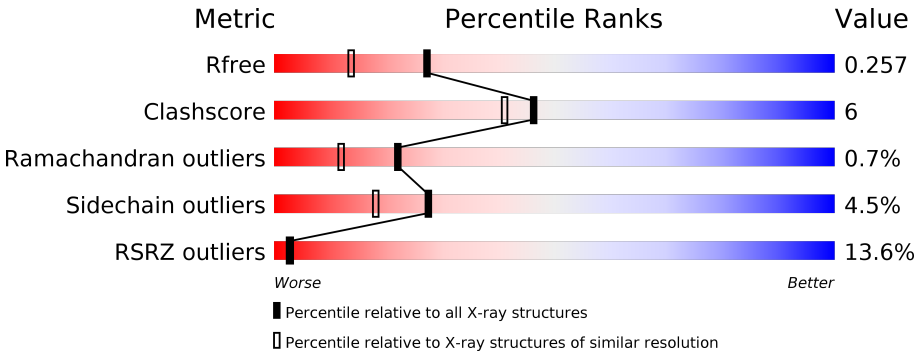
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.13.1
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (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 1.90 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	6207 (1.90-1.90)
Clashscore	141614	6847 (1.90-1.90)
Ramachandran outliers	138981	6760 (1.90-1.90)
Sidechain outliers	138945	6760 (1.90-1.90)
RSRZ outliers	127900	6082 (1.90-1.90)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments 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	432	6% 87% 11%
1	B	432	26% 82% 15%
1	C	432	14% 85% 13%
1	D	432	8% 86% 13%
2	E	4	75% 25%
3	F	3	100%

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Mol	Chain	Length	Quality of chain
4	G	5	100%
4	H	5	60% 40%

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
4	BMA	G	5	-	-	-	X
7	GOL	D	1210	-	-	X	-

2 Entry composition

There are 8 unique types of molecules in this entry. The entry contains 14382 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 ENVELOPE GLYCOPROTEIN.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	431	Total	C	N	O	S	0	2	0
			3279	2036	561	653	29			
1	B	427	Total	C	N	O	S	0	0	0
			3242	2011	557	645	29			
1	C	430	Total	C	N	O	S	0	1	0
			3271	2031	561	649	30			
1	D	431	Total	C	N	O	S	0	5	0
			3296	2046	562	658	30			

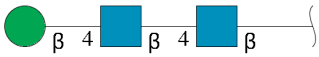
There are 12 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	688	ASP	-	expression tag	UNP A2T075
A	689	PRO	-	expression tag	UNP A2T075
A	690	GLY	-	expression tag	UNP A2T075
B	688	ASP	-	expression tag	UNP A2T075
B	689	PRO	-	expression tag	UNP A2T075
B	690	GLY	-	expression tag	UNP A2T075
C	688	ASP	-	expression tag	UNP A2T075
C	689	PRO	-	expression tag	UNP A2T075
C	690	GLY	-	expression tag	UNP A2T075
D	688	ASP	-	expression tag	UNP A2T075
D	689	PRO	-	expression tag	UNP A2T075
D	690	GLY	-	expression tag	UNP A2T075

- Molecule 2 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-glucopyranose.

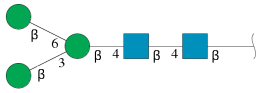
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
2	E	4	Total	C	N	O	0	0	0
			50	28	2	20			

- Molecule 3 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.



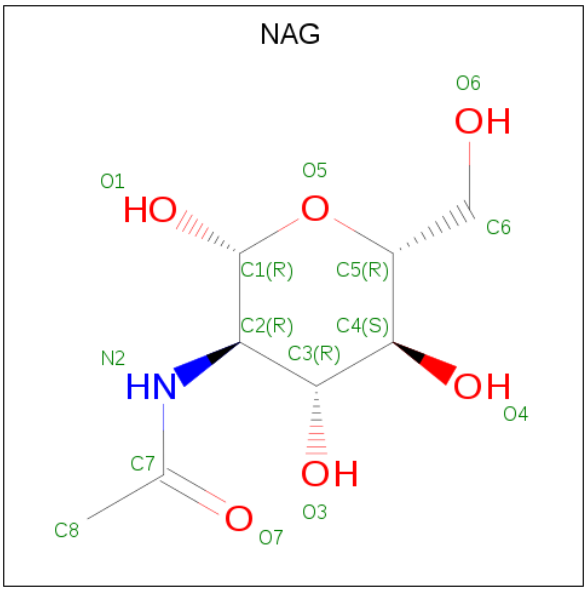
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
3	F	3	Total	C	N	O	0	0	0
			39	22	2	15			

- Molecule 4 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.



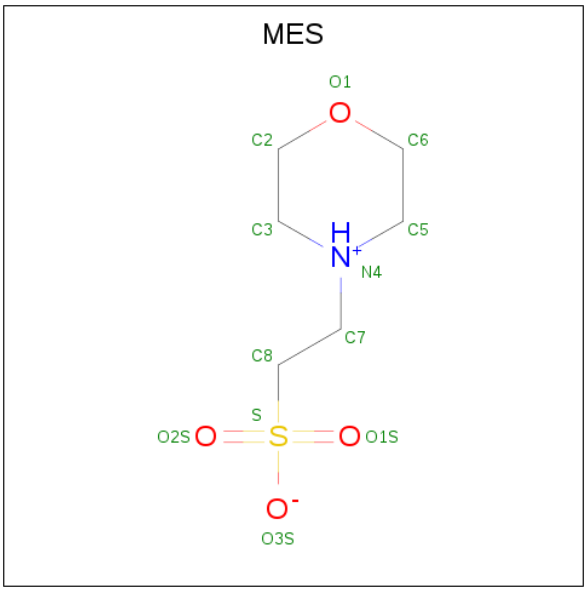
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
4	G	5	Total	C	N	O	0	0	0
			61	34	2	25			
4	H	5	Total	C	N	O	0	0	0
			61	34	2	25			

- Molecule 5 is 2-acetamido-2-deoxy-beta-D-glucopyranose (three-letter code: NAG) (formula: $C_8H_{15}NO_6$).



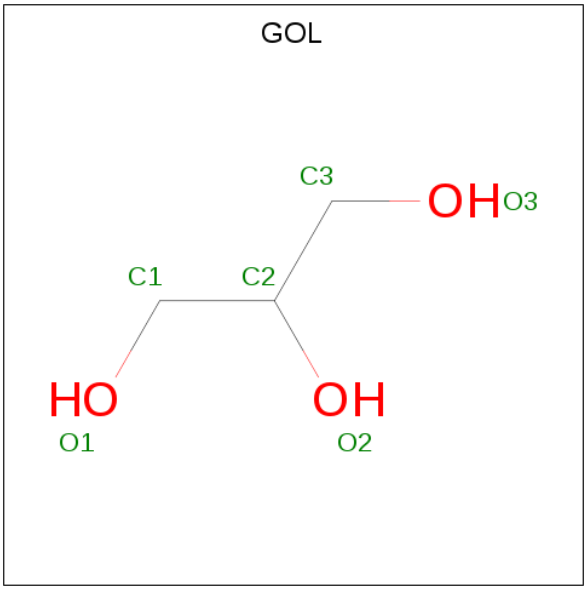
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	1	Total C N O 14 8 1 5	0	0
5	B	1	Total C N O 14 8 1 5	0	0
5	C	1	Total C N O 14 8 1 5	0	0
5	D	1	Total C N O 14 8 1 5	0	0

- Molecule 6 is 2-(N-MORPHOLINO)-ETHANESULFONIC ACID (three-letter code: MES) (formula: $C_6H_{13}NO_4S$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
6	A	1	Total	C	N	O	S	0	0
			12	6	1	4	1		
6	B	1	Total	C	N	O	S	0	0
			12	6	1	4	1		
6	C	1	Total	C	N	O	S	0	0
			12	6	1	4	1		
6	D	1	Total	C	N	O	S	0	0
			12	6	1	4	1		
6	D	1	Total	C	N	O	S	0	0
			12	6	1	4	1		

- Molecule 7 is GLYCEROL (three-letter code: GOL) (formula: $C_3H_8O_3$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
7	A	1	Total	C	O	0	0
			6	3	3		
7	B	1	Total	C	O	0	0
			6	3	3		
7	C	1	Total	C	O	0	0
			6	3	3		
7	D	1	Total	C	O	0	0
			6	3	3		
7	D	1	Total	C	O	0	0
			6	3	3		

- Molecule 8 is water.

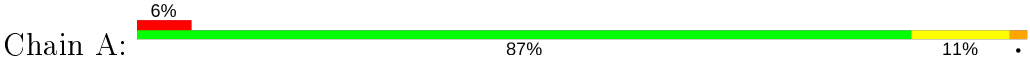
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
8	A	332	Total O 332 332	0	0
8	B	111	Total O 111 111	0	0
8	C	170	Total O 170 170	0	0
8	D	324	Total O 324 324	0	0

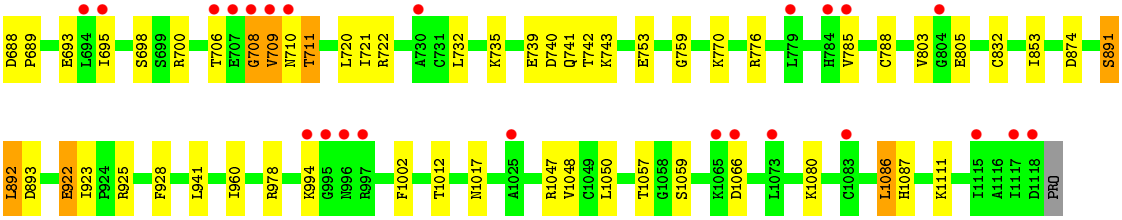
3 Residue-property plots (i)

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: ENVELOPE GLYCOPROTEIN

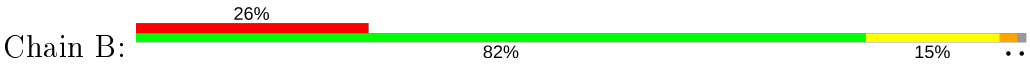
Chain A:

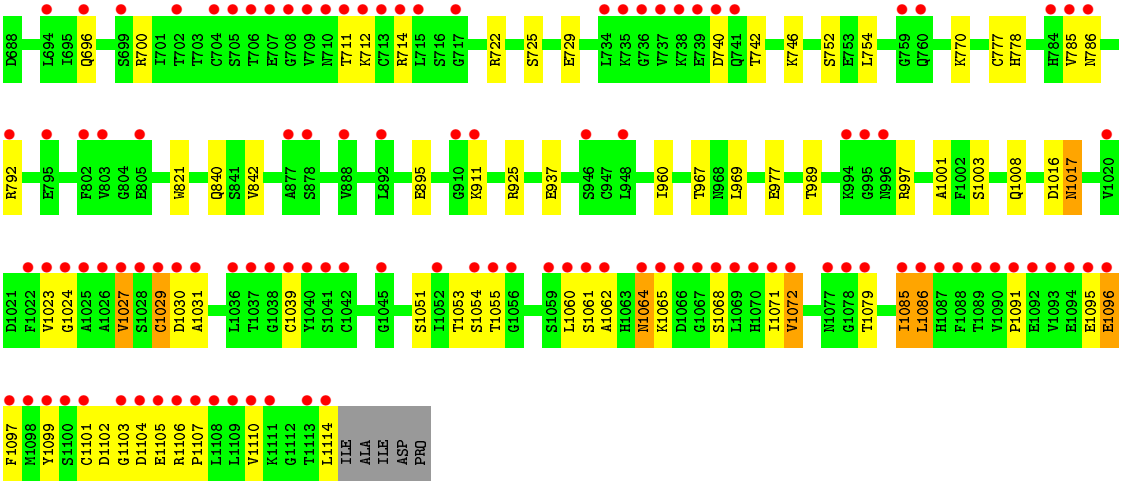




- Molecule 1: ENVELOPE GLYCOPROTEIN

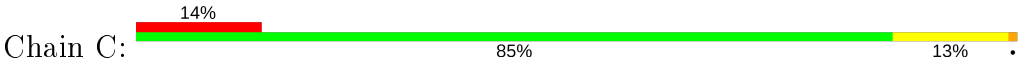
Chain B:

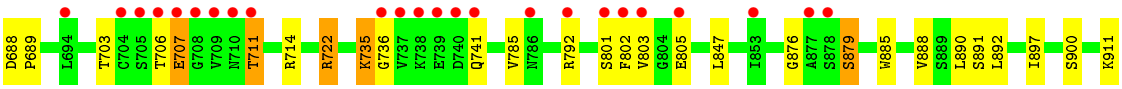


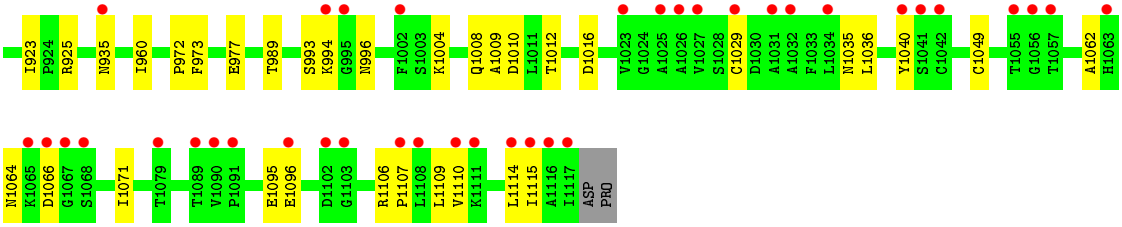


- Molecule 1: ENVELOPE GLYCOPROTEIN

Chain C:

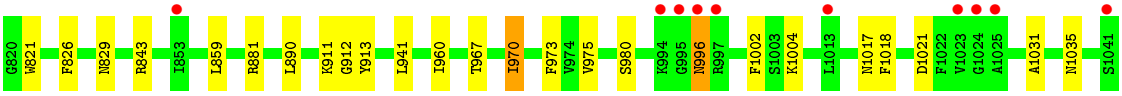


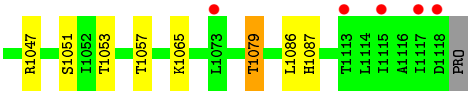




• Molecule 1: ENVELOPE GLYCOPROTEIN

Chain D:



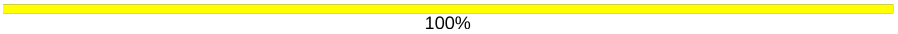


• Molecule 2: beta-D-mannopyranose-(1-6)-beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain E:

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

Chain F:



• Molecule 4: 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 G:

• Molecule 4: 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 H:

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	128.68Å 56.37Å 140.19Å 90.00° 96.55° 90.00°	Depositor
Resolution (Å)	29.76 – 1.90 29.75 – 1.90	Depositor EDS
% Data completeness (in resolution range)	97.3 (29.76-1.90) 97.4 (29.75-1.90)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.65 (at 1.91Å)	Xtriage
Refinement program	REFMAC 5.6.0117	Depositor
R, R_{free}	0.214 , 0.255 0.215 , 0.257	Depositor DCC
R_{free} test set	7722 reflections (5.01%)	wwPDB-VP
Wilson B-factor (Å^2)	33.0	Xtriage
Anisotropy	0.330	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.35 , 50.8	EDS
L-test for twinning[2]	$< \|L\| > = 0.50$, $< L^2 > = 0.34$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.96	EDS
Total number of atoms	14382	wwPDB-VP
Average B, all atoms (Å^2)	56.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 42.67 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 1.9715e-04. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

[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: GOL, BMA, NAG, MES

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	0.51	0/3345	0.69	1/4523 (0.0%)
1	B	0.39	1/3302 (0.0%)	0.56	0/4463
1	C	0.40	0/3331	0.59	0/4502
1	D	0.51	0/3368	0.66	2/4553 (0.0%)
All	All	0.45	1/13346 (0.0%)	0.63	3/18041 (0.0%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	1097	PHE	CG-CD2	-6.11	1.29	1.38

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	1047	ARG	NE-CZ-NH2	-6.47	117.06	120.30
1	D	772	LEU	CA-CB-CG	5.33	127.55	115.30
1	D	881	ARG	NE-CZ-NH1	5.02	122.81	120.30

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	3279	0	3155	39	0
1	B	3242	0	3111	39	0
1	C	3271	0	3145	36	0
1	D	3296	0	3168	52	0
2	E	50	0	43	1	0
3	F	39	0	34	0	0
4	G	61	0	52	0	0
4	H	61	0	52	3	0
5	A	14	0	13	0	0
5	B	14	0	13	0	0
5	C	14	0	13	0	0
5	D	14	0	13	0	0
6	A	12	0	13	1	0
6	B	12	0	13	0	0
6	C	12	0	13	0	0
6	D	24	0	26	3	0
7	A	6	0	8	0	0
7	B	6	0	8	0	0
7	C	6	0	8	0	0
7	D	12	0	16	10	0
8	A	332	0	0	12	0
8	B	111	0	0	1	0
8	C	170	0	0	7	0
8	D	324	0	0	11	0
All	All	14382	0	12917	166	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 6.

All (166) 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:D:912:GLY:HA3	7:D:1210:GOL:H11	1.41	1.02
1:B:1060:LEU:HA	1:B:1101:CYS:HB3	1.53	0.89
1:B:1104:ASP:HB3	1:B:1105:GLU:HA	1.53	0.89
1:B:1102:ASP:HB3	1:B:1104:ASP:N	1.90	0.83
1:A:753:GLU:HG2	1:A:1002:PHE:CE1	2.13	0.82
1:D:1004:LYS:HE3	4:H:5:BMA:O3	1.81	0.81
1:B:1039:CYS:HA	1:B:1114:LEU:HG	1.61	0.80
1:D:1087:HIS:HD2	8:D:1422:HOH:O	1.66	0.78
1:D:753[A]:GLU:HG2	1:D:1002:PHE:CE1	2.20	0.77
1:B:1104:ASP:CB	1:B:1105:GLU:HA	2.12	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:711:THR:HG21	1:D:741:GLN:HE22	1.54	0.73
1:A:735:LYS:HD2	1:A:742[A]:THR:HG22	1.71	0.73
1:A:805:GLU:HG2	8:A:1516:HOH:O	1.89	0.72
1:B:1060:LEU:O	1:B:1072:VAL:HA	1.89	0.71
1:B:792:ARG:HG2	1:B:792:ARG:HH11	1.53	0.71
7:D:1210:GOL:O3	8:D:1621:HOH:O	2.09	0.71
1:D:696:GLN:NE2	1:D:735:LYS:HD3	2.06	0.71
1:B:1065:LYS:HD2	1:B:1068:SER:HB2	1.72	0.70
1:A:688:ASP:N	1:A:689:PRO:HD3	2.07	0.69
1:D:753[A]:GLU:HG2	1:D:1002:PHE:CD1	2.27	0.69
1:A:892:LEU:CD2	8:A:1632:HOH:O	2.41	0.69
1:A:891:SER:HB2	1:A:1012:THR:OG1	1.93	0.68
1:B:778:HIS:NE2	1:B:785:VAL:HG23	2.09	0.67
1:A:892:LEU:C	1:A:892:LEU:HD23	2.14	0.67
1:A:706:THR:HG22	1:A:711:THR:HB	1.77	0.67
1:B:1062:ALA:HA	1:B:1099:TYR:HA	1.75	0.67
1:D:707:GLU:HG3	1:D:708:GLY:N	2.10	0.67
1:D:700:ARG:HG3	1:D:700:ARG:HH11	1.59	0.66
1:C:722:ARG:HD2	8:C:1366:HOH:O	1.94	0.66
1:D:778:HIS:CE1	6:D:1208:MES:H72	2.30	0.66
1:B:1104:ASP:HB3	1:B:1105:GLU:CA	2.23	0.65
1:A:803:VAL:HG12	8:A:1542:HOH:O	1.97	0.64
1:A:695:ILE:HG12	1:A:721:ILE:HD12	1.80	0.64
1:B:754:LEU:HD11	1:B:895:GLU:O	1.98	0.63
1:A:688:ASP:N	2:E:4:BMA:HO6	1.96	0.62
1:C:805:GLU:HG2	8:C:1444:HOH:O	2.00	0.62
1:D:970:ILE:HD11	1:D:975:VAL:HG21	1.82	0.61
1:A:695:ILE:HG13	1:A:732:LEU:HD12	1.81	0.61
1:D:912:GLY:CA	7:D:1210:GOL:H11	2.25	0.61
1:C:897:ILE:HB	1:C:900:SER:HB3	1.82	0.61
1:B:1029:CYS:HB3	1:B:1054:SER:HB2	1.81	0.60
1:D:707:GLU:HG3	1:D:708:GLY:H	1.65	0.60
1:B:1029:CYS:HB3	1:B:1054:SER:CB	2.31	0.60
1:C:688:ASP:N	1:C:689:PRO:HD3	2.16	0.60
1:A:892:LEU:HD23	1:A:893:ASP:N	2.16	0.60
1:A:753:GLU:HG2	1:A:1002:PHE:HE1	1.67	0.60
1:D:970:ILE:CD1	1:D:975:VAL:HG21	2.33	0.59
1:A:688:ASP:N	1:A:689:PRO:CD	2.65	0.59
1:B:792:ARG:HG2	1:B:792:ARG:NH1	2.15	0.59
1:C:891:SER:HB2	1:C:1012:THR:OG1	2.03	0.59
1:D:700:ARG:HG3	1:D:700:ARG:NH1	2.16	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:973:PHE:O	1:C:977:GLU:HG2	2.02	0.58
1:D:980[B]:SER:OG	7:D:1210:GOL:H31	2.03	0.58
1:C:885:TRP:HH2	1:C:888:VAL:HG22	1.68	0.58
1:B:1060:LEU:HA	1:B:1101:CYS:CB	2.31	0.58
1:B:1031:ALA:HA	1:B:1051:SER:O	2.04	0.58
1:A:892:LEU:CD1	8:A:1632:HOH:O	2.51	0.58
1:D:912:GLY:HA3	7:D:1210:GOL:C1	2.27	0.58
1:D:980[A]:SER:HB2	7:D:1210:GOL:H31	1.86	0.57
1:D:913:TYR:O	7:D:1210:GOL:H32	2.04	0.57
1:A:892:LEU:HD22	8:A:1632:HOH:O	2.02	0.57
1:C:935:ASN:HB2	8:C:1334:HOH:O	2.05	0.56
1:D:1087:HIS:CD2	8:D:1422:HOH:O	2.49	0.55
1:C:703:THR:HG23	8:C:1352:HOH:O	2.05	0.55
1:A:698:SER:OG	1:A:700:ARG:HG2	2.07	0.55
1:C:1008:GLN:NE2	8:C:1470:HOH:O	2.38	0.55
1:A:1048:VAL:HG11	1:A:1086:LEU:HD22	1.88	0.55
1:A:708:GLY:O	1:A:709:VAL:HG22	2.07	0.54
1:C:892:LEU:HB3	1:C:1010:ASP:HB2	1.90	0.54
1:D:970:ILE:CD1	1:D:975:VAL:CG2	2.87	0.53
1:D:758[B]:GLU:HG3	1:D:759:GLY:N	2.20	0.53
1:D:1053:THR:HG23	1:D:1079:THR:HG22	1.91	0.52
1:C:1062:ALA:HB3	1:C:1071:ILE:HB	1.92	0.52
1:A:776:ARG:HD3	6:A:1206:MES:O1S	2.09	0.52
1:A:892:LEU:C	1:A:892:LEU:CD2	2.78	0.52
1:C:1035:ASN:OD1	1:C:1049:CYS:HB2	2.11	0.51
1:C:735:LYS:O	1:C:735:LYS:HE2	2.11	0.51
1:D:769:PRO:HG3	1:D:967:THR:HG23	1.91	0.51
1:D:911:LYS:HE2	8:D:1621:HOH:O	2.11	0.51
1:B:1103:GLY:O	1:B:1104:ASP:HB2	2.09	0.50
1:D:821:TRP:CZ2	1:D:826:PHE:HA	2.46	0.50
1:D:913:TYR:H	7:D:1210:GOL:C1	2.25	0.50
1:A:1087:HIS:HD2	8:A:1449:HOH:O	1.95	0.49
1:C:688:ASP:N	1:C:689:PRO:CD	2.75	0.49
1:D:707:GLU:HG2	1:D:709:VAL:HG12	1.95	0.49
1:A:753:GLU:HG2	1:A:1002:PHE:CD1	2.46	0.49
1:B:1053:THR:HG22	1:B:1079:THR:HA	1.95	0.49
1:C:707:GLU:HG3	1:C:707:GLU:O	2.12	0.49
1:D:778:HIS:HE1	6:D:1208:MES:H72	1.75	0.48
1:B:785:VAL:HA	1:B:786:ASN:HA	1.67	0.48
1:C:892:LEU:O	1:C:1009:ALA:HA	2.14	0.48
1:B:1095:GLU:HB3	1:B:1110:VAL:HG22	1.96	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:1106:ARG:HB2	1:C:1107:PRO:HD2	1.96	0.47
1:C:923:ILE:O	1:C:925:ARG:HG3	2.14	0.47
1:D:859:LEU:HD23	1:D:890:LEU:HD21	1.96	0.47
1:A:711:THR:HG21	1:A:741:GLN:HE22	1.79	0.47
1:B:1064:ASN:ND2	1:B:1096:GLU:O	2.47	0.47
1:D:699:SER:HA	8:D:1435:HOH:O	2.13	0.47
1:A:759:GLY:HA3	1:A:853:ILE:HG23	1.95	0.47
1:C:736:GLY:HA3	1:C:741:GLN:HE21	1.80	0.47
1:D:711:THR:HG21	1:D:741:GLN:NE2	2.25	0.46
1:C:989:THR:OG1	1:C:1004:LYS:HD2	2.15	0.46
1:B:729:GLU:OE2	1:B:746:LYS:HB3	2.16	0.46
1:B:1061:SER:HA	1:B:1071:ILE:O	2.15	0.46
1:D:913:TYR:O	7:D:1210:GOL:C3	2.63	0.46
1:B:1102:ASP:HB3	1:B:1103:GLY:C	2.35	0.46
1:A:693:GLU:HG2	8:A:1395:HOH:O	2.16	0.46
1:A:770:LYS:HD3	8:A:1618:HOH:O	2.16	0.46
1:C:847:LEU:HD12	1:C:972:PRO:HB2	1.98	0.46
1:B:1023:VAL:HA	1:B:1024:GLY:HA2	1.72	0.45
1:A:925:ARG:HG2	1:A:928:PHE:CD1	2.52	0.45
1:A:978:ARG:HD3	8:A:1350:HOH:O	2.15	0.45
1:D:711:THR:CG2	1:D:741:GLN:NE2	2.80	0.45
1:B:1105:GLU:O	1:B:1106:ARG:HG2	2.16	0.45
1:D:1004:LYS:HE3	4:H:5:BMA:HO3	1.80	0.45
1:A:922:GLU:HG2	1:A:922:GLU:H	1.53	0.44
1:B:1085:ILE:O	1:B:1086:LEU:HD12	2.18	0.44
1:C:1040:TYR:HB3	1:C:1114:LEU:HD23	1.99	0.44
1:C:876:GLY:H	1:C:879:SER:HB2	1.81	0.44
1:D:743:LYS:HD2	1:D:1021:ASP:O	2.18	0.44
1:D:709:VAL:HG13	1:D:710:ASN:OD1	2.17	0.44
1:A:788:CYS:HB2	1:A:832:CYS:SG	2.58	0.44
1:B:752:SER:HB3	1:B:1003:SER:HB2	2.00	0.44
1:C:1095:GLU:HB2	1:C:1110:VAL:CG2	2.47	0.44
1:A:742[B]:THR:HB	1:A:1059:SER:HG	1.81	0.44
1:B:770:LYS:HG3	1:B:840:GLN:OE1	2.17	0.44
1:B:777:CYS:HB3	8:B:1404:HOH:O	2.17	0.44
1:C:1109:LEU:HG	8:C:1455:HOH:O	2.17	0.44
1:C:1095:GLU:HB2	1:C:1110:VAL:HG23	2.00	0.43
1:D:735:LYS:HG2	8:D:1496:HOH:O	2.18	0.43
1:D:785:VAL:HG11	6:D:1208:MES:H32	1.99	0.43
1:D:753[A]:GLU:HG2	1:D:1002:PHE:HE1	1.80	0.43
1:B:722:ARG:NH2	1:B:1008:GLN:HA	2.32	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:967:THR:HB	1:B:969:LEU:HG	1.99	0.43
1:D:688:ASP:N	8:D:1606:HOH:O	2.52	0.43
1:A:892:LEU:HD13	8:A:1632:HOH:O	2.18	0.43
1:C:706:THR:HG23	1:C:711:THR:HG22	2.01	0.43
1:C:1008:GLN:HE22	1:D:819:GLY:H	1.67	0.43
1:D:1035:ASN:HD22	4:H:1:NAG:H83	1.84	0.42
1:D:700:ARG:NH2	8:D:1430:HOH:O	2.52	0.42
1:C:1115:ILE:HG13	1:C:1115:ILE:H	1.74	0.42
1:A:1057:THR:HG23	8:A:1310:HOH:O	2.20	0.42
1:A:722:ARG:NH1	8:A:1632:HOH:O	2.35	0.42
1:B:989:THR:O	1:B:1001:ALA:HA	2.19	0.42
1:D:819:GLY:HA3	1:D:829:ASN:O	2.20	0.42
1:A:693:GLU:OE2	1:B:821:TRP:HD1	2.02	0.42
1:A:735:LYS:NZ	1:A:739:GLU:O	2.53	0.42
1:D:714:ARG:HA	1:D:1018:PHE:O	2.20	0.41
1:B:1102:ASP:N	1:B:1103:GLY:HA2	2.35	0.41
1:C:885:TRP:CH2	1:C:888:VAL:HG22	2.52	0.41
1:C:1064:ASN:HA	1:C:1096:GLU:O	2.20	0.41
1:C:801:SER:C	1:C:803:VAL:H	2.24	0.41
7:D:1210:GOL:H12	8:D:1577:HOH:O	2.20	0.41
1:D:1031:ALA:HA	1:D:1051:SER:O	2.20	0.41
1:B:1027:VAL:HG21	1:B:1055:THR:HB	2.02	0.41
1:D:693:GLU:HG2	8:D:1434:HOH:O	2.20	0.41
1:B:1017:ASN:HD22	1:B:1017:ASN:HA	1.59	0.41
1:B:1085:ILE:H	1:B:1085:ILE:HG13	1.69	0.41
1:C:714:ARG:NH2	8:C:1377:HOH:O	2.54	0.41
1:D:996:ASN:ND2	8:D:1577:HOH:O	2.53	0.41
1:D:753[A]:GLU:OE1	1:D:1002:PHE:HE1	2.04	0.40
1:A:1066:ASP:OD1	1:A:1066:ASP:N	2.55	0.40
1:D:791:TRP:CE2	1:D:795:GLU:HG3	2.57	0.40
1:C:890:LEU:CD2	1:C:1009:ALA:HB1	2.51	0.40
1:C:993:SER:HB3	1:C:996:ASN:HB3	2.03	0.40
1:D:843:ARG:HD2	1:D:973:PHE:CE1	2.57	0.40

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	431/432 (100%)	417 (97%)	10 (2%)	4 (1%)	17 7
1	B	425/432 (98%)	404 (95%)	17 (4%)	4 (1%)	17 7
1	C	429/432 (99%)	413 (96%)	13 (3%)	3 (1%)	22 12
1	D	434/432 (100%)	422 (97%)	11 (2%)	1 (0%)	47 38
All	All	1719/1728 (100%)	1656 (96%)	51 (3%)	12 (1%)	22 12

All (12) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	960	ILE
1	B	960	ILE
1	C	785	VAL
1	C	960	ILE
1	D	960	ILE
1	A	708	GLY
1	A	709	VAL
1	B	1091	PRO
1	C	802	PHE
1	B	1107	PRO
1	B	1027	VAL
1	A	785	VAL

5.3.2 Protein sidechains (i)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	A	373/372 (100%)	356 (95%)	17 (5%)	27 17
1	B	368/372 (99%)	345 (94%)	23 (6%)	18 8
1	C	371/372 (100%)	359 (97%)	12 (3%)	39 30
1	D	376/372 (101%)	361 (96%)	15 (4%)	31 22
All	All	1488/1488 (100%)	1421 (96%)	67 (4%)	27 18

All (67) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	710	ASN
1	A	711	THR
1	A	720	LEU
1	A	740	ASP
1	A	743	LYS
1	A	874	ASP
1	A	891	SER
1	A	892	LEU
1	A	922	GLU
1	A	923	ILE
1	A	941	LEU
1	A	994	LYS
1	A	1017	ASN
1	A	1050	LEU
1	A	1080	LYS
1	A	1086	LEU
1	A	1111	LYS
1	B	696	GLN
1	B	700	ARG
1	B	711	THR
1	B	712	LYS
1	B	714	ARG
1	B	725	SER
1	B	740	ASP
1	B	742	THR
1	B	842	VAL
1	B	911	LYS
1	B	925	ARG
1	B	937	GLU
1	B	977	GLU
1	B	997	ARG
1	B	1016	ASP
1	B	1017	ASN

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Mol	Chain	Res	Type
1	B	1029	CYS
1	B	1030	ASP
1	B	1064	ASN
1	B	1072	VAL
1	B	1085	ILE
1	B	1086	LEU
1	B	1096	GLU
1	C	707	GLU
1	C	711	THR
1	C	722	ARG
1	C	735	LYS
1	C	792	ARG
1	C	879	SER
1	C	911	LYS
1	C	994	LYS
1	C	1016	ASP
1	C	1029	CYS
1	C	1036	LEU
1	C	1066	ASP
1	D	700	ARG
1	D	711	THR
1	D	737	VAL
1	D	740	ASP
1	D	761	SER
1	D	772	LEU
1	D	941	LEU
1	D	970	ILE
1	D	996	ASN
1	D	1017	ASN
1	D	1047	ARG
1	D	1057	THR
1	D	1065	LYS
1	D	1079	THR
1	D	1086	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (14) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	710	ASN
1	A	1043	ASN
1	B	996	ASN
1	B	1017	ASN

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Mol	Chain	Res	Type
1	B	1063	HIS
1	B	1064	ASN
1	C	741	GLN
1	C	1008	GLN
1	D	696	GLN
1	D	778	HIS
1	D	784	HIS
1	D	829	ASN
1	D	996	ASN
1	D	1017	ASN

5.3.3 RNA

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates

17 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	$\#\|Z\| > 2$
2	NAG	E	1	1,2	14,14,15	0.64	0	17,19,21	1.25	3 (17%)
2	NAG	E	2	2	14,14,15	0.74	0	17,19,21	1.31	2 (11%)
2	BMA	E	3	2	11,11,12	0.82	0	15,15,17	1.48	3 (20%)
2	BMA	E	4	2	11,11,12	0.75	1 (9%)	15,15,17	1.94	4 (26%)
3	NAG	F	1	1,3	14,14,15	0.59	0	17,19,21	1.35	2 (11%)
3	NAG	F	2	3	14,14,15	0.43	0	17,19,21	1.72	6 (35%)
3	BMA	F	3	3	11,11,12	1.10	1 (9%)	15,15,17	1.25	2 (13%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
4	NAG	G	1	1,4	14,14,15	0.49	0	17,19,21	1.46	4 (23%)
4	NAG	G	2	4	14,14,15	0.58	0	17,19,21	1.28	1 (5%)
4	BMA	G	3	4	11,11,12	0.51	0	15,15,17	1.10	1 (6%)
4	BMA	G	4	4	11,11,12	0.49	0	15,15,17	1.33	1 (6%)
4	BMA	G	5	4	11,11,12	0.52	0	15,15,17	2.09	3 (20%)
4	NAG	H	1	1,4	14,14,15	0.52	0	17,19,21	1.21	3 (17%)
4	NAG	H	2	4	14,14,15	0.80	0	17,19,21	1.39	1 (5%)
4	BMA	H	3	4	11,11,12	0.92	1 (9%)	15,15,17	3.40	6 (40%)
4	BMA	H	4	4	11,11,12	0.67	0	15,15,17	2.69	6 (40%)
4	BMA	H	5	4	11,11,12	0.51	0	15,15,17	2.00	3 (20%)

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

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	F	3	BMA	O5-C1	3.17	1.48	1.43
4	H	3	BMA	O5-C1	2.32	1.47	1.43
2	E	4	BMA	O4-C4	2.00	1.47	1.43

All (51) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	H	3	BMA	O5-C1-C2	6.69	121.10	110.77
4	H	3	BMA	O5-C5-C6	6.26	117.03	107.20
4	G	5	BMA	C1-O5-C5	5.80	120.05	112.19
4	H	5	BMA	C1-O5-C5	-5.74	104.42	112.19
4	H	4	BMA	C1-O5-C5	5.69	119.90	112.19
4	H	3	BMA	C3-C4-C5	-5.62	100.21	110.24
4	H	4	BMA	O5-C1-C2	5.23	118.84	110.77
4	H	3	BMA	O3-C3-C4	4.53	120.83	110.35
4	H	4	BMA	C3-C4-C5	4.25	117.81	110.24
4	H	3	BMA	O3-C3-C2	4.16	117.95	109.99
4	G	4	BMA	C1-O5-C5	4.06	117.69	112.19
2	E	4	BMA	C1-C2-C3	3.90	114.46	109.67
4	H	2	NAG	O4-C4-C5	-3.86	99.70	109.30
4	H	4	BMA	C1-C2-C3	3.73	114.26	109.67
2	E	3	BMA	O5-C5-C6	-3.73	101.35	107.20
4	G	5	BMA	C3-C4-C5	3.73	116.89	110.24
2	E	4	BMA	O5-C1-C2	3.69	116.47	110.77
3	F	2	NAG	C3-C4-C5	3.66	116.77	110.24
2	E	4	BMA	C1-O5-C5	3.43	116.84	112.19
4	H	5	BMA	O5-C5-C6	3.37	112.48	107.20
4	G	2	NAG	C4-C3-C2	3.36	115.95	111.02
4	G	1	NAG	C4-C3-C2	-3.34	106.12	111.02
3	F	1	NAG	O5-C1-C2	-3.13	106.35	111.29
4	G	3	BMA	O5-C5-C6	3.12	112.10	107.20
4	H	3	BMA	C1-C2-C3	-3.10	105.85	109.67
4	G	5	BMA	O5-C5-C4	3.05	118.25	110.83
3	F	3	BMA	C1-C2-C3	-3.05	105.92	109.67
2	E	2	NAG	O4-C4-C5	-2.87	102.16	109.30
3	F	2	NAG	C1-O5-C5	2.82	116.02	112.19
2	E	4	BMA	O5-C5-C6	2.66	111.37	107.20
2	E	3	BMA	C6-C5-C4	2.61	119.12	113.00
2	E	1	NAG	O7-C7-C8	-2.55	117.31	122.06
4	H	1	NAG	C8-C7-N2	2.53	120.39	116.10
2	E	2	NAG	O5-C5-C6	2.40	110.96	107.20
3	F	2	NAG	O5-C1-C2	-2.38	107.52	111.29
4	H	4	BMA	C2-C3-C4	2.35	114.97	110.89

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	F	2	NAG	C6-C5-C4	-2.34	107.53	113.00
4	H	5	BMA	O5-C1-C2	2.33	114.36	110.77
4	G	1	NAG	C8-C7-N2	2.31	120.02	116.10
3	F	3	BMA	O5-C5-C6	2.29	110.79	107.20
4	H	1	NAG	O7-C7-C8	-2.28	117.83	122.06
4	G	1	NAG	O5-C1-C2	-2.26	107.72	111.29
2	E	1	NAG	C8-C7-N2	2.25	119.91	116.10
2	E	1	NAG	C1-C2-N2	-2.23	106.69	110.49
3	F	2	NAG	C4-C3-C2	2.21	114.25	111.02
4	H	1	NAG	O5-C1-C2	-2.12	107.94	111.29
3	F	1	NAG	C8-C7-N2	2.09	119.63	116.10
2	E	3	BMA	C1-C2-C3	-2.05	107.14	109.67
4	G	1	NAG	C1-C2-N2	2.02	113.93	110.49
4	H	4	BMA	O5-C5-C4	2.01	115.72	110.83
3	F	2	NAG	O5-C5-C4	2.01	115.71	110.83

There are no chirality outliers.

All (27) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	E	3	BMA	C4-C5-C6-O6
2	E	3	BMA	O5-C5-C6-O6
4	G	5	BMA	O5-C5-C6-O6
4	H	3	BMA	O5-C5-C6-O6
4	G	4	BMA	O5-C5-C6-O6
4	G	2	NAG	O5-C5-C6-O6
3	F	1	NAG	O5-C5-C6-O6
2	E	4	BMA	O5-C5-C6-O6
4	G	4	BMA	C4-C5-C6-O6
4	H	3	BMA	C4-C5-C6-O6
4	H	1	NAG	C8-C7-N2-C2
4	H	1	NAG	O7-C7-N2-C2
4	G	1	NAG	C8-C7-N2-C2
4	G	1	NAG	O7-C7-N2-C2
2	E	1	NAG	C8-C7-N2-C2
2	E	1	NAG	O7-C7-N2-C2
3	F	1	NAG	C8-C7-N2-C2
3	F	1	NAG	O7-C7-N2-C2
4	H	4	BMA	O5-C5-C6-O6
4	G	2	NAG	C4-C5-C6-O6
4	G	5	BMA	C4-C5-C6-O6
2	E	4	BMA	C4-C5-C6-O6

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Mol	Chain	Res	Type	Atoms
3	F	1	NAG	C4-C5-C6-O6
3	F	3	BMA	C4-C5-C6-O6
3	F	3	BMA	O5-C5-C6-O6
3	F	2	NAG	C4-C5-C6-O6
4	H	4	BMA	C4-C5-C6-O6

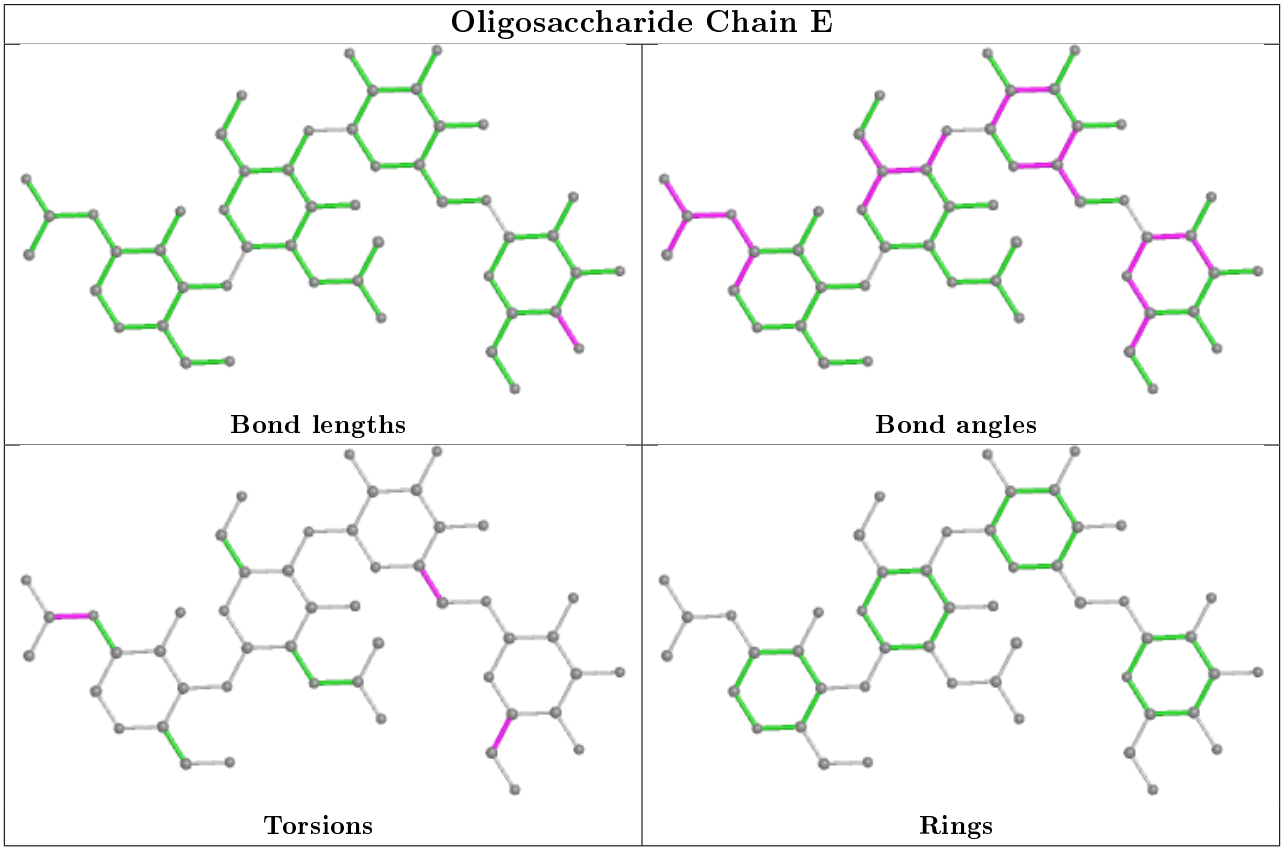
All (1) ring outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	G	4	BMA	C1-C2-C3-C4-C5-O5

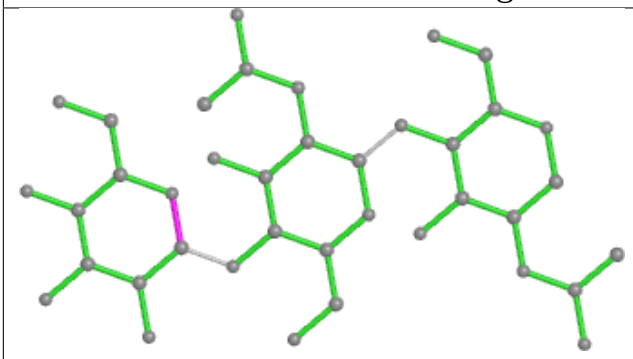
3 monomers are involved in 4 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	H	5	BMA	2	0
4	H	1	NAG	1	0
2	E	4	BMA	1	0

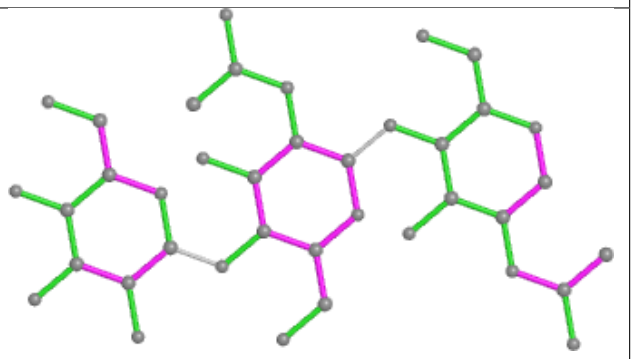
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for oligosaccharide.



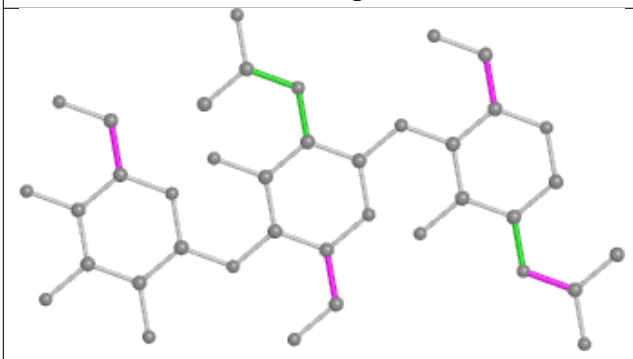
Oligosaccharide Chain F



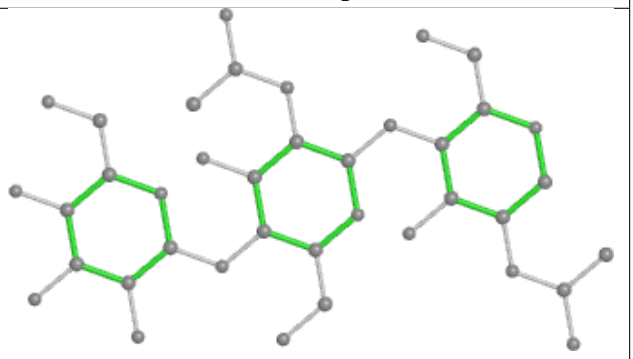
Bond lengths



Bond angles

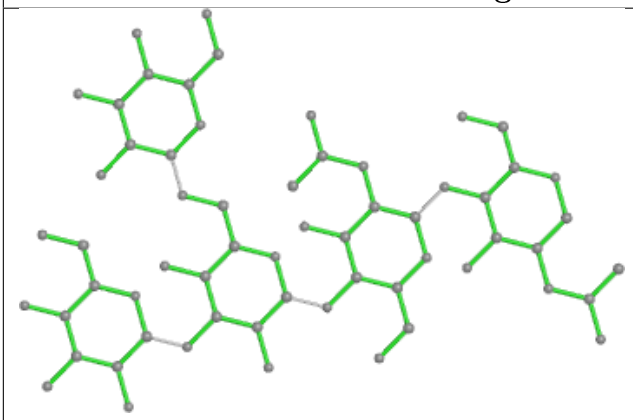


Torsions

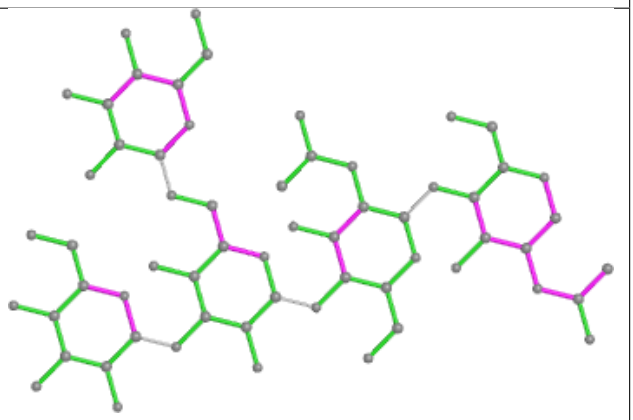


Rings

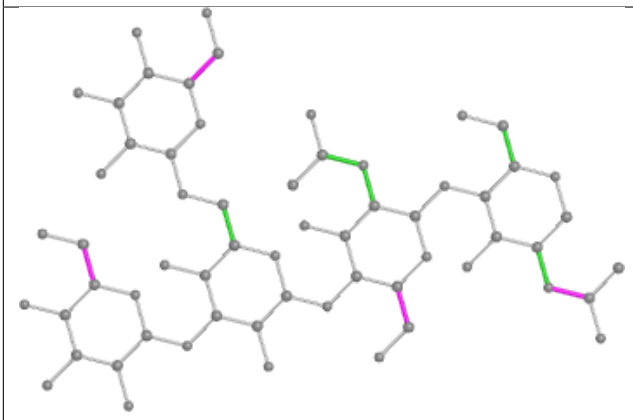
Oligosaccharide Chain G



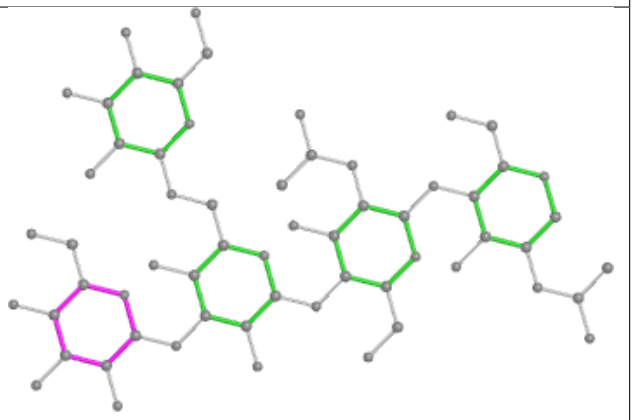
Bond lengths



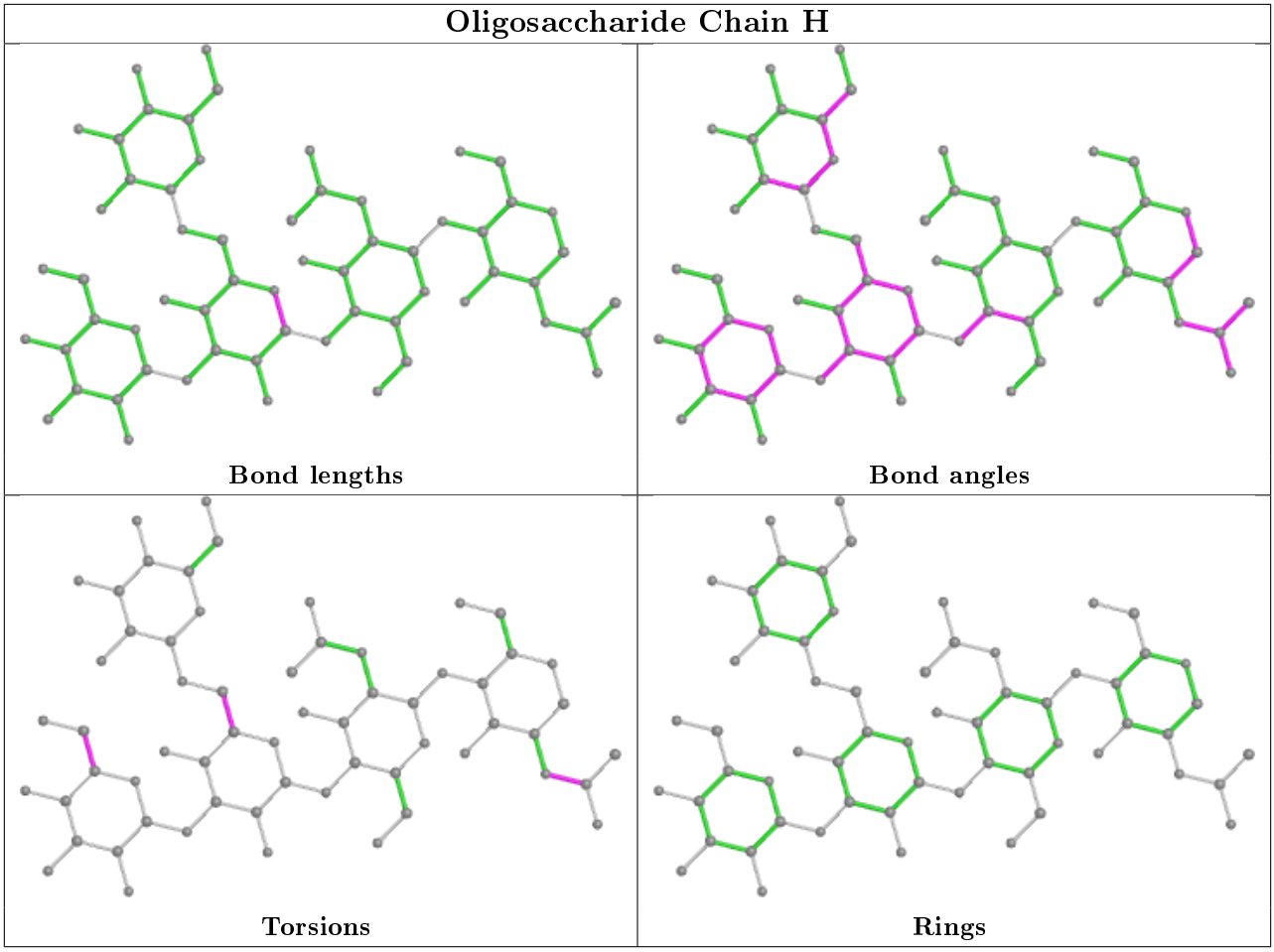
Bond angles



Torsions



Rings



5.6 Ligand geometry (i)

14 ligands are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
7	GOL	B	1206	-	5,5,5	0.33	0	5,5,5	0.34	0
6	MES	C	1207	-	12,12,12	2.39	1 (8%)	14,16,16	6.09	5 (35%)
5	NAG	C	1201	1	14,14,15	0.54	0	17,19,21	1.08	0
5	NAG	A	1201	1	14,14,15	0.52	0	17,19,21	1.26	2 (11%)
7	GOL	C	1208	-	5,5,5	0.20	0	5,5,5	0.44	0
6	MES	B	1205	-	12,12,12	2.09	1 (8%)	14,16,16	1.71	1 (7%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
6	MES	D	1208	-	12,12,12	2.14	1 (8%)	14,16,16	7.11	5 (35%)
7	GOL	D	1210	-	5,5,5	0.09	0	5,5,5	0.56	0
7	GOL	A	1207	-	5,5,5	0.21	0	5,5,5	0.62	0
5	NAG	D	1201	1	14,14,15	0.48	0	17,19,21	0.96	1 (5%)
7	GOL	D	1209	-	5,5,5	0.38	0	5,5,5	0.50	0
5	NAG	B	1201	1	14,14,15	0.49	0	17,19,21	1.10	0
6	MES	A	1206	-	12,12,12	2.26	1 (8%)	14,16,16	7.00	9 (64%)
6	MES	D	1207	-	12,12,12	2.40	1 (8%)	14,16,16	6.49	8 (57%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
7	GOL	B	1206	-	-	1/4/4/4	-
6	MES	C	1207	-	-	2/6/14/14	0/1/1/1
5	NAG	C	1201	1	-	2/6/23/26	0/1/1/1
5	NAG	A	1201	1	-	2/6/23/26	0/1/1/1
7	GOL	C	1208	-	-	0/4/4/4	-
6	MES	B	1205	-	-	4/6/14/14	0/1/1/1
6	MES	D	1208	-	-	4/6/14/14	0/1/1/1
7	GOL	D	1210	-	-	2/4/4/4	-
7	GOL	A	1207	-	-	0/4/4/4	-
5	NAG	D	1201	1	-	2/6/23/26	0/1/1/1
7	GOL	D	1209	-	-	0/4/4/4	-
5	NAG	B	1201	1	-	4/6/23/26	0/1/1/1
6	MES	A	1206	-	-	3/6/14/14	0/1/1/1
6	MES	D	1207	-	-	5/6/14/14	0/1/1/1

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	C	1207	MES	C8-S	-8.11	1.66	1.77
6	D	1207	MES	C8-S	-8.00	1.66	1.77
6	A	1206	MES	C8-S	-7.49	1.66	1.77
6	D	1208	MES	C8-S	-7.08	1.67	1.77
6	B	1205	MES	C8-S	-6.84	1.67	1.77

All (31) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
6	A	1206	MES	O3S-S-C8	-13.41	84.08	105.77
6	D	1208	MES	O3S-S-C8	-13.28	84.28	105.77
6	C	1207	MES	O2S-S-C8	13.00	122.57	106.92
6	D	1208	MES	O2S-S-C8	12.75	122.27	106.92
6	D	1207	MES	O3S-S-O1S	-11.99	81.97	111.27
6	D	1208	MES	O3S-S-O2S	-11.87	82.26	111.27
6	A	1206	MES	O1S-S-C8	11.52	120.78	106.92
6	C	1207	MES	O1S-S-C8	11.42	120.67	106.92
6	D	1207	MES	O3S-S-C8	-11.12	87.79	105.77
6	A	1206	MES	O3S-S-O2S	-11.09	84.17	111.27
6	D	1208	MES	O1S-S-C8	10.63	119.72	106.92
6	D	1207	MES	O3S-S-O2S	-10.34	86.00	111.27
6	A	1206	MES	O3S-S-O1S	-10.31	86.08	111.27
6	A	1206	MES	O2S-S-C8	10.28	119.29	106.92
6	D	1208	MES	O3S-S-O1S	-10.19	86.37	111.27
6	D	1207	MES	O2S-S-C8	9.75	118.65	106.92
6	C	1207	MES	O3S-S-C8	-9.68	90.10	105.77
6	D	1207	MES	O1S-S-C8	9.28	118.09	106.92
6	C	1207	MES	O3S-S-O1S	-8.63	90.18	111.27
6	C	1207	MES	O3S-S-O2S	-6.50	95.40	111.27
6	B	1205	MES	O3S-S-C8	5.18	114.15	105.77
6	D	1207	MES	C2-C3-N4	-3.73	104.44	110.10
6	A	1206	MES	C5-N4-C3	3.48	116.66	108.83
6	D	1207	MES	C6-C5-N4	-2.94	105.64	110.10
6	A	1206	MES	C6-C5-N4	2.47	113.84	110.10
6	A	1206	MES	C7-N4-C3	-2.34	105.26	111.23
5	A	1201	NAG	C2-N2-C7	2.31	126.19	122.90
5	D	1201	NAG	C8-C7-N2	2.11	119.67	116.10
6	D	1207	MES	O2S-S-O1S	2.10	121.20	113.95
5	A	1201	NAG	C8-C7-N2	2.05	119.57	116.10
6	A	1206	MES	C7-N4-C5	-2.03	106.04	111.23

There are no chirality outliers.

All (31) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
6	C	1207	MES	C7-C8-S-O2S
6	B	1205	MES	C7-C8-S-O2S
6	B	1205	MES	C7-C8-S-O3S
7	D	1210	GOL	O1-C1-C2-C3
6	A	1206	MES	N4-C7-C8-S

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Mol	Chain	Res	Type	Atoms
6	A	1206	MES	C7-C8-S-O1S
5	C	1201	NAG	C8-C7-N2-C2
5	C	1201	NAG	O7-C7-N2-C2
5	A	1201	NAG	C8-C7-N2-C2
5	A	1201	NAG	O7-C7-N2-C2
5	D	1201	NAG	C8-C7-N2-C2
5	D	1201	NAG	O7-C7-N2-C2
5	B	1201	NAG	C8-C7-N2-C2
5	B	1201	NAG	O7-C7-N2-C2
6	C	1207	MES	C7-C8-S-O3S
6	A	1206	MES	C7-C8-S-O3S
6	D	1207	MES	C7-C8-S-O3S
5	B	1201	NAG	C4-C5-C6-O6
5	B	1201	NAG	O5-C5-C6-O6
7	D	1210	GOL	O1-C1-C2-O2
6	D	1208	MES	C7-C8-S-O3S
6	B	1205	MES	N4-C7-C8-S
6	D	1207	MES	N4-C7-C8-S
6	D	1208	MES	C8-C7-N4-C5
6	B	1205	MES	C7-C8-S-O1S
6	D	1208	MES	C7-C8-S-O2S
6	D	1207	MES	C7-C8-S-O2S
6	D	1208	MES	C8-C7-N4-C3
6	D	1207	MES	C8-C7-N4-C3
6	D	1207	MES	C8-C7-N4-C5
7	B	1206	GOL	O1-C1-C2-O2

There are no ring outliers.

3 monomers are involved in 14 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	D	1208	MES	3	0
7	D	1210	GOL	10	0
6	A	1206	MES	1	0

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

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	431/432 (99%)	0.33	24 (5%) 24 27	22, 37, 68, 100	0
1	B	427/432 (98%)	1.57	113 (26%) 0 0	35, 70, 169, 214	0
1	C	430/432 (99%)	0.67	62 (14%) 2 2	28, 52, 110, 139	0
1	D	431/432 (99%)	0.45	34 (7%) 12 14	21, 39, 71, 128	0
All	All	1719/1728 (99%)	0.75	233 (13%) 3 3	21, 49, 120, 214	0

All (233) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	706	THR	13.7
1	B	709	VAL	13.1
1	B	1023	VAL	12.2
1	B	1067	GLY	10.6
1	B	737	VAL	10.4
1	B	1088	PHE	10.1
1	A	709	VAL	9.5
1	D	709	VAL	9.2
1	B	1025	ALA	9.0
1	D	708	GLY	8.9
1	B	1024	GLY	8.7
1	B	1101	CYS	8.6
1	B	1100	SER	8.4
1	C	709	VAL	8.2
1	B	1099	TYR	8.2
1	B	710	ASN	8.2
1	C	802	PHE	7.9
1	B	708	GLY	7.7
1	B	711	THR	7.7
1	B	785	VAL	7.6
1	B	1041	SER	7.5

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Mol	Chain	Res	Type	RSRZ
1	B	1107	PRO	7.5
1	B	704	CYS	7.4
1	B	1098	MET	7.4
1	B	1114	LEU	6.8
1	C	1027	VAL	6.7
1	C	706	THR	6.6
1	B	1029	CYS	6.6
1	B	1091	PRO	6.5
1	B	1106	ARG	6.4
1	A	996	ASN	6.4
1	B	1055	THR	6.4
1	B	1056	GLY	6.4
1	B	878	SER	6.3
1	B	712	LYS	6.3
1	B	1090	VAL	6.2
1	C	708	GLY	6.2
1	B	803	VAL	6.2
1	B	805	GLU	6.1
1	A	995	GLY	6.1
1	B	705	SER	6.0
1	B	1113	THR	5.9
1	B	1040	TYR	5.9
1	B	802	PHE	5.8
1	A	708	GLY	5.6
1	B	1110	VAL	5.6
1	D	995	GLY	5.6
1	D	710	ASN	5.6
1	B	1069	LEU	5.5
1	A	779	LEU	5.5
1	C	1032	ALA	5.5
1	D	707	GLU	5.4
1	B	1108	LEU	5.3
1	C	1117	ILE	5.3
1	B	1060	LEU	5.3
1	B	713	CYS	5.2
1	C	1096	GLU	5.1
1	C	1111	LYS	5.0
1	B	1052	ILE	5.0
1	B	1027	VAL	5.0
1	D	1025	ALA	5.0
1	B	1030	ASP	4.9
1	C	1090	VAL	4.9

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Mol	Chain	Res	Type	RSRZ
1	D	706	THR	4.9
1	C	737	VAL	4.9
1	B	736	GLY	4.9
1	C	1110	VAL	4.8
1	B	1103	GLY	4.8
1	B	1078	GLY	4.7
1	B	1028	SER	4.7
1	B	738	LYS	4.6
1	B	1105	GLU	4.6
1	B	994	LYS	4.5
1	B	1111	LYS	4.5
1	C	1025	ALA	4.5
1	B	1071	ILE	4.3
1	D	694	LEU	4.3
1	B	995	GLY	4.3
1	D	996	ASN	4.2
1	D	1023	VAL	4.2
1	D	994	LYS	4.2
1	B	1059	SER	4.2
1	B	1064	ASN	4.2
1	D	802	PHE	4.1
1	B	1094	GLU	4.1
1	A	710	ASN	4.0
1	B	715	LEU	4.0
1	B	1066	ASP	4.0
1	C	803	VAL	4.0
1	B	1095	GLU	4.0
1	B	1070	HIS	4.0
1	B	1092	GLU	3.9
1	B	1089	THR	3.9
1	C	1065	LYS	3.9
1	C	710	ASN	3.8
1	C	1026	ALA	3.8
1	C	738	LYS	3.8
1	B	1068	SER	3.8
1	B	1086	LEU	3.8
1	C	1116	ALA	3.7
1	B	735	LYS	3.7
1	B	1065	LYS	3.7
1	D	789	LEU	3.7
1	B	694	LEU	3.6
1	A	785	VAL	3.6

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Mol	Chain	Res	Type	RSRZ
1	C	707	GLU	3.6
1	C	1056	GLY	3.6
1	B	1109	LEU	3.6
1	D	805	GLU	3.6
1	D	1041	SER	3.6
1	C	1114	LEU	3.6
1	B	1026	ALA	3.5
1	B	1031	ALA	3.5
1	B	1062	ALA	3.5
1	C	1089	THR	3.4
1	C	1034	LEU	3.4
1	B	1039	CYS	3.4
1	C	1079	THR	3.4
1	B	911	LYS	3.3
1	C	1002	PHE	3.3
1	D	803	VAL	3.3
1	C	705	SER	3.3
1	C	853	ILE	3.3
1	B	702	THR	3.3
1	C	704	CYS	3.3
1	B	910	GLY	3.2
1	B	1097	PHE	3.2
1	C	1055	THR	3.2
1	A	994	LYS	3.2
1	A	694	LEU	3.2
1	B	739	GLU	3.2
1	B	1054	SER	3.1
1	B	740	ASP	3.1
1	A	707	GLU	3.1
1	D	695	ILE	3.1
1	B	1079	THR	3.0
1	A	1073	LEU	3.0
1	B	696	GLN	3.0
1	D	705	SER	3.0
1	B	1093	VAL	3.0
1	B	1022	PHE	2.9
1	B	707	GLU	2.9
1	D	997	ARG	2.9
1	C	995	GLY	2.9
1	D	1118	ASP	2.9
1	B	741	GLN	2.9
1	B	734	LEU	2.9

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Mol	Chain	Res	Type	RSRZ
1	C	1041	SER	2.8
1	B	792	ARG	2.8
1	A	706	THR	2.8
1	B	759	GLY	2.8
1	A	1066	ASP	2.8
1	A	804	GLY	2.7
1	B	948	LEU	2.7
1	B	1042	CYS	2.7
1	B	1020	VAL	2.7
1	C	1023	VAL	2.7
1	D	737	VAL	2.7
1	C	1068	SER	2.7
1	D	1115	ILE	2.7
1	C	1063	HIS	2.7
1	B	1087	HIS	2.7
1	B	699	SER	2.7
1	B	1045	GLY	2.7
1	C	994	LYS	2.7
1	A	730	ALA	2.6
1	B	1061	SER	2.6
1	B	996	ASN	2.6
1	A	695	ILE	2.6
1	A	1115	ILE	2.6
1	B	1104	ASP	2.6
1	C	1103	GLY	2.6
1	A	997	ARG	2.6
1	C	711	THR	2.6
1	C	1066	ASP	2.6
1	A	1025	ALA	2.6
1	C	740	ASP	2.6
1	D	1073	LEU	2.5
1	C	1091	PRO	2.5
1	C	1108	LEU	2.5
1	C	741	GLN	2.5
1	B	877	ALA	2.5
1	C	739	GLU	2.5
1	A	1118	ASP	2.5
1	C	1115	ILE	2.5
1	C	694	LEU	2.5
1	A	1065	LYS	2.4
1	B	1085	ILE	2.4
1	C	1040	TYR	2.4

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Mol	Chain	Res	Type	RSRZ
1	D	1024	GLY	2.4
1	C	1042	CYS	2.4
1	B	717	GLY	2.4
1	B	888	VAL	2.4
1	B	1036	LEU	2.4
1	C	1029	CYS	2.4
1	D	1117	ILE	2.4
1	C	935	ASN	2.3
1	C	792	ARG	2.3
1	D	700	ARG	2.3
1	D	721	ILE	2.3
1	B	786	ASN	2.2
1	B	946	SER	2.2
1	B	1072	VAL	2.2
1	C	1067	GLY	2.2
1	D	1113	THR	2.2
1	A	784	HIS	2.2
1	B	784	HIS	2.2
1	C	736	GLY	2.2
1	D	804	GLY	2.2
1	B	714	ARG	2.2
1	C	801	SER	2.2
1	C	878	SER	2.2
1	D	704	CYS	2.2
1	C	877	ALA	2.1
1	B	1096	GLU	2.1
1	B	1037	THR	2.1
1	D	853	ILE	2.1
1	B	1077	ASN	2.1
1	C	786	ASN	2.1
1	C	1102	ASP	2.1
1	A	1083	CYS	2.1
1	C	1107	PRO	2.1
1	B	760	GLN	2.1
1	D	711	THR	2.1
1	A	1117	ILE	2.1
1	C	1031	ALA	2.1
1	D	720	LEU	2.1
1	D	1013	LEU	2.1
1	C	1057	THR	2.1
1	B	795	GLU	2.0
1	B	1038	GLY	2.0

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Mol	Chain	Res	Type	RSRZ
1	B	892	LEU	2.0
1	C	805	GLU	2.0

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

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

6.3 Carbohydrates (i)

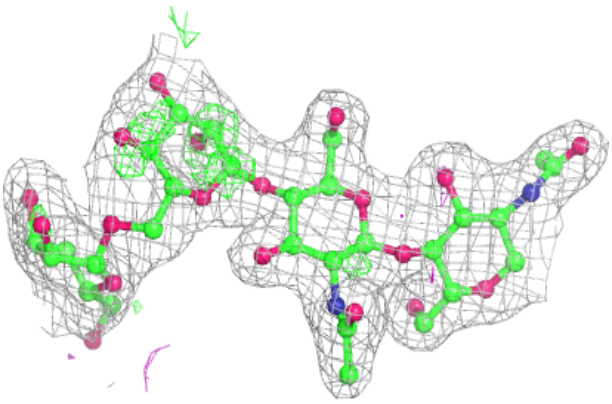
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9'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

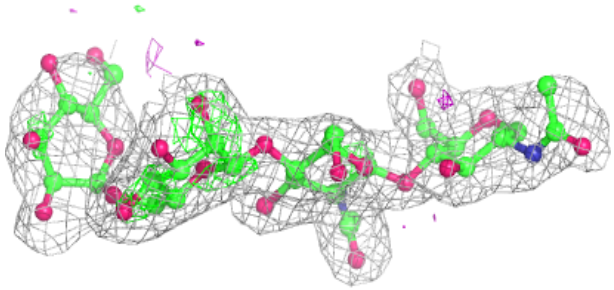
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
3	BMA	F	3	11/12	0.59	0.14	88,93,96,99	0
4	BMA	G	4	11/12	0.63	0.29	105,110,113,115	0
4	BMA	G	5	11/12	0.64	0.44	108,113,115,116	0
4	BMA	H	4	11/12	0.66	0.21	64,73,76,76	0
2	BMA	E	3	11/12	0.79	0.20	101,104,105,106	0
4	BMA	H	5	11/12	0.79	0.35	94,103,107,109	0
3	NAG	F	1	14/15	0.80	0.13	79,83,91,92	0
4	BMA	G	3	11/12	0.81	0.27	98,102,107,109	0
4	NAG	G	2	14/15	0.81	0.14	69,78,84,92	0
4	BMA	H	3	11/12	0.81	0.17	51,64,73,84	0
2	BMA	E	4	11/12	0.83	0.18	102,103,104,104	0
4	NAG	G	1	14/15	0.83	0.17	75,78,90,93	0
3	NAG	F	2	14/15	0.87	0.12	75,81,83,88	0
2	NAG	E	2	14/15	0.92	0.11	34,38,46,51	0
4	NAG	H	2	14/15	0.94	0.10	35,36,44,44	0
4	NAG	H	1	14/15	0.94	0.10	37,38,48,53	0
2	NAG	E	1	14/15	0.95	0.10	37,39,52,57	0

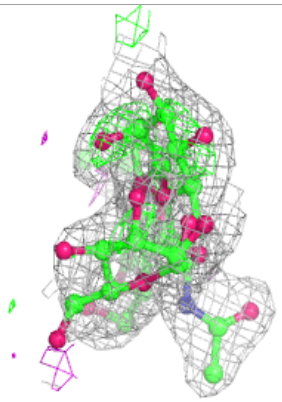
The following is a graphical depiction of the model fit to experimental electron density for oligosaccharide. Each fit is shown from different orientation to approximate a three-dimensional view.

Electron density around Chain E:

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

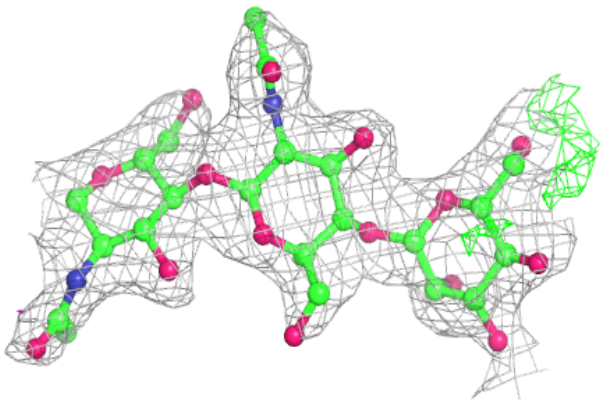


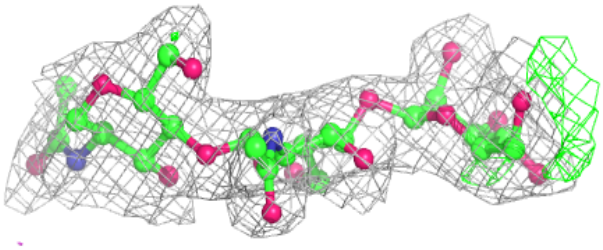


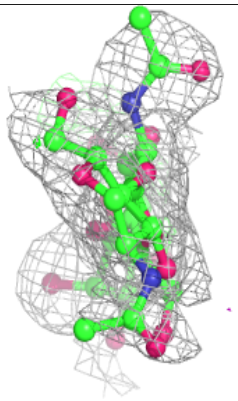


Electron density around Chain F:

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

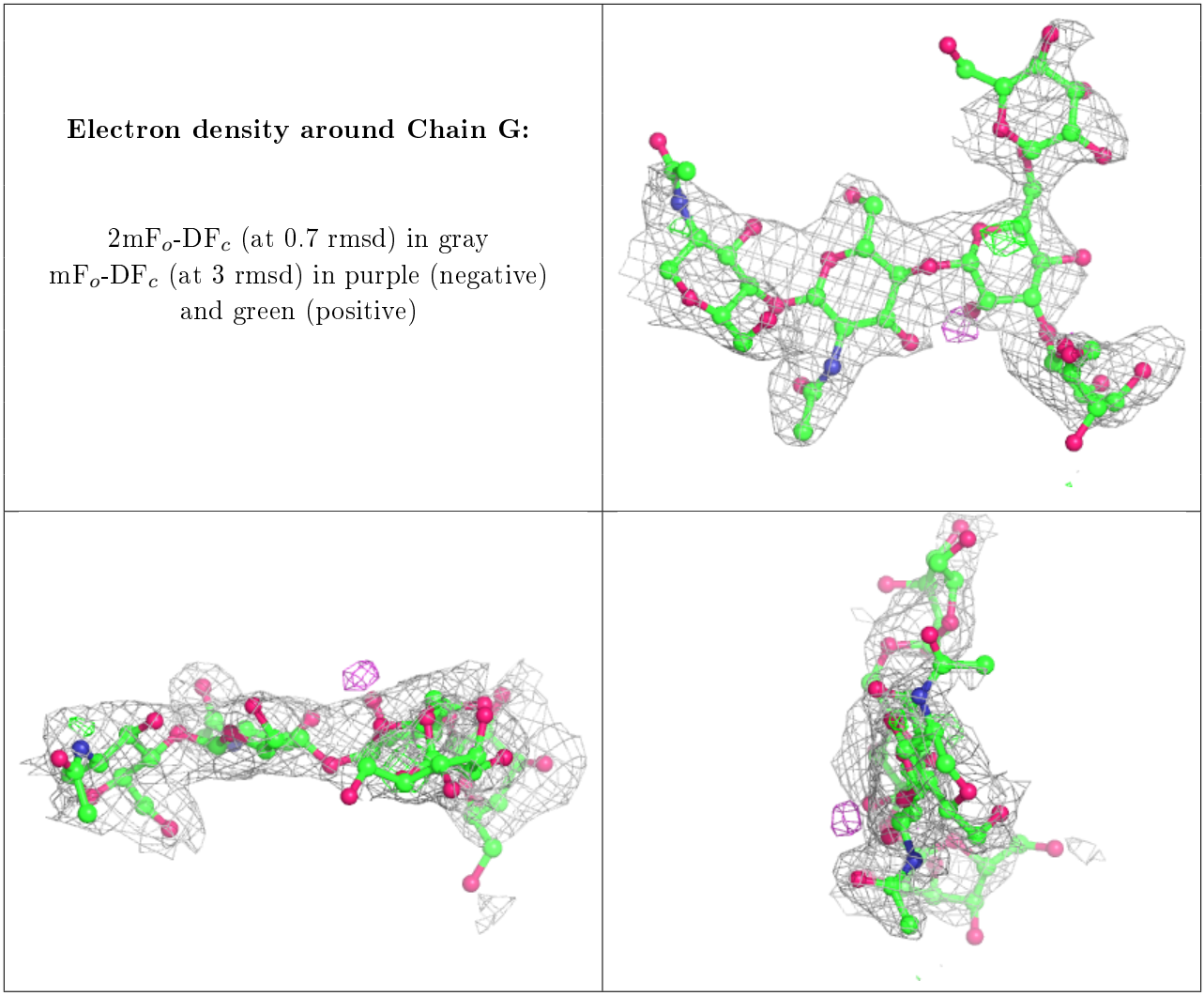






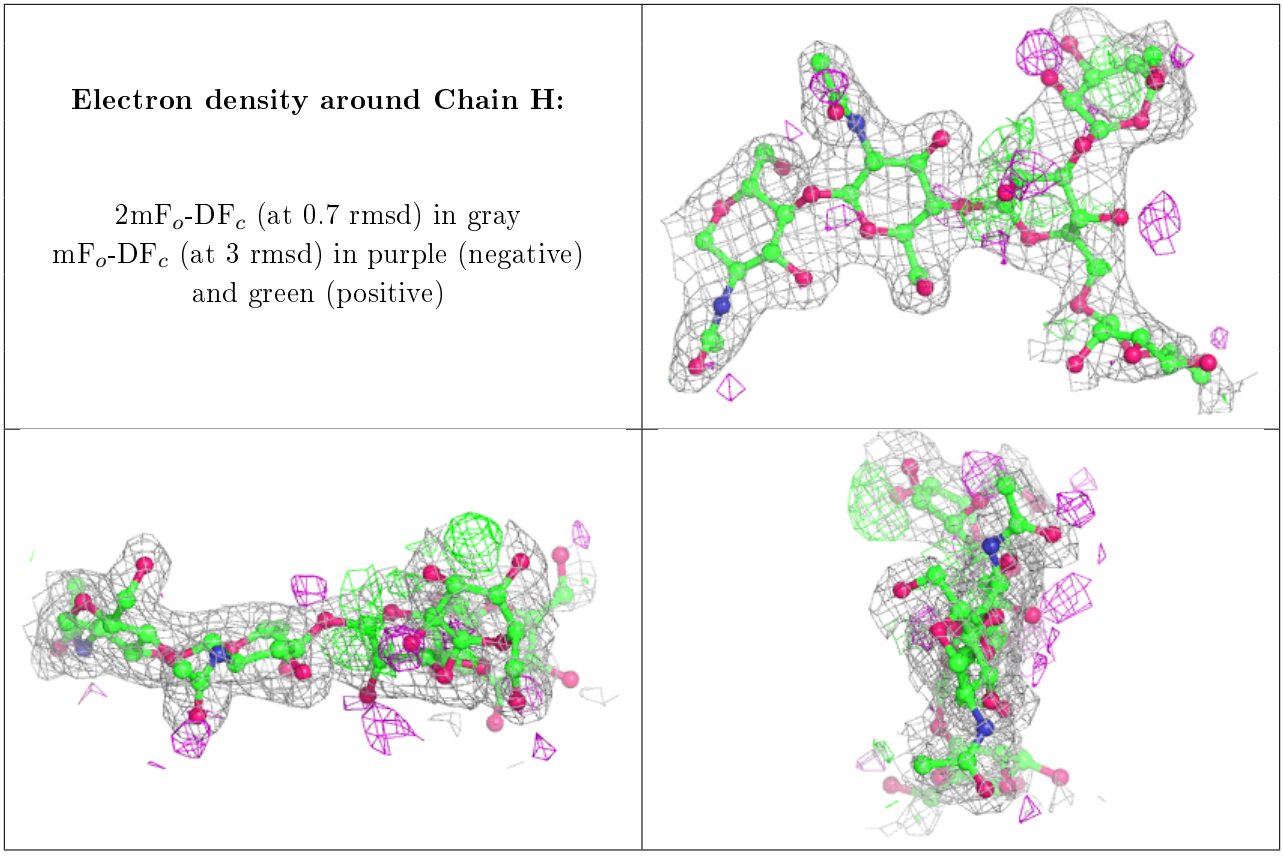
Electron density around Chain G:

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



Electron density around Chain H:

$2mF_o$-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
5	NAG	B	1201	14/15	0.64	0.33	129,141,158,160	0
5	NAG	C	1201	14/15	0.71	0.37	103,110,114,115	0
7	GOL	D	1210	6/6	0.79	0.33	33,39,47,47	0
5	NAG	D	1201	14/15	0.81	0.28	79,89,94,95	0
5	NAG	A	1201	14/15	0.83	0.31	82,96,99,100	0
7	GOL	B	1206	6/6	0.90	0.13	69,70,71,71	0
6	MES	A	1206	12/12	0.91	0.18	52,57,60,60	12
6	MES	D	1208	12/12	0.93	0.19	55,63,70,71	12
6	MES	C	1207	12/12	0.94	0.15	33,40,49,49	12
7	GOL	D	1209	6/6	0.94	0.09	35,39,40,43	0
7	GOL	A	1207	6/6	0.94	0.08	35,36,39,41	0
7	GOL	C	1208	6/6	0.95	0.08	47,54,57,62	0
6	MES	D	1207	12/12	0.95	0.12	69,76,81,81	0
6	MES	B	1205	12/12	0.96	0.17	59,67,74,75	0

6.5 Other polymers (i)

There are no such residues in this entry.