Full wwPDB X-ray Structure Validation Report ⓘ

Aug 9, 2020 – 08:54 AM BST

PDB ID	:	6FYU
Title	:	Structure of H7(A/Shanghai/2/2013) Influenza Hemagglutinin in complex SD36
Authors	:	Laursen, N.S.; Wilson, I.A.
Deposited on	:	2018-03-12
Resolution	:	2.64 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:

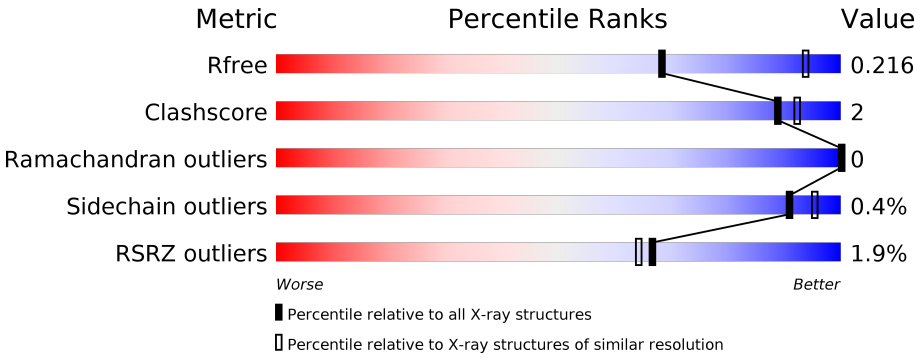
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.13.1
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (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 2.64 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	1426 (2.66-2.62)
Clashscore	141614	1472 (2.66-2.62)
Ramachandran outliers	138981	1446 (2.66-2.62)
Sidechain outliers	138945	1446 (2.66-2.62)
RSRZ outliers	127900	1408 (2.66-2.62)

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	321	94% 5%
1	D	321	4% 92% 7%
1	G	321	2% 91% 8%
2	B	183	% 91% 6%
2	E	183	2% 89% 8%
2	H	183	2% 88% 8%

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Mol	Chain	Length	Quality of chain
3	C	122	95% 5%
3	F	122	94% 6%
3	I	122	2% 96%
4	J	2	100%
4	K	2	50% 50%
4	L	2	100%

2 Entry composition

There are 7 unique types of molecules in this entry. The entry contains 14796 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.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	319	Total	C	N	O	S	0	0	0
			2436	1515	440	466	15			
1	D	318	Total	C	N	O	S	0	0	0
			2427	1509	438	465	15			
1	G	318	Total	C	N	O	S	0	0	0
			2427	1509	438	465	15			

- Molecule 2 is a protein called Hemagglutinin.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	172	Total	C	N	O	S	0	0	0
			1396	862	244	283	7			
2	E	168	Total	C	N	O	S	0	0	0
			1369	843	240	279	7			
2	H	168	Total	C	N	O	S	0	0	0
			1364	840	239	278	7			

There are 21 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	177	SER	-	expression tag	UNP A0A0C4ZTH5
B	178	GLY	-	expression tag	UNP A0A0C4ZTH5
B	179	ARG	-	expression tag	UNP A0A0C4ZTH5
B	180	LEU	-	expression tag	UNP A0A0C4ZTH5
B	181	VAL	-	expression tag	UNP A0A0C4ZTH5
B	182	PRO	-	expression tag	UNP A0A0C4ZTH5
B	183	ARG	-	expression tag	UNP A0A0C4ZTH5
E	177	SER	-	expression tag	UNP A0A0C4ZTH5
E	178	GLY	-	expression tag	UNP A0A0C4ZTH5
E	179	ARG	-	expression tag	UNP A0A0C4ZTH5
E	180	LEU	-	expression tag	UNP A0A0C4ZTH5
E	181	VAL	-	expression tag	UNP A0A0C4ZTH5

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Chain	Residue	Modelled	Actual	Comment	Reference
E	182	PRO	-	expression tag	UNP A0A0C4ZTH5
E	183	ARG	-	expression tag	UNP A0A0C4ZTH5
H	177	SER	-	expression tag	UNP A0A0C4ZTH5
H	178	GLY	-	expression tag	UNP A0A0C4ZTH5
H	179	ARG	-	expression tag	UNP A0A0C4ZTH5
H	180	LEU	-	expression tag	UNP A0A0C4ZTH5
H	181	VAL	-	expression tag	UNP A0A0C4ZTH5
H	182	PRO	-	expression tag	UNP A0A0C4ZTH5
H	183	ARG	-	expression tag	UNP A0A0C4ZTH5

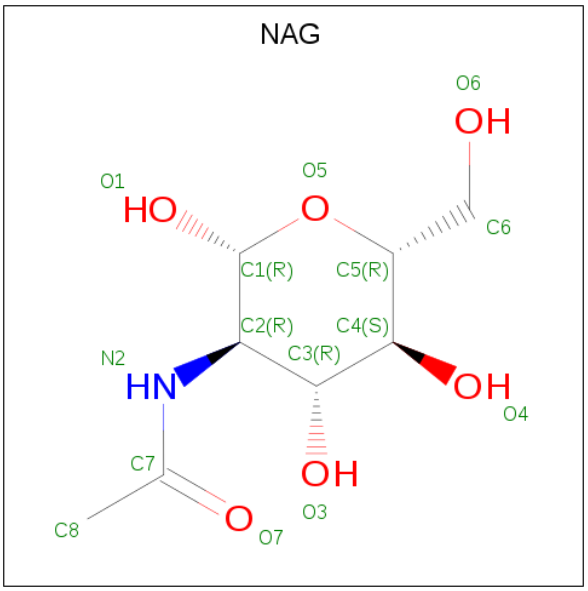
- Molecule 3 is a protein called Single domain antibody SD36.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	C	122	Total	C	N	O	S	0	0	0
			939	588	165	182	4			
3	F	122	Total	C	N	O	S	0	0	0
			939	588	165	182	4			
3	I	121	Total	C	N	O	S	0	0	0
			930	583	164	179	4			

- 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	J	2	Total	C	N	O	0	0	0
			28	16	2	10			
4	K	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	B	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	D	1	Total C N O 14 8 1 5	0	0
5	E	1	Total C N O 14 8 1 5	0	0
5	E	1	Total C N O 14 8 1 5	0	0
5	G	1	Total C N O 14 8 1 5	0	0
5	G	1	Total C N O 14 8 1 5	0	0
5	H	1	Total C N O 14 8 1 5	0	0
5	H	1	Total C N O 14 8 1 5	0	0

- Molecule 6 is SODIUM ION (three-letter code: NA) (formula: Na).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	G	2	Total Na 2 2	0	0
6	D	1	Total Na 1 1	0	0
6	E	1	Total Na 1 1	0	0

- Molecule 7 is water.

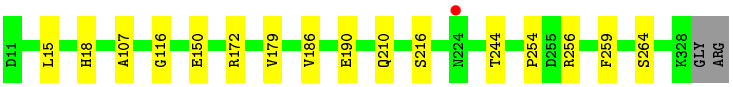
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
7	A	103	Total O 103 103	0	0
7	B	51	Total O 51 51	0	0
7	C	28	Total O 28 28	0	0
7	D	37	Total O 37 37	0	0
7	E	28	Total O 28 28	0	0
7	F	35	Total O 35 35	0	0
7	G	42	Total O 42 42	0	0
7	H	26	Total O 26 26	0	0
7	I	5	Total O 5 5	0	0

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.

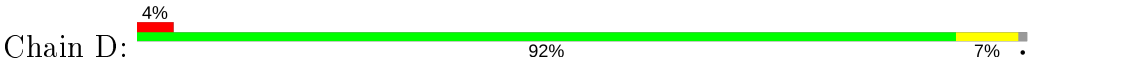
- Molecule 1: Hemagglutinin

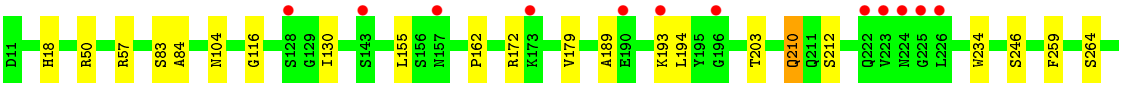
Chain A:

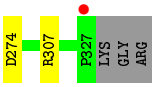


- Molecule 1: Hemagglutinin

Chain D:

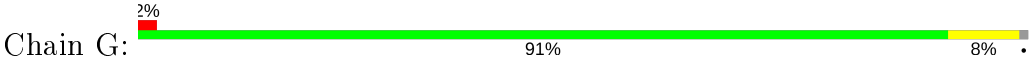


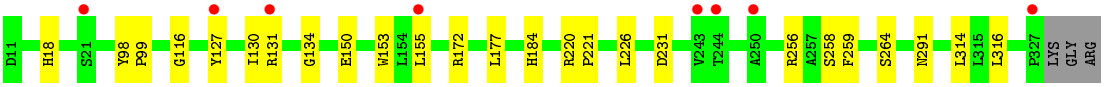




- Molecule 1: Hemagglutinin

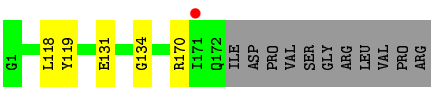
Chain G:





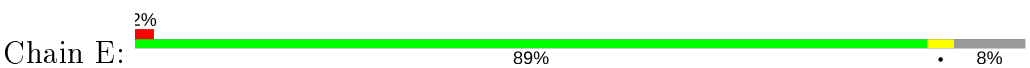
- Molecule 2: Hemagglutinin

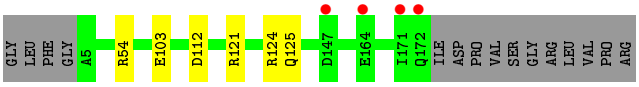
Chain B:



- Molecule 2: Hemagglutinin

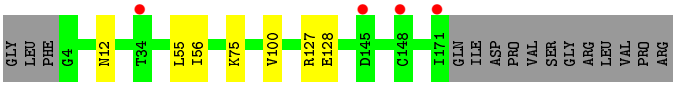
Chain E:





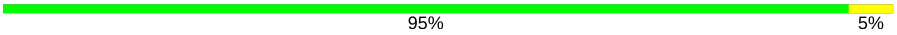
• Molecule 2: Hemagglutinin

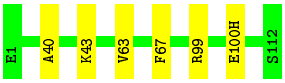
Chain H:



• Molecule 3: Single domain antibody SD36

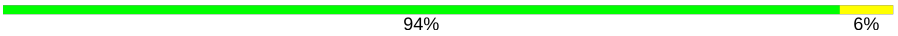
Chain C:





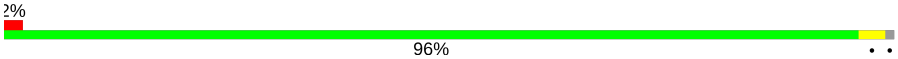
• Molecule 3: Single domain antibody SD36

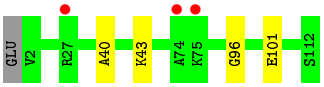
Chain F:



• Molecule 3: Single domain antibody SD36

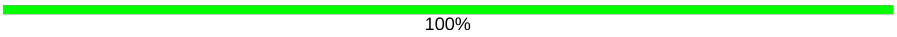
Chain I:





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

Chain J:

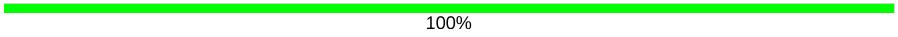


• Molecule 4: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain K:

• 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 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	101.42Å 128.16Å 192.10Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	48.03 – 2.64 48.03 – 2.64	Depositor EDS
% Data completeness (in resolution range)	99.4 (48.03-2.64) 99.4 (48.03-2.64)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.14	Depositor
$< I/\sigma(I) >$ [1]	2.75 (at 2.65Å)	Xtriage
Refinement program	PHENIX dev_1839	Depositor
R, R_{free}	0.186 , 0.216 0.187 , 0.216	Depositor DCC
R_{free} test set	2000 reflections (2.72%)	wwPDB-VP
Wilson B-factor (Å^2)	46.4	Xtriage
Anisotropy	0.164	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.31 , 37.5	EDS
L-test for twinning[2]	$< \|L\| > = 0.48$, $< L^2 > = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.94	EDS
Total number of atoms	14796	wwPDB-VP
Average B, all atoms (Å^2)	53.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.51% 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: NA, NAG

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#$\|Z\|>5$	RMSZ	#$\|Z\|>5$
1	A	0.22	0/2483	0.43	0/3356
1	D	0.23	0/2474	0.43	0/3345
1	G	0.22	0/2474	0.42	0/3345
2	B	0.22	0/1420	0.41	0/1913
2	E	0.22	0/1392	0.42	1/1876 (0.1%)
2	H	0.22	0/1387	0.40	0/1869
3	C	0.23	0/959	0.41	0/1299
3	F	0.23	0/959	0.42	0/1299
3	I	0.22	0/950	0.39	0/1287
All	All	0.22	0/14498	0.42	1/19589 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	E	112	ASP	CB-CG-OD2	5.18	122.97	118.30

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	2436	0	2400	11	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	D	2427	0	2387	15	0
1	G	2427	0	2387	16	0
2	B	1396	0	1298	4	0
2	E	1369	0	1269	3	0
2	H	1364	0	1264	5	0
3	C	939	0	899	4	0
3	F	939	0	899	4	0
3	I	930	0	890	2	0
4	J	28	0	25	0	0
4	K	28	0	25	1	0
4	L	28	0	25	0	0
5	B	28	0	26	0	0
5	D	14	0	13	0	0
5	E	28	0	26	0	0
5	G	28	0	26	0	0
5	H	28	0	26	0	0
6	D	1	0	0	0	0
6	E	1	0	0	0	0
6	G	2	0	0	0	0
7	A	103	0	0	0	0
7	B	51	0	0	0	0
7	C	28	0	0	0	0
7	D	37	0	0	1	0
7	E	28	0	0	0	0
7	F	35	0	0	1	0
7	G	42	0	0	0	0
7	H	26	0	0	0	0
7	I	5	0	0	0	0
All	All	14796	0	13885	54	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 2.

All (54) 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)
3:I:96:GLY:N	3:I:101:GLU:OE2	2.06	0.89
1:D:130:ILE:HD11	1:D:162:PRO:HD2	1.65	0.77
3:C:40:ALA:HB3	3:C:43:LYS:HD2	1.66	0.75
3:I:40:ALA:HB3	3:I:43:LYS:HD2	1.68	0.74
1:G:150:GLU:OE2	1:G:256:ARG:HD3	1.97	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:15:LEU:HD13	2:B:119:TYR:HA	1.82	0.62
1:A:244:THR:HB	1:G:221:PRO:HD3	1.82	0.61
1:A:116:GLY:HA2	1:A:264:SER:HB3	1.82	0.61
3:C:99:ARG:NH2	3:C:100(H):GLU:O	2.38	0.57
3:F:63:VAL:HG13	3:F:67:PHE:HB2	1.87	0.56
1:D:57:ARG:HH12	1:D:84:ALA:N	2.06	0.54
1:G:127:TYR:HB3	1:G:130:ILE:HD11	1.91	0.53
1:A:186:VAL:HG12	1:A:190:GLU:OE1	2.10	0.52
1:D:172:ARG:HD3	1:D:259:PHE:CZ	2.45	0.52
1:G:131:ARG:HB2	1:G:155:LEU:HB2	1.93	0.51
1:D:307:ARG:NH2	7:D:606:HOH:O	2.43	0.50
1:G:316:LEU:HD22	2:H:55:LEU:HD22	1.93	0.50
1:G:116:GLY:HA2	1:G:264:SER:HB3	1.94	0.49
2:E:121:ARG:O	2:E:125:GLN:HG3	2.13	0.48
3:F:56:ARG:NH1	7:F:202:HOH:O	2.40	0.48
1:D:203:THR:OG1	1:D:246:SER:HB2	2.14	0.48
1:A:150:GLU:OE1	1:A:256:ARG:HD3	2.13	0.47
1:G:98:TYR:CD1	1:G:226:LEU:HD13	2.50	0.47
1:A:15:LEU:HD22	2:B:118:LEU:HG	1.96	0.47
1:A:210:GLN:NE2	1:G:231:ASP:OD1	2.47	0.47
3:C:99:ARG:HD2	4:K:1:NAG:H61	1.97	0.47
1:D:155:LEU:HD22	1:D:194:LEU:HD22	1.96	0.46
2:B:131:GLU:OE2	2:B:170:ARG:HD2	2.15	0.46
1:G:314:LEU:HB3	2:H:100:VAL:HG21	1.98	0.46
1:G:177:LEU:HB3	1:G:258:SER:HB2	1.98	0.46
1:D:50:ARG:NE	1:D:274:ASP:OD2	2.48	0.46
1:A:172:ARG:HD3	1:A:259:PHE:CZ	2.51	0.45
1:G:291:ASN:HB3	2:H:56:ILE:HG23	1.99	0.45
1:D:57:ARG:NH1	1:D:83:SER:HB3	2.32	0.44
1:G:134:GLY:HA3	1:G:153:TRP:HB3	2.00	0.44
1:D:57:ARG:NH1	1:D:84:ALA:N	2.65	0.44
1:G:150:GLU:OE2	1:G:256:ARG:HB2	2.18	0.43
1:A:107:ALA:HB1	2:H:75:LYS:HB3	2.00	0.43
3:C:63:VAL:HG13	3:C:67:PHE:HB2	2.01	0.42
1:D:130:ILE:HD11	1:D:162:PRO:CD	2.45	0.42
1:D:210:GLN:O	1:D:210:GLN:HG2	2.20	0.42
1:D:179:VAL:HG22	1:D:234:TRP:HB3	2.00	0.42
1:G:172:ARG:HD2	1:G:259:PHE:CZ	2.55	0.42
2:E:54:ARG:NH2	2:E:103:GLU:OE2	2.42	0.42
1:D:116:GLY:HA2	1:D:264:SER:HB3	2.01	0.41
1:G:98:TYR:HA	1:G:99:PRO:HD3	1.94	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:179:VAL:O	1:A:254:PRO:HB3	2.20	0.41
1:G:184:HIS:HB3	1:G:220:ARG:HH12	1.85	0.41
1:D:189:ALA:O	1:D:193:LYS:HG3	2.21	0.41
3:F:22:CYS:HB3	3:F:78:GLU:HB3	2.03	0.41
1:A:216:SER:HB2	1:D:212:SER:OG	2.20	0.40
2:B:134:GLY:HA2	2:E:124:ARG:HD3	2.02	0.40
2:H:127:ARG:HB3	2:H:128:GLU:H	1.64	0.40
3:F:40:ALA:HB3	3:F:43:LYS:HD2	2.03	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	317/321 (99%)	311 (98%)	6 (2%)	0	100	100
1	D	316/321 (98%)	308 (98%)	8 (2%)	0	100	100
1	G	316/321 (98%)	309 (98%)	7 (2%)	0	100	100
2	B	170/183 (93%)	165 (97%)	5 (3%)	0	100	100
2	E	166/183 (91%)	164 (99%)	2 (1%)	0	100	100
2	H	166/183 (91%)	162 (98%)	4 (2%)	0	100	100
3	C	120/122 (98%)	119 (99%)	1 (1%)	0	100	100
3	F	120/122 (98%)	119 (99%)	1 (1%)	0	100	100
3	I	119/122 (98%)	118 (99%)	1 (1%)	0	100	100
All	All	1810/1878 (96%)	1775 (98%)	35 (2%)	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	268/269 (100%)	267 (100%)	1 (0%)	91 95
1	D	267/269 (99%)	264 (99%)	3 (1%)	73 85
1	G	267/269 (99%)	266 (100%)	1 (0%)	91 95
2	B	147/157 (94%)	147 (100%)	0	100 100
2	E	145/157 (92%)	145 (100%)	0	100 100
2	H	144/157 (92%)	143 (99%)	1 (1%)	84 91
3	C	94/94 (100%)	94 (100%)	0	100 100
3	F	94/94 (100%)	94 (100%)	0	100 100
3	I	93/94 (99%)	93 (100%)	0	100 100
All	All	1519/1560 (97%)	1513 (100%)	6 (0%)	91 95

All (6) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	18	HIS
1	D	18	HIS
1	D	104	ASN
1	D	210	GLN
1	G	18	HIS
2	H	12	ASN

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (1) such sidechains are listed below:

Mol	Chain	Res	Type
1	D	210	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)

6 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	$\#\|Z\|>2$
4	NAG	J	1	1,4	14,14,15	0.37	0	17,19,21	0.46	0
4	NAG	J	2	4	14,14,15	0.27	0	17,19,21	0.39	0
4	NAG	K	1	1,4	14,14,15	0.38	0	17,19,21	0.42	0
4	NAG	K	2	4	14,14,15	0.33	0	17,19,21	0.41	0
4	NAG	L	1	1,4	14,14,15	0.34	0	17,19,21	0.41	0
4	NAG	L	2	4	14,14,15	0.23	0	17,19,21	0.36	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
4	NAG	J	1	1,4	-	2/6/23/26	0/1/1/1
4	NAG	J	2	4	-	2/6/23/26	0/1/1/1
4	NAG	K	1	1,4	-	2/6/23/26	0/1/1/1
4	NAG	K	2	4	-	0/6/23/26	0/1/1/1
4	NAG	L	1	1,4	-	2/6/23/26	0/1/1/1
4	NAG	L	2	4	-	1/6/23/26	0/1/1/1

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (9) torsion outliers are listed below:

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

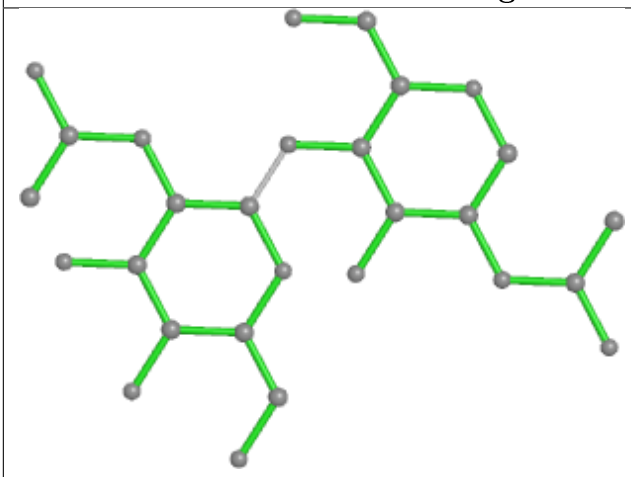
There are no ring outliers.

1 monomer is involved in 1 short contact:

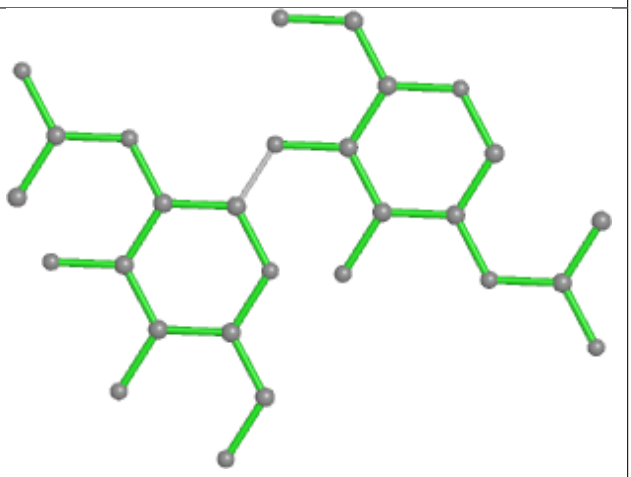
Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	K	1	NAG	1	0

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

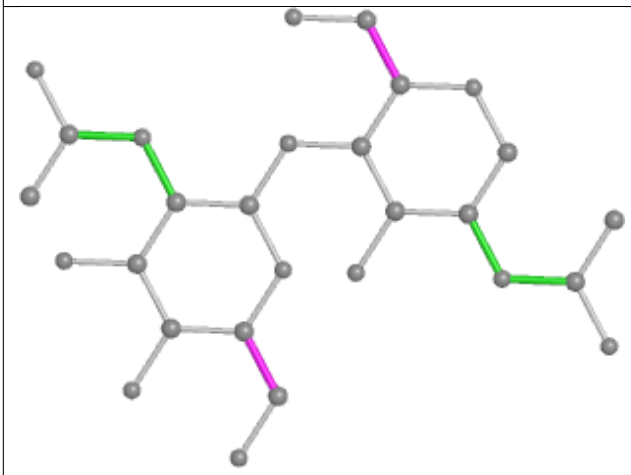
Oligosaccharide Chain J



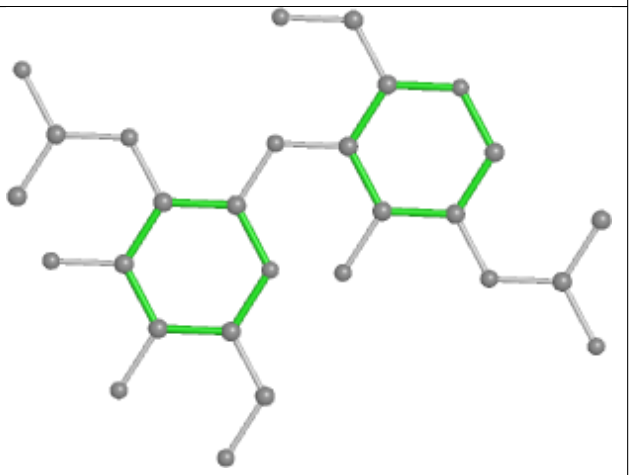
Bond lengths



Bond angles

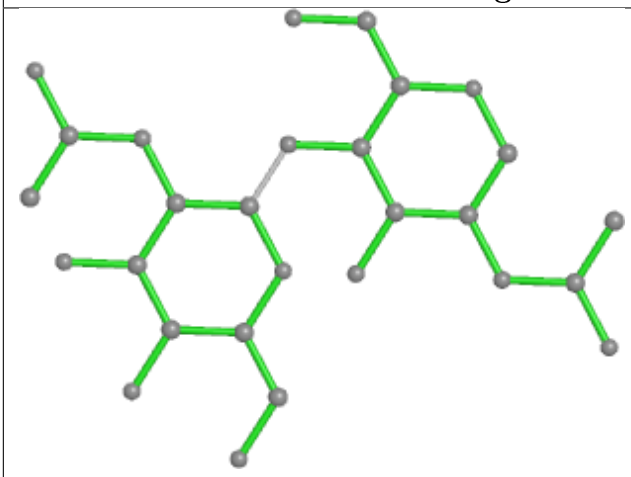


Torsions

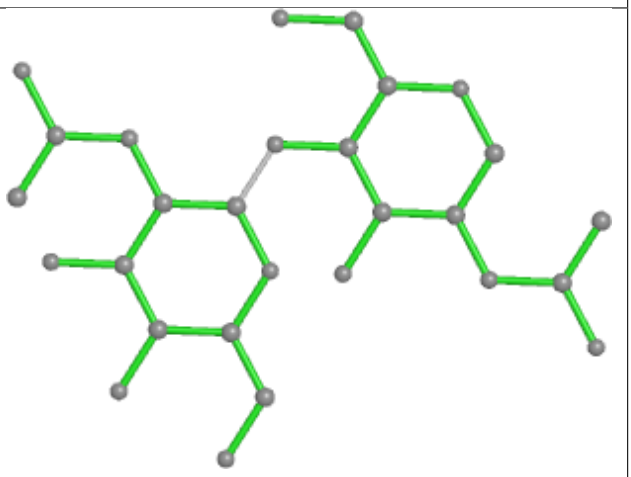


Rings

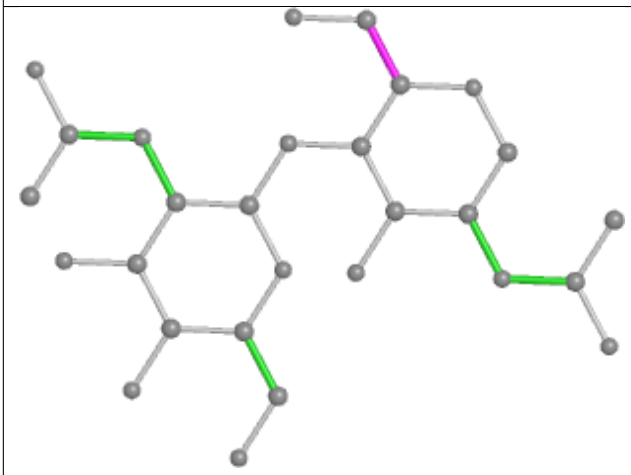
Oligosaccharide Chain K



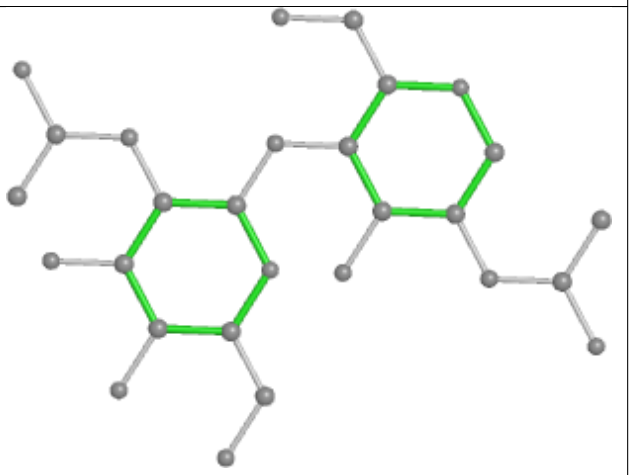
Bond lengths



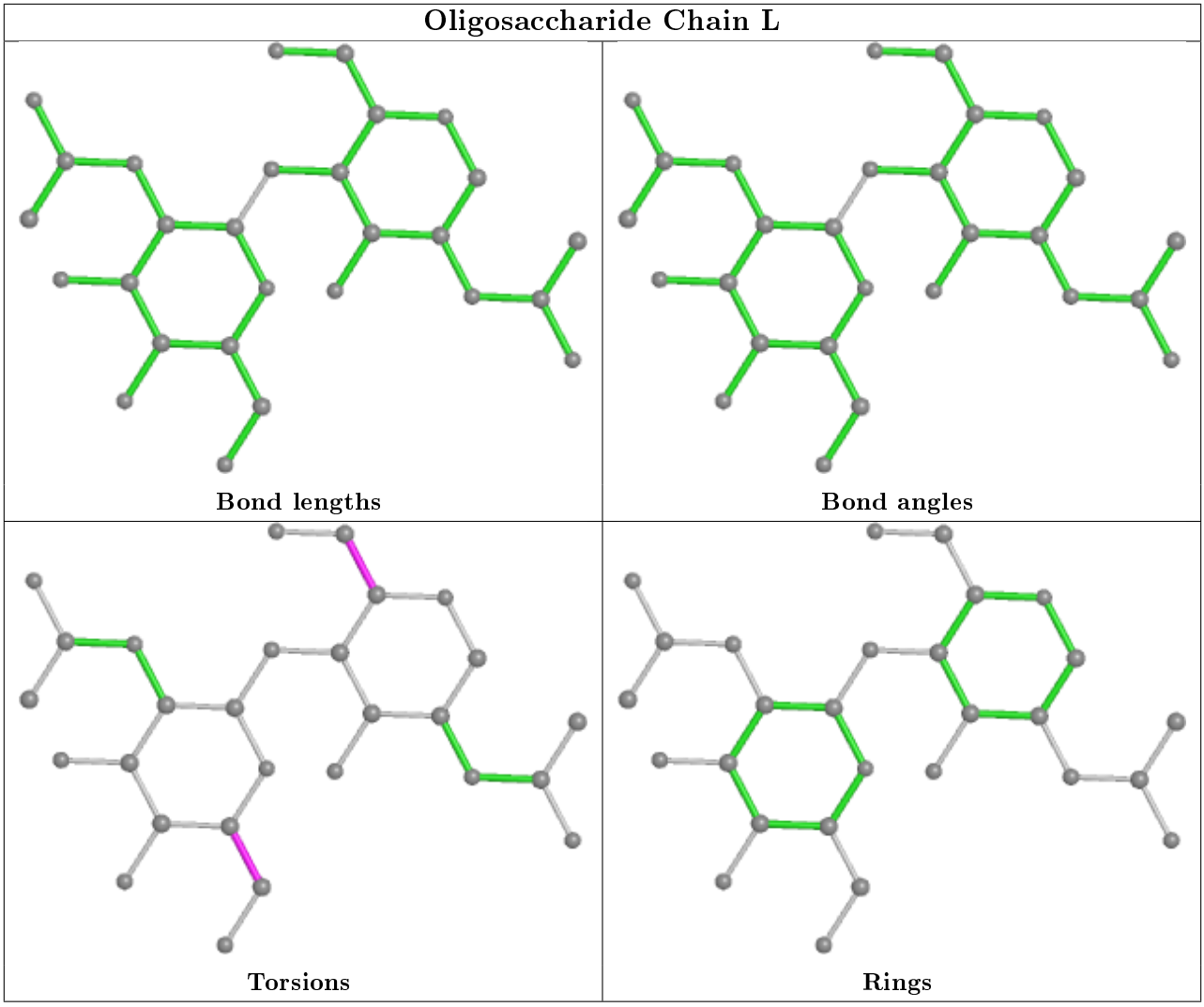
Bond angles



Torsions



Rings



5.6 Ligand geometry

Of 13 ligands modelled in this entry, 4 are monoatomic - leaving 9 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
5	NAG	H	500	2	14,14,15	0.40	0	17,19,21	0.49	0
5	NAG	G	402	1	14,14,15	0.26	0	17,19,21	0.38	0
5	NAG	H	501	2	14,14,15	0.27	0	17,19,21	0.46	0
5	NAG	E	201	2	14,14,15	0.34	0	17,19,21	0.52	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
5	NAG	D	500	1	14,14,15	0.49	0	17,19,21	0.86	1 (5%)
5	NAG	E	202	2	14,14,15	0.31	0	17,19,21	0.36	0
5	NAG	G	401	1	14,14,15	0.34	0	17,19,21	0.51	0
5	NAG	B	500	2	14,14,15	0.38	0	17,19,21	0.52	0
5	NAG	B	501	2	14,14,15	0.23	0	17,19,21	0.42	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
5	NAG	H	500	2	-	2/6/23/26	0/1/1/1
5	NAG	G	402	1	-	2/6/23/26	0/1/1/1
5	NAG	H	501	2	-	0/6/23/26	0/1/1/1
5	NAG	E	201	2	-	2/6/23/26	0/1/1/1
5	NAG	D	500	1	-	1/6/23/26	0/1/1/1
5	NAG	E	202	2	-	0/6/23/26	0/1/1/1
5	NAG	G	401	1	-	2/6/23/26	0/1/1/1
5	NAG	B	500	2	-	2/6/23/26	0/1/1/1
5	NAG	B	501	2	-	0/6/23/26	0/1/1/1

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
5	D	500	NAG	C1-O5-C5	2.12	115.06	112.19

There are no chirality outliers.

All (11) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	G	402	NAG	O5-C5-C6-O6
5	G	402	NAG	C4-C5-C6-O6
5	E	201	NAG	O5-C5-C6-O6
5	E	201	NAG	C4-C5-C6-O6
5	H	500	NAG	O5-C5-C6-O6
5	H	500	NAG	C4-C5-C6-O6
5	D	500	NAG	C1-C2-N2-C7
5	G	401	NAG	C4-C5-C6-O6

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Mol	Chain	Res	Type	Atoms
5	G	401	NAG	O5-C5-C6-O6
5	B	500	NAG	C4-C5-C6-O6
5	B	500	NAG	O5-C5-C6-O6

There are no ring outliers.

No monomer is involved in short contacts.

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	319/321 (99%)	-0.31	1 (0%) 94 95	22, 35, 58, 80	2 (0%)
1	D	318/321 (99%)	0.07	13 (4%) 37 33	25, 62, 93, 113	2 (0%)
1	G	318/321 (99%)	-0.05	8 (2%) 57 53	24, 58, 100, 117	1 (0%)
2	B	172/183 (93%)	-0.13	1 (0%) 89 88	24, 44, 76, 101	0
2	E	168/183 (91%)	-0.08	4 (2%) 59 55	26, 50, 77, 108	0
2	H	168/183 (91%)	0.08	4 (2%) 59 55	23, 56, 87, 95	0
3	C	122/122 (100%)	-0.23	0 100 100	24, 43, 68, 84	0
3	F	122/122 (100%)	-0.28	0 100 100	28, 44, 71, 86	0
3	I	121/122 (99%)	0.05	3 (2%) 57 53	36, 65, 88, 96	0
All	All	1828/1878 (97%)	-0.09	34 (1%) 66 64	22, 50, 88, 117	5 (0%)

All (34) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	190	GLU	5.0
1	D	224	ASN	3.9
1	G	155	LEU	3.8
3	I	74	ALA	3.5
2	E	164	GLU	3.1
2	H	34	THR	3.0
1	D	226	LEU	2.8
1	G	243	VAL	2.6
1	G	327	PRO	2.6
1	D	143	SER	2.6
1	D	173	LYS	2.5
3	I	75	LYS	2.5
1	D	327	PRO	2.5
1	D	222	GLN	2.4
2	E	172	GLN	2.4

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Mol	Chain	Res	Type	RSRZ
1	D	223	VAL	2.4
2	H	171	ILE	2.3
1	D	196	GLY	2.2
2	H	148	CYS	2.2
1	D	128	SER	2.2
1	G	127	TYR	2.2
3	I	27	ARG	2.2
1	D	193	LYS	2.2
1	D	157	ASN	2.2
2	B	171	ILE	2.1
1	G	250	ALA	2.1
1	G	244	THR	2.1
2	E	147	ASP	2.1
1	G	21	SER	2.1
1	A	224	ASN	2.1
2	H	145	ASP	2.1
2	E	171	ILE	2.0
1	D	225	GLY	2.0
1	G	131	ARG	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)

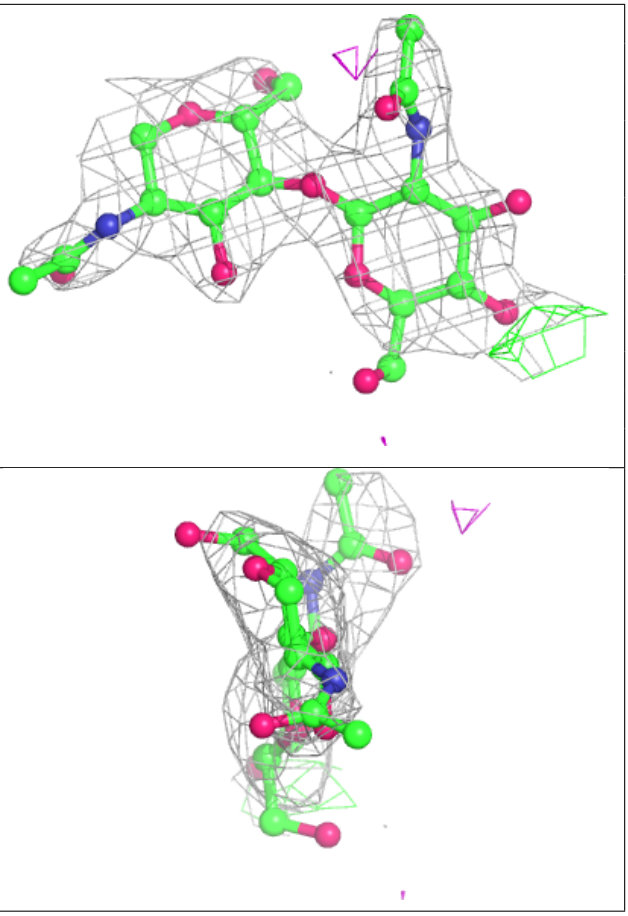
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9'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

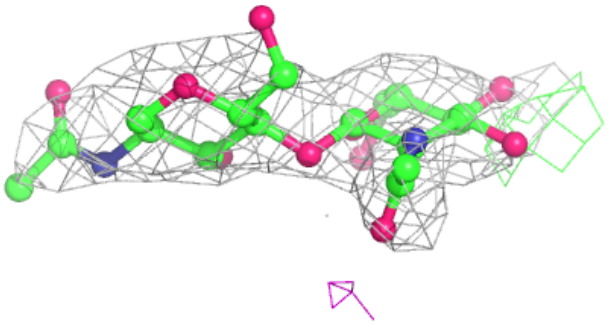
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
4	NAG	L	2	14/15	0.81	0.42	109,116,119,119	0
4	NAG	K	2	14/15	0.82	0.29	94,99,102,102	0
4	NAG	J	2	14/15	0.82	0.35	94,108,116,118	0
4	NAG	L	1	14/15	0.86	0.33	77,94,103,106	0
4	NAG	K	1	14/15	0.88	0.15	66,76,84,90	0
4	NAG	J	1	14/15	0.92	0.32	87,94,99,99	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 J:

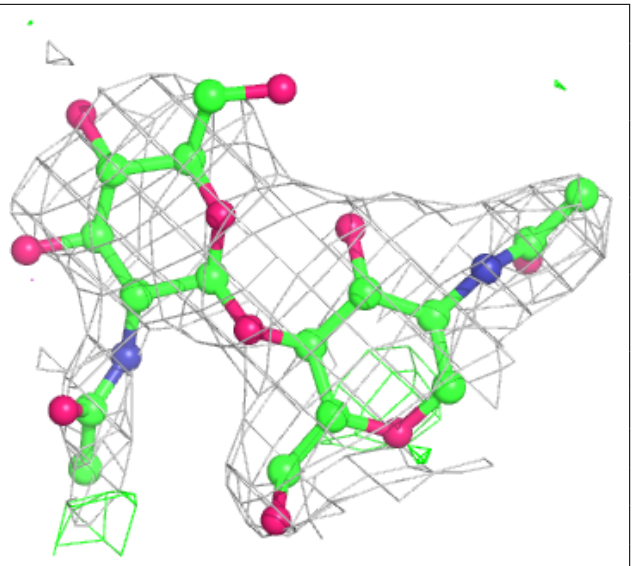
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

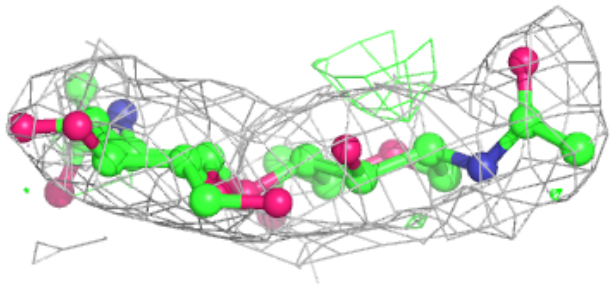


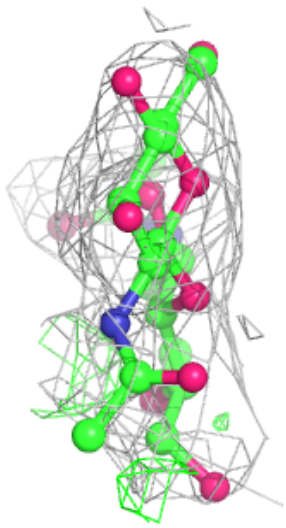


Electron density around Chain K:

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

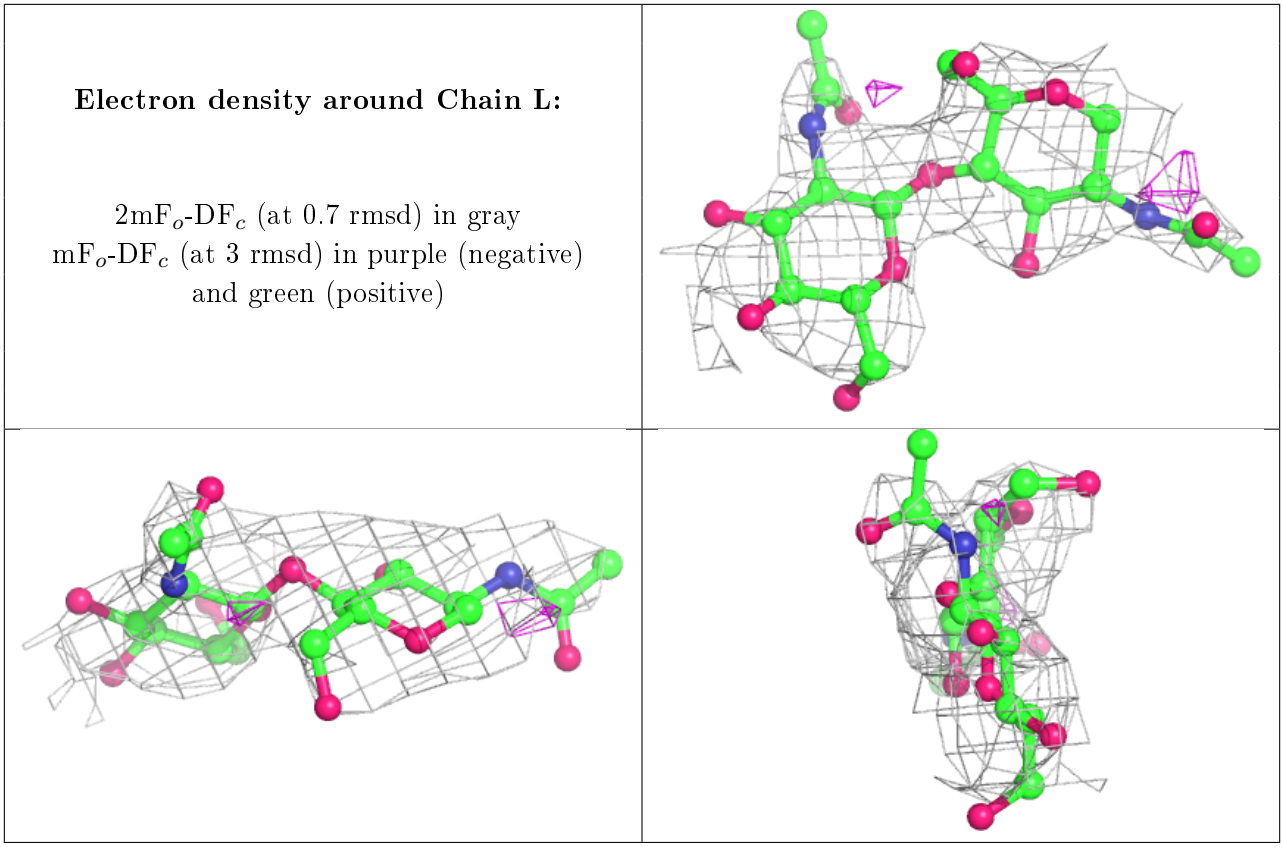






Electron density around Chain L:

$2mF_o$-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	E	201	14/15	0.73	0.30	70,79,92,94	0
5	NAG	H	500	14/15	0.78	0.33	71,79,89,91	0
5	NAG	D	500	14/15	0.79	0.26	82,97,107,108	0
5	NAG	G	401	14/15	0.79	0.36	76,88,97,98	0
5	NAG	B	501	14/15	0.80	0.27	74,86,92,94	0
5	NAG	H	501	14/15	0.82	0.26	77,86,94,95	0
5	NAG	G	402	14/15	0.84	0.33	86,99,106,106	0
5	NAG	E	202	14/15	0.86	0.31	68,79,83,84	0
6	NA	G	404	1/1	0.88	0.16	62,62,62,62	0
5	NAG	B	500	14/15	0.89	0.24	58,74,84,84	0
6	NA	G	403	1/1	0.94	0.14	65,65,65,65	0
6	NA	D	503	1/1	0.96	0.13	66,66,66,66	0
6	NA	E	203	1/1	0.98	0.25	51,51,51,51	0

6.5 Other polymers (i)

There are no such residues in this entry.