Full wwPDB X-ray Structure Validation Report (i)

Sep 4, 2023 – 08:51 PM EDT

PDB ID	:	3U7Y
Title	:	Structure of NIH45-46 Fab in complex with gp120 of 93TH057 HIV
Authors	:	Diskin, R.; Bjorkman, P.J.
Deposited on	:	2011-10-14
Resolution	:	2.45 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 (i) 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 (i)) were used in the production of this report:

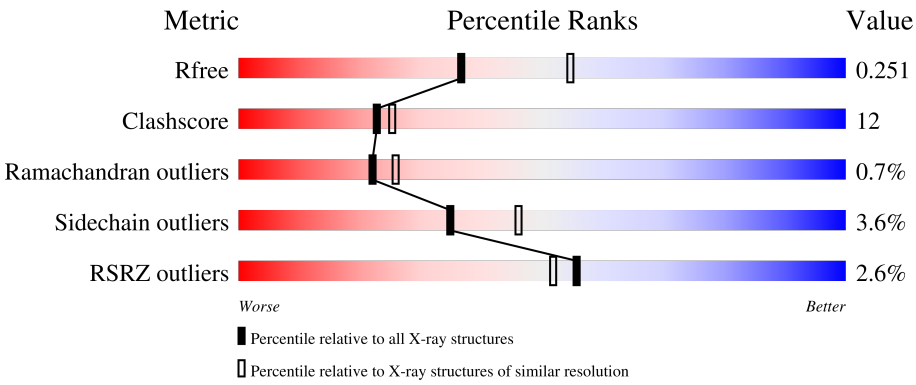
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.35
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.35

1 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 2.45 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	1564 (2.46-2.42)
Clashscore	141614	1631 (2.46-2.42)
Ramachandran outliers	138981	1617 (2.46-2.42)
Sidechain outliers	138945	1617 (2.46-2.42)
RSRZ outliers	127900	1547 (2.46-2.42)

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	H	229	% 76% 19% • •
2	G	361	4% 68% 23% • 6%
3	L	210	78% 20% • •
4	A	4	50% 50%

2 Entry composition (i)

There are 8 unique types of molecules in this entry. The entry contains 6204 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 NIH45-46 heavy chain, Ig gamma-1 chain C region.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	H	222	1718	1084	303	321	10	0	1	0

- Molecule 2 is a protein called Envelope glycoprotein gp160.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
2	G	340	2669	1674	463	508	24	0	1	0

There are 18 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
G	65	CYS	VAL	engineered mutation	UNP Q0ED31
G	115	CYS	SER	engineered mutation	UNP Q0ED31
G	124	GLY	-	linker	UNP Q0ED31
G	198	GLY	-	linker	UNP Q0ED31
G	318	GLY	-	linker	UNP Q0ED31
G	319	GLY	-	linker	UNP Q0ED31
G	320	SER	-	linker	UNP Q0ED31
G	321	GLY	-	linker	UNP Q0ED31
G	322	SER	-	linker	UNP Q0ED31
G	323	GLY	-	linker	UNP Q0ED31
G	493	GLY	-	expression tag	UNP Q0ED31
G	494	SER	-	expression tag	UNP Q0ED31
G	495	HIS	-	expression tag	UNP Q0ED31
G	496	HIS	-	expression tag	UNP Q0ED31
G	497	HIS	-	expression tag	UNP Q0ED31
G	498	HIS	-	expression tag	UNP Q0ED31
G	499	HIS	-	expression tag	UNP Q0ED31
G	500	HIS	-	expression tag	UNP Q0ED31

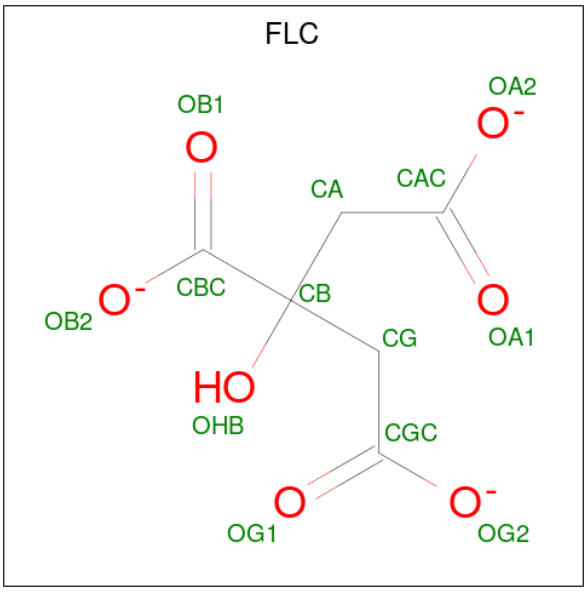
- Molecule 3 is a protein called NIH45-46 light chain, Ig kappa chain C region.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
3	L	208	1602	1000	274	323	5	0	0	0

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

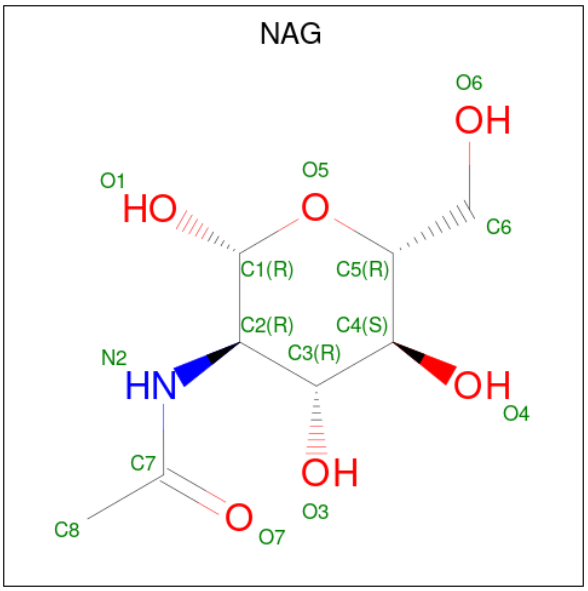
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
			Total	C	N	O			
4	A	4	50	28	2	20	0	0	0

- Molecule 5 is CITRATE ANION (three-letter code: FLC) (formula: $C_6H_5O_7$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	C	O		
5	H	1	13	6	7	0	0

- Molecule 6 is 2-acetamido-2-deoxy-beta-D-glucopyranose (three-letter code: NAG) (formula: $C_8H_{15}NO_6$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	C	N	O		
6	G	1	14	8	1	5	0	0
			Total	C	N	O		
6	G	1	14	8	1	5	0	0
			Total	C	N	O		
6	G	1	14	8	1	5	0	0
			Total	C	N	O		
6	G	1	14	8	1	5	0	0
			Total	C	N	O		
6	G	1	14	8	1	5	0	0
			Total	C	N	O		
6	L	1	14	8	1	5	0	0

- Molecule 7 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	Cl		
7	G	1	1	1	0	0

- Molecule 8 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
8	H	25	25	25	0	0
			Total	O		
8	G	29	29	29	0	0

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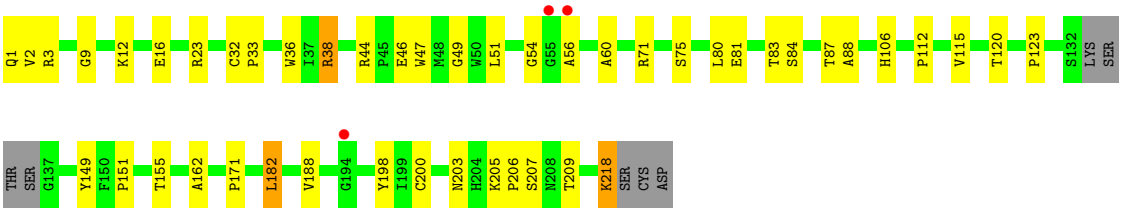
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
8	L	13	13	13	0	0

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.

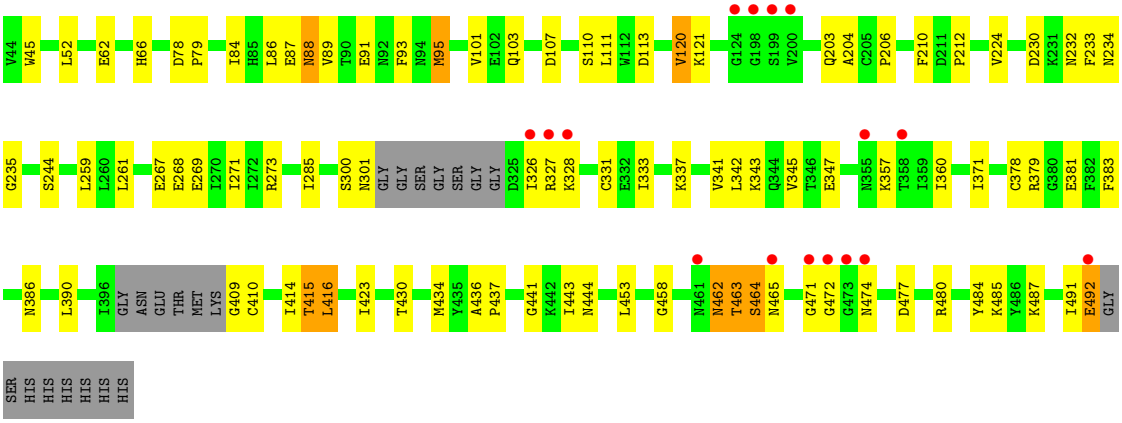
• Molecule 1: NIH45-46 heavy chain, Ig gamma-1 chain C region

Chain H:



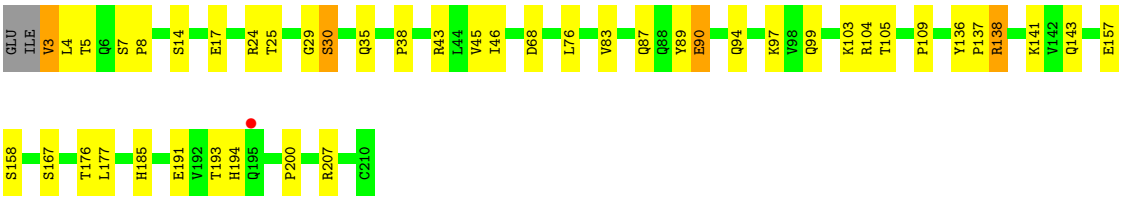
• Molecule 2: Envelope glycoprotein gp160

Chain G:



• Molecule 3: NIH45-46 light chain, Ig kappa chain C region

Chain L:



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

Chain A:

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	69.13Å 70.50Å 217.74Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	37.05 – 2.45 37.05 – 2.45	Depositor EDS
% Data completeness (in resolution range)	97.1 (37.05-2.45) 89.6 (37.05-2.45)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	3.32 (at 2.45Å)	Xtriage
Refinement program	PHENIX (phenix.refine: dev_805)	Depositor
R, R_{free}	0.207 , 0.256 0.200 , 0.251	Depositor DCC
R_{free} test set	2116 reflections (5.42%)	wwPDB-VP
Wilson B-factor (Å^2)	57.1	Xtriage
Anisotropy	0.704	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.28 , 43.8	EDS
L-test for twinning[2]	$< \|L\| > = 0.47$, $< L^2 > = 0.31$	Xtriage
Estimated twinning fraction	0.036 for k,h,-l	Xtriage
F_o,F_c correlation	0.95	EDS
Total number of atoms	6204	wwPDB-VP
Average B, all atoms (Å^2)	80.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.76% 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 (i)

5.1 Standard geometry (i)

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

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	H	0.26	0/1760	0.46	0/2393
2	G	0.25	0/2728	0.43	0/3703
3	L	0.25	0/1637	0.42	0/2221
All	All	0.25	0/6125	0.44	0/8317

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts (i)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	H	1718	0	1676	34	0
2	G	2669	0	2599	79	0
3	L	1602	0	1539	31	0
4	A	50	0	43	1	0
5	H	13	0	5	0	0
6	G	70	0	65	6	0
6	L	14	0	13	0	0
7	G	1	0	0	0	0
8	G	29	0	0	2	0
8	H	25	0	0	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
8	L	13	0	0	2	0
All	All	6204	0	5940	139	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 12.

All (139) 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)
2:G:463:THR:HA	2:G:464:SER:HB3	1.37	1.06
3:L:185:HIS:O	3:L:207:ARG:NH1	2.04	0.91
2:G:390:LEU:HD11	2:G:416:LEU:HD21	1.53	0.91
2:G:463:THR:HA	2:G:464:SER:CB	2.02	0.89
2:G:463:THR:HG23	2:G:465:ASN:H	1.36	0.88
3:L:99:GLN:OE1	3:L:138:ARG:NH1	2.10	0.84
2:G:120:VAL:HG22	2:G:434:MET:HB2	1.56	0.84
2:G:95:MET:HE1	2:G:273:ARG:HB3	1.61	0.82
3:L:143:GLN:HB3	3:L:191:GLU:HB3	1.66	0.76
2:G:267:GLU:OE1	2:G:267:GLU:N	2.15	0.74
2:G:463:THR:CA	2:G:464:SER:HB3	2.15	0.74
2:G:379:ARG:NH1	2:G:444:ASN:O	2.20	0.73
2:G:423:ILE:HG12	2:G:434:MET:HG2	1.71	0.72
1:H:23:ARG:HH12	1:H:75:SER:HB2	1.54	0.72
1:H:84:SER:HA	1:H:115:VAL:HG23	1.73	0.70
1:H:56:ALA:HB2	2:G:371:ILE:HD13	1.73	0.70
2:G:378:CYS:HB3	2:G:383:PHE:CE2	2.28	0.68
2:G:87:GLU:HG2	6:G:506:NAG:H62	1.75	0.66
2:G:269:GLU:HB2	6:G:503:NAG:H61	1.74	0.66
2:G:95:MET:CE	2:G:235:GLY:HA3	2.25	0.66
3:L:35:GLN:OE1	3:L:43:ARG:HD3	1.97	0.63
1:H:12:LYS:HB2	1:H:115:VAL:HG12	1.79	0.63
2:G:390:LEU:H	2:G:390:LEU:HD12	1.63	0.63
3:L:104:ARG:NH1	3:L:105:THR:O	2.32	0.63
2:G:121:LYS:HE3	2:G:203:GLN:HE22	1.64	0.62
1:H:9:GLY:HA3	1:H:112:PRO:HD2	1.82	0.62
3:L:87:GLN:NE2	3:L:89:TYR:O	2.33	0.60
1:H:38:ARG:HG3	1:H:46:GLU:HB2	1.81	0.60
2:G:232:ASN:HD21	2:G:268:GLU:HG2	1.67	0.60
3:L:17:GLU:O	3:L:76:LEU:HD13	2.03	0.59
1:H:80:LEU:HD23	1:H:80:LEU:C	2.24	0.58
1:H:155:THR:CG2	1:H:203:ASN:HB3	2.33	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:G:101:VAL:HG21	2:G:480:ARG:HG3	1.86	0.58
2:G:88:ASN:HD22	6:G:506:NAG:C7	2.12	0.57
2:G:462:ASN:O	2:G:463:THR:HG22	2.05	0.57
2:G:84:ILE:HG13	2:G:84:ILE:O	2.05	0.57
3:L:5:THR:HA	3:L:94:GLN:HE22	1.70	0.57
2:G:328:LYS:HB3	8:G:18:HOH:O	2.04	0.56
2:G:414:ILE:HD12	2:G:414:ILE:O	2.04	0.56
2:G:95:MET:HE2	2:G:235:GLY:HA3	1.87	0.56
1:H:182:LEU:C	1:H:182:LEU:HD12	2.26	0.56
2:G:95:MET:HE3	2:G:235:GLY:HA3	1.89	0.54
2:G:45:TRP:NE1	2:G:91:GLU:OE2	2.34	0.54
2:G:86:LEU:HB2	2:G:89:VAL:HG11	1.90	0.54
3:L:29:GLY:O	3:L:30:SER:C	2.46	0.54
1:H:23:ARG:NH1	1:H:75:SER:HB2	2.21	0.53
2:G:66:HIS:ND1	2:G:212:PRO:HA	2.22	0.53
2:G:121:LYS:HE3	2:G:203:GLN:NE2	2.23	0.53
3:L:99:GLN:CD	3:L:138:ARG:HH12	2.07	0.53
3:L:97:LYS:HZ2	3:L:99:GLN:HB3	1.73	0.53
2:G:93:PHE:HB2	2:G:233:PHE:HZ	1.73	0.53
3:L:24:ARG:NH1	3:L:68:ASP:OD1	2.42	0.52
1:H:44:ARG:HH22	3:L:94:GLN:HE21	1.55	0.52
2:G:337:LYS:O	2:G:341:VAL:HG23	2.09	0.52
2:G:342:LEU:HA	2:G:345:VAL:HG12	1.91	0.52
3:L:3:VAL:HG12	3:L:4:LEU:H	1.75	0.52
4:A:3:BMA:O2	4:A:4:MAN:H2	2.10	0.52
2:G:463:THR:OG1	2:G:464:SER:HB3	2.09	0.52
2:G:93:PHE:HB2	2:G:233:PHE:CZ	2.45	0.52
1:H:87:THR:O	1:H:88:ALA:HB2	2.10	0.52
1:H:218:LYS:HE3	1:H:218:LYS:C	2.31	0.51
2:G:390:LEU:HD11	2:G:416:LEU:CD2	2.33	0.51
3:L:104:ARG:HD2	3:L:167:SER:HB2	1.90	0.51
3:L:136:TYR:CG	3:L:137:PRO:HA	2.44	0.51
1:H:47:TRP:CZ2	1:H:49:GLY:HA2	2.46	0.51
1:H:83:THR:O	1:H:115:VAL:HG21	2.11	0.51
1:H:123:PRO:HB3	1:H:149:TYR:HB3	1.93	0.51
2:G:204:ALA:C	2:G:206:PRO:HD3	2.31	0.51
1:H:54:GLY:HA3	2:G:371:ILE:HD11	1.93	0.50
2:G:269:GLU:HB2	6:G:503:NAG:C6	2.39	0.50
2:G:273:ARG:HB2	2:G:285:ILE:HB	1.93	0.50
3:L:14:SER:OG	3:L:103:LYS:HD3	2.10	0.50
3:L:141:LYS:HB3	3:L:193:THR:OG1	2.11	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:G:491:ILE:O	2:G:492:GLU:HB2	2.12	0.50
2:G:379:ARG:NH1	2:G:444:ASN:H	2.09	0.49
2:G:62:GLU:OE1	8:G:24:HOH:O	2.20	0.49
1:H:155:THR:HG22	1:H:203:ASN:HB3	1.94	0.49
1:H:162:ALA:O	8:H:230:HOH:O	2.20	0.48
3:L:94:GLN:H	3:L:94:GLN:CD	2.17	0.48
1:H:32:CYS:HB2	1:H:33:PRO:CD	2.43	0.48
2:G:78:ASP:OD1	2:G:79:PRO:HD2	2.13	0.48
3:L:193:THR:HG22	3:L:200:PRO:HG3	1.96	0.48
2:G:84:ILE:HG12	2:G:244:SER:HB3	1.95	0.48
2:G:52:LEU:O	2:G:103:GLN:NE2	2.46	0.48
1:H:12:LYS:HE3	1:H:16:GLU:OE2	2.13	0.47
1:H:2:VAL:O	1:H:3:ARG:HD3	2.14	0.47
1:H:120:THR:HG22	1:H:151:PRO:HD3	1.96	0.47
2:G:101:VAL:HG21	2:G:480:ARG:CG	2.44	0.47
3:L:4:LEU:CD2	3:L:25:THR:HG22	2.44	0.47
2:G:357:LYS:HD2	2:G:464:SER:H	1.80	0.47
3:L:176:THR:O	3:L:177:LEU:HD23	2.14	0.47
1:H:2:VAL:HB	1:H:106:HIS:CE1	2.49	0.47
3:L:90:GLU:H	3:L:90:GLU:HG3	1.42	0.47
2:G:52:LEU:N	2:G:103:GLN:HE22	2.13	0.47
2:G:333:ILE:HB	2:G:414:ILE:HD11	1.97	0.46
2:G:230:ASP:HB2	2:G:233:PHE:HB2	1.96	0.46
2:G:381:GLU:HG3	2:G:443:ILE:HD13	1.98	0.46
1:H:60:ALA:HA	2:G:458:GLY:O	2.16	0.46
3:L:138:ARG:HD3	8:L:220:HOH:O	2.16	0.46
2:G:453:LEU:O	2:G:471:GLY:N	2.45	0.46
2:G:409:GLY:O	2:G:410:CYS:HB2	2.15	0.46
2:G:386:ASN:O	2:G:416:LEU:HG	2.15	0.45
1:H:188:VAL:HG11	1:H:198:TYR:CE1	2.50	0.45
2:G:484:TYR:CE2	2:G:485:LYS:HB3	2.51	0.45
3:L:7:SER:HB2	3:L:8:PRO:HA	1.99	0.45
3:L:157:GLU:HG3	8:L:218:HOH:O	2.16	0.45
2:G:111:LEU:HD21	2:G:210:PHE:CE1	2.53	0.44
2:G:269:GLU:O	2:G:271:ILE:HG13	2.18	0.44
3:L:45:VAL:HG12	3:L:46:ILE:HG13	1.99	0.44
2:G:87:GLU:O	2:G:88:ASN:C	2.56	0.44
3:L:97:LYS:NZ	3:L:99:GLN:HB3	2.32	0.44
1:H:205:LYS:N	1:H:206:PRO:CD	2.81	0.44
1:H:218:LYS:HE3	1:H:218:LYS:CA	2.48	0.44
2:G:234:ASN:ND2	6:G:505:NAG:C7	2.81	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:G:300:SER:HB3	2:G:441:GLY:C	2.39	0.43
2:G:87:GLU:HG2	6:G:506:NAG:C6	2.45	0.43
1:H:207:SER:OG	1:H:209:THR:HG23	2.19	0.43
2:G:390:LEU:HD12	2:G:390:LEU:N	2.33	0.43
2:G:111:LEU:HD21	2:G:210:PHE:HE1	1.84	0.43
2:G:474:ASN:O	2:G:477:ASP:HB2	2.19	0.43
2:G:343:LYS:O	2:G:347:GLU:HB2	2.19	0.43
2:G:204:ALA:O	2:G:206:PRO:HD3	2.19	0.42
2:G:471:GLY:HA2	2:G:472:GLY:HA2	1.88	0.42
2:G:333:ILE:N	2:G:333:ILE:HD12	2.35	0.42
1:H:80:LEU:HD23	1:H:81:GLU:N	2.34	0.42
2:G:300:SER:O	2:G:301:ASN:HB2	2.20	0.41
2:G:436:ALA:HB1	2:G:437:PRO:HD2	2.01	0.41
1:H:171:PRO:HD2	3:L:158:SER:OG	2.20	0.41
1:H:36:TRP:CG	1:H:80:LEU:HD12	2.55	0.41
3:L:109:PRO:HD3	3:L:194:HIS:ND1	2.36	0.41
2:G:52:LEU:H	2:G:103:GLN:HE22	1.68	0.41
1:H:44:ARG:NH2	3:L:94:GLN:HE21	2.18	0.41
1:H:38:ARG:CG	1:H:46:GLU:HB2	2.49	0.40
2:G:66:HIS:HA	2:G:111:LEU:HD11	2.03	0.40
2:G:107:ASP:O	2:G:110:SER:HB3	2.20	0.40
2:G:331:CYS:O	2:G:415:THR:HA	2.21	0.40
2:G:93:PHE:CE1	2:G:487:LYS:HG2	2.55	0.40
2:G:232:ASN:OD1	2:G:268:GLU:HB3	2.21	0.40
2:G:390:LEU:HD11	2:G:416:LEU:HD11	2.04	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	H	219/229 (96%)	211 (96%)	8 (4%)	0	100 100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	G	335/361 (93%)	316 (94%)	16 (5%)	3 (1%)	17	20
3	L	206/210 (98%)	196 (95%)	8 (4%)	2 (1%)	15	16
All	All	760/800 (95%)	723 (95%)	32 (4%)	5 (1%)	22	26

All (5) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	G	88	ASN
2	G	464	SER
3	L	30	SER
2	G	326	ILE
3	L	38	PRO

5.3.2 Protein sidechains (i)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	H	188/194 (97%)	182 (97%)	6 (3%)	39	50
2	G	305/318 (96%)	291 (95%)	14 (5%)	27	35
3	L	179/181 (99%)	175 (98%)	4 (2%)	52	64
All	All	672/693 (97%)	648 (96%)	24 (4%)	35	46

All (24) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	H	38	ARG
1	H	51	LEU
1	H	71	ARG
1	H	182	LEU
1	H	200	CYS
1	H	218	LYS
2	G	95	MET
2	G	113	ASP
2	G	120	VAL

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Mol	Chain	Res	Type
2	G	224	VAL
2	G	259	LEU
2	G	261	LEU
2	G	327	ARG
2	G	360	ILE
2	G	415	THR
2	G	416	LEU
2	G	430	THR
2	G	462	ASN
2	G	463	THR
2	G	492	GLU
3	L	3	VAL
3	L	83	VAL
3	L	90	GLU
3	L	138	ARG

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

Mol	Chain	Res	Type
2	G	203	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)

1 non-standard protein/DNA/RNA residue is 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	$\#\|Z\| > 2$
1	PCA	H	1	1	7,8,9	1.85	1 (14%)	9,10,12	2.35	5 (55%)

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
1	PCA	H	1	1	-	0/0/11/13	0/1/1/1

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	H	1	PCA	CD-N	4.76	1.47	1.34

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	H	1	PCA	CB-CA-C	-3.53	107.85	112.70
1	H	1	PCA	OE-CD-CG	-3.20	121.18	126.76
1	H	1	PCA	CA-N-CD	-3.05	103.13	113.58
1	H	1	PCA	CB-CA-N	2.60	110.77	103.30
1	H	1	PCA	CG-CD-N	2.53	114.94	108.39

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.5 Carbohydrates (i)

4 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	A	1	2,4	14,14,15	1.68	3 (21%)	17,19,21	1.47	3 (17%)
4	NAG	A	2	4	14,14,15	1.67	2 (14%)	17,19,21	1.70	4 (23%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
4	BMA	A	3	4	11,11,12	2.27	3 (27%)	15,15,17	1.16	1 (6%)
4	MAN	A	4	4	11,11,12	0.64	0	15,15,17	0.89	1 (6%)

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	A	1	2,4	-	2/6/23/26	0/1/1/1
4	NAG	A	2	4	-	2/6/23/26	0/1/1/1
4	BMA	A	3	4	-	0/2/19/22	0/1/1/1
4	MAN	A	4	4	-	1/2/19/22	0/1/1/1

All (8) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	3	BMA	C4-C3	-5.05	1.39	1.52
4	A	2	NAG	C1-C2	4.17	1.58	1.52
4	A	3	BMA	C2-C3	-3.80	1.46	1.52
4	A	1	NAG	C1-C2	3.69	1.57	1.52
4	A	3	BMA	O5-C1	-3.19	1.38	1.43
4	A	2	NAG	O5-C5	-2.71	1.38	1.43
4	A	1	NAG	C3-C2	2.68	1.58	1.52
4	A	1	NAG	O5-C5	-2.48	1.38	1.43

All (9) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	A	2	NAG	C2-N2-C7	-4.07	117.11	122.90
4	A	2	NAG	O5-C1-C2	-3.40	105.91	111.29
4	A	1	NAG	O5-C1-C2	-3.33	106.03	111.29
4	A	1	NAG	C2-N2-C7	-3.17	118.39	122.90
4	A	2	NAG	O4-C4-C3	-2.44	104.71	110.35
4	A	1	NAG	O4-C4-C3	-2.38	104.86	110.35
4	A	3	BMA	O4-C4-C3	-2.21	105.24	110.35
4	A	4	MAN	O5-C1-C2	-2.21	107.37	110.77
4	A	2	NAG	C4-C3-C2	-2.15	107.87	111.02

There are no chirality outliers.

All (5) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	A	1	NAG	O5-C5-C6-O6
4	A	1	NAG	C4-C5-C6-O6
4	A	4	MAN	O5-C5-C6-O6
4	A	2	NAG	O5-C5-C6-O6
4	A	2	NAG	C4-C5-C6-O6

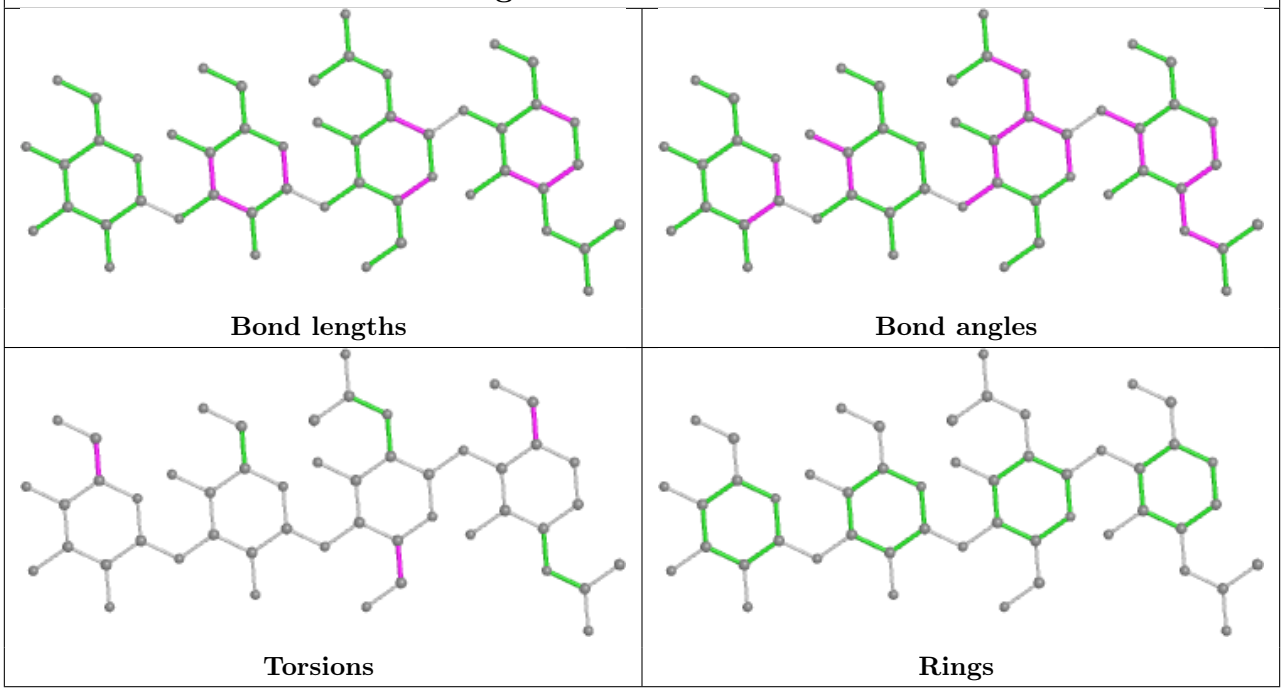
There are no ring outliers.

2 monomers are involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	3	BMA	1	0
4	A	4	MAN	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 A



5.6 Ligand geometry (i)

Of 8 ligands modelled in this entry, 1 is monoatomic - leaving 7 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	$\#\|Z\| > 2$
6	NAG	G	502	2	14,14,15	1.67	3 (21%)	17,19,21	1.55	3 (17%)
6	NAG	G	503	2	14,14,15	1.60	2 (14%)	17,19,21	1.66	3 (17%)
6	NAG	L	211	3	14,14,15	1.51	2 (14%)	17,19,21	1.58	3 (17%)
6	NAG	G	501	2	14,14,15	2.12	4 (28%)	17,19,21	1.37	3 (17%)
5	FLC	H	222	-	12,12,12	1.99	4 (33%)	17,17,17	1.57	2 (11%)
6	NAG	G	506	2	14,14,15	1.72	3 (21%)	17,19,21	1.50	2 (11%)
6	NAG	G	505	2	14,14,15	1.69	4 (28%)	17,19,21	1.59	3 (17%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
6	NAG	G	502	2	-	0/6/23/26	0/1/1/1
6	NAG	G	503	2	-	0/6/23/26	0/1/1/1
6	NAG	L	211	3	-	2/6/23/26	0/1/1/1
6	NAG	G	501	2	-	2/6/23/26	0/1/1/1
5	FLC	H	222	-	-	2/16/16/16	-
6	NAG	G	506	2	-	2/6/23/26	0/1/1/1
6	NAG	G	505	2	-	1/6/23/26	0/1/1/1

All (22) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	G	501	NAG	C1-C2	5.70	1.60	1.52
6	G	506	NAG	C1-C2	4.13	1.58	1.52
6	G	503	NAG	C1-C2	3.81	1.58	1.52
5	H	222	FLC	CB-CBC	-3.48	1.49	1.53
6	G	505	NAG	C1-C2	3.35	1.57	1.52
6	G	502	NAG	C1-C2	3.32	1.57	1.52
6	G	501	NAG	O5-C5	-3.31	1.36	1.43
5	H	222	FLC	CA-CB	-3.27	1.49	1.53
6	G	502	NAG	O5-C5	-3.10	1.37	1.43
5	H	222	FLC	CG-CB	-3.00	1.50	1.53
6	G	505	NAG	C4-C5	2.96	1.59	1.53
6	L	211	NAG	O5-C5	-2.94	1.37	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	G	506	NAG	O5-C5	-2.93	1.37	1.43
6	L	211	NAG	C1-C2	2.72	1.56	1.52
6	G	501	NAG	C3-C2	2.72	1.58	1.52
6	G	503	NAG	O5-C5	-2.60	1.38	1.43
5	H	222	FLC	OHB-CB	-2.48	1.38	1.43
6	G	506	NAG	C3-C2	2.23	1.57	1.52
6	G	502	NAG	C3-C2	2.16	1.57	1.52
6	G	505	NAG	O5-C5	-2.14	1.39	1.43
6	G	505	NAG	C4-C3	2.11	1.57	1.52
6	G	501	NAG	C7-N2	2.01	1.41	1.34

All (19) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
5	H	222	FLC	OB2-CBC-CB	4.26	120.44	113.05
6	G	503	NAG	C2-N2-C7	-3.97	117.26	122.90
6	G	505	NAG	C2-N2-C7	-3.70	117.64	122.90
6	L	211	NAG	C2-N2-C7	-3.65	117.70	122.90
6	G	502	NAG	C2-N2-C7	-3.65	117.70	122.90
6	G	506	NAG	C2-N2-C7	-3.61	117.77	122.90
6	L	211	NAG	O5-C1-C2	-3.31	106.06	111.29
6	G	505	NAG	O5-C1-C2	-3.16	106.29	111.29
6	G	503	NAG	O5-C1-C2	-3.07	106.45	111.29
6	G	506	NAG	O5-C1-C2	-2.92	106.67	111.29
6	G	502	NAG	O5-C1-C2	-2.90	106.70	111.29
6	G	501	NAG	C2-N2-C7	-2.69	119.07	122.90
6	G	503	NAG	C4-C3-C2	-2.47	107.41	111.02
5	H	222	FLC	CB-CG-CGC	2.29	119.37	113.81
6	G	501	NAG	O5-C5-C4	-2.21	105.46	110.83
6	L	211	NAG	O4-C4-C3	-2.16	105.36	110.35
6	G	502	NAG	O4-C4-C3	-2.16	105.37	110.35
6	G	501	NAG	O3-C3-C2	-2.15	105.03	109.47
6	G	505	NAG	C1-O5-C5	2.12	115.07	112.19

There are no chirality outliers.

All (9) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
6	L	211	NAG	C4-C5-C6-O6
6	L	211	NAG	O5-C5-C6-O6
6	G	506	NAG	C4-C5-C6-O6
6	G	501	NAG	O5-C5-C6-O6

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Mol	Chain	Res	Type	Atoms
6	G	506	NAG	O5-C5-C6-O6
6	G	501	NAG	C4-C5-C6-O6
5	H	222	FLC	CBC-CB-CG-CGC
6	G	505	NAG	C4-C5-C6-O6
5	H	222	FLC	OHB-CB-CG-CGC

There are no ring outliers.

3 monomers are involved in 6 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	G	503	NAG	2	0
6	G	506	NAG	3	0
6	G	505	NAG	1	0

5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

6 Fit of model and data (i)

6.1 Protein, DNA and RNA chains (i)

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, 95th 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	H	221/229 (96%)	-0.22	3 (1%)	75	73	48, 71, 108, 142	0
2	G	340/361 (94%)	0.17	16 (4%)	31	29	51, 79, 124, 159	0
3	L	208/210 (99%)	-0.26	1 (0%)	91	91	58, 80, 100, 146	0
All	All	769/800 (96%)	-0.06	20 (2%)	56	52	48, 77, 116, 159	0

All (20) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	G	326	ILE	4.5
2	G	198	GLY	4.2
2	G	199	SER	3.6
2	G	473	GLY	3.3
2	G	200	VAL	3.2
2	G	465	ASN	2.8
2	G	472	GLY	2.8
2	G	328	LYS	2.8
1	H	56	ALA	2.6
2	G	327	ARG	2.6
2	G	358	THR	2.5
1	H	55	GLY	2.5
2	G	124	GLY	2.5
2	G	355	ASN	2.4
2	G	492	GLU	2.3
1	H	194	GLY	2.2
2	G	471	GLY	2.2
3	L	195	GLN	2.2
2	G	461	ASN	2.2
2	G	474	ASN	2.1

6.2 Non-standard residues in protein, DNA, RNA chains (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, 95th 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
1	PCA	H	1	8/9	0.93	0.20	69,82,88,92	0

6.3 Carbohydrates (i)

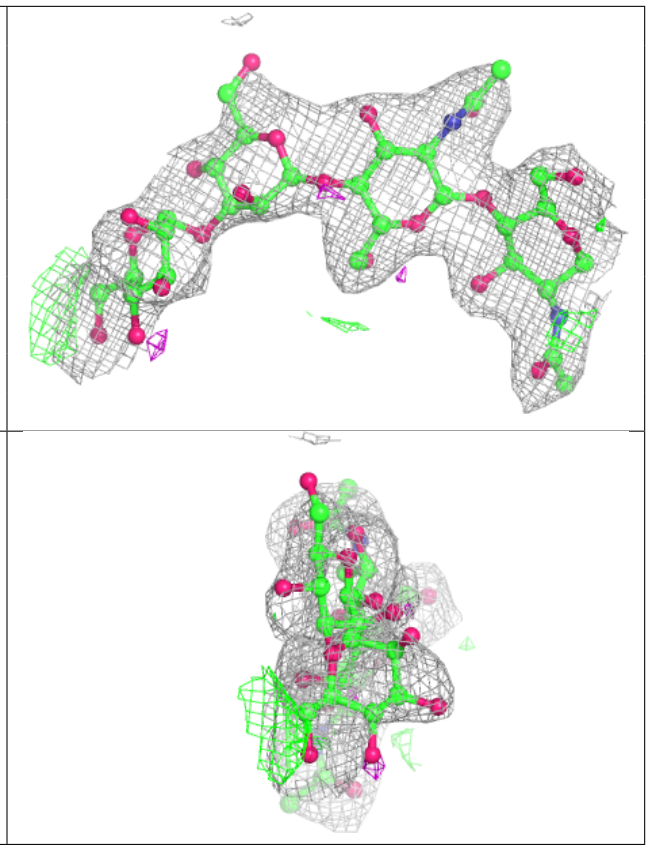
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists 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	MAN	A	4	11/12	0.71	0.23	133,138,140,141	0
4	BMA	A	3	11/12	0.82	0.26	130,132,136,138	0
4	NAG	A	2	14/15	0.92	0.13	80,83,123,127	0
4	NAG	A	1	14/15	0.96	0.10	54,65,80,88	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 A:

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



6.4 Ligands (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, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
6	NAG	G	506	14/15	0.72	0.28	90,111,172,172	0
6	NAG	G	505	14/15	0.80	0.28	75,98,117,118	0
6	NAG	L	211	14/15	0.82	0.36	81,134,142,143	0
5	FLC	H	222	13/13	0.88	0.34	88,97,100,102	0
6	NAG	G	502	14/15	0.90	0.24	61,79,96,97	0
6	NAG	G	503	14/15	0.91	0.24	76,106,153,154	0
6	NAG	G	501	14/15	0.93	0.13	78,84,91,92	0
7	CL	G	504	1/1	0.97	0.18	55,55,55,55	0

6.5 Other polymers (i)

There are no such residues in this entry.