Full wwPDB X-ray Structure Validation Report ⓘ

Aug 10, 2020 – 08:58 AM BST

PDB ID	:	3S11
Title	:	Crystal structure of H5N1 influenza virus hemagglutinin, strain 437-10
Authors	:	DuBois, R.M.; Zaraket, H.; Reddivari, M.; Heath, R.J.; White, S.W.; Russell, C.J.
Deposited on	:	2011-05-14
Resolution	:	2.50 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:

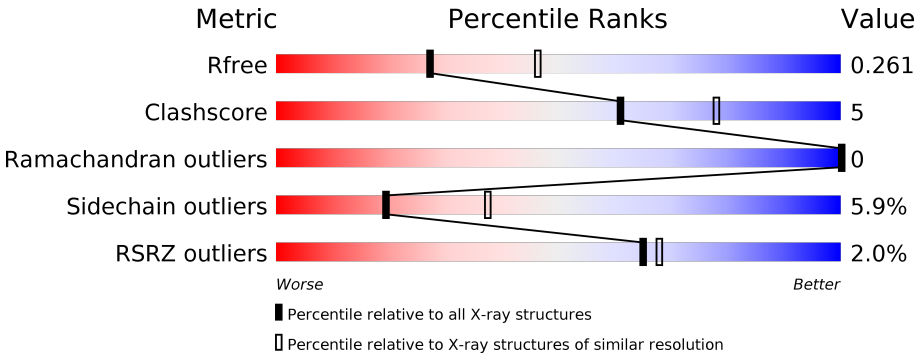
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.13.1
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (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 2.50 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	4661 (2.50-2.50)
Clashscore	141614	5346 (2.50-2.50)
Ramachandran outliers	138981	5231 (2.50-2.50)
Sidechain outliers	138945	5233 (2.50-2.50)
RSRZ outliers	127900	4559 (2.50-2.50)

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	331	81% 15% • •
1	C	331	% 82% 15% • •
1	E	331	87% 9% • •
2	B	182	7% 77% 13% • 7%
2	D	182	3% 82% 11% • 5%
2	F	182	4% 74% 17% • 5%

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Mol	Chain	Length	Quality of chain
3	G	2	
3	I	2	
4	H	3	

2 Entry composition

There are 8 unique types of molecules in this entry. The entry contains 12093 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 Hemagglutinin HA1 chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	322	Total	C	N	O	S	0	0	0
			2542	1604	439	484	15			
1	C	321	Total	C	N	O	S	0	0	0
			2535	1599	438	483	15			
1	E	322	Total	C	N	O	S	0	0	0
			2542	1604	439	484	15			

There are 24 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	3	ASP	-	expression tag	UNP Q9EA62
A	4	LEU	-	expression tag	UNP Q9EA62
A	5	GLY	-	expression tag	UNP Q9EA62
A	6	SER	-	expression tag	UNP Q9EA62
A	7	ALA	-	expression tag	UNP Q9EA62
A	8	ASP	-	expression tag	UNP Q9EA62
A	9	PRO	-	expression tag	UNP Q9EA62
A	10	GLY	-	expression tag	UNP Q9EA62
C	3	ASP	-	expression tag	UNP Q9EA62
C	4	LEU	-	expression tag	UNP Q9EA62
C	5	GLY	-	expression tag	UNP Q9EA62
C	6	SER	-	expression tag	UNP Q9EA62
C	7	ALA	-	expression tag	UNP Q9EA62
C	8	ASP	-	expression tag	UNP Q9EA62
C	9	PRO	-	expression tag	UNP Q9EA62
C	10	GLY	-	expression tag	UNP Q9EA62
E	3	ASP	-	expression tag	UNP Q9EA62
E	4	LEU	-	expression tag	UNP Q9EA62
E	5	GLY	-	expression tag	UNP Q9EA62
E	6	SER	-	expression tag	UNP Q9EA62
E	7	ALA	-	expression tag	UNP Q9EA62
E	8	ASP	-	expression tag	UNP Q9EA62
E	9	PRO	-	expression tag	UNP Q9EA62

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Chain	Residue	Modelled	Actual	Comment	Reference
E	10	GLY	-	expression tag	UNP Q9EA62

- Molecule 2 is a protein called Hemagglutinin HA2 chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	170	Total	C	N	O	S	0	0	0
			1377	857	239	273	8			
2	D	172	Total	C	N	O	S	0	0	0
			1395	867	241	279	8			
2	F	173	Total	C	N	O	S	0	0	0
			1403	873	242	280	8			

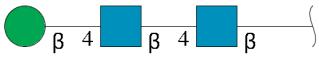
There are 18 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	177	ARG	-	expression tag	UNP Q9EA62
B	178	SER	-	expression tag	UNP Q9EA62
B	179	LEU	-	expression tag	UNP Q9EA62
B	180	VAL	-	expression tag	UNP Q9EA62
B	181	PRO	-	expression tag	UNP Q9EA62
B	182	ARG	-	expression tag	UNP Q9EA62
D	177	ARG	-	expression tag	UNP Q9EA62
D	178	SER	-	expression tag	UNP Q9EA62
D	179	LEU	-	expression tag	UNP Q9EA62
D	180	VAL	-	expression tag	UNP Q9EA62
D	181	PRO	-	expression tag	UNP Q9EA62
D	182	ARG	-	expression tag	UNP Q9EA62
F	177	ARG	-	expression tag	UNP Q9EA62
F	178	SER	-	expression tag	UNP Q9EA62
F	179	LEU	-	expression tag	UNP Q9EA62
F	180	VAL	-	expression tag	UNP Q9EA62
F	181	PRO	-	expression tag	UNP Q9EA62
F	182	ARG	-	expression tag	UNP Q9EA62

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

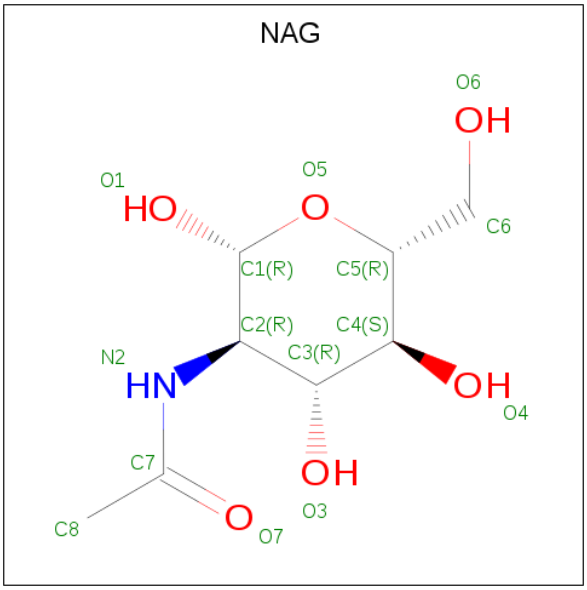
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf	Trace
3	G	2	Total C N O 28 16 2 10	0	0	0
3	I	2	Total C N O 28 16 2 10	0	0	0

- Molecule 4 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.



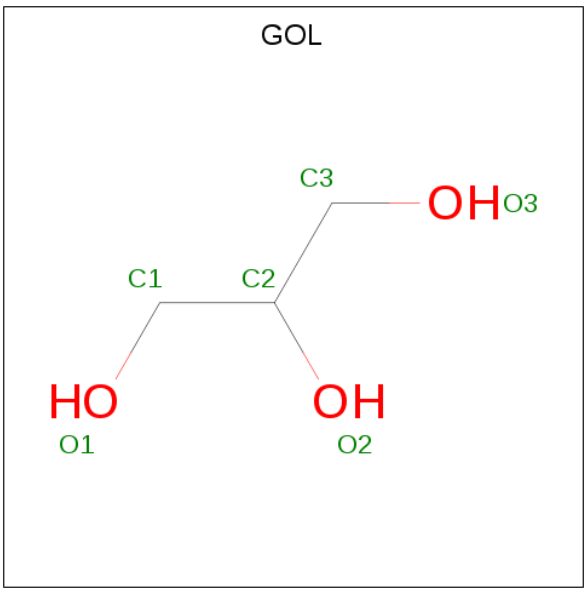
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf	Trace
4	H	3	Total C N O 39 22 2 15	0	0	0

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



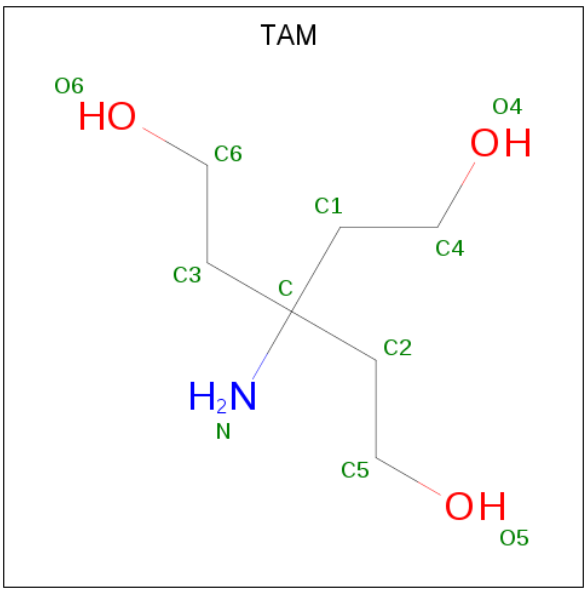
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	1	Total C N O 14 8 1 5	0	0
5	C	1	Total C N O 14 8 1 5	0	0
5	E	1	Total C N O 14 8 1 5	0	0

- Molecule 6 is GLYCEROL (three-letter code: GOL) (formula: $C_3H_8O_3$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	A	1	Total C O 6 3 3	0	0
6	C	1	Total C O 6 3 3	0	0
6	E	1	Total C O 6 3 3	0	0

- Molecule 7 is TRIS(HYDROXYETHYL)AMINOMETHANE (three-letter code: TAM) (formula: $C_7H_{17}NO_3$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
7	A	1	Total C N O 11 7 1 3	0	0

- Molecule 8 is water.

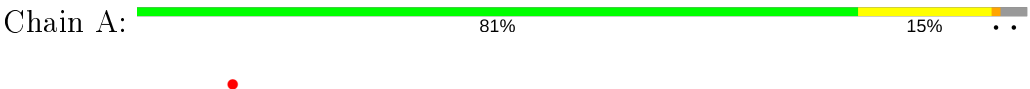
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
8	A	38	Total O 38 38	0	0
8	B	16	Total O 16 16	0	0
8	C	43	Total O 43 43	0	0
8	D	9	Total O 9 9	0	0
8	E	18	Total O 18 18	0	0
8	F	9	Total O 9 9	0	0

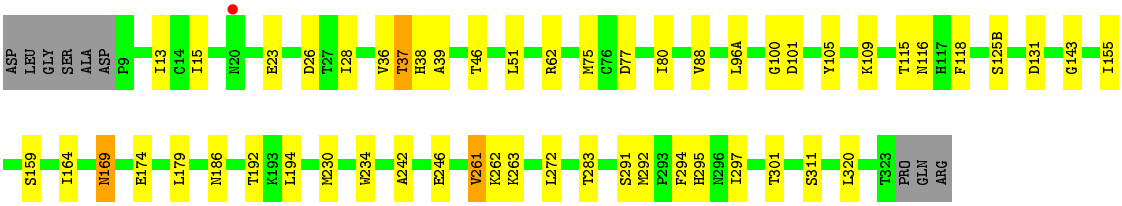
3 Residue-property plots (i)

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: Hemagglutinin HA1 chain

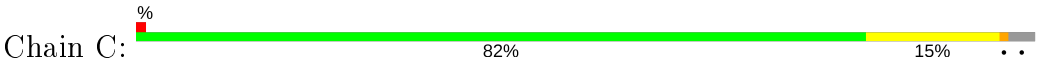
Chain A:

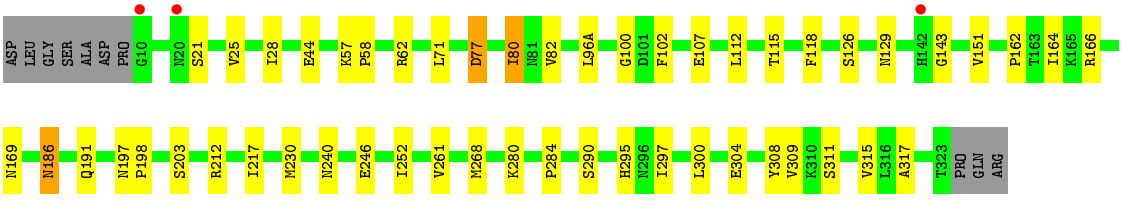




- Molecule 1: Hemagglutinin HA1 chain

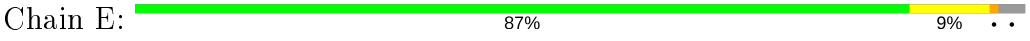
Chain C:

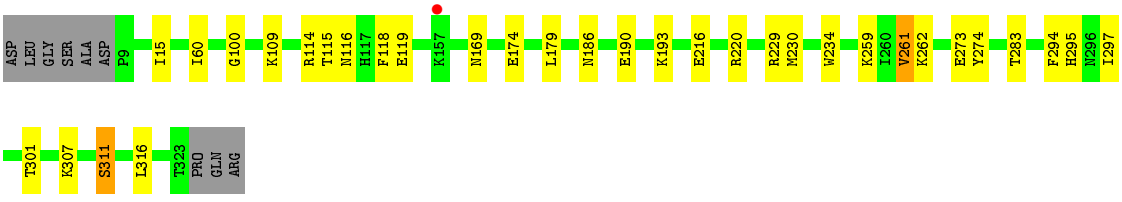




- Molecule 1: Hemagglutinin HA1 chain

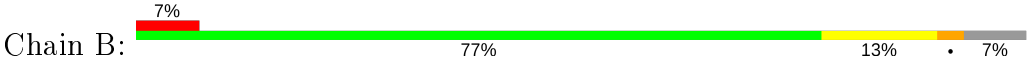
Chain E:

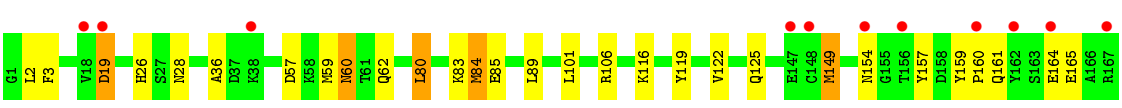


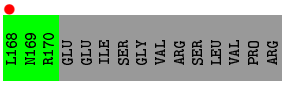


- Molecule 2: Hemagglutinin HA2 chain

Chain B:

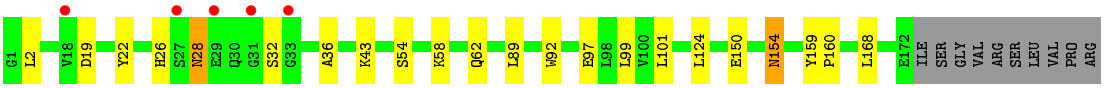






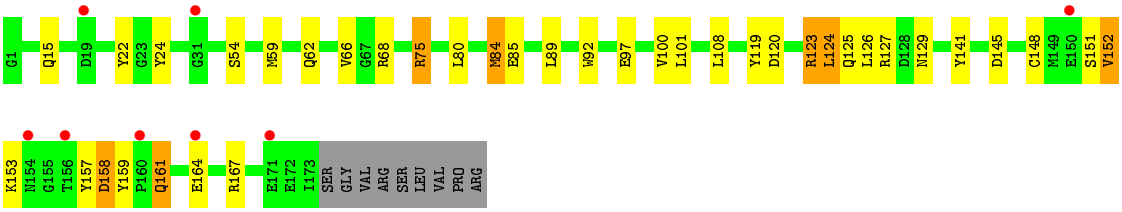
• Molecule 2: Hemagglutinin HA2 chain

Chain D:



• Molecule 2: Hemagglutinin HA2 chain

Chain F:



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

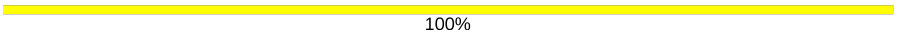
Chain G:

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

Chain I:

• Molecule 4: 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	69.36Å 241.05Å 70.06Å 90.00° 116.69° 90.00°	Depositor
Resolution (Å)	49.07 – 2.50 49.07 – 2.50	Depositor EDS
% Data completeness (in resolution range)	95.9 (49.07-2.50) 95.9 (49.07-2.50)	Depositor EDS
R_{merge}	0.10	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.63 (at 2.51Å)	Xtriage
Refinement program	REFMAC	Depositor
R, R_{free}	0.221 , 0.265 0.219 , 0.261	Depositor DCC
R_{free} test set	3457 reflections (5.10%)	wwPDB-VP
Wilson B-factor (Å^2)	43.3	Xtriage
Anisotropy	0.032	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.36 , 34.0	EDS
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.32$	Xtriage
Estimated twinning fraction	0.028 for l,-k,h	Xtriage
F_o,F_c correlation	0.93	EDS
Total number of atoms	12093	wwPDB-VP
Average B, all atoms (Å^2)	41.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.82% 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: GOL, BMA, NAG, TAM

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	0.38	0/2606	0.52	0/3542
1	C	0.38	0/2598	0.55	1/3531 (0.0%)
1	E	0.35	0/2606	0.51	0/3542
2	B	0.36	0/1404	0.49	1/1888 (0.1%)
2	D	0.38	0/1422	0.49	0/1912
2	F	0.39	0/1430	0.53	1/1923 (0.1%)
All	All	0.37	0/12066	0.52	3/16338 (0.0%)

There are no bond length outliers.

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	F	80	LEU	CA-CB-CG	5.49	127.93	115.30
2	B	80	LEU	CA-CB-CG	5.46	127.86	115.30
1	C	143	GLY	N-CA-C	-5.25	99.96	113.10

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	2542	0	2470	27	0
1	C	2535	0	2462	28	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	E	2542	0	2470	17	0
2	B	1377	0	1284	18	0
2	D	1395	0	1296	13	0
2	F	1403	0	1307	25	0
3	G	28	0	25	1	0
3	I	28	0	25	0	0
4	H	39	0	34	0	0
5	A	14	0	13	0	0
5	C	14	0	13	0	0
5	E	14	0	13	0	0
6	A	6	0	8	1	0
6	C	6	0	8	1	0
6	E	6	0	8	0	0
7	A	11	0	17	1	0
8	A	38	0	0	0	0
8	B	16	0	0	0	0
8	C	43	0	0	1	0
8	D	9	0	0	0	0
8	E	18	0	0	0	0
8	F	9	0	0	0	0
All	All	12093	0	11453	106	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 5.

All (106) 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:C:151:VAL:HG13	1:C:252:ILE:HG22	1.50	0.94
2:F:123:ARG:HH11	2:F:123:ARG:HG3	1.35	0.90
1:E:116:ASN:HB2	1:E:262:LYS:HG2	1.61	0.80
1:A:28:ILE:HD13	2:B:101:LEU:HD23	1.63	0.79
1:C:311:SER:HB3	2:D:97:GLU:OE2	1.86	0.76
1:C:308:TYR:CD2	2:D:89:LEU:HD21	2.24	0.73
1:C:212:ARG:HD2	1:E:216:GLU:HG2	1.71	0.71
1:C:308:TYR:HD2	2:D:89:LEU:HD21	1.57	0.70
1:C:295:HIS:HD2	1:C:297:ILE:H	1.38	0.69
1:A:26:ASP:HB2	6:A:328:GOL:H11	1.75	0.68
1:A:23:GLU:HG2	1:A:39:ALA:HB3	1.75	0.68
1:A:283:THR:HG22	1:A:301:THR:HG22	1.76	0.67
1:C:151:VAL:HG13	1:C:252:ILE:CG2	2.23	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:220:ARG:HD3	1:E:229:ARG:HG2	1.75	0.67
1:A:28:ILE:CD1	2:B:101:LEU:HD23	2.24	0.66
1:A:37:THR:HG23	1:A:38:HIS:ND1	2.13	0.63
1:E:15:ILE:HD13	2:F:119:TYR:HA	1.82	0.61
1:A:295:HIS:HD2	1:A:297:ILE:H	1.48	0.61
2:F:123:ARG:HH11	2:F:123:ARG:CG	2.12	0.61
2:F:127:ARG:HG3	2:F:159:TYR:CD1	2.36	0.60
1:C:151:VAL:CG1	1:C:252:ILE:HG22	2.28	0.60
2:F:120:ASP:O	2:F:124:LEU:HG	2.00	0.59
1:E:283:THR:HG22	1:E:301:THR:HG22	1.84	0.58
1:A:15:ILE:HD11	2:B:122:VAL:HG21	1.84	0.58
2:D:19:ASP:HB3	2:D:36:ALA:HB2	1.86	0.58
2:F:126:LEU:O	2:F:129:ASN:HB2	2.06	0.56
1:A:115:THR:HG21	1:A:118:PHE:CE1	2.40	0.56
1:A:143:GLY:O	7:A:329:TAM:H21	2.06	0.56
1:C:280:LYS:HB3	1:C:304:GLU:HG3	1.87	0.55
2:D:62:GLN:HG3	2:D:92:TRP:CD2	2.42	0.55
2:B:84:MET:HG3	2:B:85:GLU:N	2.22	0.55
2:D:150:GLU:O	2:D:154:ASN:HB2	2.06	0.55
1:A:169:ASN:ND2	1:A:242:ALA:HB2	2.22	0.54
1:E:115:THR:HG21	1:E:118:PHE:CE1	2.43	0.54
1:A:15:ILE:HG13	2:B:119:TYR:HA	1.89	0.53
1:E:294:PHE:HZ	2:F:59:MET:HG3	1.73	0.53
1:A:179:LEU:HD23	1:A:234:TRP:HB3	1.91	0.53
1:C:151:VAL:CG1	1:C:252:ILE:CG2	2.86	0.53
1:C:268:MET:HE3	1:C:284:PRO:HA	1.91	0.53
2:F:125:GLN:HG2	2:F:157:TYR:HB3	1.89	0.53
1:E:100:GLY:HA3	1:E:230:MET:O	2.08	0.52
1:E:174:GLU:HG2	1:E:261:VAL:HA	1.91	0.52
2:F:62:GLN:HB2	2:F:92:TRP:CD2	2.44	0.52
1:C:115:THR:HG21	1:C:118:PHE:CE1	2.44	0.52
1:E:311:SER:HB3	2:F:97:GLU:OE2	2.09	0.52
2:B:83:LYS:HE2	2:F:66:VAL:HG21	1.90	0.52
1:C:77:ASP:HA	1:C:80:ILE:HD12	1.92	0.51
2:F:158:ASP:HB3	2:F:161:GLN:HG2	1.93	0.51
1:E:307:LYS:HD2	2:F:62:GLN:HG2	1.93	0.50
1:C:191:GLN:HG2	1:C:217:ILE:HD11	1.92	0.50
1:A:77:ASP:HA	1:A:80:ILE:HG12	1.94	0.50
2:B:159:TYR:HB3	2:B:160:PRO:HD3	1.94	0.49
2:F:127:ARG:HB2	2:F:159:TYR:CE1	2.47	0.49
1:A:174:GLU:HG2	1:A:261:VAL:HA	1.94	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:24:TYR:CD2	2:F:153:LYS:HG2	2.48	0.48
2:F:148:CYS:O	2:F:151:SER:HB3	2.12	0.48
2:B:83:LYS:HG3	2:F:68:ARG:NH2	2.28	0.48
1:A:100:GLY:HA3	1:A:230:MET:O	2.14	0.47
1:C:284:PRO:HD3	1:C:300:LEU:O	2.14	0.47
2:D:159:TYR:HB3	2:D:160:PRO:HD3	1.96	0.47
1:E:179:LEU:HD23	1:E:234:TRP:HB3	1.96	0.47
2:F:164:GLU:O	2:F:167:ARG:HG2	2.14	0.47
1:A:115:THR:HG21	1:A:118:PHE:HE1	1.78	0.47
1:E:119:GLU:HB3	1:E:259:LYS:HB2	1.95	0.47
1:A:28:ILE:HD13	2:B:101:LEU:CD2	2.38	0.47
1:E:295:HIS:HD2	1:E:297:ILE:H	1.63	0.47
1:A:116:ASN:HB2	1:A:262:LYS:HG2	1.96	0.47
2:B:164:GLU:HG3	2:B:165:GLU:H	1.80	0.46
2:F:129:ASN:O	2:F:141:TYR:HB2	2.15	0.46
1:C:164:ILE:O	1:C:246:GLU:HA	2.16	0.46
1:E:186:ASN:ND2	1:E:190:GLU:OE1	2.48	0.46
1:A:169:ASN:HD21	3:G:1:NAG:C7	2.29	0.46
2:B:19:ASP:HB3	2:B:36:ALA:HB2	1.97	0.46
2:F:84:MET:HG3	2:F:85:GLU:N	2.30	0.46
1:A:131:ASP:HB3	1:A:155:ILE:HB	1.97	0.46
1:A:105:TYR:CE2	1:A:109:LYS:HE2	2.51	0.45
1:C:315:VAL:H	6:C:2:GOL:H2	1.81	0.45
1:C:44:GLU:HG2	1:C:290:SER:OG	2.17	0.44
1:C:197:ASN:HA	1:C:198:PRO:HD3	1.90	0.44
1:C:25:VAL:HG21	1:C:317:ALA:HB2	2.00	0.44
1:C:129:ASN:HB3	1:C:162:PRO:HG2	1.99	0.44
2:D:28:ASN:HD22	2:D:28:ASN:C	2.20	0.44
2:B:57:ASP:O	2:B:60:ASN:ND2	2.47	0.43
1:C:308:TYR:CE2	2:D:89:LEU:HD21	2.52	0.43
2:F:123:ARG:CG	2:F:123:ARG:NH1	2.77	0.43
1:C:77:ASP:HA	1:C:80:ILE:CD1	2.48	0.43
1:A:164:ILE:O	1:A:246:GLU:HA	2.19	0.43
2:D:26:HIS:O	2:D:32:SER:HA	2.18	0.43
2:B:26:HIS:HB2	2:B:149:MET:SD	2.59	0.43
2:F:126:LEU:HD21	2:F:152:VAL:HG11	2.01	0.43
1:A:13:ILE:HB	2:B:149:MET:HE1	2.01	0.42
1:E:60:ILE:HD13	1:E:274:TYR:HB2	2.01	0.42
2:B:3:PHE:CZ	2:D:2:LEU:HG	2.54	0.42
1:A:51:LEU:HD13	1:A:88:VAL:HG21	2.02	0.42
2:B:83:LYS:HE2	2:F:66:VAL:CG2	2.48	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:316:LEU:HD13	2:F:100:VAL:HG22	2.02	0.42
1:A:294:PHE:HZ	2:B:59:MET:HG3	1.85	0.41
2:B:125:GLN:HG2	2:B:157:TYR:HB3	2.02	0.41
1:C:107:GLU:OE2	2:F:75:ARG:N	2.44	0.41
1:C:186:ASN:HB3	8:C:368:HOH:O	2.19	0.41
2:D:28:ASN:ND2	2:D:28:ASN:H	2.18	0.41
1:C:126:SER:O	1:C:166:ARG:NH2	2.54	0.41
1:A:263:LYS:HB2	1:A:263:LYS:NZ	2.36	0.41
2:D:54:SER:O	2:D:58:LYS:HG2	2.21	0.41
1:C:100:GLY:HA3	1:C:230:MET:O	2.20	0.41
1:C:57:LYS:HG2	1:C:58:PRO:HD2	2.02	0.41

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	320/331 (97%)	311 (97%)	9 (3%)	0	100	100
1	C	319/331 (96%)	307 (96%)	12 (4%)	0	100	100
1	E	320/331 (97%)	307 (96%)	13 (4%)	0	100	100
2	B	168/182 (92%)	162 (96%)	6 (4%)	0	100	100
2	D	170/182 (93%)	166 (98%)	4 (2%)	0	100	100
2	F	171/182 (94%)	164 (96%)	7 (4%)	0	100	100
All	All	1468/1539 (95%)	1417 (96%)	51 (4%)	0	100	100

There are no Ramachandran outliers to report.

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	286/293 (98%)	267 (93%)	19 (7%)	16 32
1	C	285/293 (97%)	269 (94%)	16 (6%)	21 40
1	E	286/293 (98%)	279 (98%)	7 (2%)	49 74
2	B	145/156 (93%)	132 (91%)	13 (9%)	9 19
2	D	147/156 (94%)	139 (95%)	8 (5%)	22 42
2	F	148/156 (95%)	134 (90%)	14 (10%)	8 17
All	All	1297/1347 (96%)	1220 (94%)	77 (6%)	19 37

All (77) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	36	VAL
1	A	37	THR
1	A	46	THR
1	A	62	ARG
1	A	75	MET
1	A	96(A)	LEU
1	A	101	ASP
1	A	125(B)	SER
1	A	159	SER
1	A	169	ASN
1	A	186	ASN
1	A	192	THR
1	A	194	LEU
1	A	261	VAL
1	A	272	LEU
1	A	291	SER
1	A	292	MET
1	A	311	SER
1	A	320	LEU
2	B	2	LEU
2	B	19	ASP
2	B	28	ASN

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Mol	Chain	Res	Type
2	B	60	ASN
2	B	62	GLN
2	B	80	LEU
2	B	84	MET
2	B	89	LEU
2	B	106	ARG
2	B	116	LYS
2	B	149	MET
2	B	154	ASN
2	B	161	GLN
1	C	21	SER
1	C	28	ILE
1	C	62	ARG
1	C	71	LEU
1	C	77	ASP
1	C	80	ILE
1	C	82	VAL
1	C	96(A)	LEU
1	C	102	PHE
1	C	112	LEU
1	C	169	ASN
1	C	186	ASN
1	C	203	SER
1	C	240	ASN
1	C	261	VAL
1	C	309	VAL
2	D	22	TYR
2	D	28	ASN
2	D	43	LYS
2	D	99	LEU
2	D	101	LEU
2	D	124	LEU
2	D	154	ASN
2	D	168	LEU
1	E	109	LYS
1	E	114	ARG
1	E	169	ASN
1	E	193	LYS
1	E	261	VAL
1	E	273	GLU
1	E	311	SER
2	F	15	GLN

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Mol	Chain	Res	Type
2	F	22	TYR
2	F	54	SER
2	F	75	ARG
2	F	84	MET
2	F	89	LEU
2	F	101	LEU
2	F	108	LEU
2	F	123	ARG
2	F	124	LEU
2	F	145	ASP
2	F	152	VAL
2	F	158	ASP
2	F	161	GLN

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (33) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	12	GLN
1	A	104	ASN
1	A	196	GLN
1	A	289	ASN
1	A	295	HIS
1	A	312	ASN
2	B	28	ASN
2	B	95	ASN
2	B	114	ASN
2	B	129	ASN
2	B	146	ASN
2	B	154	ASN
1	C	12	GLN
1	C	129	ASN
1	C	211	GLN
1	C	289	ASN
1	C	295	HIS
2	D	28	ASN
2	D	95	ASN
2	D	114	ASN
2	D	129	ASN
2	D	146	ASN
1	E	20	ASN
1	E	129	ASN
1	E	142	HIS

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Mol	Chain	Res	Type
1	E	240	ASN
1	E	289	ASN
1	E	295	HIS
2	F	15	GLN
2	F	95	ASN
2	F	114	ASN
2	F	125	GLN
2	F	129	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)

7 monosaccharides are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
3	NAG	G	1	1,3	14,14,15	0.51	0	17,19,21	1.11	2 (11%)
3	NAG	G	2	3	14,14,15	0.49	0	17,19,21	0.70	0
4	NAG	H	1	1,4	14,14,15	0.49	0	17,19,21	1.26	2 (11%)
4	NAG	H	2	4	14,14,15	0.54	0	17,19,21	1.11	1 (5%)
4	BMA	H	3	4	11,11,12	0.41	0	15,15,17	1.14	1 (6%)
3	NAG	I	1	1,3	14,14,15	0.51	0	17,19,21	0.85	0
3	NAG	I	2	3	14,14,15	0.50	0	17,19,21	1.05	1 (5%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	NAG	G	1	1,3	-	0/6/23/26	0/1/1/1
3	NAG	G	2	3	-	2/6/23/26	0/1/1/1
4	NAG	H	1	1,4	-	0/6/23/26	0/1/1/1
4	NAG	H	2	4	-	1/6/23/26	0/1/1/1
4	BMA	H	3	4	-	0/2/19/22	0/1/1/1
3	NAG	I	1	1,3	-	0/6/23/26	0/1/1/1
3	NAG	I	2	3	-	2/6/23/26	0/1/1/1

There are no bond length outliers.

All (7) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	I	2	NAG	C1-O5-C5	3.65	117.14	112.19
4	H	3	BMA	C1-O5-C5	-3.34	107.67	112.19
3	G	1	NAG	O5-C5-C6	2.64	111.34	107.20
4	H	1	NAG	O5-C5-C6	2.53	111.17	107.20
4	H	1	NAG	C1-O5-C5	2.24	115.23	112.19
4	H	2	NAG	C1-O5-C5	2.24	115.22	112.19
3	G	1	NAG	O5-C1-C2	-2.13	107.92	111.29

There are no chirality outliers.

All (5) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	I	2	NAG	O5-C5-C6-O6
3	I	2	NAG	C4-C5-C6-O6
3	G	2	NAG	O5-C5-C6-O6
4	H	2	NAG	C4-C5-C6-O6
3	G	2	NAG	C4-C5-C6-O6

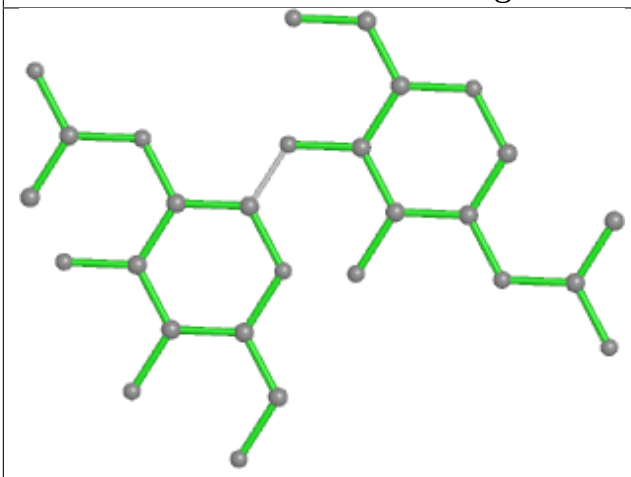
There are no ring outliers.

1 monomer is involved in 1 short contact:

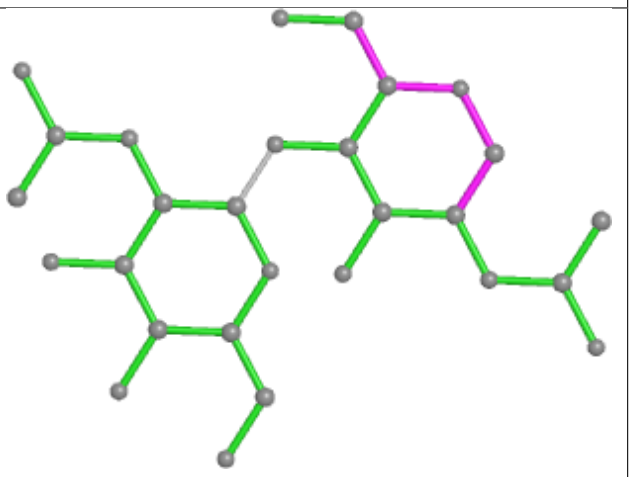
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	G	1	NAG	1	0

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

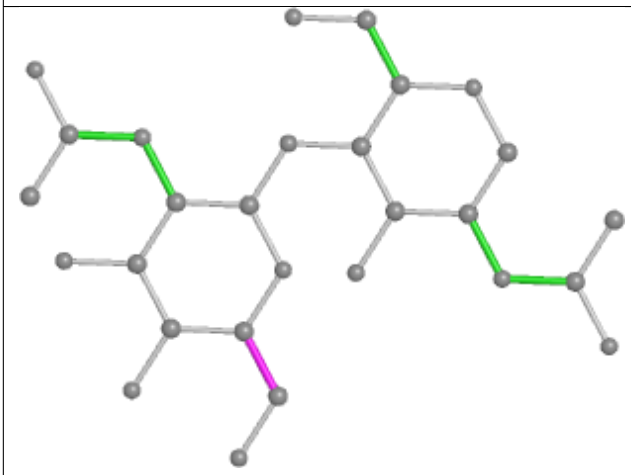
Oligosaccharide Chain G



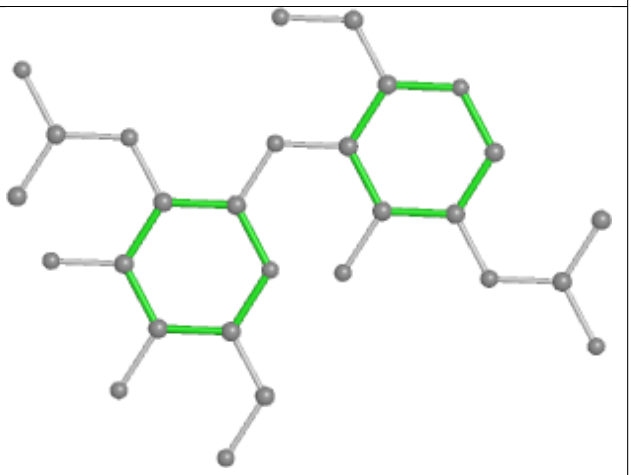
Bond lengths



Bond angles

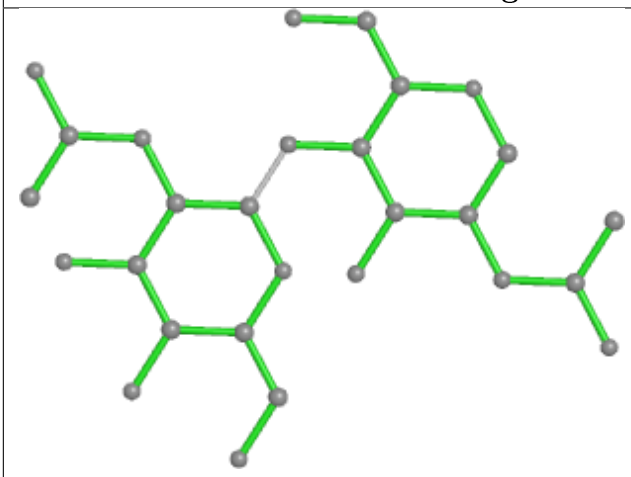


Torsions

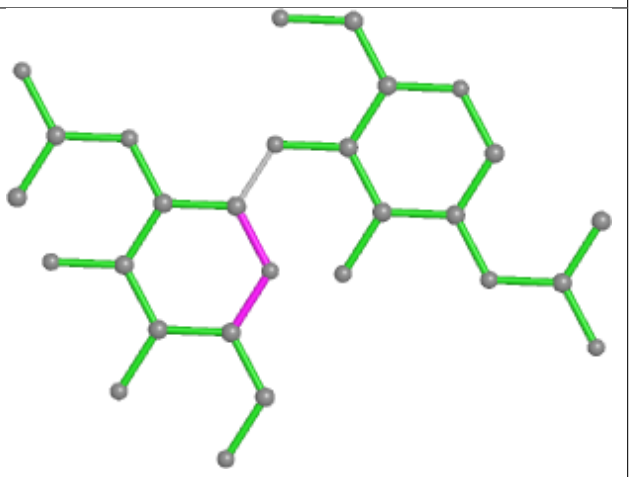


Rings

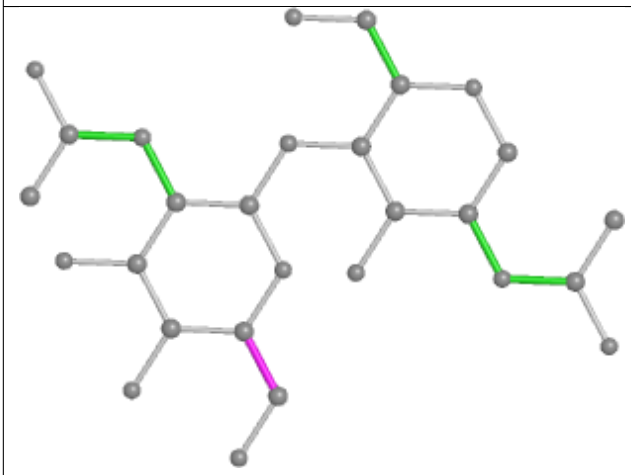
Oligosaccharide Chain I



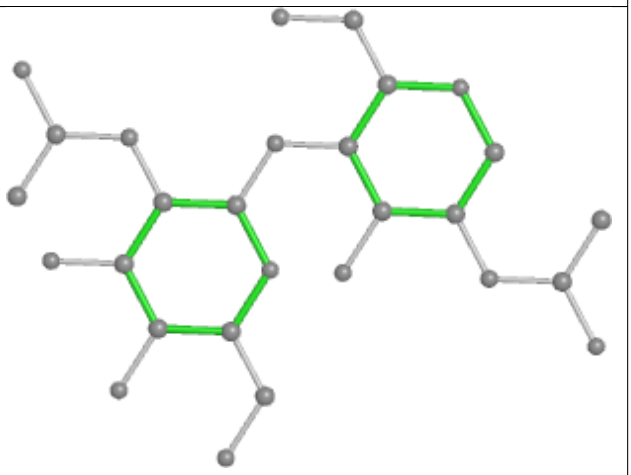
Bond lengths



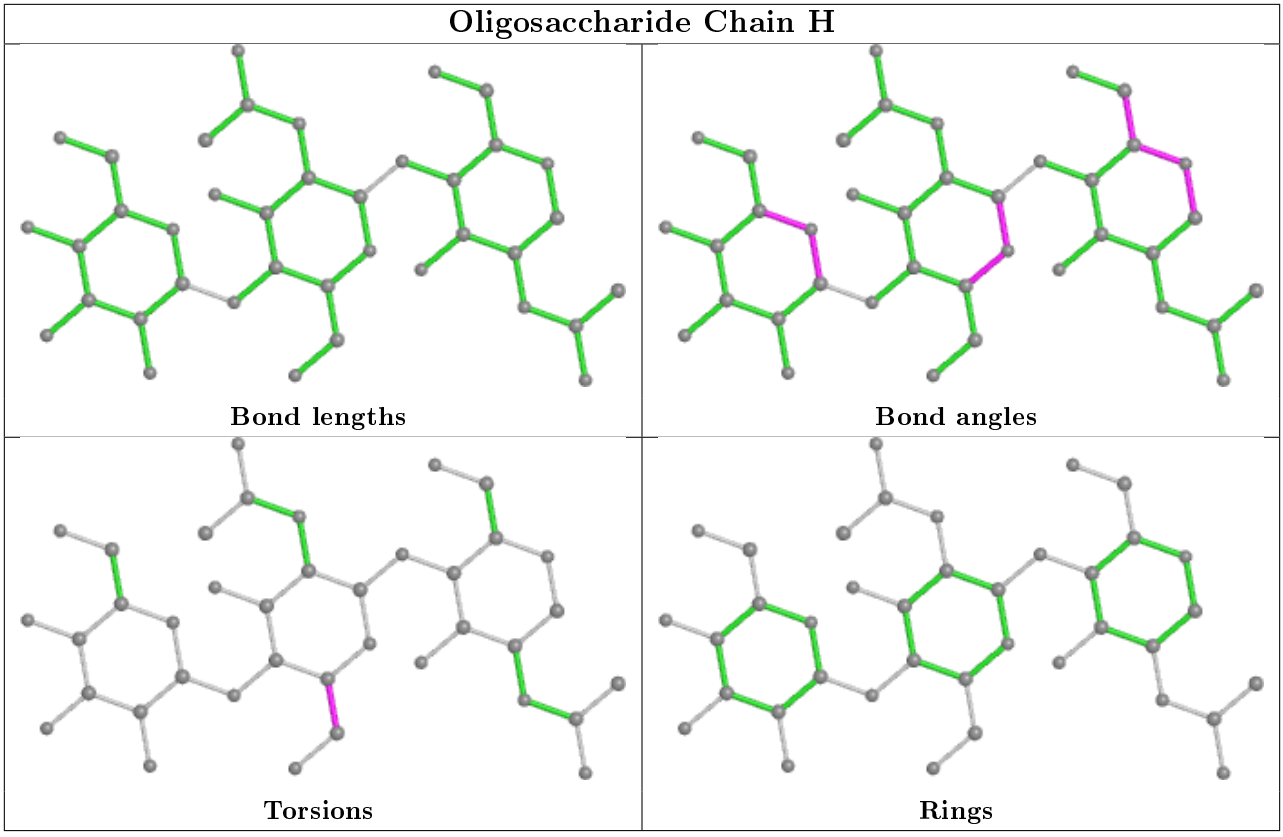
Bond angles



Torsions



Rings



5.6 Ligand geometry

7 ligands are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
7	TAM	A	329	-	7,10,10	0.76	0	9,12,12	0.69	0
6	GOL	E	330	-	5,5,5	0.43	0	5,5,5	0.48	0
5	NAG	C	327	1	14,14,15	0.56	0	17,19,21	0.66	0
5	NAG	E	327	1	14,14,15	0.56	0	17,19,21	0.66	0
6	GOL	A	328	-	5,5,5	0.41	0	5,5,5	0.16	0
5	NAG	A	1	1	14,14,15	1.53	2 (14%)	17,19,21	2.63	5 (29%)
6	GOL	C	2	-	5,5,5	0.36	0	5,5,5	0.30	0

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
7	TAM	A	329	-	-	6/12/12/12	-
6	GOL	E	330	-	-	0/4/4/4	-
5	NAG	C	327	1	-	2/6/23/26	0/1/1/1
5	NAG	E	327	1	-	2/6/23/26	0/1/1/1
6	GOL	A	328	-	-	2/4/4/4	-
5	NAG	A	1	1	-	2/6/23/26	0/1/1/1
6	GOL	C	2	-	-	2/4/4/4	-

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	A	1	NAG	C1-C2	-3.30	1.47	1.52
5	A	1	NAG	O5-C1	-2.80	1.39	1.43

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
5	A	1	NAG	O5-C1-C2	-8.57	97.75	111.29
5	A	1	NAG	C1-O5-C5	-3.68	107.21	112.19
5	A	1	NAG	O5-C5-C6	3.20	112.21	107.20
5	A	1	NAG	C2-N2-C7	2.28	126.14	122.90
5	A	1	NAG	C3-C4-C5	2.03	113.86	110.24

There are no chirality outliers.

All (16) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
7	A	329	TAM	C1-C-C2-C5
7	A	329	TAM	C3-C-C2-C5
7	A	329	TAM	N-C-C2-C5
7	A	329	TAM	C1-C-C3-C6
5	E	327	NAG	O5-C5-C6-O6
5	A	1	NAG	O5-C5-C6-O6
5	C	327	NAG	O5-C5-C6-O6
5	E	327	NAG	C4-C5-C6-O6
5	C	327	NAG	C4-C5-C6-O6
6	C	2	GOL	O1-C1-C2-C3

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Mol	Chain	Res	Type	Atoms
5	A	1	NAG	C4-C5-C6-O6
7	A	329	TAM	C2-C-C3-C6
6	A	328	GOL	O1-C1-C2-O2
6	C	2	GOL	O1-C1-C2-O2
7	A	329	TAM	N-C-C3-C6
6	A	328	GOL	O1-C1-C2-C3

There are no ring outliers.

3 monomers are involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
7	A	329	TAM	1	0
6	A	328	GOL	1	0
6	C	2	GOL	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	322/331 (97%)	-0.08	1 (0%)	94	94	25, 38, 48, 63	0
1	C	321/331 (96%)	-0.03	3 (0%)	84	86	27, 37, 48, 57	0
1	E	322/331 (97%)	-0.02	1 (0%)	94	94	28, 40, 50, 54	0
2	B	170/182 (93%)	0.61	12 (7%)	16	16	26, 51, 83, 85	0
2	D	172/182 (94%)	0.35	5 (2%)	51	55	27, 44, 59, 63	0
2	F	173/182 (95%)	0.51	8 (4%)	32	34	26, 45, 72, 74	0
All	All	1480/1539 (96%)	0.14	30 (2%)	65	68	25, 40, 62, 85	0

All (30) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	F	160	PRO	4.3
2	B	160	PRO	4.0
2	D	29	GLU	3.7
2	B	168	LEU	3.3
2	B	154	ASN	3.1
2	B	164	GLU	3.1
2	F	19	ASP	3.1
2	B	38	LYS	3.1
2	B	148	CYS	3.0
2	D	31	GLY	3.0
2	B	156	THR	2.9
2	D	18	VAL	2.7
2	B	162	TYR	2.7
2	F	164	GLU	2.7
1	A	20	ASN	2.7
2	B	167	ARG	2.6
2	B	147	GLU	2.6
2	B	19	ASP	2.6
2	D	33	GLY	2.5

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Mol	Chain	Res	Type	RSRZ
1	C	10	GLY	2.5
2	F	31	GLY	2.5
1	C	20	ASN	2.5
2	F	154	ASN	2.4
2	D	27	SER	2.4
2	B	18	VAL	2.4
2	F	156	THR	2.2
1	C	142	HIS	2.1
1	E	157	LYS	2.1
2	F	171	GLU	2.0
2	F	150	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)

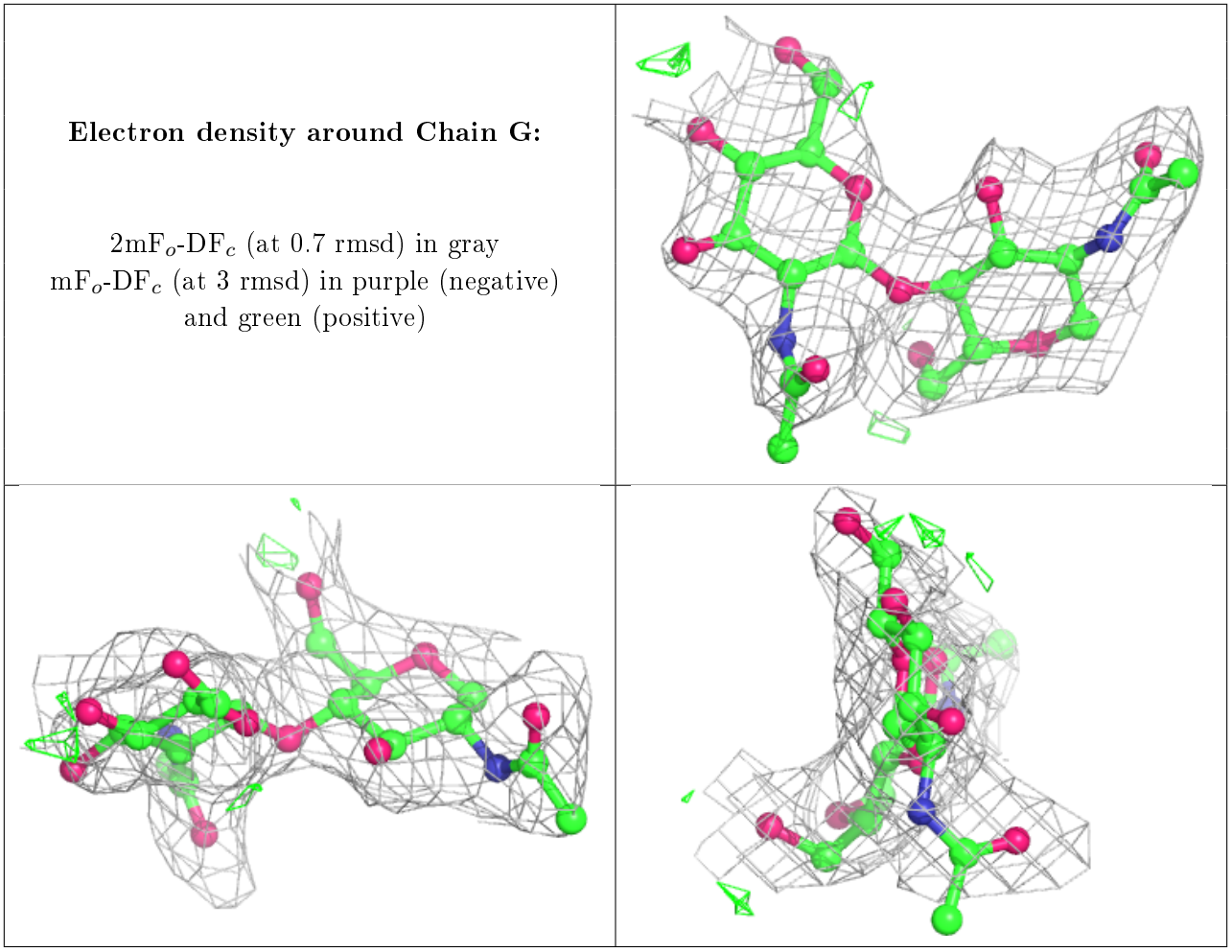
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' 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
4	BMA	H	3	11/12	0.72	0.26	20,20,20,20	0
3	NAG	G	2	14/15	0.79	0.30	59,61,62,62	0
3	NAG	I	2	14/15	0.85	0.28	62,63,64,64	0
3	NAG	I	1	14/15	0.87	0.15	54,56,58,60	0
3	NAG	G	1	14/15	0.89	0.17	50,53,55,57	0
4	NAG	H	2	14/15	0.91	0.22	47,49,49,51	0
4	NAG	H	1	14/15	0.93	0.13	37,40,42,45	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.

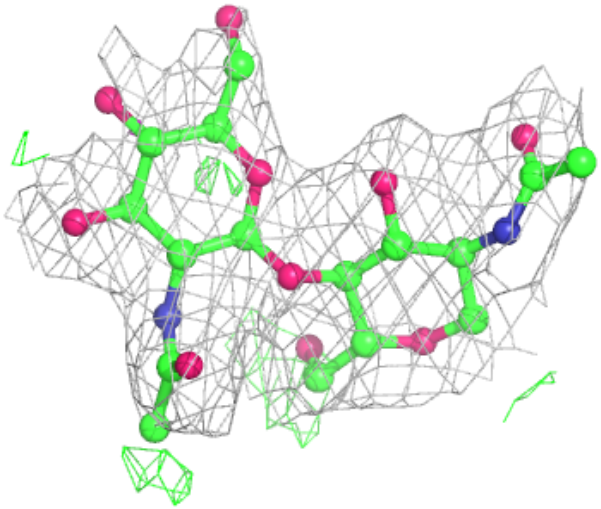
Electron density around Chain G:

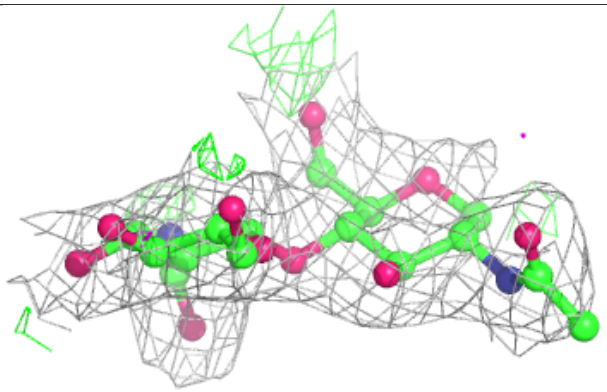
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

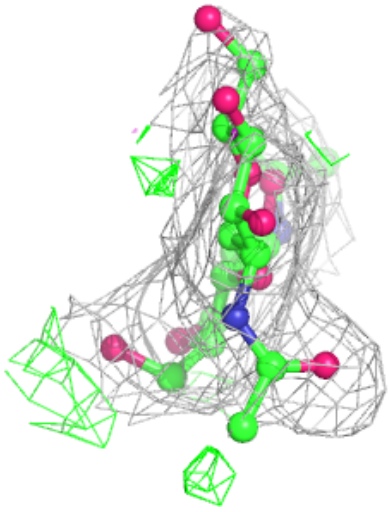


Electron density around Chain I:

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

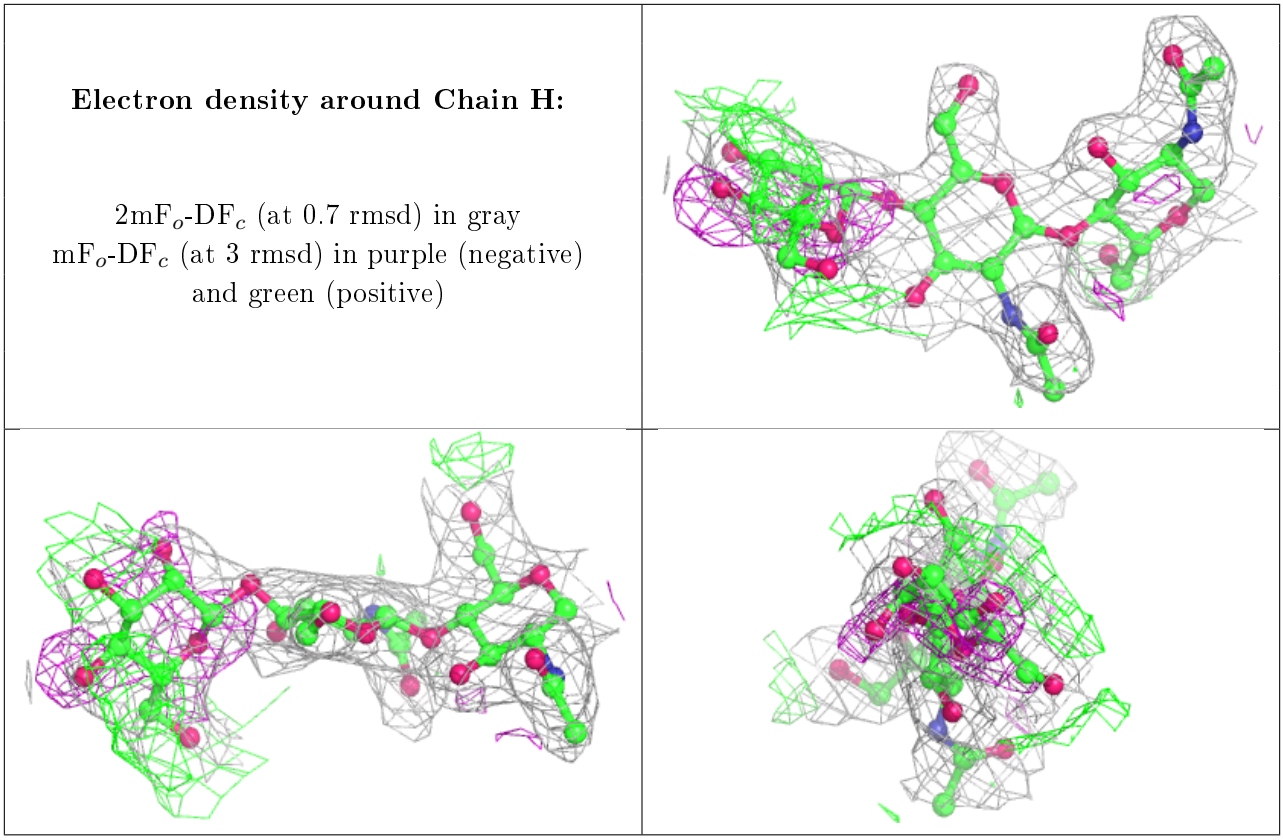






Electron density around Chain H:

$2mF_o$-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
7	TAM	A	329	11/11	0.79	0.20	50,50,51,51	0
5	NAG	E	327	14/15	0.82	0.27	58,61,63,63	0
5	NAG	C	327	14/15	0.85	0.36	65,67,68,68	0
6	GOL	A	328	6/6	0.88	0.25	52,54,55,56	0
5	NAG	A	1	14/15	0.90	0.42	20,20,20,20	0
6	GOL	E	330	6/6	0.94	0.23	41,41,42,43	0
6	GOL	C	2	6/6	0.94	0.19	60,60,60,61	0

6.5 Other polymers

There are no such residues in this entry.