Full wwPDB X-ray Structure Validation Report (i)

Sep 17, 2023 – 11:28 PM EDT

PDB ID	:	4XNZ
Title	:	Crystal structure of broadly and potently neutralizing antibody VRC06B in complex with HIV-1 clade A/E strain 93TH057 gp120
Authors	:	Zhou, T.; Srivatsan, S.; Kwong, P.D.
Deposited on	:	2015-01-16
Resolution	:	3.39 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:

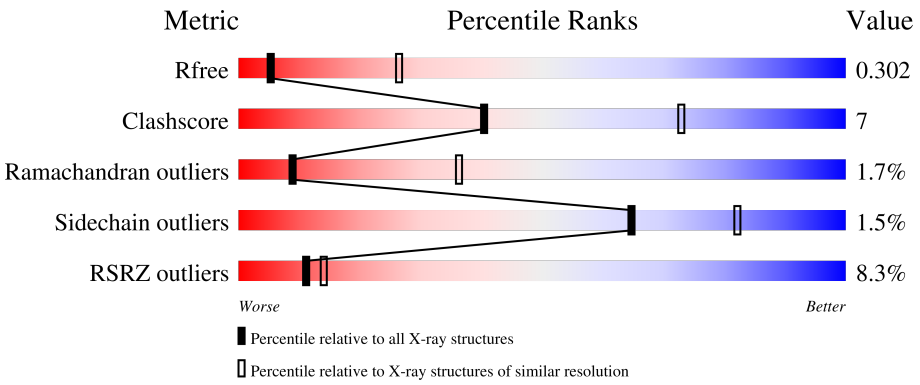
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.35.1
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (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 3.39 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	1691 (3.46-3.30)
Clashscore	141614	1762 (3.46-3.30)
Ramachandran outliers	138981	1732 (3.46-3.30)
Sidechain outliers	138945	1731 (3.46-3.30)
RSRZ outliers	127900	1635 (3.46-3.30)

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	353	9% 75% 22% •
1	D	353	7% 74% 19% • 7%
1	G	353	14% 75% 21% •
2	B	234	7% 79% 14% • 5%
2	E	234	9% 75% 18% • 6%

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Mol	Chain	Length	Quality of chain
2	H	234	8% 77% 17% 5%
3	C	209	3% 79% 18%
3	F	209	6% 76% 21%
3	L	209	3% 78% 21%
4	I	3	67% 33%
4	J	3	67% 33%
4	K	3	33% 67%

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
4	NAG	I	2	-	-	-	X
4	FUC	I	3	-	-	-	X
4	FUC	K	3	X	-	-	-
5	NAG	G	504	-	-	-	X
5	NAG	G	506	-	-	-	X

2 Entry composition (i)

There are 5 unique types of molecules in this entry. The entry contains 18134 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called Envelope glycoprotein gp160,Envelope glycoprotein gp160.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	G	340	2667	1674	463	509	21	0	0	0
1	A	341	2665	1669	463	511	22	0	0	0
1	D	330	2598	1634	452	492	20	0	0	0

There are 24 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
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
A	124	GLY	-	linker	UNP Q0ED31
A	198	GLY	-	linker	UNP Q0ED31
A	318	GLY	-	linker	UNP Q0ED31
A	319	GLY	-	linker	UNP Q0ED31
A	320	SER	-	linker	UNP Q0ED31
A	321	GLY	-	linker	UNP Q0ED31
A	322	SER	-	linker	UNP Q0ED31
A	323	GLY	-	linker	UNP Q0ED31
D	124	GLY	-	linker	UNP Q0ED31
D	198	GLY	-	linker	UNP Q0ED31
D	318	GLY	-	linker	UNP Q0ED31
D	319	GLY	-	linker	UNP Q0ED31
D	320	SER	-	linker	UNP Q0ED31
D	321	GLY	-	linker	UNP Q0ED31
D	322	SER	-	linker	UNP Q0ED31

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Chain	Residue	Modelled	Actual	Comment	Reference
D	323	GLY	-	linker	UNP Q0ED31

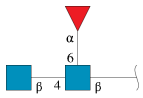
- Molecule 2 is a protein called HEAVY CHAIN OF ANTIBODY VRC06B.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
2	H	222	1686	1070	293	313	10	0	0	0
2	B	222	1687	1071	294	312	10	0	0	0
2	E	220	1670	1062	291	307	10	0	0	0

- Molecule 3 is a protein called LIGHT CHAIN OF ANTIBODY VRC06B.

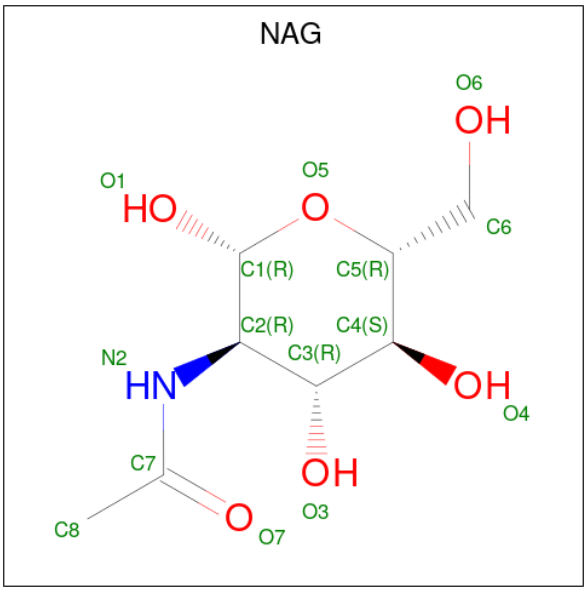
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
3	L	207	1604	1006	276	318	4	0	0	0
3	C	206	1596	999	275	318	4	0	0	0
3	F	206	1595	1001	275	315	4	0	0	0

- Molecule 4 is an oligosaccharide called 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-[alpha-L-fucopyranose-(1-6)]2-acetamido-2-deoxy-beta-D-glucopyranose.



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
			Total	C	N	O			
4	I	3	38	22	2	14	0	0	0
4	J	3	38	22	2	14	0	0	0
4	K	3	38	22	2	14	0	0	0

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



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

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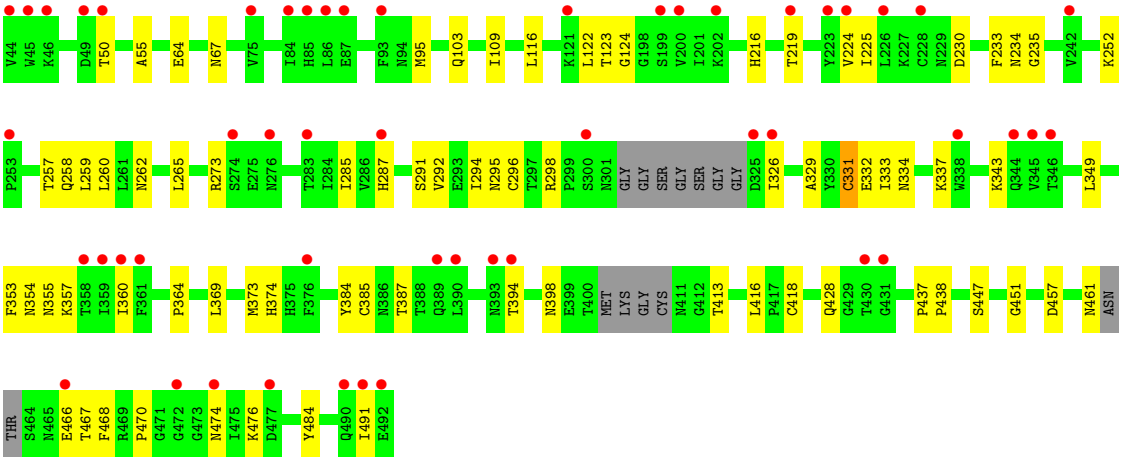
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	C	N	O		
5	D	1	14	8	1	5	0	0
			Total	C	N	O		
5	D	1	14	8	1	5	0	0
			Total	C	N	O		
5	D	1	14	8	1	5	0	0
			Total	C	N	O		
5	D	1	14	8	1	5	0	0

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.

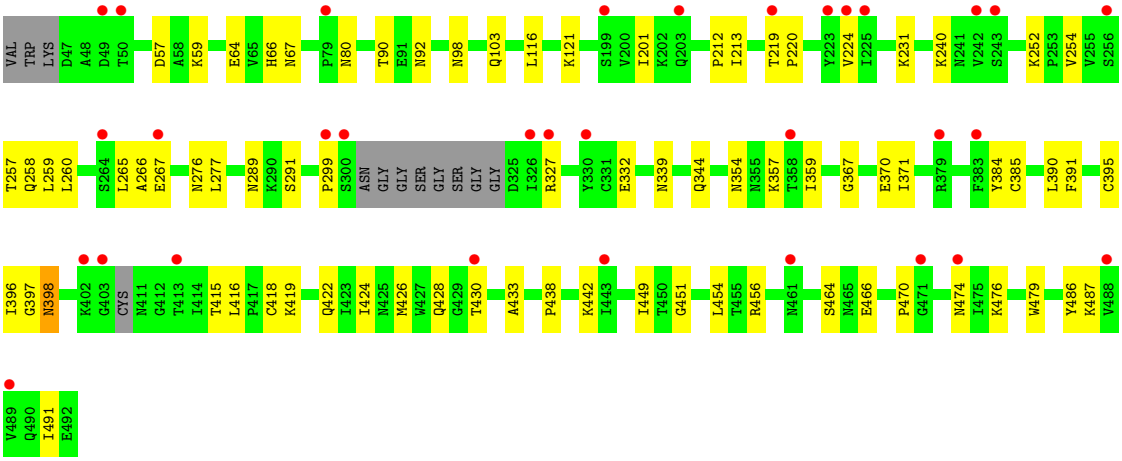
• Molecule 1: Envelope glycoprotein gp160,Envelope glycoprotein gp160

Chain G: 14% 75% 21%



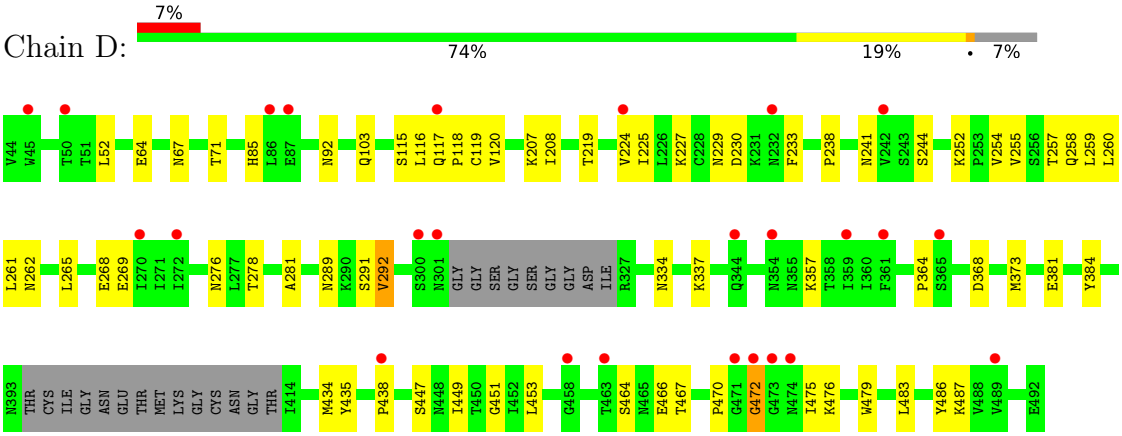
• Molecule 1: Envelope glycoprotein gp160,Envelope glycoprotein gp160

Chain A: 9% 75% 22%



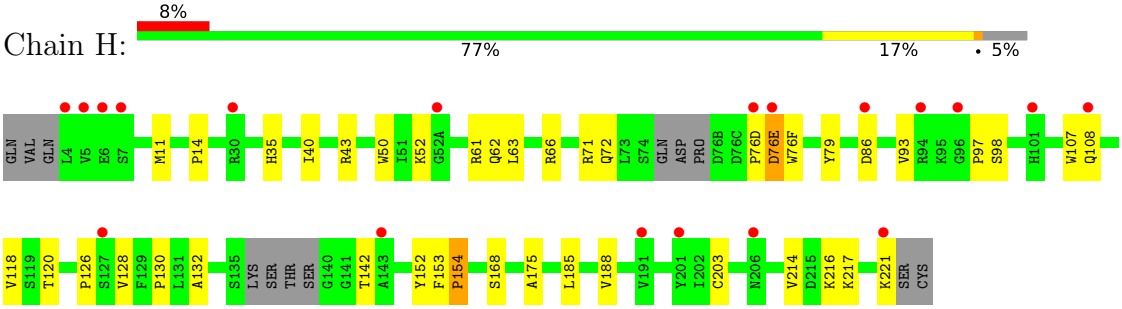
• Molecule 1: Envelope glycoprotein gp160,Envelope glycoprotein gp160

Chain D:



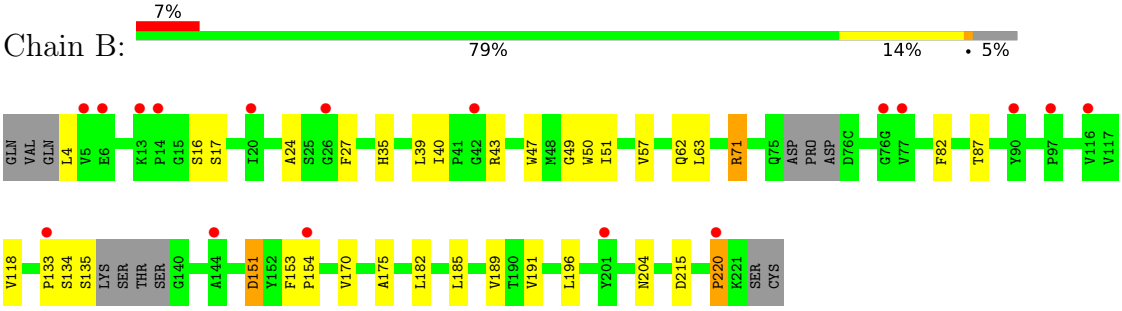
• Molecule 2: HEAVY CHAIN OF ANTIBODY VRC06B

Chain H:



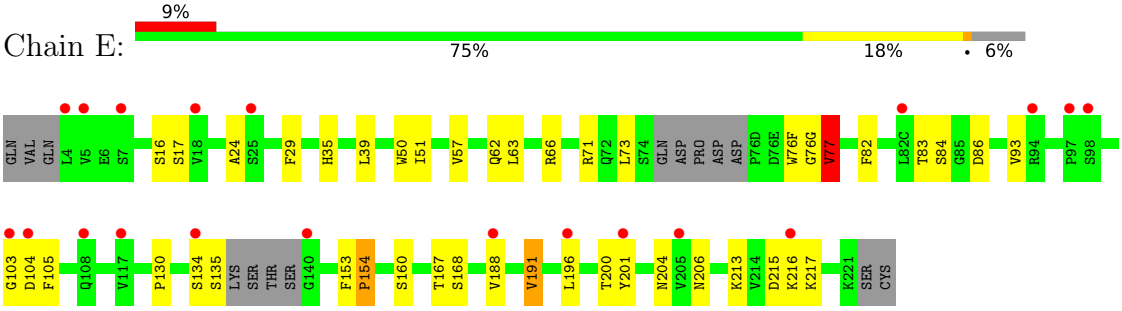
• Molecule 2: HEAVY CHAIN OF ANTIBODY VRC06B

Chain B:



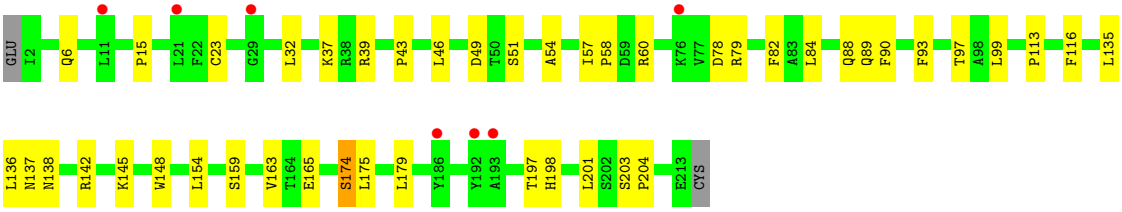
• Molecule 2: HEAVY CHAIN OF ANTIBODY VRC06B

Chain E:



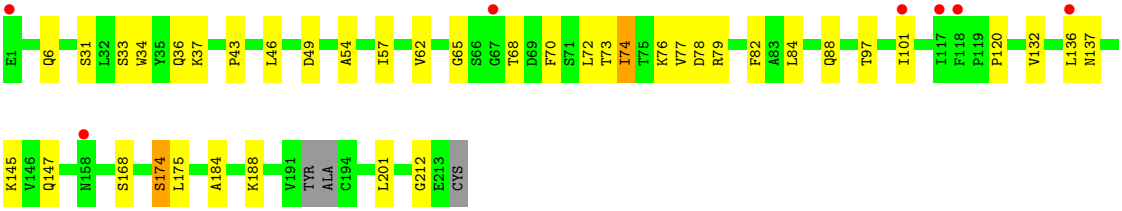
• Molecule 3: LIGHT CHAIN OF ANTIBODY VRC06B

Chain L:



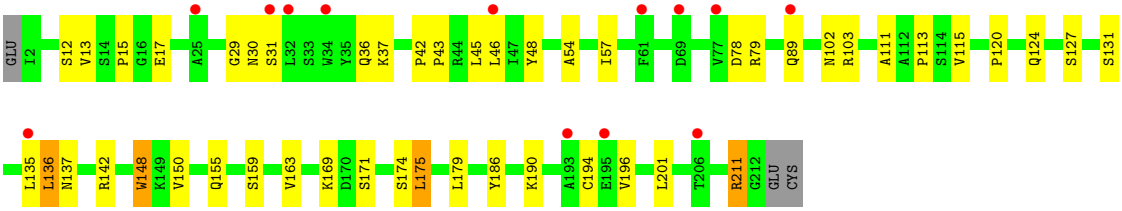
• Molecule 3: LIGHT CHAIN OF ANTIBODY VRC06B

Chain C:



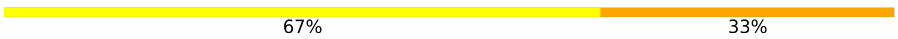
• Molecule 3: LIGHT CHAIN OF ANTIBODY VRC06B

Chain F:



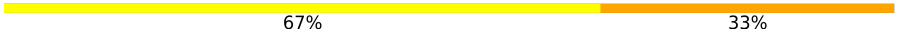
• Molecule 4: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-[alpha-L-fucopyranose-(1-6)]2-acetamido-2-deoxy-beta-D-glucopyranose

Chain I:



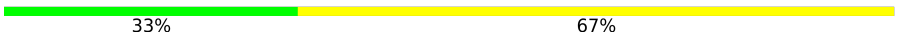
• Molecule 4: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-[alpha-L-fucopyranose-(1-6)]2-acetamido-2-deoxy-beta-D-glucopyranose

Chain J:



• Molecule 4: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-[alpha-L-fucopyranose-(1-6)]2-acetamido-2-deoxy-beta-D-glucopyranose

Chain K:



NAG1
NAG2
FUC3

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	68.31Å 189.44Å 219.94Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	39.90 – 3.39 39.90 – 3.39	Depositor EDS
% Data completeness (in resolution range)	86.0 (39.90-3.39) 82.0 (39.90-3.39)	Depositor EDS
R_{merge}	0.10	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.91 (at 3.40Å)	Xtriage
Refinement program	PHENIX	Depositor
R, R_{free}	0.244 , 0.301 0.247 , 0.302	Depositor DCC
R_{free} test set	1736 reflections (4.97%)	wwPDB-VP
Wilson B-factor (Å^2)	100.3	Xtriage
Anisotropy	0.527	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.25 , 63.4	EDS
L-test for twinning[2]	$< \|L\| > = 0.45$, $< L^2 > = 0.27$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.89	EDS
Total number of atoms	18134	wwPDB-VP
Average B, all atoms (Å^2)	144.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.46% 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: NAG, FUC

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	0.21	0/2719	0.39	0/3689
1	D	0.20	0/2654	0.37	0/3603
1	G	0.20	0/2722	0.38	0/3694
2	B	0.20	0/1735	0.37	0/2358
2	E	0.21	0/1718	0.41	0/2334
2	H	0.21	0/1734	0.38	0/2357
3	C	0.21	0/1628	0.37	0/2203
3	F	0.21	0/1629	0.38	0/2207
3	L	0.21	0/1638	0.38	0/2219
All	All	0.21	0/18177	0.38	0/24664

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	A	2665	0	2601	44	0
1	D	2598	0	2540	37	0
1	G	2667	0	2601	42	0
2	B	1687	0	1638	23	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	E	1670	0	1627	23	0
2	H	1686	0	1634	22	0
3	C	1596	0	1553	19	1
3	F	1595	0	1553	29	0
3	L	1604	0	1559	23	0
4	I	38	0	34	0	1
4	J	38	0	34	1	0
4	K	38	0	34	1	0
5	A	98	0	91	1	0
5	D	70	0	65	2	0
5	G	84	0	78	0	0
All	All	18134	0	17642	256	1

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 7.

All (256) 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:E:76(G):GLY:HA2	2:E:77:VAL:HB	1.70	0.72
2:E:62:GLN:HG2	2:E:63:LEU:HD12	1.76	0.67
2:H:132:ALA:HB1	2:H:221:LYS:H	1.60	0.66
3:C:74:ILE:HD11	3:C:77:VAL:HG22	1.78	0.66
1:G:374:HIS:HB3	1:G:385:CYS:HB2	1.79	0.65
1:A:357:LYS:HD2	1:A:466:GLU:HG2	1.79	0.65
3:F:163:VAL:HB	3:F:175:LEU:HD12	1.80	0.64
1:D:85:HIS:NE2	1:D:241:ASN:OD1	2.31	0.64
1:D:120:VAL:HB	1:D:434:MET:HB3	1.79	0.64
3:C:82:PHE:HB3	3:C:101:ILE:HG12	1.80	0.64
1:A:212:PRO:O	1:A:252:LYS:NZ	2.30	0.63
2:B:62:GLN:HG2	2:B:63:LEU:HD12	1.81	0.63
1:D:254:VAL:HG11	1:D:261:LEU:HB2	1.81	0.63
2:E:24:ALA:H	2:E:77:VAL:H	1.47	0.63
1:A:90:THR:HG22	1:A:240:LYS:HG2	1.81	0.62
1:G:333:ILE:O	1:G:413:THR:OG1	2.17	0.62
3:F:190:LYS:HD2	3:F:211:ARG:HB3	1.79	0.62
2:B:87:THR:HG22	2:B:118:VAL:H	1.63	0.62
3:F:113:PRO:HB2	3:F:136:LEU:HB2	1.80	0.62
1:G:295:ASN:HB3	1:G:332:GLU:HB3	1.82	0.61
1:G:353:PHE:O	1:G:355:ASN:N	2.33	0.61
1:A:424:ILE:O	1:A:433:ALA:N	2.31	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:294:ILE:HG22	1:G:333:ILE:HG12	1.83	0.61
1:A:426:MET:SD	1:A:430:THR:OG1	2.59	0.61
3:F:103:ARG:HD2	3:F:171:SER:HB2	1.81	0.60
1:G:343:LYS:HD3	1:G:398:ASN:HB3	1.84	0.59
1:A:357:LYS:HG3	1:A:464:SER:HB3	1.84	0.59
1:A:370:GLU:HA	1:A:384:TYR:HE2	1.67	0.59
2:E:35:HIS:HB2	2:E:93:VAL:HG23	1.83	0.59
2:H:175:ALA:HB2	2:H:185:LEU:HD23	1.86	0.58
3:C:79:ARG:NH1	3:C:168:SER:O	2.36	0.58
1:G:360:ILE:HG12	1:G:394:THR:HG23	1.86	0.57
1:D:357:LYS:HG3	1:D:464:SER:HB3	1.86	0.57
1:G:474:ASN:HD21	1:G:476:LYS:HE3	1.70	0.57
3:L:136:LEU:HD11	3:L:175:LEU:HD22	1.86	0.57
2:B:175:ALA:HB2	2:B:185:LEU:HD23	1.85	0.57
5:D:503:NAG:O4	3:F:29:GLY:O	2.22	0.57
3:C:33:SER:HB2	3:C:88:GLN:HB3	1.87	0.57
3:F:30:ASN:ND2	3:F:31:SER:O	2.38	0.57
3:F:37:LYS:HD2	3:F:43:PRO:HG3	1.85	0.57
1:A:265:LEU:HD21	1:A:291:SER:HB2	1.87	0.56
3:F:120:PRO:HB3	3:F:131:SER:H	1.70	0.56
1:G:64:GLU:HB3	1:G:67:ASN:HD22	1.69	0.56
3:L:159:SER:HB3	3:L:179:LEU:HD23	1.88	0.56
2:E:39:LEU:HD22	3:F:37:LYS:HE2	1.86	0.56
1:D:207:LYS:NZ	1:D:381:GLU:OE2	2.33	0.56
1:G:466:GLU:OE1	2:H:61:ARG:NH2	2.38	0.56
1:G:50:THR:O	1:G:103:GLN:NE2	2.37	0.56
2:B:24:ALA:HB1	2:B:27:PHE:HE1	1.69	0.56
1:D:453:LEU:HD22	1:D:472:GLY:HA2	1.88	0.55
1:G:298:ARG:NH1	1:G:326:ILE:O	2.40	0.55
2:E:66:ARG:NH2	2:E:86:ASP:OD2	2.40	0.55
1:D:265:LEU:HD21	1:D:291:SER:HB3	1.89	0.55
3:C:137:ASN:HA	3:C:174:SER:HA	1.89	0.54
3:C:62:VAL:HB	3:C:73:THR:HG23	1.89	0.54
3:L:116:PHE:HD2	3:L:135:LEU:HD23	1.72	0.54
1:A:92:ASN:O	1:A:487:LYS:NZ	2.31	0.54
1:D:276:ASN:OD1	1:D:278:THR:OG1	2.23	0.54
1:A:332:GLU:HG2	1:A:415:THR:HG22	1.89	0.54
1:G:252:LYS:HD3	1:G:262:ASN:HB3	1.90	0.54
1:A:260:LEU:HD12	1:A:451:GLY:HA3	1.90	0.54
1:A:64:GLU:OE1	1:A:67:ASN:ND2	2.42	0.53
1:G:294:ILE:HD11	1:G:447:SER:HB2	1.90	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:F:78:ASP:OD1	3:F:79:ARG:N	2.38	0.53
3:F:12:SER:HB3	3:F:102:ASN:HB2	1.89	0.53
2:B:196:LEU:HD21	2:B:220:PRO:HG3	1.91	0.52
2:H:40:ILE:HG23	2:H:43:ARG:HB2	1.91	0.52
3:C:37:LYS:HD2	3:C:43:PRO:HG3	1.91	0.52
2:E:103:GLY:O	2:E:105:PHE:N	2.33	0.52
3:L:39:ARG:NH1	3:L:165:GLU:OE2	2.43	0.52
1:A:339:ASN:O	1:A:398:ASN:ND2	2.42	0.52
2:B:51:ILE:HD11	2:B:71:ARG:HD2	1.92	0.52
2:B:170:VAL:HG22	2:B:189:VAL:HG22	1.90	0.52
3:F:13:VAL:HG13	3:F:17:GLU:HB3	1.92	0.52
2:H:72:GLN:HB2	2:H:79:TYR:HE2	1.75	0.52
3:L:137:ASN:HA	3:L:174:SER:HA	1.90	0.52
1:A:367:GLY:HA3	1:A:371:ILE:HD11	1.91	0.52
3:C:31:SER:HB2	3:C:49:ASP:HA	1.91	0.52
3:F:148:TRP:HA	3:F:194:CYS:HA	1.92	0.52
1:G:457:ASP:HB3	1:G:467:THR:HB	1.91	0.52
1:D:52:LEU:O	1:D:103:GLN:NE2	2.41	0.51
1:D:64:GLU:OE1	1:D:67:ASN:ND2	2.36	0.51
3:F:159:SER:HB3	3:F:179:LEU:HG	1.92	0.51
1:D:268:GLU:HG2	1:D:269:GLU:HG2	1.93	0.51
3:F:137:ASN:HA	3:F:174:SER:HA	1.92	0.51
1:A:121:LYS:HB3	1:A:201:ILE:HB	1.92	0.51
1:D:227:LYS:NZ	1:D:229:ASN:OD1	2.44	0.51
1:D:257:THR:O	1:D:259:LEU:N	2.43	0.51
2:B:151:ASP:HA	2:B:182:LEU:HB3	1.92	0.51
2:E:200:THR:HG23	2:E:217:LYS:HE3	1.93	0.51
1:A:66:HIS:HB3	1:A:213:ILE:HG12	1.92	0.50
3:L:78:ASP:OD1	3:L:79:ARG:N	2.41	0.50
1:G:257:THR:O	1:G:259:LEU:N	2.43	0.50
2:H:98:SER:OG	2:H:108:GLN:OE1	2.26	0.50
3:C:54:ALA:HB3	3:C:57:ILE:HD12	1.93	0.50
2:H:35:HIS:HB2	2:H:93:VAL:HG23	1.93	0.50
1:A:390:LEU:HG	1:A:416:LEU:HD21	1.94	0.50
3:L:37:LYS:HD2	3:L:43:PRO:HG3	1.93	0.50
3:L:6:GLN:HE21	3:L:97:THR:HG23	1.76	0.50
1:A:231:LYS:HE2	1:A:267:GLU:HG3	1.94	0.50
2:H:107:TRP:HZ3	3:L:93:PHE:HZ	1.60	0.50
1:G:387:THR:HG22	1:G:416:LEU:HD13	1.94	0.49
3:L:54:ALA:H	3:L:57:ILE:HD12	1.77	0.49
3:L:163:VAL:HA	3:L:175:LEU:HA	1.94	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:265:LEU:HD21	1:G:291:SER:HB2	1.92	0.49
1:A:476:LYS:HA	1:A:479:TRP:CD1	2.47	0.49
1:D:483:LEU:HD12	1:D:486:TYR:HD2	1.78	0.49
1:A:224:VAL:HG23	1:A:491:ILE:HD11	1.93	0.49
1:A:257:THR:O	1:A:259:LEU:N	2.43	0.49
3:C:120:PRO:HD3	3:C:132:VAL:HG22	1.95	0.49
1:A:64:GLU:HB3	1:A:67:ASN:HD22	1.78	0.49
1:G:64:GLU:OE1	1:G:67:ASN:ND2	2.46	0.48
2:E:71:ARG:HE	2:E:73:LEU:HD13	1.78	0.48
2:H:76(D):PRO:O	2:H:76(F):TRP:N	2.47	0.48
1:D:364:PRO:HD3	1:D:470:PRO:HG2	1.94	0.48
2:H:216:LYS:NZ	2:H:217:LYS:O	2.46	0.48
3:C:6:GLN:HE21	3:C:97:THR:HG23	1.78	0.48
3:C:145:LYS:NZ	3:C:147:GLN:OE1	2.45	0.48
1:G:230:ASP:HB3	1:G:233:PHE:HB2	1.94	0.48
1:A:98:ASN:ND2	1:A:486:TYR:O	2.47	0.48
1:D:252:LYS:HD3	1:D:262:ASN:HB3	1.95	0.48
3:F:163:VAL:HA	3:F:175:LEU:HA	1.94	0.48
3:C:78:ASP:OD1	3:C:79:ARG:N	2.46	0.48
1:D:118:PRO:HG3	1:D:435:TYR:CZ	2.48	0.48
1:G:234:ASN:O	1:G:273:ARG:NH2	2.42	0.48
1:G:428:GLN:OE1	1:G:428:GLN:N	2.45	0.48
1:G:273:ARG:HB2	1:G:285:ILE:HB	1.96	0.47
1:G:55:ALA:N	1:G:216:HIS:O	2.39	0.47
1:A:428:GLN:N	1:A:428:GLN:OE1	2.47	0.47
2:B:204:ASN:ND2	2:B:215:ASP:OD1	2.48	0.47
2:E:130:PRO:HD3	2:E:216:LYS:HE3	1.95	0.47
2:B:189:VAL:HG12	2:B:191:VAL:HG23	1.97	0.47
2:E:51:ILE:HG22	2:E:57:VAL:HG12	1.95	0.47
1:G:329:ALA:HB3	1:G:418:CYS:HB2	1.96	0.47
3:F:142:ARG:HE	3:F:163:VAL:HG21	1.79	0.47
1:G:292:VAL:HG13	1:G:337:LYS:HE3	1.97	0.47
2:H:14:PRO:HG3	2:H:120:THR:HG22	1.97	0.47
1:G:122:LEU:HG	1:G:124:GLY:H	1.80	0.47
2:H:11:MET:SD	2:H:154:PRO:HG3	2.54	0.47
3:L:82:PHE:HA	3:L:99:LEU:HB3	1.97	0.46
2:B:40:ILE:HB	2:B:43:ARG:HB3	1.96	0.46
3:F:103:ARG:HH12	3:F:111:ALA:HB2	1.80	0.46
1:D:92:ASN:HA	1:D:238:PRO:HA	1.97	0.46
1:D:373:MET:SD	1:D:384:TYR:HB3	2.55	0.46
2:E:83:THR:OG1	2:E:84:SER:N	2.47	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:206:ASN:HD21	2:E:213:LYS:HE3	1.80	0.46
3:L:113:PRO:HD3	3:L:198:HIS:HD2	1.81	0.46
1:A:277:LEU:O	1:A:456:ARG:NH1	2.48	0.46
2:E:191:VAL:HG11	2:E:201:TYR:CE2	2.50	0.46
1:G:461:ASN:OD1	1:G:461:ASN:N	2.45	0.46
1:D:230:ASP:HB2	1:D:233:PHE:HB2	1.98	0.46
3:L:32:LEU:HD12	3:L:89:GLN:HG3	1.98	0.46
1:A:384:TYR:CZ	1:A:424:ILE:HD11	2.51	0.45
3:F:54:ALA:H	3:F:57:ILE:HD12	1.81	0.45
1:G:373:MET:SD	1:G:384:TYR:HB3	2.56	0.45
4:K:2:NAG:C8	4:K:3:FUC:H2	2.45	0.45
1:A:327:ARG:HD3	1:A:419:LYS:HE3	1.99	0.45
2:B:39:LEU:HD22	3:C:37:LYS:HE2	1.98	0.45
2:E:204:ASN:ND2	2:E:215:ASP:OD1	2.42	0.45
1:G:219:THR:HG23	1:G:225:ILE:HG13	1.99	0.45
1:G:334:ASN:HB3	1:G:337:LYS:HG2	1.99	0.45
1:G:357:LYS:HD2	1:G:466:GLU:HG2	1.99	0.45
2:H:130:PRO:HD3	2:H:216:LYS:HE3	1.99	0.45
2:B:16:SER:OG	2:B:17:SER:N	2.48	0.45
1:D:67:ASN:O	1:D:71:THR:OG1	2.27	0.45
1:D:292:VAL:HG13	1:D:449:ILE:HD11	1.98	0.44
2:B:24:ALA:HB1	2:B:27:PHE:CE1	2.49	0.44
3:L:142:ARG:HH21	3:L:163:VAL:HG11	1.82	0.44
2:B:47:TRP:CZ2	2:B:49:GLY:HA2	2.52	0.44
1:D:281:ALA:HA	2:E:50:TRP:CZ2	2.52	0.44
3:F:30:ASN:OD1	3:F:89:GLN:NE2	2.50	0.44
1:A:424:ILE:HD12	1:A:424:ILE:HA	1.76	0.44
2:E:16:SER:OG	2:E:17:SER:N	2.49	0.44
3:C:65:GLY:HA3	3:C:70:PHE:HA	2.00	0.44
2:E:188:VAL:HG21	3:F:135:LEU:HD11	1.99	0.44
1:A:299:PRO:HA	1:A:442:LYS:HD2	1.98	0.44
1:A:344:GLN:HB3	5:A:505:NAG:H62	2.00	0.44
1:A:474:ASN:HD21	1:A:476:LYS:HE2	1.82	0.44
1:D:260:LEU:HD12	1:D:451:GLY:HA3	1.99	0.44
1:G:224:VAL:HG23	1:G:491:ILE:HD11	2.00	0.44
1:A:57:ASP:O	1:A:59:LYS:NZ	2.48	0.44
3:C:34:TRP:CD2	3:C:72:LEU:HB2	2.53	0.44
3:F:45:LEU:HD21	3:F:48:TYR:HB3	2.00	0.44
3:C:34:TRP:CE2	3:C:72:LEU:HB2	2.53	0.44
2:H:203:CYS:SG	2:H:216:LYS:HB3	2.58	0.44
1:D:219:THR:HG23	1:D:225:ILE:HG12	2.00	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:269:GLU:HA	1:D:289:ASN:HD22	1.83	0.43
3:F:79:ARG:NH1	3:F:169:LYS:O	2.50	0.43
2:H:50:TRP:CZ3	2:H:52:LYS:HG2	2.52	0.43
3:L:145:LYS:HE2	3:L:197:THR:HB	1.99	0.43
1:G:349:LEU:HD13	1:G:468:PHE:CE2	2.54	0.43
2:B:153:PHE:HA	2:B:154:PRO:HA	1.71	0.43
2:H:128:VAL:HG21	2:H:214:VAL:HG11	1.99	0.43
1:A:266:ALA:HB3	1:A:289:ASN:HB3	2.00	0.43
1:D:476:LYS:HA	1:D:479:TRP:CD1	2.54	0.43
3:F:150:VAL:HB	3:F:155:GLN:HE22	1.84	0.43
1:A:80:ASN:OD1	1:A:80:ASN:N	2.51	0.43
2:B:35:HIS:CG	2:B:50:TRP:HB3	2.54	0.43
2:B:40:ILE:HG21	2:B:43:ARG:HE	1.84	0.43
1:D:447:SER:HB3	5:D:502:NAG:HN2	1.84	0.43
2:H:76(E):ASP:OD1	2:H:76(F):TRP:N	2.51	0.43
1:D:92:ASN:O	1:D:487:LYS:NZ	2.40	0.43
2:E:76(G):GLY:CA	2:E:77:VAL:HB	2.46	0.43
2:H:62:GLN:HG2	2:H:63:LEU:HD12	2.01	0.42
2:B:35:HIS:ND1	2:B:50:TRP:HB3	2.33	0.42
2:H:66:ARG:NH2	2:H:86:ASP:OD2	2.52	0.42
1:A:391:PHE:CD2	1:A:470:PRO:HG3	2.54	0.42
3:F:186:TYR:O	3:F:211:ARG:NH2	2.52	0.42
3:L:46:LEU:HA	3:L:57:ILE:HD13	2.01	0.42
1:A:422:GLN:HE21	1:A:438:PRO:HD3	1.84	0.42
3:F:115:VAL:HG22	3:F:136:LEU:HB3	2.01	0.42
1:D:368:ASP:CG	2:E:71:ARG:HH12	2.23	0.42
2:E:134:SER:OG	2:E:135:SER:N	2.52	0.42
2:E:153:PHE:HA	2:E:154:PRO:HA	1.74	0.42
1:G:260:LEU:HD12	1:G:451:GLY:HA3	2.01	0.42
3:L:88:GLN:NE2	3:L:90:PHE:O	2.53	0.42
1:A:474:ASN:OD1	1:A:476:LYS:HB2	2.18	0.42
3:F:42:PRO:HA	3:F:43:PRO:HD3	1.91	0.42
1:G:364:PRO:HD3	1:G:470:PRO:HG2	2.00	0.42
2:H:126:PRO:HB3	2:H:152:TYR:HB3	2.02	0.42
1:A:454:LEU:HA	1:A:470:PRO:HA	2.01	0.42
3:L:203:SER:HA	3:L:204:PRO:HD3	1.94	0.42
2:B:134:SER:OG	2:B:135:SER:N	2.53	0.42
1:A:252:LYS:HB3	1:A:254:VAL:HG23	2.02	0.41
3:F:124:GLN:O	3:F:127:SER:OG	2.32	0.41
1:G:109:ILE:HG13	1:G:428:GLN:HG3	2.01	0.41
1:G:296:CYS:HA	1:G:331:CYS:HA	2.01	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:133:PRO:HD2	2:B:220:PRO:HA	2.02	0.41
1:A:219:THR:HA	1:A:220:PRO:HD3	1.91	0.41
1:D:381:GLU:OE2	1:D:438:PRO:HA	2.20	0.41
3:L:58:PRO:HB2	3:L:60:ARG:HG2	2.03	0.41
1:A:385:CYS:HA	1:A:418:CYS:HA	2.02	0.41
1:G:437:PRO:HA	1:G:438:PRO:HD3	1.96	0.41
3:C:184:ALA:O	3:C:188:LYS:HG2	2.21	0.41
2:B:35:HIS:HA	2:B:50:TRP:HA	2.03	0.41
1:D:224:VAL:HG11	1:D:244:SER:HB2	2.03	0.41
3:F:36:GLN:HB2	3:F:46:LEU:HD11	2.02	0.41
1:G:95:MET:HB3	1:G:484:TYR:HA	2.03	0.41
1:G:369:LEU:O	1:G:373:MET:HG2	2.20	0.41
2:H:188:VAL:HG21	3:L:135:LEU:HD11	2.03	0.41
1:A:121:LYS:O	1:A:201:ILE:N	2.44	0.41
3:C:36:GLN:HB2	3:C:46:LEU:HD11	2.03	0.41
1:D:254:VAL:HG21	1:D:262:ASN:HB2	2.03	0.41
2:E:160:SER:O	2:E:204:ASN:N	2.42	0.41
2:H:153:PHE:HA	2:H:154:PRO:HA	1.78	0.41
1:D:357:LYS:NZ	1:D:466:GLU:OE2	2.44	0.40
3:L:49:ASP:O	3:L:51:SER:N	2.51	0.40
4:J:1:NAG:H61	4:J:2:NAG:HN2	1.86	0.40
1:D:334:ASN:HD21	1:D:337:LYS:HD3	1.87	0.40
1:D:475:ILE:H	1:D:475:ILE:HG12	1.71	0.40
1:G:234:ASN:OD1	1:G:235:GLY:N	2.54	0.40
3:L:6:GLN:HE21	3:L:6:GLN:HB3	1.70	0.40
1:A:259:LEU:HD13	1:A:449:ILE:HD13	2.03	0.40
2:B:51:ILE:HB	2:B:57:VAL:HG12	2.02	0.40
1:D:115:SER:O	1:D:117:GLN:N	2.55	0.40
1:A:359:ILE:HB	1:A:395:CYS:SG	2.61	0.40

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:68:THR:OG1	4:I:3:FUC:O4[3_545]	1.86	0.34

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	335/353 (95%)	311 (93%)	18 (5%)	6 (2%)	8	35
1	D	324/353 (92%)	309 (95%)	12 (4%)	3 (1%)	17	51
1	G	332/353 (94%)	306 (92%)	23 (7%)	3 (1%)	17	51
2	B	216/234 (92%)	195 (90%)	19 (9%)	2 (1%)	17	51
2	E	214/234 (92%)	193 (90%)	16 (8%)	5 (2%)	6	31
2	H	216/234 (92%)	194 (90%)	17 (8%)	5 (2%)	6	31
3	C	202/209 (97%)	178 (88%)	19 (9%)	5 (2%)	5	29
3	F	204/209 (98%)	176 (86%)	24 (12%)	4 (2%)	7	33
3	L	205/209 (98%)	176 (86%)	24 (12%)	5 (2%)	6	30
All	All	2248/2388 (94%)	2038 (91%)	172 (8%)	38 (2%)	9	36

All (38) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	G	354	ASN
2	H	76(E)	ASP
1	A	354	ASN
1	A	396	ILE
2	E	76(F)	TRP
2	H	168	SER
2	B	151	ASP
2	E	104	ASP
2	E	168	SER
1	G	116	LEU
3	L	148	TRP
3	L	201	LEU
1	A	398	ASN
2	B	220	PRO
3	C	76	LYS
3	C	201	LEU

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Mol	Chain	Res	Type
1	D	116	LEU
2	E	77	VAL
3	F	148	TRP
3	F	201	LEU
1	G	258	GLN
2	H	142	THR
3	F	175	LEU
3	L	138	ASN
1	A	116	LEU
1	A	258	GLN
1	D	258	GLN
3	L	174	SER
3	C	174	SER
3	C	175	LEU
3	C	212	GLY
3	F	15	PRO
3	L	15	PRO
1	A	397	GLY
2	H	97	PRO
1	D	472	GLY
2	E	154	PRO
2	H	154	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	A	304/311 (98%)	302 (99%)	2 (1%)	84 92
1	D	296/311 (95%)	291 (98%)	5 (2%)	60 80
1	G	304/311 (98%)	301 (99%)	3 (1%)	76 87
2	B	186/198 (94%)	183 (98%)	3 (2%)	62 81
2	E	184/198 (93%)	178 (97%)	6 (3%)	38 67
2	H	186/198 (94%)	184 (99%)	2 (1%)	73 86
3	C	180/182 (99%)	177 (98%)	3 (2%)	60 80

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
3	F	179/182 (98%)	176 (98%)	3 (2%)	60	80
3	L	180/182 (99%)	177 (98%)	3 (2%)	60	80
All	All	1999/2073 (96%)	1969 (98%)	30 (2%)	65	82

All (30) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	G	123	THR
1	G	287	HIS
1	G	331	CYS
2	H	71	ARG
2	H	118	VAL
3	L	23	CYS
3	L	84	LEU
3	L	154	LEU
1	A	103	GLN
1	A	276	ASN
2	B	4	LEU
2	B	71	ARG
2	B	82	PHE
3	C	74	ILE
3	C	84	LEU
3	C	136	LEU
1	D	119	CYS
1	D	208	ILE
1	D	255	VAL
1	D	292	VAL
1	D	467	THR
2	E	29	PHE
2	E	77	VAL
2	E	82	PHE
2	E	167	THR
2	E	191	VAL
2	E	196	LEU
3	F	136	LEU
3	F	196	VAL
3	F	211	ARG

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

Mol	Chain	Res	Type
3	F	30	ASN
3	F	89	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)

9 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	I	1	3,4	14,14,15	0.58	0	17,19,21	0.78	1 (5%)
4	NAG	I	2	4	14,14,15	0.34	0	17,19,21	0.67	1 (5%)
4	FUC	I	3	4	10,10,11	0.43	0	14,14,16	1.46	2 (14%)
4	NAG	J	1	3,4	14,14,15	0.27	0	17,19,21	0.70	1 (5%)
4	NAG	J	2	4	14,14,15	0.27	0	17,19,21	0.31	0
4	FUC	J	3	4	10,10,11	0.91	1 (10%)	14,14,16	1.41	2 (14%)
4	NAG	K	1	3,4	14,14,15	0.25	0	17,19,21	0.51	0
4	NAG	K	2	4	14,14,15	0.33	0	17,19,21	0.65	0
4	FUC	K	3	4	10,10,11	0.73	0	14,14,16	0.97	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	I	1	3,4	-	0/6/23/26	0/1/1/1
4	NAG	I	2	4	-	4/6/23/26	0/1/1/1
4	FUC	I	3	4	-	-	0/1/1/1
4	NAG	J	1	3,4	-	0/6/23/26	0/1/1/1
4	NAG	J	2	4	-	2/6/23/26	0/1/1/1
4	FUC	J	3	4	-	-	0/1/1/1
4	NAG	K	1	3,4	-	2/6/23/26	0/1/1/1
4	NAG	K	2	4	-	3/6/23/26	0/1/1/1
4	FUC	K	3	4	1/1/4/5	-	0/1/1/1

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	J	3	FUC	O5-C1	-2.26	1.40	1.43

All (7) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	J	3	FUC	C1-O5-C5	3.34	120.34	112.78
4	I	3	FUC	C3-C4-C5	2.83	114.18	109.77
4	I	2	NAG	C1-O5-C5	2.33	115.35	112.19
4	J	1	NAG	C1-O5-C5	2.33	115.35	112.19
4	I	3	FUC	O5-C1-C2	-2.20	107.37	110.77
4	J	3	FUC	O5-C1-C2	2.10	114.01	110.77
4	I	1	NAG	O4-C4-C5	-2.01	104.31	109.30

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
4	K	3	FUC	C1

All (11) torsion outliers are listed below:

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

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Mol	Chain	Res	Type	Atoms
4	I	2	NAG	C4-C5-C6-O6
4	I	2	NAG	C1-C2-N2-C7
4	K	2	NAG	C3-C2-N2-C7
4	I	2	NAG	C3-C2-N2-C7

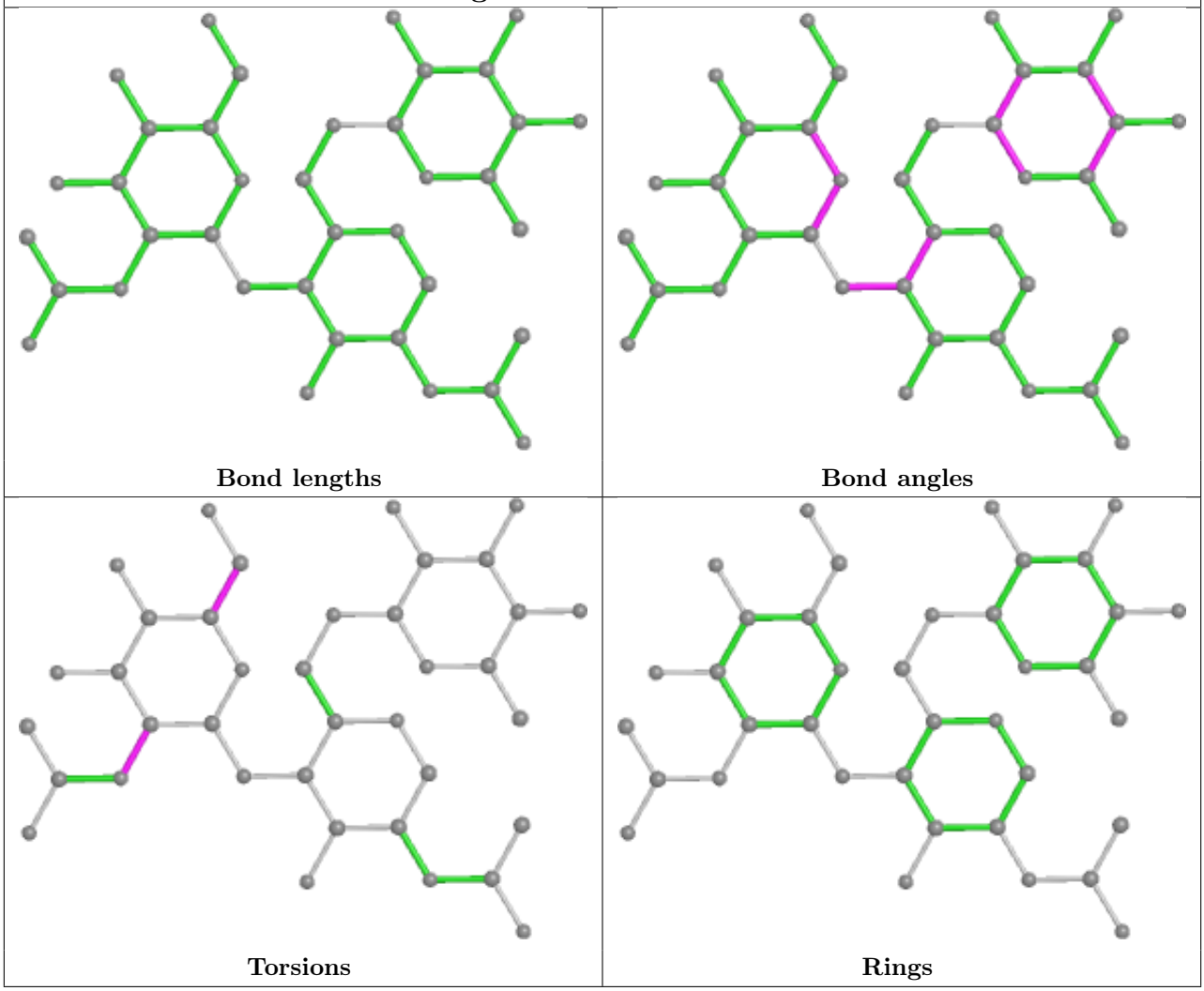
There are no ring outliers.

5 monomers are involved in 3 short contacts:

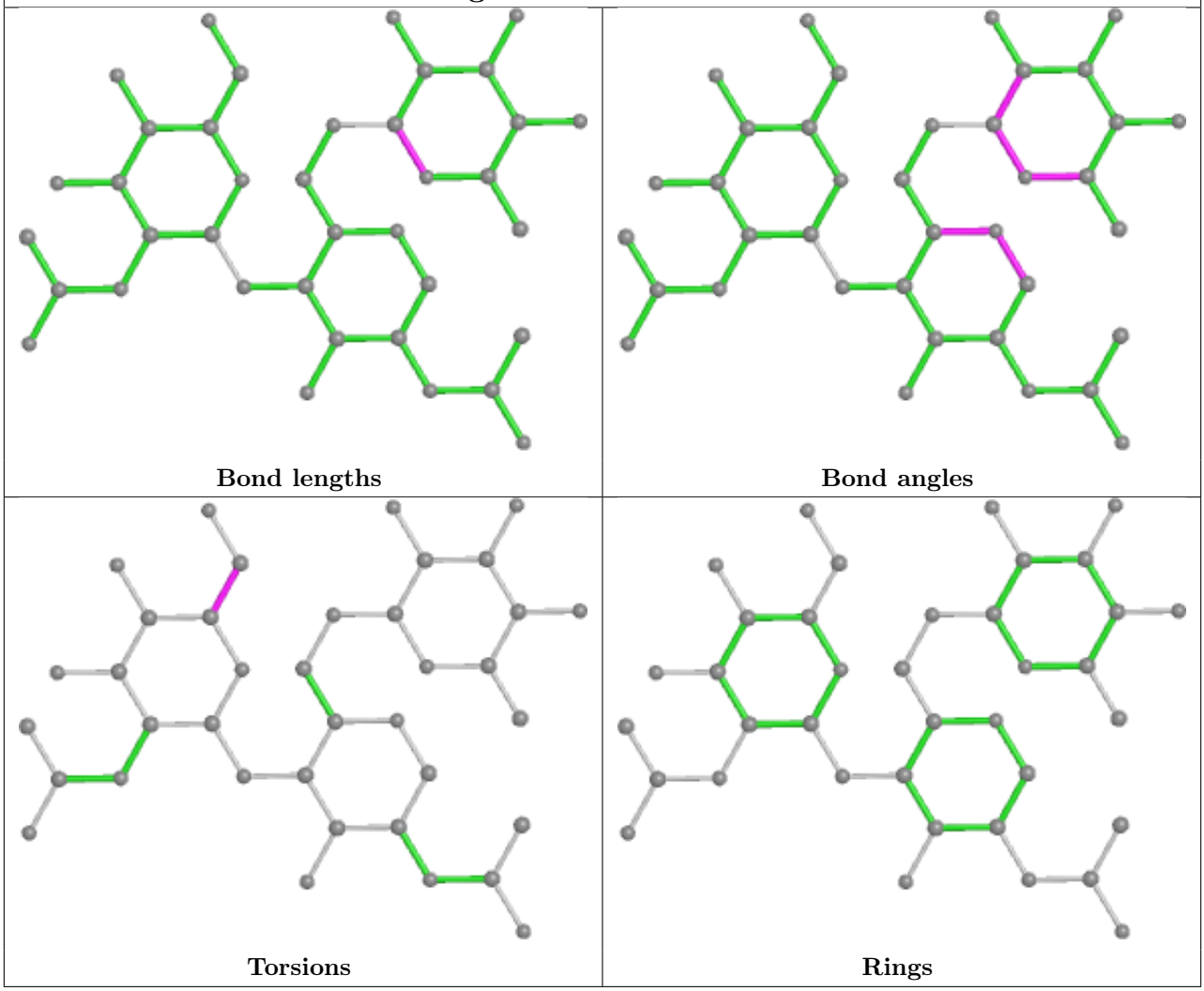
Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	K	3	FUC	1	0
4	J	1	NAG	1	0
4	I	3	FUC	0	1
4	K	2	NAG	1	0
4	J	2	NAG	1	0

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

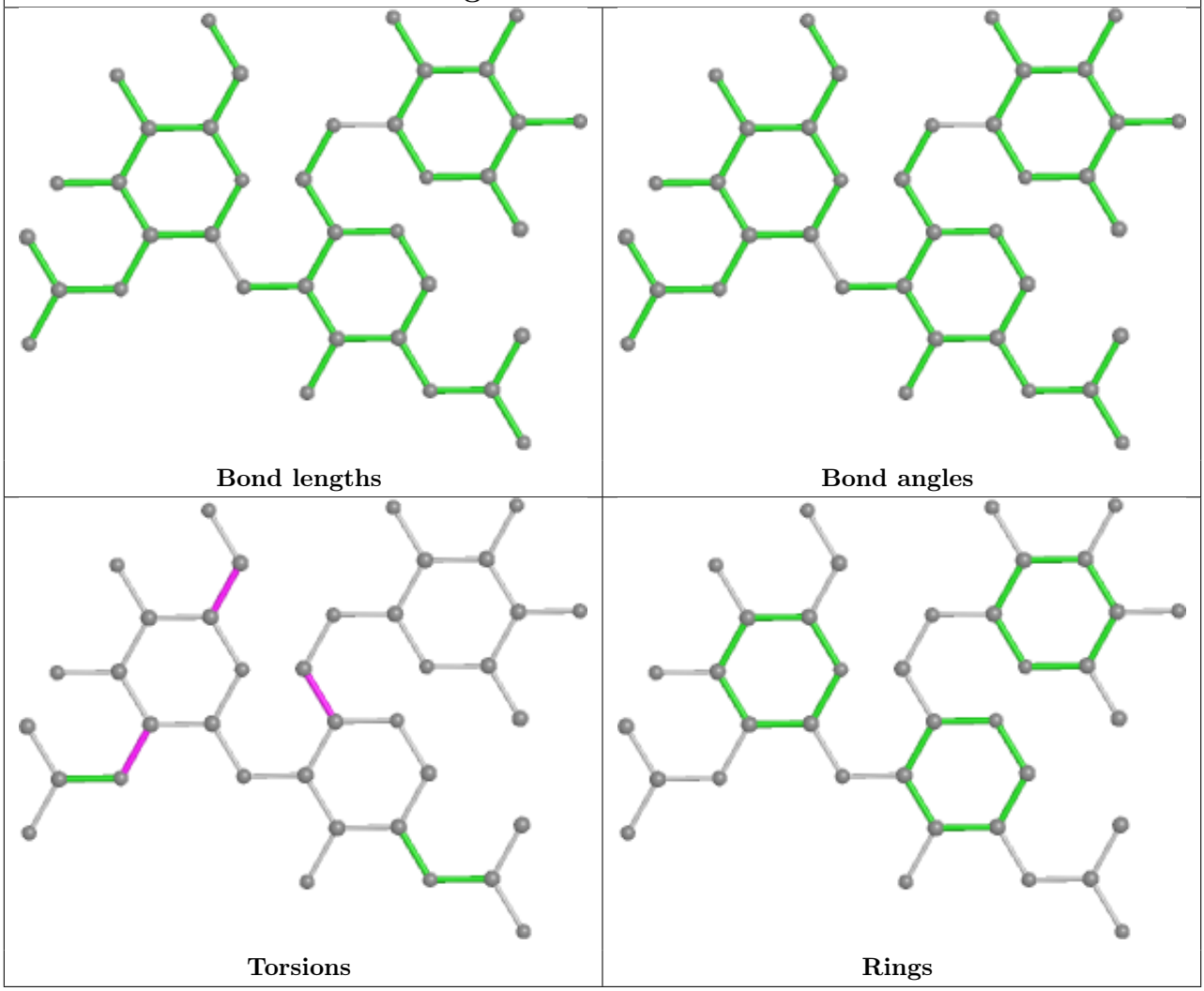
Oligosaccharide Chain I



Oligosaccharide Chain J



Oligosaccharide Chain K



5.6 Ligand geometry (i)

18 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	502	1	14,14,15	0.31	0	17,19,21	0.45	0
5	NAG	G	502	1	14,14,15	0.23	0	17,19,21	0.46	0
5	NAG	G	501	1	14,14,15	0.20	0	17,19,21	0.38	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
5	NAG	A	506	1	14,14,15	0.26	0	17,19,21	0.44	0
5	NAG	D	502	1	14,14,15	0.22	0	17,19,21	0.44	0
5	NAG	D	503	1	14,14,15	0.24	0	17,19,21	0.42	0
5	NAG	A	503	1	14,14,15	0.25	0	17,19,21	0.42	0
5	NAG	A	505	1	14,14,15	0.19	0	17,19,21	0.44	0
5	NAG	G	504	1	14,14,15	0.24	0	17,19,21	0.36	0
5	NAG	A	501	1	14,14,15	0.19	0	17,19,21	0.42	0
5	NAG	D	505	1	14,14,15	0.29	0	17,19,21	0.47	0
5	NAG	D	504	1	14,14,15	0.28	0	17,19,21	0.43	0
5	NAG	G	506	1	14,14,15	0.24	0	17,19,21	0.46	0
5	NAG	G	505	1	14,14,15	0.27	0	17,19,21	0.41	0
5	NAG	D	501	1	14,14,15	0.20	0	17,19,21	0.39	0
5	NAG	G	503	1	14,14,15	0.23	0	17,19,21	0.39	0
5	NAG	A	507	1	14,14,15	0.23	0	17,19,21	0.40	0
5	NAG	A	504	1	14,14,15	0.24	0	17,19,21	0.44	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	A	502	1	-	0/6/23/26	0/1/1/1
5	NAG	G	502	1	-	2/6/23/26	0/1/1/1
5	NAG	G	501	1	-	2/6/23/26	0/1/1/1
5	NAG	A	506	1	-	4/6/23/26	0/1/1/1
5	NAG	D	502	1	-	2/6/23/26	0/1/1/1
5	NAG	D	503	1	-	1/6/23/26	0/1/1/1
5	NAG	A	503	1	-	2/6/23/26	0/1/1/1
5	NAG	A	505	1	-	0/6/23/26	0/1/1/1
5	NAG	G	504	1	-	2/6/23/26	0/1/1/1
5	NAG	A	501	1	-	2/6/23/26	0/1/1/1
5	NAG	D	505	1	-	2/6/23/26	0/1/1/1
5	NAG	D	504	1	-	2/6/23/26	0/1/1/1
5	NAG	G	506	1	-	4/6/23/26	0/1/1/1
5	NAG	G	505	1	-	3/6/23/26	0/1/1/1
5	NAG	D	501	1	-	2/6/23/26	0/1/1/1
5	NAG	G	503	1	-	2/6/23/26	0/1/1/1
5	NAG	A	507	1	-	4/6/23/26	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	NAG	A	504	1	-	2/6/23/26	0/1/1/1

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (38) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	G	502	NAG	O5-C5-C6-O6
5	A	504	NAG	O5-C5-C6-O6
5	A	503	NAG	O5-C5-C6-O6
5	D	505	NAG	O5-C5-C6-O6
5	A	501	NAG	O5-C5-C6-O6
5	A	506	NAG	O5-C5-C6-O6
5	D	501	NAG	O5-C5-C6-O6
5	G	501	NAG	O5-C5-C6-O6
5	A	503	NAG	C4-C5-C6-O6
5	A	501	NAG	C4-C5-C6-O6
5	A	504	NAG	C4-C5-C6-O6
5	A	506	NAG	C4-C5-C6-O6
5	D	501	NAG	C4-C5-C6-O6
5	G	505	NAG	C8-C7-N2-C2
5	G	505	NAG	O7-C7-N2-C2
5	G	506	NAG	C8-C7-N2-C2
5	G	506	NAG	O7-C7-N2-C2
5	A	506	NAG	C8-C7-N2-C2
5	A	506	NAG	O7-C7-N2-C2
5	A	507	NAG	C8-C7-N2-C2
5	A	507	NAG	O7-C7-N2-C2
5	D	504	NAG	C8-C7-N2-C2
5	D	504	NAG	O7-C7-N2-C2
5	G	506	NAG	O5-C5-C6-O6
5	G	501	NAG	C4-C5-C6-O6
5	G	502	NAG	C4-C5-C6-O6
5	G	503	NAG	O5-C5-C6-O6
5	D	505	NAG	C4-C5-C6-O6
5	A	507	NAG	O5-C5-C6-O6
5	G	504	NAG	O5-C5-C6-O6
5	G	503	NAG	C4-C5-C6-O6
5	G	506	NAG	C4-C5-C6-O6
5	D	502	NAG	C4-C5-C6-O6

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Mol	Chain	Res	Type	Atoms
5	A	507	NAG	C4-C5-C6-O6
5	D	503	NAG	O5-C5-C6-O6
5	D	502	NAG	O5-C5-C6-O6
5	G	504	NAG	C4-C5-C6-O6
5	G	505	NAG	C4-C5-C6-O6

There are no ring outliers.

3 monomers are involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	D	502	NAG	1	0
5	D	503	NAG	1	0
5	A	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	A	341/353 (96%)	0.60	32 (9%)	8	11	86, 142, 228, 331	0
1	D	330/353 (93%)	0.45	25 (7%)	13	17	92, 148, 217, 300	0
1	G	340/353 (96%)	0.68	51 (15%)	2	3	93, 151, 224, 305	0
2	B	222/234 (94%)	0.37	17 (7%)	13	16	77, 145, 225, 262	0
2	E	220/234 (94%)	0.40	20 (9%)	9	12	86, 128, 221, 268	0
2	H	222/234 (94%)	0.36	19 (8%)	10	13	82, 133, 224, 285	0
3	C	206/209 (98%)	0.20	7 (3%)	45	48	69, 140, 212, 269	0
3	F	206/209 (98%)	0.45	13 (6%)	20	23	95, 143, 202, 265	0
3	L	207/209 (99%)	0.10	7 (3%)	45	48	67, 114, 173, 230	0
All	All	2294/2388 (96%)	0.43	191 (8%)	11	14	67, 141, 219, 331	0

All (191) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	E	4	LEU	7.8
1	A	224	VAL	7.0
2	E	134	SER	5.8
1	G	430	THR	5.2
1	A	300	SER	4.7
1	D	473	GLY	4.7
3	C	67	GLY	4.7
2	H	4	LEU	4.5
1	G	492	GLU	4.4
1	G	359	ILE	4.4
1	G	345	VAL	4.3
2	B	220	PRO	4.3
1	G	474	ASN	4.1
1	G	87	GLU	4.1
1	D	463	THR	4.0

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Mol	Chain	Res	Type	RSRZ
1	G	326	ILE	4.0
1	A	326	ILE	3.9
1	D	232	ASN	3.8
2	E	104	ASP	3.8
1	G	390	LEU	3.8
3	C	158	ASN	3.8
1	A	50	THR	3.7
1	G	338	TRP	3.6
1	G	490	GLN	3.5
1	D	301	ASN	3.5
2	H	86	ASP	3.5
2	E	205	VAL	3.5
1	G	472	GLY	3.5
2	H	5	VAL	3.5
3	F	61	PHE	3.5
2	B	5	VAL	3.4
1	G	491	ILE	3.4
1	G	393	ASN	3.4
1	G	202	LYS	3.4
3	F	195	GLU	3.4
1	A	223	TYR	3.3
1	G	360	ILE	3.3
1	G	274	SER	3.3
3	L	192	TYR	3.3
2	B	154	PRO	3.2
2	E	98	SER	3.2
1	A	267	GLU	3.2
1	D	300	SER	3.2
2	E	97	PRO	3.2
1	G	346	THR	3.2
2	H	201	TYR	3.2
3	C	118	PHE	3.1
1	D	87	GLU	3.1
1	A	225	ILE	3.1
1	A	256	SER	3.1
3	F	32	LEU	3.1
1	A	299	PRO	3.1
2	B	201	TYR	3.1
2	E	7	SER	3.1
3	F	206	THR	3.1
1	D	86	LEU	3.1
1	G	300	SER	3.0

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Mol	Chain	Res	Type	RSRZ
1	A	199	SER	3.0
1	D	474	ASN	3.0
2	B	26	GLY	3.0
1	D	489	VAL	3.0
1	G	93	PHE	3.0
2	B	97	PRO	3.0
1	A	489	VAL	2.9
1	G	75	VAL	2.9
2	E	25	SER	2.9
1	G	45	TRP	2.9
1	G	389	GLN	2.9
1	A	474	ASN	2.9
1	G	325	ASP	2.9
1	G	394	THR	2.9
1	A	49	ASP	2.9
1	G	242	VAL	2.8
1	G	224	VAL	2.8
2	B	77	VAL	2.8
2	H	143	ALA	2.8
1	D	354	ASN	2.8
1	G	50	THR	2.8
2	E	140	GLY	2.8
3	C	136	LEU	2.8
2	B	133	PRO	2.8
2	H	94	ARG	2.8
2	B	76(G)	GLY	2.8
1	A	488	VAL	2.8
2	H	6	GLU	2.8
1	G	44	VAL	2.7
2	H	206	ASN	2.7
1	A	471	GLY	2.7
1	G	276	ASN	2.7
1	G	46	LYS	2.7
1	D	438	PRO	2.7
2	E	5	VAL	2.7
2	E	201	TYR	2.7
1	G	86	LEU	2.7
2	E	117	VAL	2.6
1	A	79	PRO	2.6
1	D	50	THR	2.6
1	G	219	THR	2.6
1	G	121	LYS	2.6

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Mol	Chain	Res	Type	RSRZ
1	G	477	ASP	2.6
1	G	358	THR	2.6
3	F	193	ALA	2.5
1	G	200	VAL	2.5
1	A	461	ASN	2.5
1	A	203	GLN	2.5
1	A	330	TYR	2.5
1	D	344	GLN	2.5
1	A	402	LYS	2.5
1	G	85	HIS	2.5
2	H	101	HIS	2.5
2	H	76(D)	PRO	2.4
1	G	199	SER	2.4
2	H	7	SER	2.4
2	E	82(C)	LEU	2.4
1	A	443	ILE	2.4
1	D	45	TRP	2.4
2	H	30	ARG	2.4
1	G	431	GLY	2.4
1	D	272	ILE	2.3
1	A	379	ARG	2.3
1	D	224	VAL	2.3
2	E	216	LYS	2.3
1	D	270	ILE	2.3
3	F	31	SER	2.3
2	B	42	GLY	2.3
1	G	344	GLN	2.3
1	G	84	ILE	2.3
1	A	219	THR	2.3
1	A	327	ARG	2.3
3	C	1	GLU	2.3
3	F	77	VAL	2.3
1	A	403	GLY	2.2
1	D	458	GLY	2.2
1	G	376	PHE	2.2
1	A	430	THR	2.2
1	A	242	VAL	2.2
2	B	14	PRO	2.2
1	A	264	SER	2.2
1	G	466	GLU	2.2
3	F	46	LEU	2.2
1	A	383	PHE	2.2

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Mol	Chain	Res	Type	RSRZ
2	E	188	VAL	2.2
3	C	101	ILE	2.2
1	G	283	THR	2.2
3	F	25	ALA	2.2
3	F	34	TRP	2.2
2	H	96	GLY	2.2
1	D	117	GLN	2.2
3	L	21	LEU	2.2
1	G	226	LEU	2.2
1	G	361	PHE	2.2
2	H	76(E)	ASP	2.2
2	H	52(A)	GLY	2.2
2	B	144	ALA	2.2
1	G	49	ASP	2.2
2	E	94	ARG	2.2
1	G	223	TYR	2.1
3	L	29	GLY	2.1
1	A	413	THR	2.1
2	H	221	LYS	2.1
2	E	108	GLN	2.1
1	A	243	SER	2.1
2	B	13	LYS	2.1
1	D	359	ILE	2.1
1	D	471	GLY	2.1
3	L	186	TYR	2.1
3	L	76	LYS	2.1
1	D	242	VAL	2.1
2	B	20	ILE	2.1
3	F	69	ASP	2.1
1	G	287	HIS	2.1
2	B	90	TYR	2.1
3	C	117	ILE	2.1
3	L	11	LEU	2.1
1	D	365	SER	2.1
3	F	89	GLN	2.1
2	H	108	GLN	2.0
1	G	228	CYS	2.0
2	B	116	VAL	2.0
1	D	361	PHE	2.0
2	H	191	VAL	2.0
1	G	253	PRO	2.0
1	D	472	GLY	2.0

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Mol	Chain	Res	Type	RSRZ
3	F	135	LEU	2.0
2	H	127	SER	2.0
3	L	193	ALA	2.0
2	E	18	VAL	2.0
2	B	6	GLU	2.0
2	E	103	GLY	2.0
1	A	358	THR	2.0
2	E	196	LEU	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)

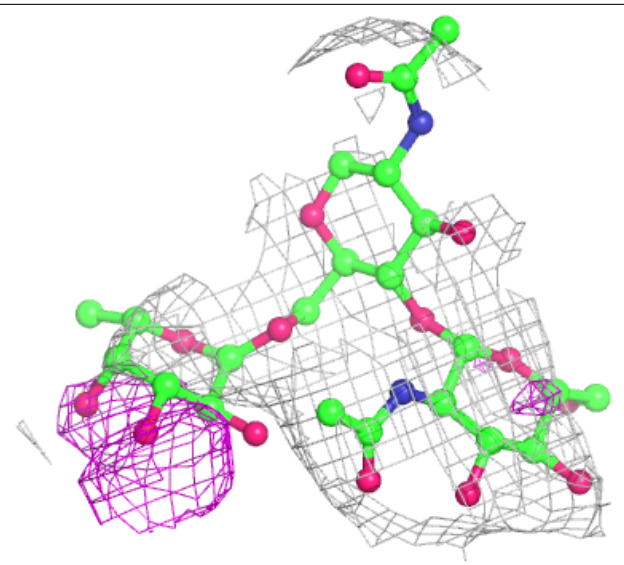
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

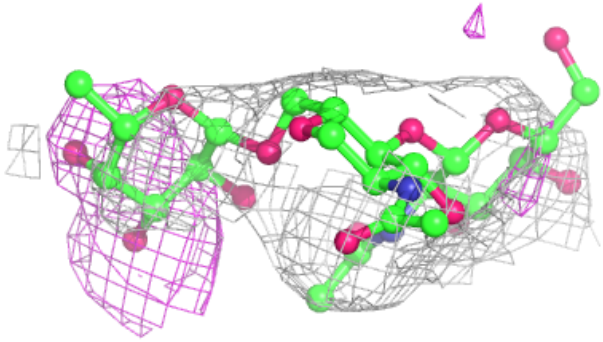
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
4	FUC	I	3	10/11	0.76	0.82	139,161,170,180	0
4	NAG	I	2	14/15	0.77	0.40	145,151,158,159	0
4	NAG	J	2	14/15	0.78	0.29	164,167,172,174	0
4	NAG	K	1	14/15	0.81	0.26	164,175,184,199	0
4	NAG	I	1	14/15	0.87	0.19	100,114,129,133	0
4	FUC	K	3	10/11	0.87	0.26	159,165,169,173	0
4	NAG	K	2	14/15	0.88	0.42	217,223,230,232	0
4	NAG	J	1	14/15	0.90	0.28	124,140,151,155	0
4	FUC	J	3	10/11	0.94	0.16	156,161,162,162	0

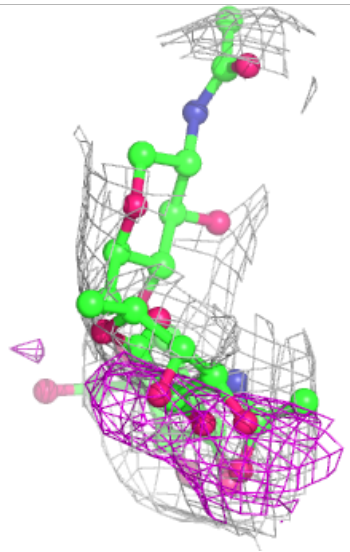
The following is a graphical depiction of the model fit to experimental electron density for oligosaccharide. Each fit is shown from different orientation to approximate a three-dimensional view.

Electron density around Chain I:

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

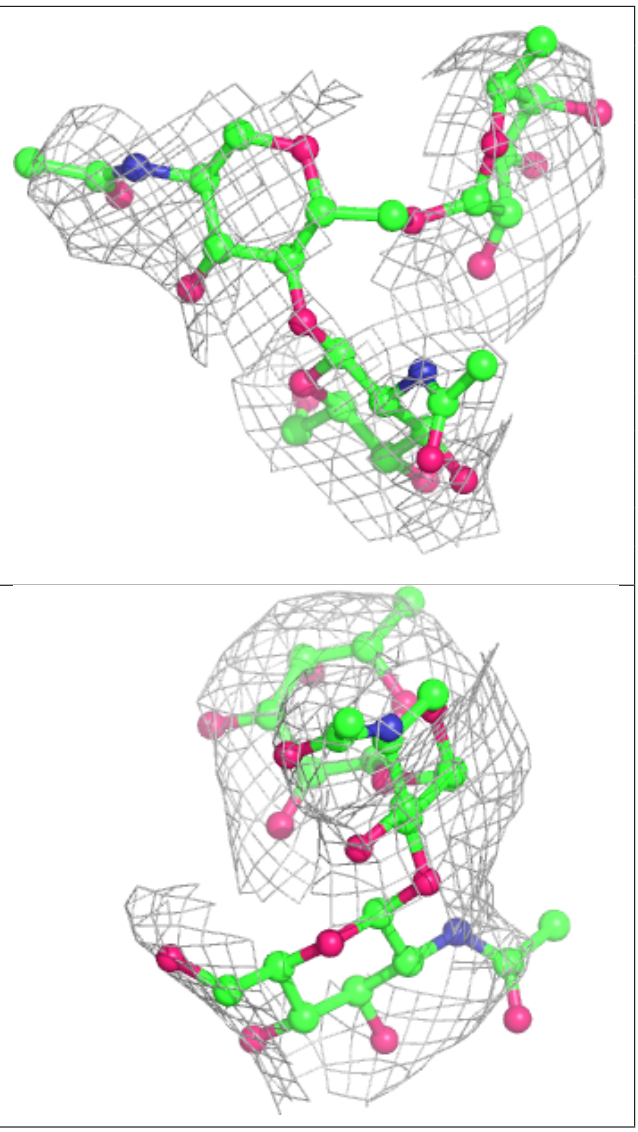






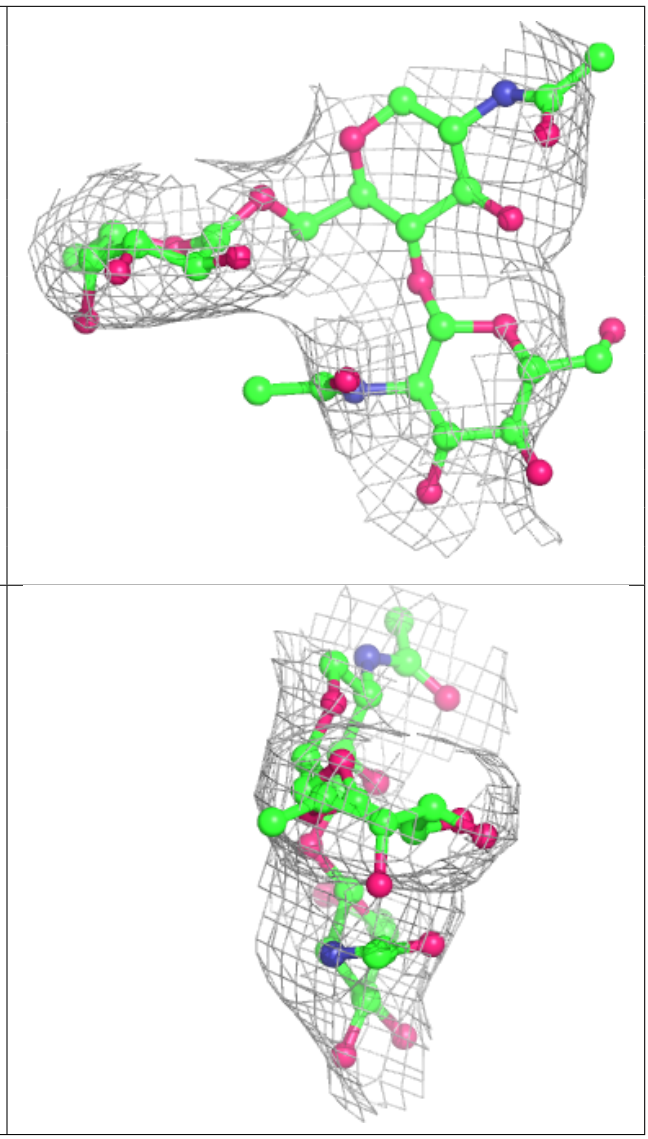
Electron density around Chain J:

$2mF_o$-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)



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
5	NAG	G	506	14/15	0.68	0.49	130,149,155,160	0
5	NAG	G	504	14/15	0.74	0.41	152,171,173,176	0
5	NAG	A	507	14/15	0.74	0.23	121,135,143,145	0
5	NAG	D	505	14/15	0.79	0.32	120,132,135,137	0
5	NAG	G	501	14/15	0.81	0.27	113,121,124,125	0
5	NAG	D	503	14/15	0.82	0.26	137,156,159,161	0
5	NAG	A	504	14/15	0.82	0.24	136,151,170,175	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
5	NAG	D	504	14/15	0.85	0.24	121,127,131,132	0
5	NAG	D	501	14/15	0.85	0.47	138,144,146,147	0
5	NAG	A	506	14/15	0.86	0.25	100,109,113,114	0
5	NAG	A	502	14/15	0.86	0.37	143,155,165,167	0
5	NAG	A	505	14/15	0.87	0.42	120,133,138,145	0
5	NAG	A	501	14/15	0.88	0.34	123,134,138,138	0
5	NAG	G	502	14/15	0.89	0.34	131,144,150,152	0
5	NAG	D	502	14/15	0.90	0.24	113,119,136,139	0
5	NAG	G	503	14/15	0.90	0.27	112,124,129,131	0
5	NAG	G	505	14/15	0.94	0.20	107,116,125,126	0
5	NAG	A	503	14/15	0.95	0.14	93,98,100,105	0

6.5 Other polymers (i)

There are no such residues in this entry.