Full wwPDB X-ray Structure Validation Report ⓘ

Sep 23, 2023 – 07:17 PM EDT

PDB ID	:	5THF
Title	:	Crystal structure of H3 hemagglutinin with insertion of two amino acids in the 150-loop from the A/Hong Kong/1/1968 (H3N2) influenza virus
Authors	:	Tzarum, N.; Wilson, I.A.
Deposited on	:	2016-09-29
Resolution	:	2.59 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 types of validation reports are described at
http://www.wwpdb.org/validation/2017/FAQs#types.

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

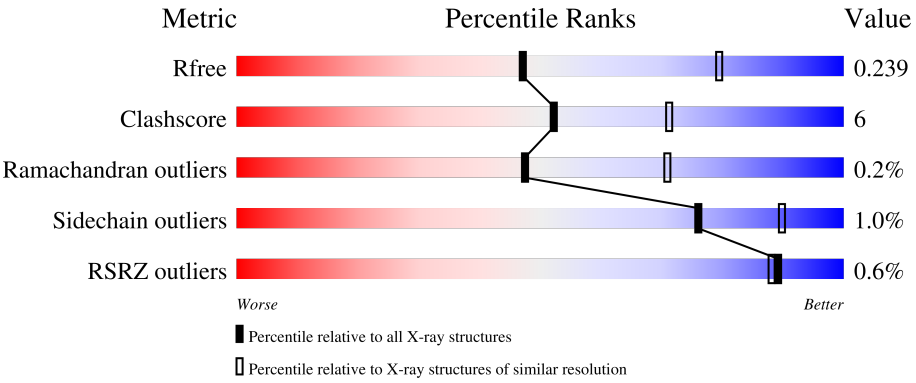
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.35.1
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.35.1

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 2.59 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	3163 (2.60-2.60)
Clashscore	141614	3518 (2.60-2.60)
Ramachandran outliers	138981	3455 (2.60-2.60)
Sidechain outliers	138945	3455 (2.60-2.60)
RSRZ outliers	127900	3104 (2.60-2.60)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=5% The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	325	86% 12%
1	C	325	89% 7%
1	E	325	83% 14%
2	B	184	84% 10% 7%
2	D	184	87% 13%

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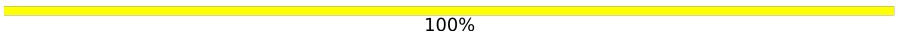
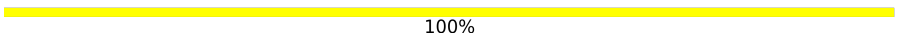
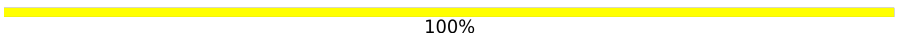
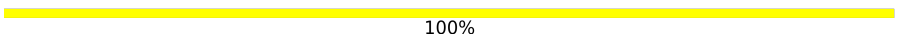
Mol	Chain	Length	Quality of chain
2	F	184	
3	G	3	
3	I	3	
3	K	3	
4	H	2	
4	J	2	
4	L	2	

2 Entry composition (i)

There are 6 unique types of molecules in this entry. The entry contains 12268 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	319	Total	C	N	O	S	0	0	0
			2458	1540	432	473	13			
1	C	318	Total	C	N	O	S	0	0	0
			2449	1535	431	470	13			
1	E	319	Total	C	N	O	S	0	0	0
			2458	1540	432	473	13			

There are 18 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	7	ALA	-	expression tag	UNP Q91MA7
A	8	ASP	-	expression tag	UNP Q91MA7
A	9	PRO	-	expression tag	UNP Q91MA7
A	10	GLY	-	expression tag	UNP Q91MA7
A	157A	SER	-	insertion	UNP Q91MA7
A	157B	LYS	-	insertion	UNP Q91MA7
C	7	ALA	-	expression tag	UNP Q91MA7
C	8	ASP	-	expression tag	UNP Q91MA7
C	9	PRO	-	expression tag	UNP Q91MA7
C	10	GLY	-	expression tag	UNP Q91MA7
C	157A	SER	-	insertion	UNP Q91MA7
C	157B	LYS	-	insertion	UNP Q91MA7
E	7	ALA	-	expression tag	UNP Q91MA7
E	8	ASP	-	expression tag	UNP Q91MA7
E	9	PRO	-	expression tag	UNP Q91MA7
E	10	GLY	-	expression tag	UNP Q91MA7
E	157A	SER	-	insertion	UNP Q91MA7
E	157B	LYS	-	insertion	UNP Q91MA7

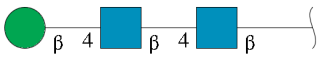
- Molecule 2 is a protein called Hemagglutinin HA2 chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	172	Total	C	N	O	S	0	0	0
			1392	865	243	278	6			
2	D	184	Total	C	N	O	S	0	0	0
			1465	907	257	295	6			
2	F	176	Total	C	N	O	S	0	0	0
			1419	882	248	283	6			

There are 27 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	123	GLY	ARG	engineered mutation	UNP Q91MA7
B	177	SER	-	expression tag	UNP Q91MA7
B	178	GLY	-	expression tag	UNP Q91MA7
B	179	GLY	-	expression tag	UNP Q91MA7
B	180	GLY	-	expression tag	UNP Q91MA7
B	181	GLY	-	expression tag	UNP Q91MA7
B	182	LEU	-	expression tag	UNP Q91MA7
B	183	ASN	-	expression tag	UNP Q91MA7
B	184	ASP	-	expression tag	UNP Q91MA7
D	123	GLY	ARG	engineered mutation	UNP Q91MA7
D	177	SER	-	expression tag	UNP Q91MA7
D	178	GLY	-	expression tag	UNP Q91MA7
D	179	GLY	-	expression tag	UNP Q91MA7
D	180	GLY	-	expression tag	UNP Q91MA7
D	181	GLY	-	expression tag	UNP Q91MA7
D	182	LEU	-	expression tag	UNP Q91MA7
D	183	ASN	-	expression tag	UNP Q91MA7
D	184	ASP	-	expression tag	UNP Q91MA7
F	123	GLY	ARG	engineered mutation	UNP Q91MA7
F	177	SER	-	expression tag	UNP Q91MA7
F	178	GLY	-	expression tag	UNP Q91MA7
F	179	GLY	-	expression tag	UNP Q91MA7
F	180	GLY	-	expression tag	UNP Q91MA7
F	181	GLY	-	expression tag	UNP Q91MA7
F	182	LEU	-	expression tag	UNP Q91MA7
F	183	ASN	-	expression tag	UNP Q91MA7
F	184	ASP	-	expression tag	UNP Q91MA7

- 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.

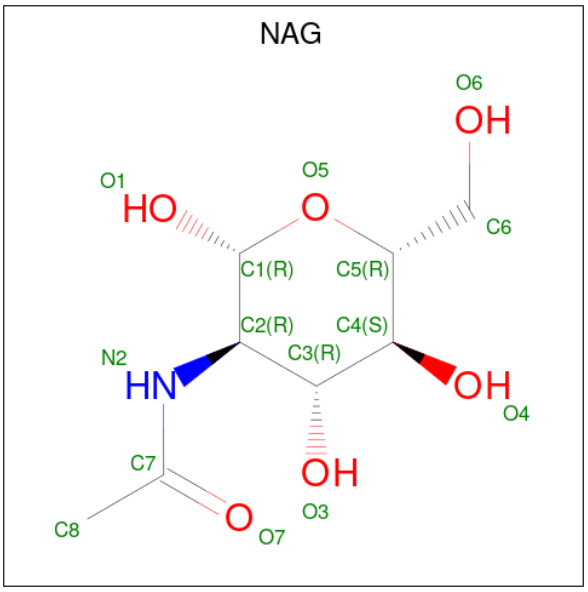


Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
3	G	3	Total	C	N	O	0	0	0
			39	22	2	15			
3	I	3	Total	C	N	O	0	0	0
			39	22	2	15			
3	K	3	Total	C	N	O	0	0	0
			39	22	2	15			

- Molecule 4 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
4	H	2	Total	C	N	O	0	0	0
			28	16	2	10			
4	J	2	Total	C	N	O	0	0	0
			28	16	2	10			
4	L	2	Total	C	N	O	0	0	0
			28	16	2	10			

- 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	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

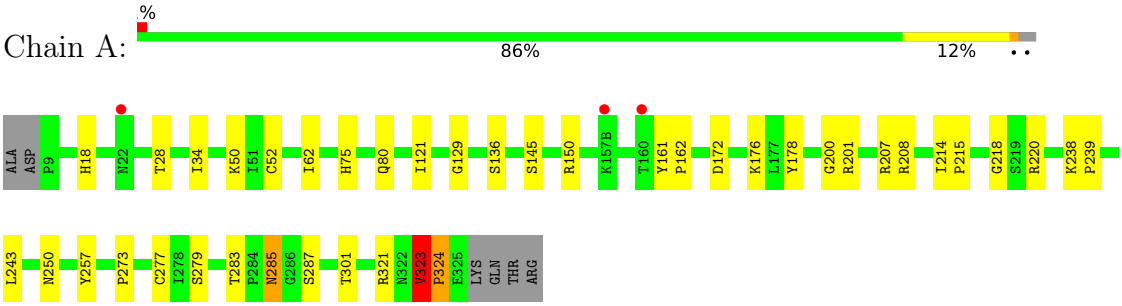
- Molecule 6 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	A	70	Total O 70 70	0	0
6	B	47	Total O 47 47	0	0
6	C	81	Total O 81 81	0	0
6	D	48	Total O 48 48	0	0
6	E	78	Total O 78 78	0	0
6	F	46	Total O 46 46	0	0

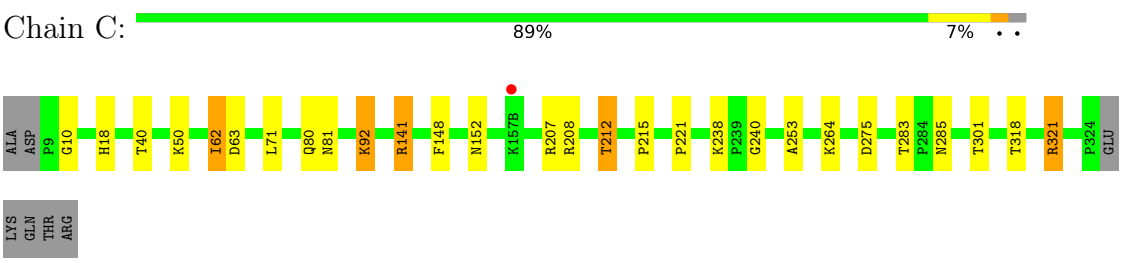
3 Residue-property plots (i)

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.

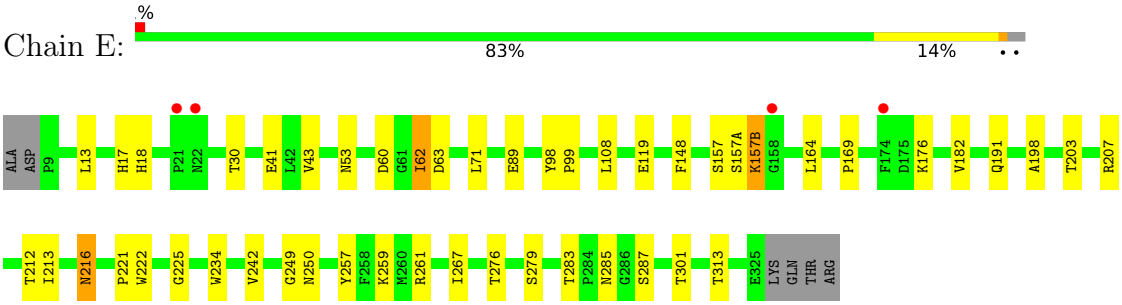
• Molecule 1: Hemagglutinin HA1 chain



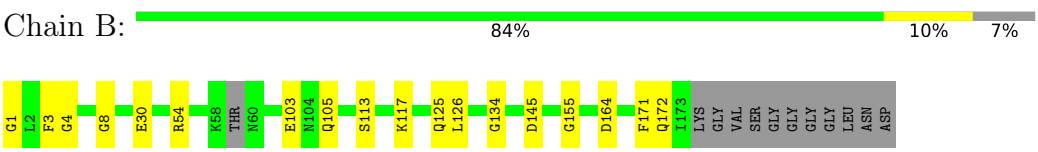
• Molecule 1: Hemagglutinin HA1 chain



• Molecule 1: Hemagglutinin HA1 chain

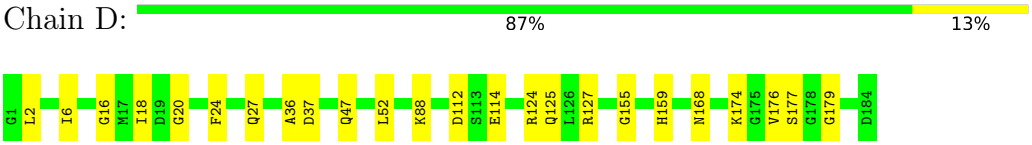


• Molecule 2: Hemagglutinin HA2 chain



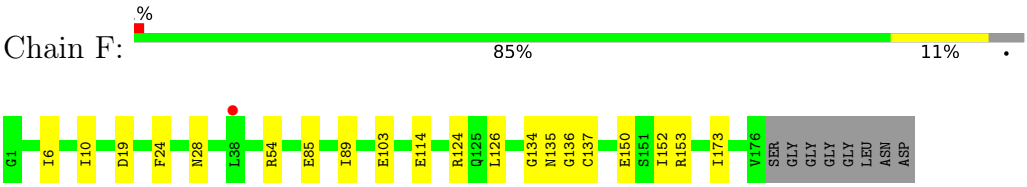
• Molecule 2: Hemagglutinin HA2 chain

Chain D:



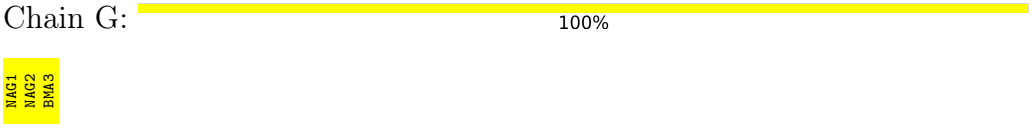
• Molecule 2: Hemagglutinin HA2 chain

Chain F:



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

Chain G:



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

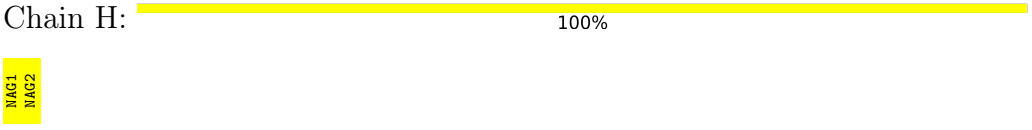
Chain I:

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

Chain K:

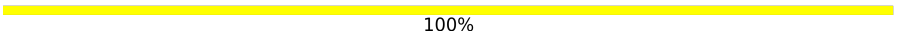
• Molecule 4: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain H:

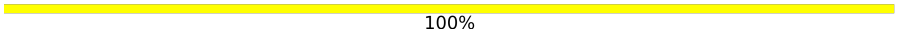


• Molecule 4: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain J:



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

Chain L: 

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	68.98Å 236.44Å 72.64Å 90.00° 116.49° 90.00°	Depositor
Resolution (Å)	48.60 – 2.59 48.60 – 2.59	Depositor EDS
% Data completeness (in resolution range)	99.3 (48.60-2.59) 92.7 (48.60-2.59)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.16	Depositor
$< I/\sigma(I) >$ [1]	1.49 (at 2.58Å)	Xtriage
Refinement program	PHENIX (1.10.1_2155: ???)	Depositor
R, R_{free}	0.187 , 0.239 0.187 , 0.239	Depositor DCC
R_{free} test set	3254 reflections (5.09%)	wwPDB-VP
Wilson B-factor (Å^2)	29.2	Xtriage
Anisotropy	0.465	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.33 , 40.5	EDS
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.32$	Xtriage
Estimated twinning fraction	0.029 for h,-k,-h-l	Xtriage
F_o,F_c correlation	0.93	EDS
Total number of atoms	12268	wwPDB-VP
Average B, all atoms (Å^2)	35.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.89% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: NAG, BMA

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	0.60	0/2515	0.73	4/3426 (0.1%)
1	C	0.59	0/2506	0.71	2/3414 (0.1%)
1	E	0.54	0/2515	0.70	0/3426
2	B	0.53	0/1415	0.66	0/1900
2	D	0.57	0/1489	0.73	1/2000 (0.1%)
2	F	0.56	0/1443	0.66	0/1939
All	All	0.57	0/11883	0.70	7/16105 (0.0%)

There are no bond length outliers.

All (7) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	324	PRO	CA-C-N	-9.48	96.35	117.20
1	A	323	VAL	O-C-N	6.58	133.61	121.10
1	A	324	PRO	CA-C-O	6.02	134.66	120.20
1	C	141	ARG	N-CA-C	-5.67	95.70	111.00
1	C	212	THR	CA-CB-CG2	-5.66	104.48	112.40
1	A	324	PRO	C-N-CA	5.12	134.49	121.70
2	D	179	GLY	N-CA-C	-5.05	100.48	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	2458	0	2409	26	0
1	C	2449	0	2401	26	0
1	E	2458	0	2408	35	0
2	B	1392	0	1310	13	0
2	D	1465	0	1381	20	0
2	F	1419	0	1343	15	0
3	G	39	0	34	3	0
3	I	39	0	34	6	0
3	K	39	0	34	2	0
4	H	28	0	25	0	0
4	J	28	0	25	0	0
4	L	28	0	25	0	0
5	A	28	0	26	0	0
5	C	14	0	13	2	0
5	E	14	0	13	0	0
6	A	70	0	0	3	0
6	B	47	0	0	1	0
6	C	81	0	0	3	0
6	D	48	0	0	3	0
6	E	78	0	0	2	0
6	F	46	0	0	3	0
All	All	12268	0	11481	129	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 (129) 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:A:52:CYS:CB	1:A:277:CYS:SG	2.32	1.17
1:A:52:CYS:SG	1:A:277:CYS:SG	1.11	1.11
1:C:92:LYS:H	1:C:92:LYS:HD2	1.37	0.89
2:F:54:ARG:NH2	2:F:103:GLU:OE2	2.10	0.85
1:A:80:GLN:HG2	1:A:150:ARG:NH2	1.94	0.82
1:C:283:THR:HG22	1:C:301:THR:HG22	1.65	0.79
1:C:212:THR:HG21	1:E:216:ASN:OD1	1.85	0.76
2:F:114:GLU:OE1	6:F:201:HOH:O	2.05	0.74
2:F:114:GLU:OE2	6:F:202:HOH:O	2.05	0.74
3:K:1:NAG:H61	3:K:2:NAG:HN2	1.52	0.74
1:C:81:ASN:HD22	5:C:401:NAG:H83	1.54	0.72
1:A:34:ILE:HD11	1:A:321:ARG:HE	1.55	0.70
2:B:54:ARG:NH2	2:B:103:GLU:OE2	2.24	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:134:GLY:HA2	2:F:124:ARG:HD3	1.75	0.69
1:A:285:ASN:N	1:A:285:ASN:OD1	2.26	0.68
2:D:114:GLU:OE1	6:D:201:HOH:O	2.12	0.68
1:C:318:THR:O	6:C:501:HOH:O	2.13	0.67
1:E:222:TRP:CZ2	1:E:225:GLY:HA2	2.30	0.67
3:K:1:NAG:H61	3:K:2:NAG:N2	2.12	0.65
2:F:28:ASN:O	6:F:203:HOH:O	2.13	0.65
3:I:1:NAG:H62	3:I:2:NAG:H82	1.79	0.65
1:C:10:GLY:O	6:C:502:HOH:O	2.15	0.64
3:I:1:NAG:C6	3:I:2:NAG:H82	2.27	0.64
2:D:125:GLN:HE22	2:D:155:GLY:HA2	1.65	0.62
1:A:201:ARG:NE	6:A:505:HOH:O	2.25	0.62
1:E:203:THR:HG23	1:E:212:THR:HG22	1.82	0.61
1:C:215:PRO:HG2	6:C:548:HOH:O	2.00	0.61
1:A:50:LYS:HG2	1:A:273:PRO:HG2	1.83	0.60
3:I:1:NAG:H61	3:I:2:NAG:N2	2.17	0.60
1:E:182:VAL:HG21	1:E:213:ILE:HB	1.84	0.59
1:A:208:ARG:NH1	1:A:238:LYS:HB2	2.18	0.58
1:C:321:ARG:HH11	1:C:321:ARG:HG3	1.68	0.57
1:A:218:GLY:O	1:A:220:ARG:NH1	2.38	0.56
2:D:124:ARG:HD3	2:F:134:GLY:HA2	1.86	0.56
2:F:135:ASN:OD1	2:F:137:CYS:HB2	2.05	0.56
2:D:47:GLN:HG2	1:E:30:THR:HG21	1.86	0.55
2:D:27:GLN:OE1	6:D:202:HOH:O	2.17	0.54
2:D:168:ASN:HB2	2:F:173:ILE:HD11	1.90	0.54
2:D:20:GLY:HA3	2:D:36:ALA:HB1	1.90	0.54
2:D:125:GLN:NE2	2:D:155:GLY:HA2	2.24	0.53
1:C:221:PRO:HA	3:G:2:NAG:O7	2.08	0.53
1:C:212:THR:HG21	1:E:216:ASN:CG	2.30	0.53
1:A:200:GLY:HA3	1:A:250:ASN:OD1	2.09	0.52
1:A:283:THR:HG22	1:A:301:THR:HG22	1.91	0.52
3:I:1:NAG:H61	3:I:2:NAG:C7	2.39	0.52
1:E:119:GLU:OE1	1:E:261:ARG:NH2	2.41	0.52
1:E:169:PRO:HA	1:E:242:VAL:HG12	1.91	0.52
1:E:259:LYS:HD3	1:E:261:ARG:NH2	2.25	0.51
2:B:172:GLN:HA	2:B:172:GLN:OE1	2.11	0.51
2:D:6:ILE:HD12	2:D:112:ASP:HA	1.93	0.50
1:E:41:GLU:OE1	1:E:313:THR:OG1	2.24	0.50
2:B:164:ASP:OD2	2:D:174:LYS:HB2	2.12	0.50
1:C:208:ARG:NH1	1:C:238:LYS:HD2	2.27	0.50
2:D:16:GLY:O	2:D:18:ILE:HG23	2.11	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:19:ASP:N	2:F:19:ASP:OD1	2.45	0.50
1:A:207:ARG:HD2	6:A:519:HOH:O	2.12	0.49
1:E:216:ASN:N	1:E:216:ASN:ND2	2.59	0.49
1:C:80:GLN:O	1:C:81:ASN:HB2	2.10	0.49
2:F:126:LEU:HD21	2:F:152:ILE:HD13	1.93	0.49
1:E:176:LYS:HE2	1:E:257:TYR:CE1	2.48	0.49
1:A:323:VAL:HG22	1:A:323:VAL:O	2.13	0.48
3:I:1:NAG:H61	3:I:2:NAG:H82	1.93	0.48
1:E:13:LEU:HD11	2:F:24:PHE:HB3	1.96	0.48
1:E:279:SER:CB	1:E:287:SER:HB3	2.43	0.48
2:B:125:GLN:OE1	2:B:155:GLY:HA2	2.14	0.47
1:E:191:GLN:HG2	1:E:198:ALA:O	2.14	0.47
1:C:221:PRO:HA	3:G:2:NAG:H81	1.96	0.47
2:D:176:VAL:O	2:D:177:SER:HB2	2.15	0.47
2:B:4:GLY:O	2:B:8:GLY:HA3	2.15	0.47
1:C:221:PRO:HB3	3:G:2:NAG:H81	1.98	0.47
1:A:52:CYS:CA	1:A:277:CYS:SG	3.03	0.46
1:A:323:VAL:HA	1:A:324:PRO:HD3	1.40	0.46
1:E:71:LEU:O	1:E:148:PHE:HB3	2.16	0.45
1:E:43:VAL:O	6:E:501:HOH:O	2.20	0.45
1:C:92:LYS:HD2	1:C:92:LYS:N	2.18	0.45
1:E:222:TRP:CE2	1:E:225:GLY:HA2	2.51	0.45
3:I:1:NAG:H61	3:I:2:NAG:HN2	1.80	0.45
1:A:136:SER:N	1:A:145:SER:HB2	2.32	0.45
2:B:113:SER:O	2:B:117:LYS:HG3	2.16	0.45
1:C:321:ARG:HG3	1:C:321:ARG:NH1	2.31	0.45
1:A:28:THR:HB	2:B:105:GLN:OE1	2.17	0.45
1:C:81:ASN:HD22	5:C:401:NAG:C8	2.28	0.45
2:F:10:ILE:HD13	2:F:136:GLY:HA3	1.99	0.45
1:C:207:ARG:HA	1:E:221:PRO:HG2	1.98	0.44
1:E:53:ASN:OD1	1:E:276:THR:HA	2.17	0.44
1:A:75:HIS:N	6:A:506:HOH:O	2.39	0.44
1:E:60:ASP:O	1:E:62:ILE:HG13	2.18	0.44
1:A:161:TYR:HA	1:A:162:PRO:HD3	1.65	0.44
1:A:172:ASP:O	1:A:239:PRO:HB3	2.18	0.44
1:A:279:SER:OG	1:A:287:SER:HB3	2.18	0.44
1:C:152:ASN:HB3	1:C:253:ALA:HB3	1.99	0.44
2:B:126:LEU:HA	2:B:126:LEU:HD23	1.71	0.44
2:D:24:PHE:CE1	2:D:37:ASP:HB2	2.53	0.44
1:E:283:THR:HG22	1:E:301:THR:HG22	1.98	0.44
2:B:3:PHE:HZ	2:D:2:LEU:HB3	1.83	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:62:ILE:HG22	1:C:63:ASP:H	1.84	0.43
1:E:157(A):SER:O	1:E:157(B):LYS:HD2	2.19	0.43
2:F:150:GLU:OE1	2:F:153:ARG:NH2	2.41	0.43
2:D:24:PHE:HE1	2:D:37:ASP:HB2	1.82	0.43
2:D:88:LYS:NZ	6:D:207:HOH:O	2.48	0.43
1:E:176:LYS:HG2	1:E:257:TYR:CD2	2.54	0.43
1:A:176:LYS:HB3	1:A:257:TYR:HB2	2.01	0.43
1:E:279:SER:HB3	1:E:287:SER:HB3	2.01	0.43
2:D:2:LEU:HD23	2:D:2:LEU:HA	1.75	0.43
1:E:62:ILE:HG22	1:E:63:ASP:H	1.84	0.43
1:C:208:ARG:H	1:C:208:ARG:HG2	1.76	0.43
1:A:129:GLY:HA3	1:A:162:PRO:HG2	2.00	0.42
1:C:50:LYS:HD3	1:C:275:ASP:HB3	2.00	0.42
1:A:214:ILE:HA	1:A:215:PRO:HD3	1.90	0.42
1:C:71:LEU:O	1:C:148:PHE:HB3	2.19	0.42
1:E:108:LEU:HB2	1:E:234:TRP:CZ3	2.54	0.42
2:B:1:GLY:N	6:B:208:HOH:O	2.38	0.42
1:A:121:ILE:HD13	1:A:257:TYR:CE2	2.54	0.42
1:E:98:TYR:CD1	1:E:99:PRO:HD2	2.54	0.42
2:D:127:ARG:HG3	2:D:159:HIS:CG	2.54	0.42
1:E:207:ARG:NE	6:E:505:HOH:O	2.42	0.42
1:A:178:TYR:CD1	1:A:243:LEU:HD22	2.54	0.41
2:D:47:GLN:HG2	1:E:30:THR:CG2	2.51	0.41
1:E:17:HIS:CD2	2:F:6:ILE:HG12	2.56	0.41
2:F:85:GLU:O	2:F:89:ILE:HG13	2.20	0.41
2:B:30:GLU:OE2	2:B:145:ASP:HB2	2.20	0.41
2:B:171:PHE:N	2:B:171:PHE:CD1	2.88	0.41
1:C:40:THR:HG21	2:D:52:LEU:HD11	2.02	0.41
1:E:249:GLY:O	1:E:250:ASN:HB2	2.21	0.41
1:E:89:GLU:HG3	1:E:267:ILE:HD11	2.03	0.40
1:E:164:LEU:HA	1:E:164:LEU:HD23	1.86	0.40
1:C:207:ARG:NH1	1:C:240:GLY:O	2.51	0.40
1:C:212:THR:O	1:C:212:THR:HG23	2.20	0.40
1:E:157:SER:C	1:E:157(B):LYS:H	2.25	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	317/325 (98%)	305 (96%)	11 (4%)	1 (0%)	41	64
1	C	316/325 (97%)	307 (97%)	8 (2%)	1 (0%)	41	64
1	E	317/325 (98%)	305 (96%)	11 (4%)	1 (0%)	41	64
2	B	168/184 (91%)	161 (96%)	7 (4%)	0	100	100
2	D	182/184 (99%)	174 (96%)	8 (4%)	0	100	100
2	F	174/184 (95%)	166 (95%)	8 (5%)	0	100	100
All	All	1474/1527 (96%)	1418 (96%)	53 (4%)	3 (0%)	47	71

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	E	62	ILE
1	A	62	ILE
1	C	62	ILE

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	280/285 (98%)	277 (99%)	3 (1%)	73	88
1	C	279/285 (98%)	273 (98%)	6 (2%)	52	76
1	E	280/285 (98%)	276 (99%)	4 (1%)	67	85
2	B	146/153 (95%)	146 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
2	D	153/153 (100%)	153 (100%)	0	100 100
2	F	149/153 (97%)	149 (100%)	0	100 100
All	All	1287/1314 (98%)	1274 (99%)	13 (1%)	76 90

All (13) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	18	HIS
1	A	285	ASN
1	A	323	VAL
1	C	18	HIS
1	C	92	LYS
1	C	141	ARG
1	C	264	LYS
1	C	285	ASN
1	C	321	ARG
1	E	18	HIS
1	E	157(B)	LYS
1	E	216	ASN
1	E	285	ASN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (2) such sidechains are listed below:

Mol	Chain	Res	Type
2	B	12	ASN
2	D	125	GLN

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates (i)

15 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	3,1	14,14,15	1.06	2 (14%)	17,19,21	1.48	3 (17%)
3	NAG	G	2	3	14,14,15	0.23	0	17,19,21	0.53	0
3	BMA	G	3	3	11,11,12	1.46	2 (18%)	15,15,17	0.90	1 (6%)
4	NAG	H	1	4,1	14,14,15	1.17	2 (14%)	17,19,21	1.21	1 (5%)
4	NAG	H	2	4	14,14,15	0.52	0	17,19,21	2.01	4 (23%)
3	NAG	I	1	3,1	14,14,15	0.97	1 (7%)	17,19,21	0.98	1 (5%)
3	NAG	I	2	3	14,14,15	0.71	1 (7%)	17,19,21	2.50	7 (41%)
3	BMA	I	3	3	11,11,12	1.45	2 (18%)	15,15,17	0.90	1 (6%)
4	NAG	J	1	4,1	14,14,15	0.98	1 (7%)	17,19,21	1.12	2 (11%)
4	NAG	J	2	4	14,14,15	0.54	0	17,19,21	1.25	3 (17%)
3	NAG	K	1	3,1	14,14,15	1.19	2 (14%)	17,19,21	1.44	2 (11%)
3	NAG	K	2	3	14,14,15	0.72	0	17,19,21	1.70	4 (23%)
3	BMA	K	3	3	11,11,12	1.47	2 (18%)	15,15,17	0.91	1 (6%)
4	NAG	L	1	4,1	14,14,15	1.12	2 (14%)	17,19,21	1.94	5 (29%)
4	NAG	L	2	4	14,14,15	0.46	0	17,19,21	2.73	5 (29%)

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	3,1	-	0/6/23/26	0/1/1/1
3	NAG	G	2	3	-	2/6/23/26	0/1/1/1
3	BMA	G	3	3	-	0/2/19/22	0/1/1/1
4	NAG	H	1	4,1	-	2/6/23/26	0/1/1/1
4	NAG	H	2	4	-	2/6/23/26	0/1/1/1
3	NAG	I	1	3,1	-	2/6/23/26	0/1/1/1
3	NAG	I	2	3	-	0/6/23/26	0/1/1/1
3	BMA	I	3	3	-	0/2/19/22	0/1/1/1
4	NAG	J	1	4,1	-	2/6/23/26	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	NAG	J	2	4	-	2/6/23/26	0/1/1/1
3	NAG	K	1	3,1	-	2/6/23/26	0/1/1/1
3	NAG	K	2	3	-	4/6/23/26	0/1/1/1
3	BMA	K	3	3	-	0/2/19/22	0/1/1/1
4	NAG	L	1	4,1	-	2/6/23/26	0/1/1/1
4	NAG	L	2	4	-	4/6/23/26	0/1/1/1

All (17) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	K	3	BMA	O5-C1	3.11	1.48	1.43
3	G	3	BMA	O5-C1	3.09	1.48	1.43
3	I	3	BMA	O5-C1	3.07	1.48	1.43
4	L	1	NAG	C2-N2	-2.88	1.41	1.46
3	K	1	NAG	C2-N2	-2.71	1.41	1.46
3	G	3	BMA	O5-C5	2.60	1.48	1.43
3	K	3	BMA	O5-C5	2.59	1.48	1.43
3	I	3	BMA	O5-C5	2.57	1.48	1.43
3	I	1	NAG	O5-C1	-2.49	1.39	1.43
3	G	1	NAG	O5-C1	-2.48	1.39	1.43
4	H	1	NAG	O5-C1	-2.39	1.39	1.43
4	L	1	NAG	O5-C1	-2.36	1.39	1.43
4	J	1	NAG	O5-C1	-2.36	1.39	1.43
4	H	1	NAG	C2-N2	-2.18	1.42	1.46
3	G	1	NAG	O7-C7	-2.12	1.18	1.23
3	K	1	NAG	O5-C1	-2.10	1.40	1.43
3	I	2	NAG	O7-C7	-2.02	1.18	1.23

All (40) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	L	2	NAG	C1-C2-N2	7.51	123.32	110.49
4	H	2	NAG	C1-C2-N2	5.98	120.70	110.49
4	L	1	NAG	O5-C5-C6	5.29	115.50	107.20
3	I	2	NAG	C2-N2-C7	4.95	129.95	122.90
4	L	2	NAG	C2-N2-C7	-4.81	116.05	122.90
3	I	2	NAG	C1-C2-N2	-4.77	102.34	110.49
3	K	1	NAG	O3-C3-C2	4.36	118.48	109.47
3	I	2	NAG	O3-C3-C2	4.35	118.47	109.47
3	I	2	NAG	O7-C7-C8	-4.27	114.13	122.06
4	L	2	NAG	O3-C3-C4	-4.02	101.06	110.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	K	2	NAG	C6-C5-C4	-3.87	103.94	113.00
4	L	2	NAG	O4-C4-C5	-3.45	100.72	109.30
3	G	1	NAG	C1-C2-N2	-3.38	104.72	110.49
4	L	2	NAG	O5-C5-C6	-3.22	102.15	107.20
3	K	2	NAG	O5-C5-C6	-3.15	102.27	107.20
4	L	1	NAG	O6-C6-C5	-3.07	100.77	111.29
3	G	1	NAG	C6-C5-C4	-3.02	105.94	113.00
4	J	1	NAG	O5-C5-C6	-3.00	102.50	107.20
3	K	2	NAG	O3-C3-C2	2.82	115.29	109.47
4	H	2	NAG	C2-N2-C7	-2.81	118.91	122.90
4	H	2	NAG	O5-C5-C6	-2.76	102.88	107.20
3	I	1	NAG	O3-C3-C2	2.75	115.16	109.47
3	K	2	NAG	C2-N2-C7	2.72	126.78	122.90
4	L	1	NAG	C1-C2-N2	-2.62	106.02	110.49
4	L	1	NAG	O3-C3-C2	2.54	114.72	109.47
3	G	1	NAG	O3-C3-C2	2.52	114.68	109.47
3	I	2	NAG	O5-C5-C6	2.44	111.04	107.20
3	I	2	NAG	O7-C7-N2	2.36	126.28	121.95
4	J	2	NAG	C2-N2-C7	-2.34	119.57	122.90
4	H	1	NAG	O5-C5-C6	-2.27	103.64	107.20
4	J	2	NAG	O3-C3-C4	-2.24	105.17	110.35
3	K	3	BMA	C1-O5-C5	2.18	115.15	112.19
4	J	2	NAG	O4-C4-C3	2.17	115.37	110.35
3	I	3	BMA	C1-O5-C5	2.15	115.10	112.19
3	G	3	BMA	C1-O5-C5	2.14	115.09	112.19
4	H	2	NAG	O4-C4-C3	2.14	115.30	110.35
4	L	1	NAG	O3-C3-C4	2.13	115.26	110.35
3	I	2	NAG	C8-C7-N2	2.06	119.59	116.10
3	K	1	NAG	C1-C2-N2	-2.04	107.00	110.49
4	J	1	NAG	C6-C5-C4	-2.04	108.23	113.00

There are no chirality outliers.

All (24) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	H	1	NAG	O5-C5-C6-O6
4	J	2	NAG	O5-C5-C6-O6
4	L	2	NAG	O5-C5-C6-O6
4	J	2	NAG	C4-C5-C6-O6
3	K	2	NAG	O5-C5-C6-O6
4	H	1	NAG	C4-C5-C6-O6
4	H	2	NAG	C4-C5-C6-O6

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Mol	Chain	Res	Type	Atoms
4	J	1	NAG	O5-C5-C6-O6
4	L	2	NAG	C4-C5-C6-O6
4	J	1	NAG	C4-C5-C6-O6
4	L	1	NAG	C4-C5-C6-O6
3	G	2	NAG	O5-C5-C6-O6
4	L	2	NAG	C8-C7-N2-C2
3	G	2	NAG	C4-C5-C6-O6
4	L	2	NAG	O7-C7-N2-C2
3	K	2	NAG	C4-C5-C6-O6
4	L	1	NAG	O5-C5-C6-O6
3	I	1	NAG	C4-C5-C6-O6
3	K	2	NAG	C8-C7-N2-C2
4	H	2	NAG	O5-C5-C6-O6
3	K	1	NAG	C8-C7-N2-C2
3	I	1	NAG	O5-C5-C6-O6
3	K	2	NAG	O7-C7-N2-C2
3	K	1	NAG	O7-C7-N2-C2

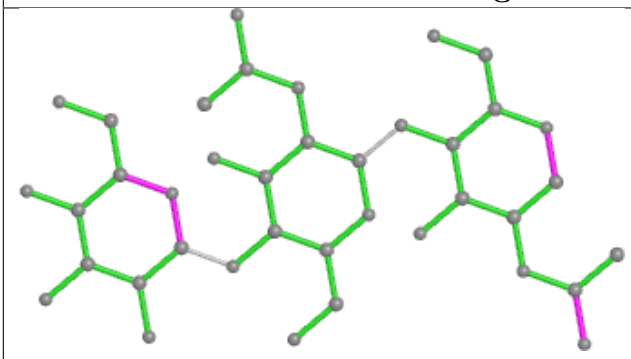
There are no ring outliers.

5 monomers are involved in 11 short contacts:

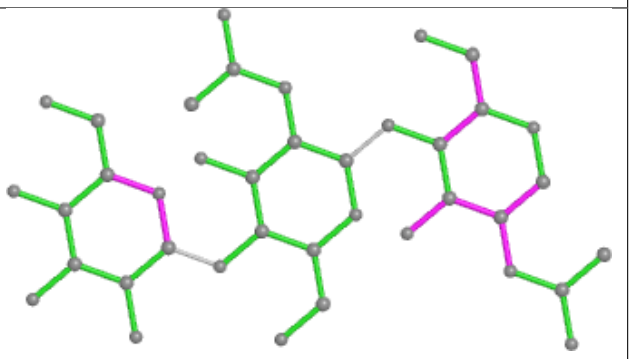
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	K	1	NAG	2	0
3	G	2	NAG	3	0
3	K	2	NAG	2	0
3	I	1	NAG	6	0
3	I	2	NAG	6	0

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

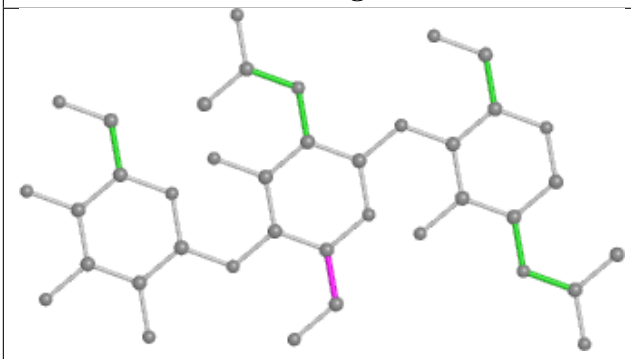
Oligosaccharide Chain G



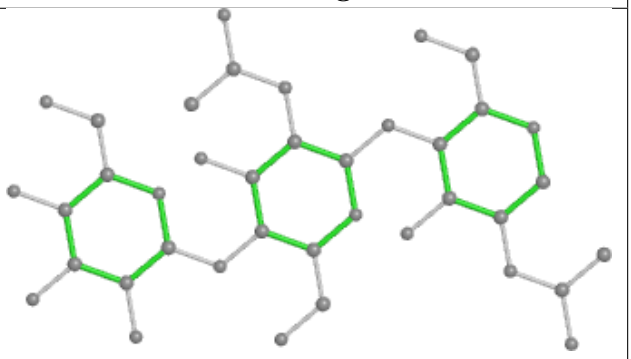
Bond lengths



Bond angles

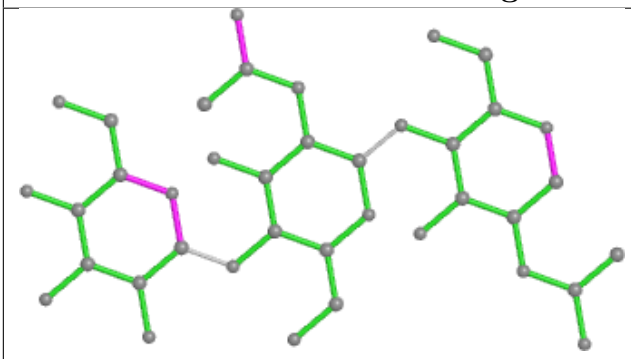


Torsions

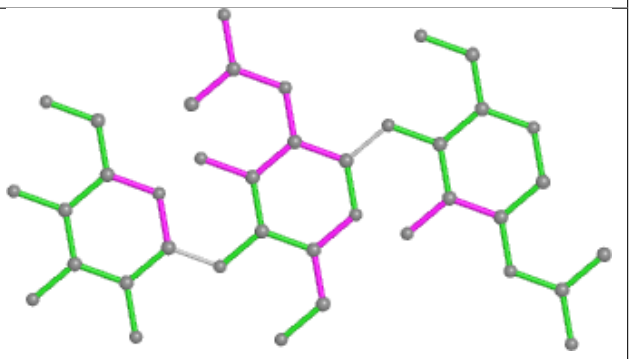


Rings

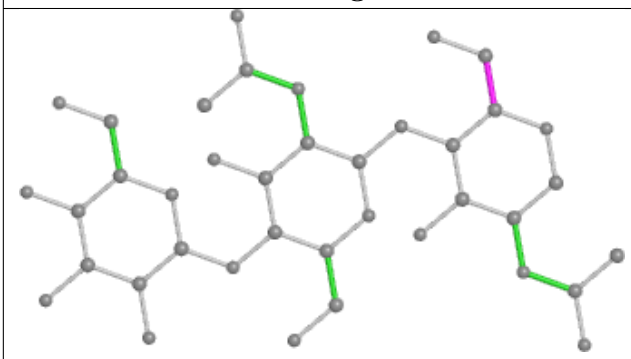
Oligosaccharide Chain I



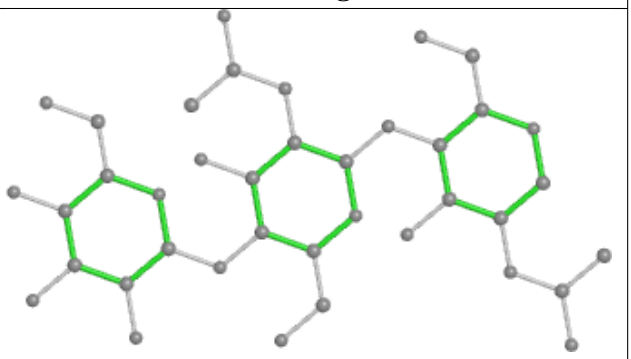
Bond lengths



Bond angles

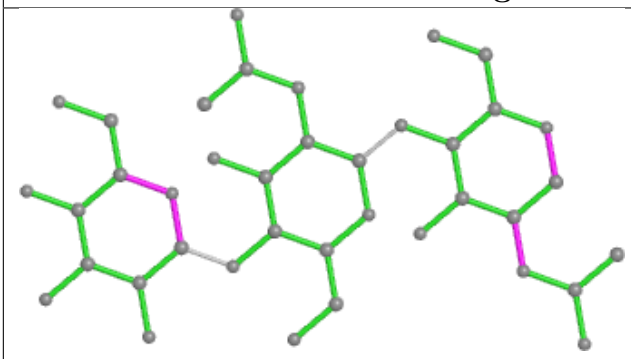


Torsions

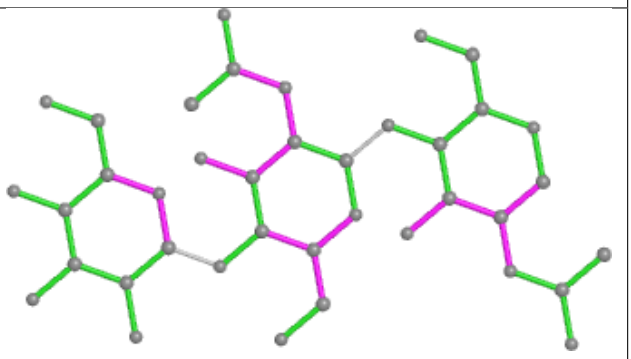


Rings

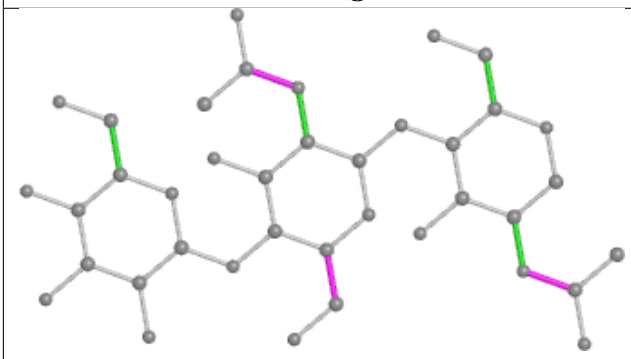
Oligosaccharide Chain K



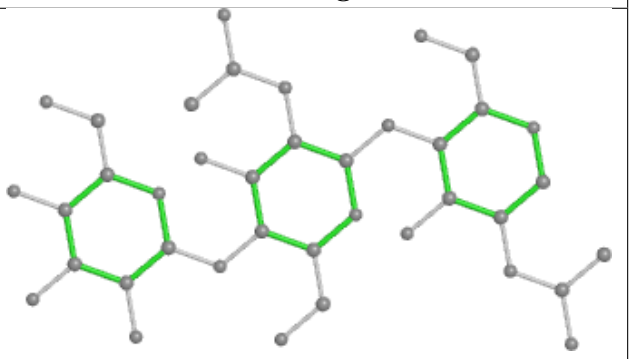
Bond lengths



Bond angles

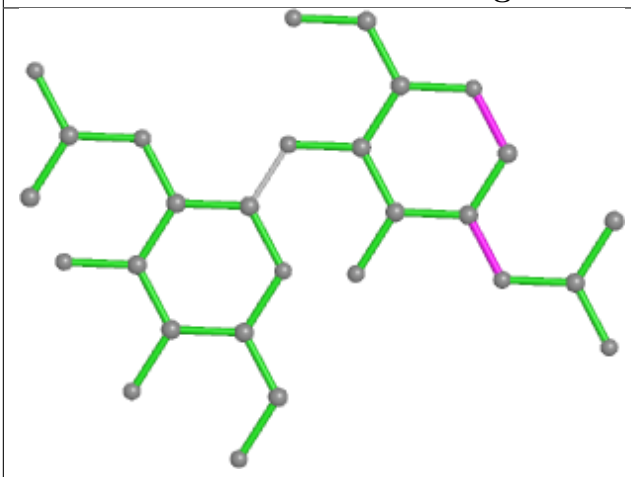


Torsions

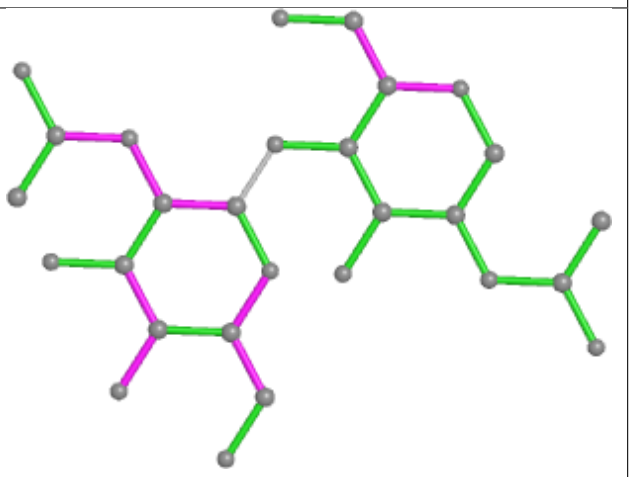


Rings

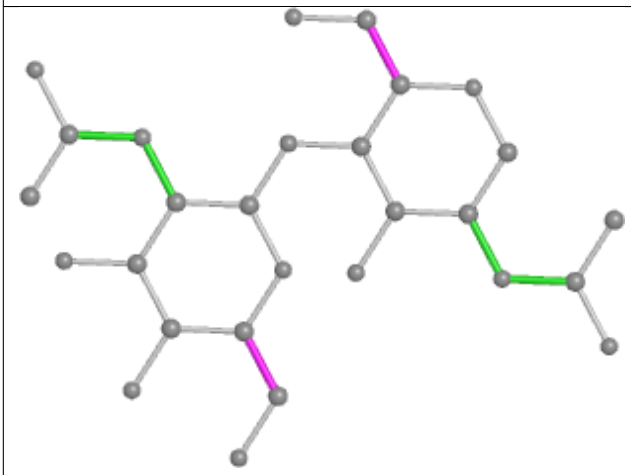
Oligosaccharide Chain H



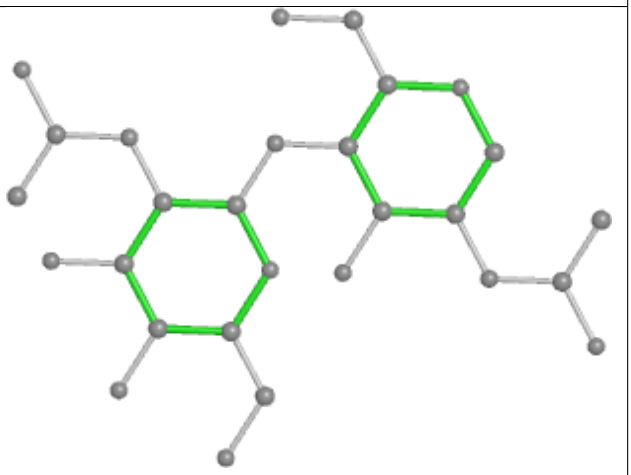
Bond lengths



Bond angles

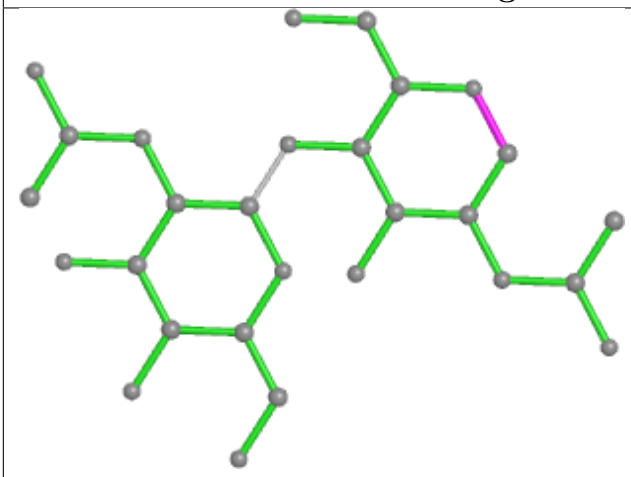


Torsions

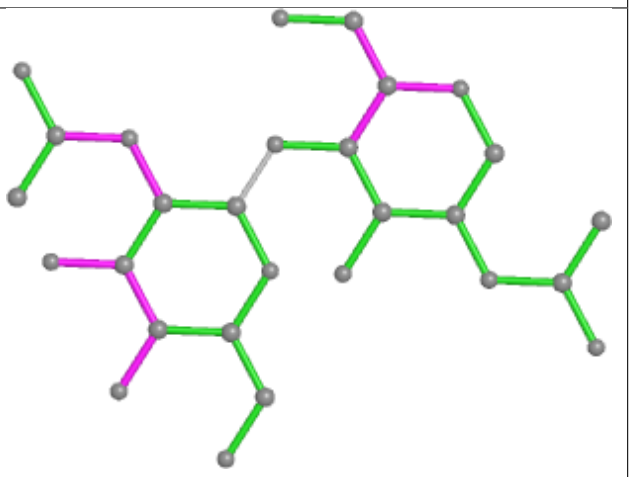


Rings

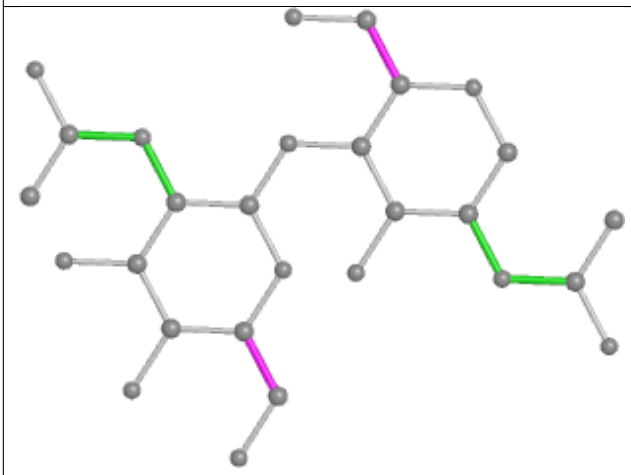
Oligosaccharide Chain J



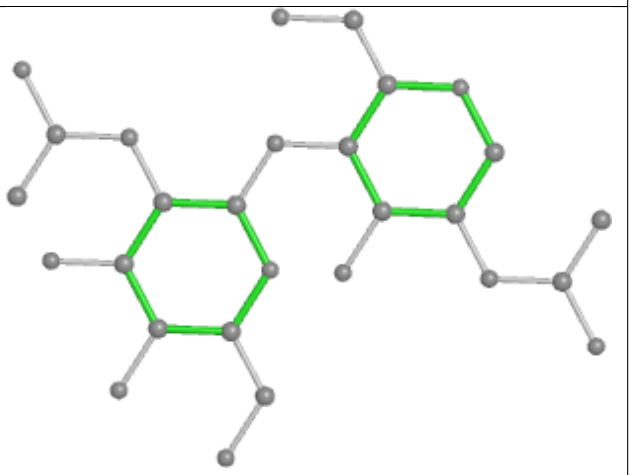
Bond lengths



Bond angles

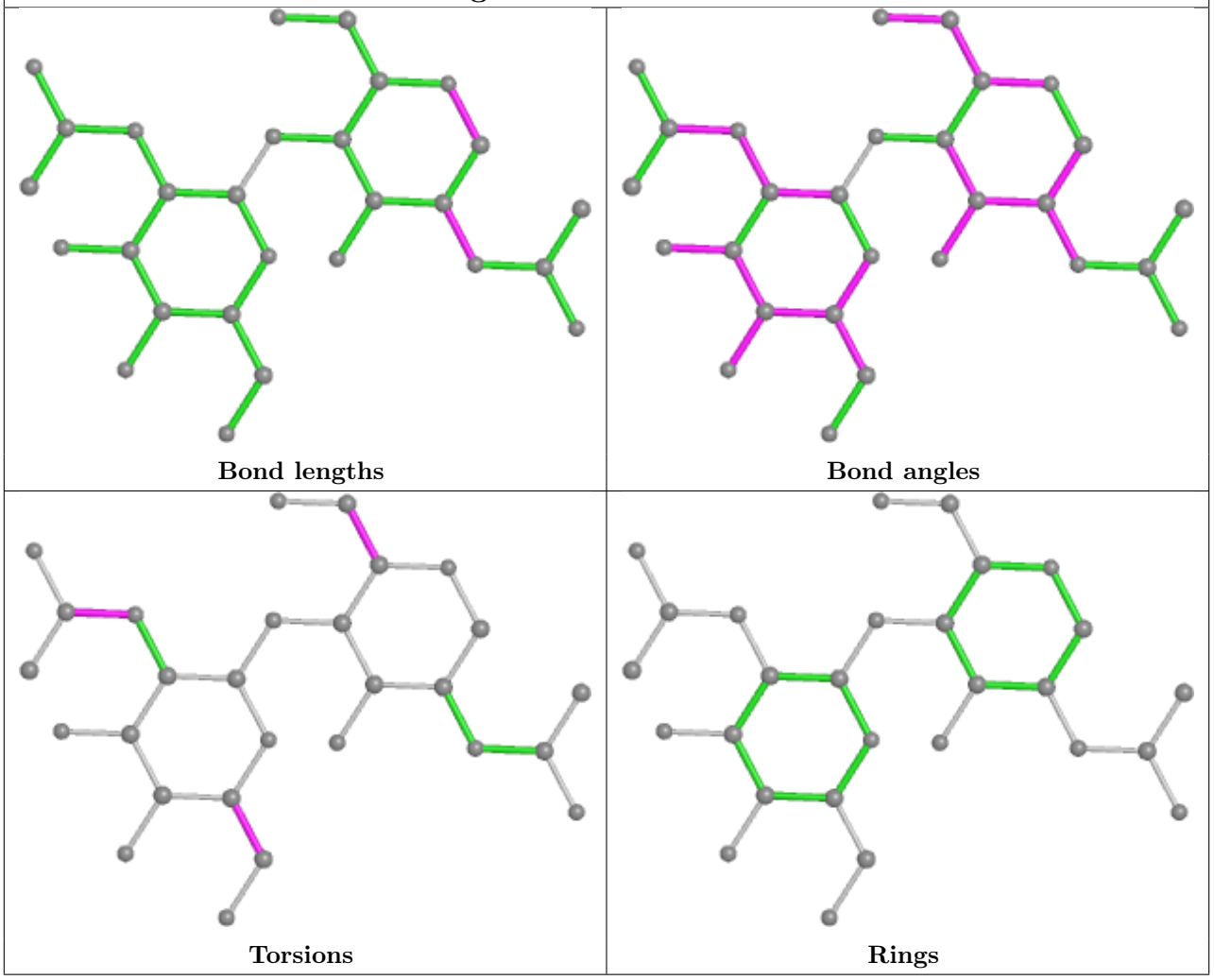


Torsions



Rings

Oligosaccharide Chain L



5.6 Ligand geometry (i)

4 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	$\#\|Z\| > 2$
5	NAG	A	402	1	14,14,15	0.91	2 (14%)	17,19,21	1.73	4 (23%)
5	NAG	E	401	1	14,14,15	0.85	1 (7%)	17,19,21	1.14	2 (11%)
5	NAG	C	401	1	14,14,15	0.72	1 (7%)	17,19,21	1.96	6 (35%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
5	NAG	A	401	1	14,14,15	0.84	1 (7%)	17,19,21	1.14	2 (11%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	NAG	A	402	1	-	4/6/23/26	0/1/1/1
5	NAG	E	401	1	-	4/6/23/26	0/1/1/1
5	NAG	C	401	1	-	4/6/23/26	0/1/1/1
5	NAG	A	401	1	-	4/6/23/26	0/1/1/1

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	C	401	NAG	O5-C1	-2.36	1.39	1.43
5	A	402	NAG	O5-C1	-2.34	1.40	1.43
5	E	401	NAG	O5-C1	-2.27	1.40	1.43
5	A	401	NAG	O5-C1	-2.27	1.40	1.43
5	A	402	NAG	C2-N2	-2.11	1.42	1.46

All (14) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
5	A	402	NAG	C1-C2-N2	-4.98	101.98	110.49
5	C	401	NAG	O5-C5-C6	-4.07	100.82	107.20
5	C	401	NAG	O3-C3-C2	3.39	116.48	109.47
5	A	402	NAG	O3-C3-C2	-3.01	103.23	109.47
5	C	401	NAG	C1-C2-N2	2.92	115.48	110.49
5	C	401	NAG	C2-N2-C7	-2.82	118.89	122.90
5	E	401	NAG	C2-N2-C7	-2.79	118.94	122.90
5	A	401	NAG	C2-N2-C7	-2.77	118.96	122.90
5	C	401	NAG	O3-C3-C4	2.44	115.99	110.35
5	A	402	NAG	O4-C4-C5	-2.30	103.58	109.30
5	C	401	NAG	O7-C7-C8	-2.29	117.81	122.06
5	A	401	NAG	C6-C5-C4	-2.26	107.70	113.00
5	E	401	NAG	C6-C5-C4	-2.25	107.72	113.00
5	A	402	NAG	O3-C3-C4	-2.08	105.54	110.35

There are no chirality outliers.

All (16) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	C	401	NAG	C8-C7-N2-C2
5	C	401	NAG	O7-C7-N2-C2
5	A	402	NAG	C4-C5-C6-O6
5	C	401	NAG	O5-C5-C6-O6
5	A	402	NAG	O5-C5-C6-O6
5	A	401	NAG	C8-C7-N2-C2
5	E	401	NAG	C8-C7-N2-C2
5	A	401	NAG	O5-C5-C6-O6
5	E	401	NAG	O5-C5-C6-O6
5	C	401	NAG	C4-C5-C6-O6
5	A	401	NAG	O7-C7-N2-C2
5	A	402	NAG	C8-C7-N2-C2
5	A	402	NAG	O7-C7-N2-C2
5	E	401	NAG	O7-C7-N2-C2
5	A	401	NAG	C4-C5-C6-O6
5	E	401	NAG	C4-C5-C6-O6

There are no ring outliers.

1 monomer is involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	C	401	NAG	2	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	319/325 (98%)	-0.18	3 (0%)	84	82	23, 35, 47, 65	0
1	C	318/325 (97%)	-0.35	1 (0%)	94	93	20, 30, 43, 76	0
1	E	319/325 (98%)	-0.17	4 (1%)	77	73	22, 35, 49, 78	0
2	B	172/184 (93%)	-0.13	0	100	100	22, 37, 51, 57	0
2	D	184/184 (100%)	-0.14	0	100	100	22, 35, 49, 56	0
2	F	176/184 (95%)	-0.09	1 (0%)	89	88	21, 38, 51, 58	0
All	All	1488/1527 (97%)	-0.19	9 (0%)	89	88	20, 34, 50, 78	0

All (9) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	157(B)	LYS	3.1
1	A	160	THR	2.6
1	E	22	ASN	2.6
1	A	157(B)	LYS	2.5
2	F	38	LEU	2.2
1	E	174	PHE	2.2
1	E	158	GLY	2.2
1	A	22	ASN	2.0
1	E	21	PRO	2.0

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)

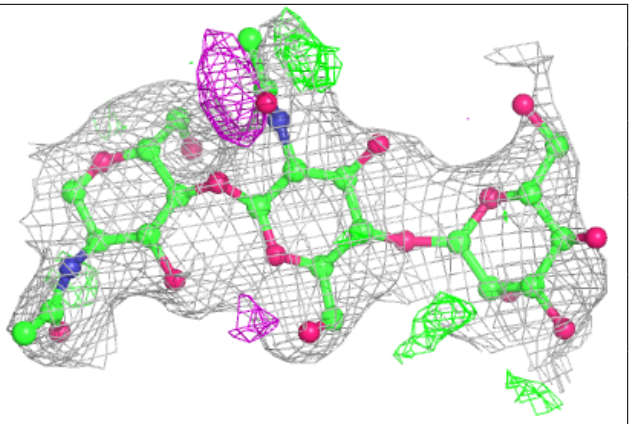
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9'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

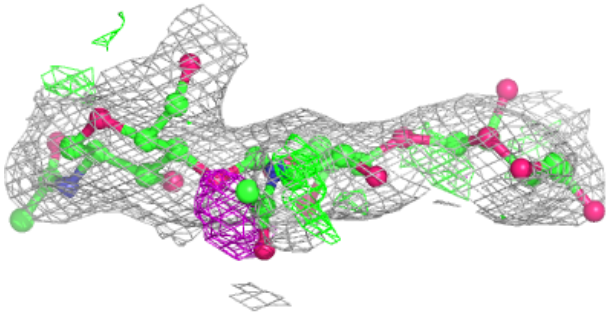
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
3	BMA	K	3	11/12	0.73	0.32	65,72,85,86	0
3	BMA	G	3	11/12	0.76	0.27	67,73,80,81	0
4	NAG	H	2	14/15	0.76	0.33	62,80,89,96	0
4	NAG	J	2	14/15	0.79	0.25	56,77,86,88	0
4	NAG	L	2	14/15	0.80	0.28	59,75,83,87	0
3	NAG	G	2	14/15	0.81	0.26	56,59,65,68	0
3	NAG	I	2	14/15	0.84	0.25	44,50,60,64	0
3	NAG	K	2	14/15	0.84	0.22	42,58,73,78	0
4	NAG	H	1	14/15	0.86	0.18	41,61,69,71	0
4	NAG	L	1	14/15	0.87	0.20	42,51,57,62	0
3	NAG	G	1	14/15	0.87	0.18	47,55,59,60	0
3	NAG	I	1	14/15	0.89	0.16	40,47,54,62	0
3	BMA	I	3	11/12	0.90	0.14	55,60,69,70	0
4	NAG	J	1	14/15	0.91	0.11	35,55,61,63	0
3	NAG	K	1	14/15	0.91	0.17	40,50,58,59	0

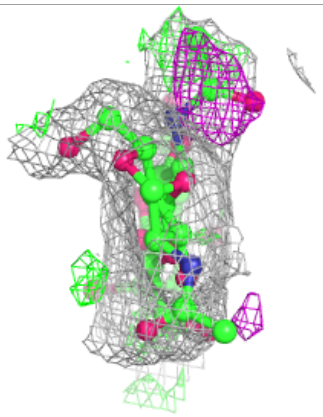
The following is a graphical depiction of the model fit to experimental electron density for oligosaccharide. Each fit is shown from different orientation to approximate a three-dimensional view.

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)

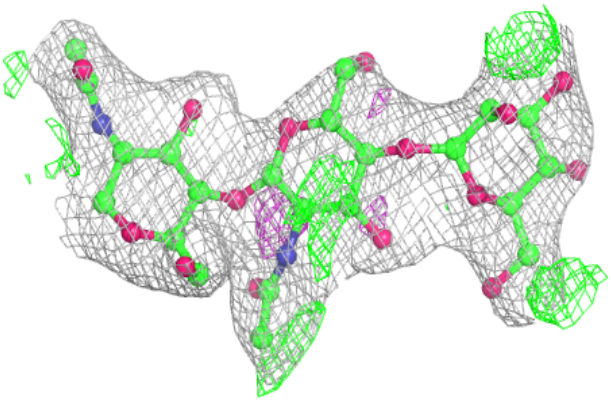


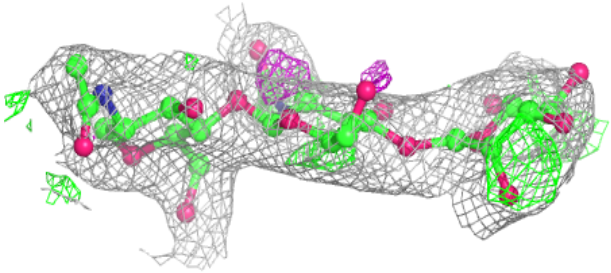


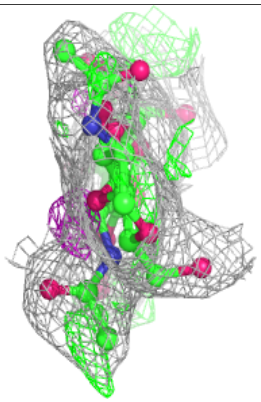


Electron density around Chain I:

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

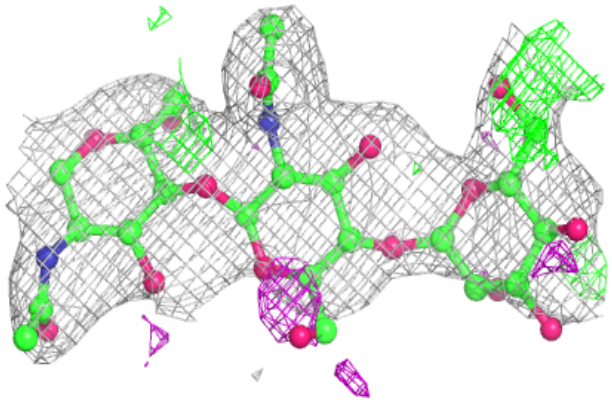


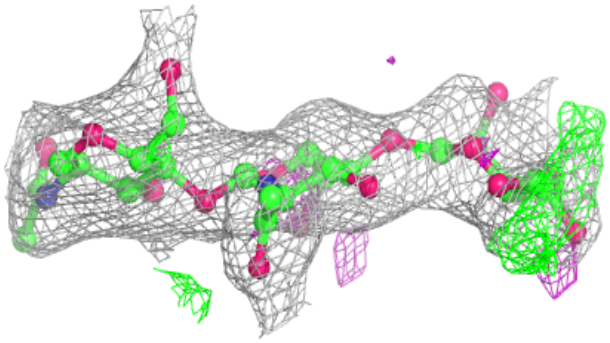


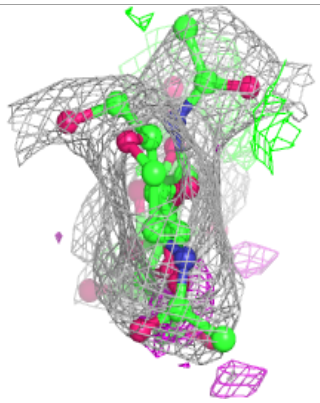


Electron density around Chain K:

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

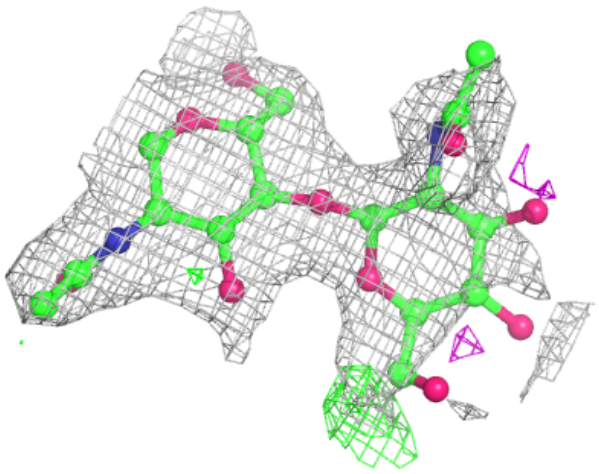


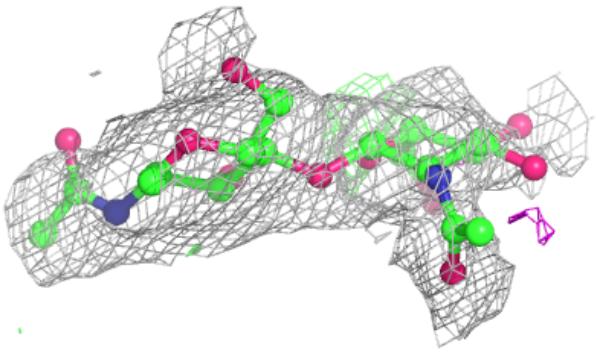


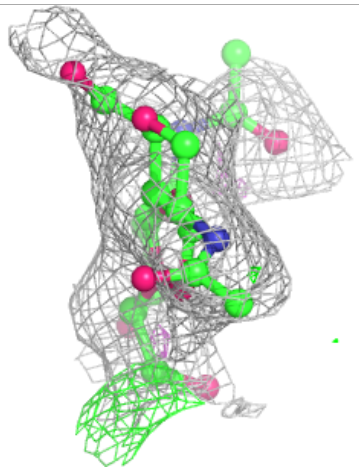


Electron density around Chain H:

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

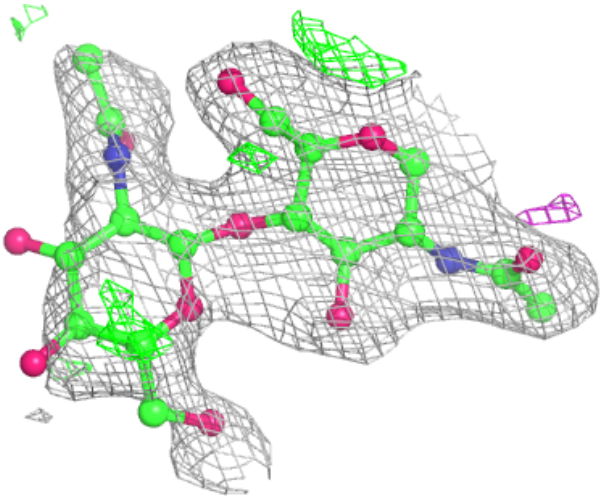


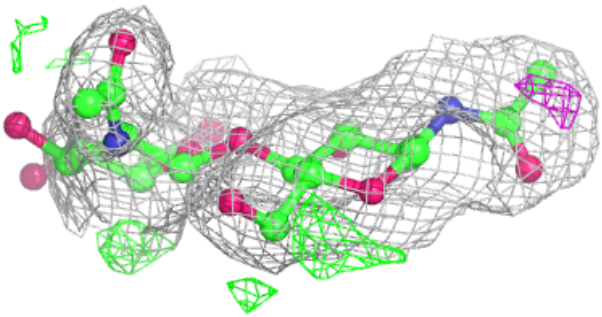


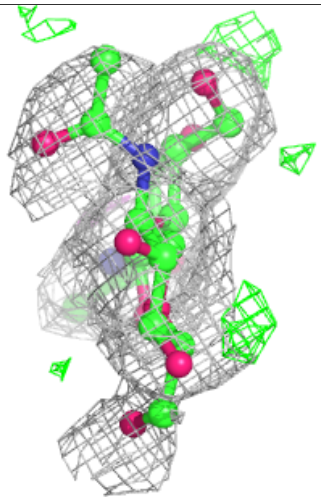


Electron density around Chain J:

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

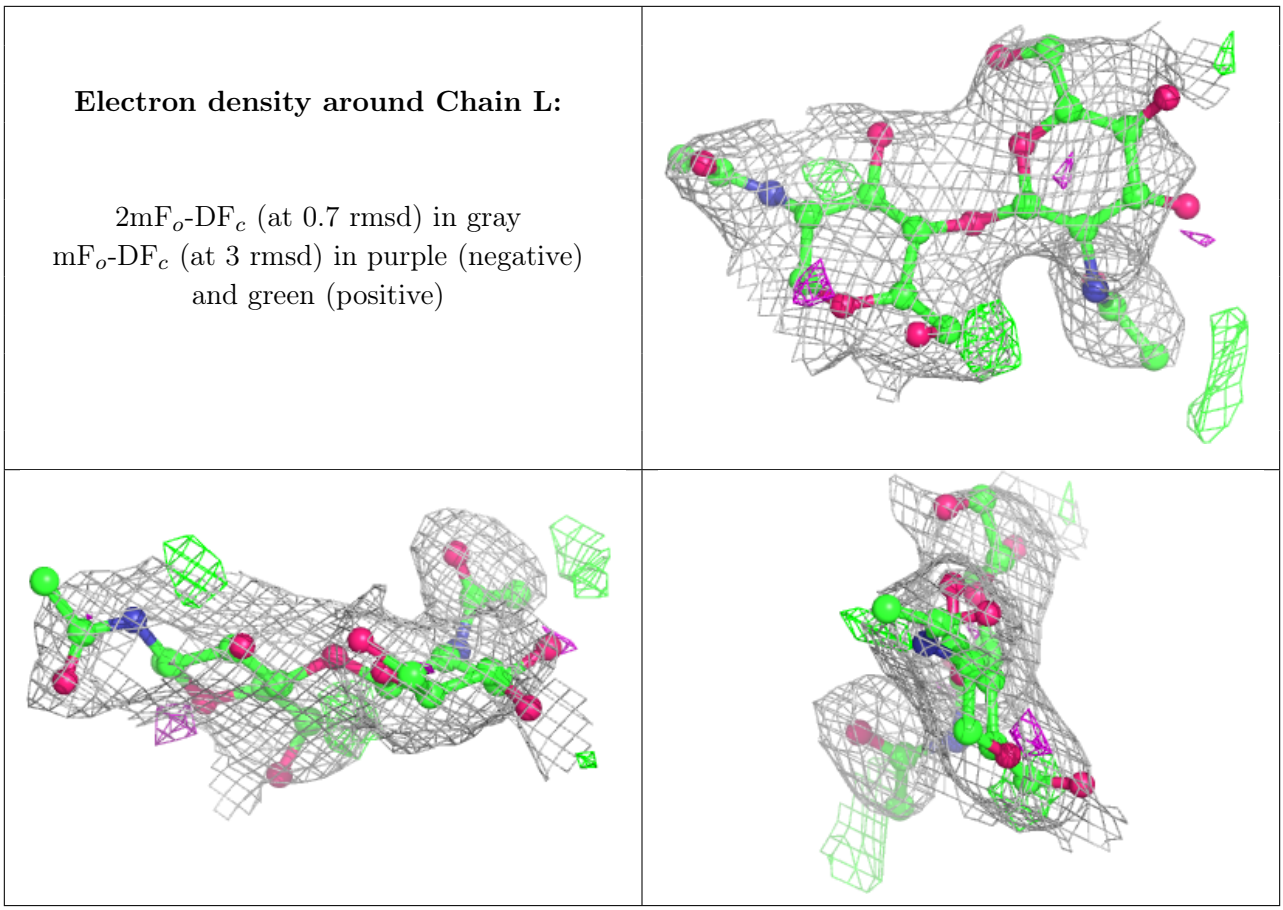






Electron density around Chain L:

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



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	A	402	14/15	0.76	0.27	58,70,78,80	0
5	NAG	A	401	14/15	0.82	0.25	57,63,72,74	0
5	NAG	E	401	14/15	0.82	0.28	59,68,77,77	0
5	NAG	C	401	14/15	0.83	0.20	47,55,58,59	0

6.5 Other polymers

There are no such residues in this entry.