Full wwPDB X-ray Structure Validation Report (i)

Jun 12, 2025 – 02:15 PM JST

PDB ID	:	9JQV / pdb_00009jqv
Title	:	The crystal structure of SFTSV Gn and SD12 antibody complex
Authors	:	Shi, W.F.; Quan, C.S.; Qi, J.X.
Deposited on	:	2024-09-28
Resolution	:	2.40 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:

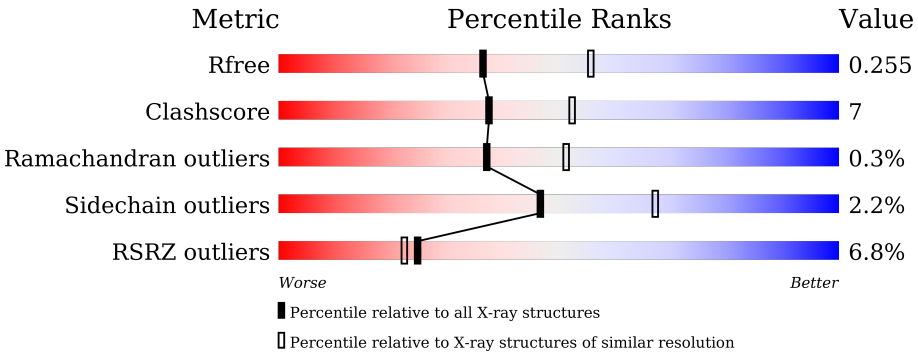
MolProbity	:	4-5-2 with Phenix2.0rc1
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	2.0rc1
EDS	:	3.0
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20231227.v01 (using entries in the PDB archive December 27th 2023)
CCP4	:	9.0.006 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.43.1

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 2.40 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}	164625	4642 (2.40-2.40)
Clashscore	180529	5218 (2.40-2.40)
Ramachandran outliers	177936	5158 (2.40-2.40)
Sidechain outliers	177891	5159 (2.40-2.40)
RSRZ outliers	164620	4642 (2.40-2.40)

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

Mol	Chain	Length	Quality of chain
1	A	325	6% 86% 12%
1	B	325	7% 77% 19%
2	C	223	4% 78% 18%
2	H	223	7% 78% 17%
3	D	214	8% 82% 16%
3	L	214	7% 78% 20%

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Mol	Chain	Length	Quality of chain
4	E	2	100%
5	F	3	67% 33%
5	G	3	67% 33%

2 Entry composition (i)

There are 7 unique types of molecules in this entry. The entry contains 11809 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 Envelopment polyprotein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	321	Total	C	N	O	S	0	1	0
			2475	1547	433	469	26			
1	B	312	Total	C	N	O	S	0	0	0
			2406	1508	421	451	26			

There are 12 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	339	HIS	-	expression tag	UNP A0A1S6K8S9
A	340	HIS	-	expression tag	UNP A0A1S6K8S9
A	341	HIS	-	expression tag	UNP A0A1S6K8S9
A	342	HIS	-	expression tag	UNP A0A1S6K8S9
A	343	HIS	-	expression tag	UNP A0A1S6K8S9
A	344	HIS	-	expression tag	UNP A0A1S6K8S9
B	339	HIS	-	expression tag	UNP A0A1S6K8S9
B	340	HIS	-	expression tag	UNP A0A1S6K8S9
B	341	HIS	-	expression tag	UNP A0A1S6K8S9
B	342	HIS	-	expression tag	UNP A0A1S6K8S9
B	343	HIS	-	expression tag	UNP A0A1S6K8S9
B	344	HIS	-	expression tag	UNP A0A1S6K8S9

- Molecule 2 is a protein called SD12 heavy chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	H	214	Total	C	N	O	S	0	0	0
			1598	1007	267	318	6			
2	C	214	Total	C	N	O	S	0	0	0
			1598	1007	267	318	6			

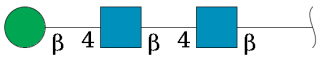
- Molecule 3 is a protein called SD12 light chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	L	211	Total	C	N	O	S	0	0	0
			1639	1026	272	336	5			
3	D	211	Total	C	N	O	S	0	0	0
			1636	1024	271	336	5			

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

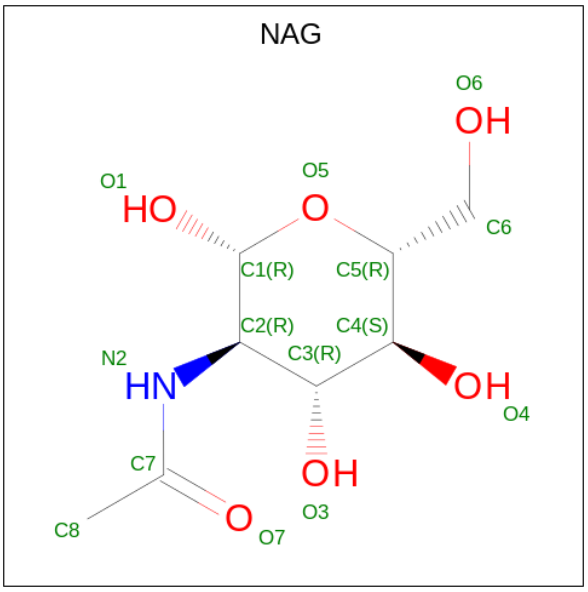
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
4	E	2	Total	C	N	O	0	0	0
			28	16	2	10			

- Molecule 5 is an oligosaccharide called beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose.



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

- Molecule 6 is 2-acetamido-2-deoxy-beta-D-glucopyranose (CCD ID: NAG) (formula: $C_8H_{15}NO_6$) (labeled as "Ligand of Interest" by depositor).



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

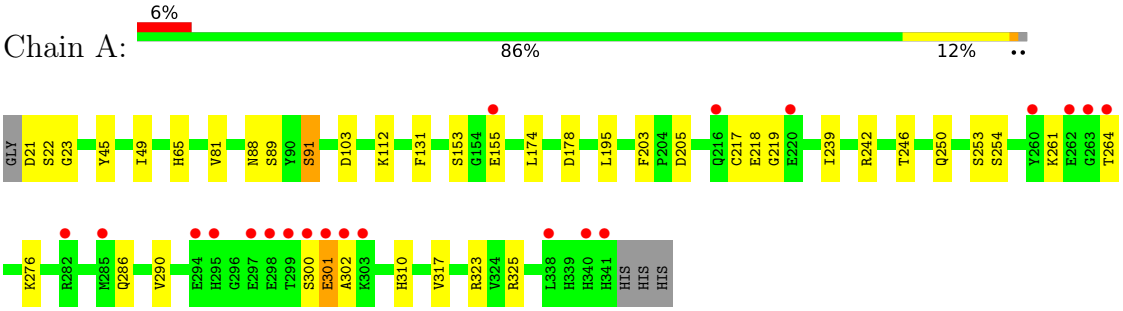
- Molecule 7 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
7	A	82	Total O 82 82	0	0
7	H	70	Total O 70 70	0	0
7	L	46	Total O 46 46	0	0
7	B	51	Total O 51 51	0	0
7	C	45	Total O 45 45	0	0
7	D	43	Total O 43 43	0	0

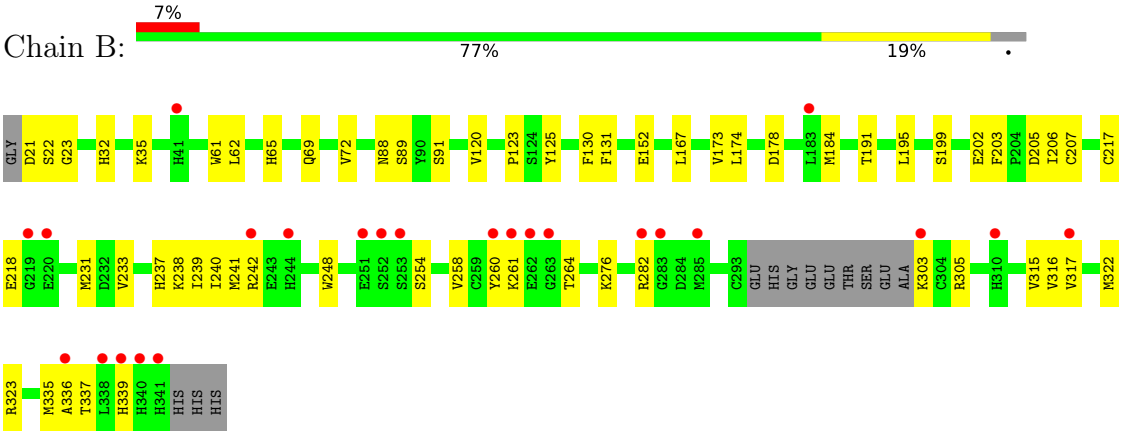
3 Residue-property plots (i)

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.

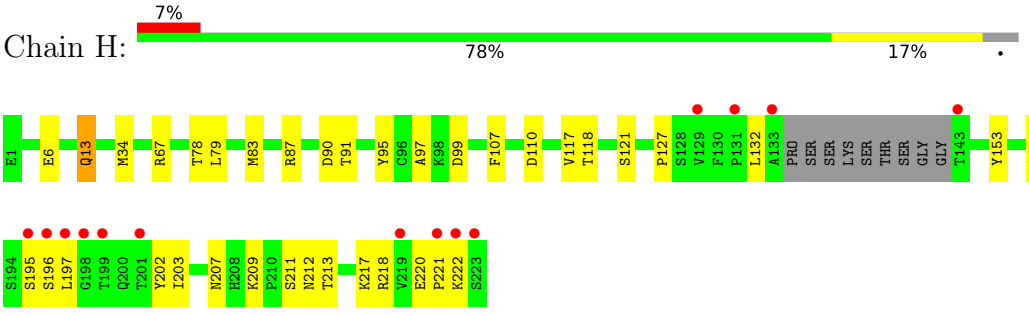
• Molecule 1: Envelopment polyprotein



• Molecule 1: Envelopment polyprotein

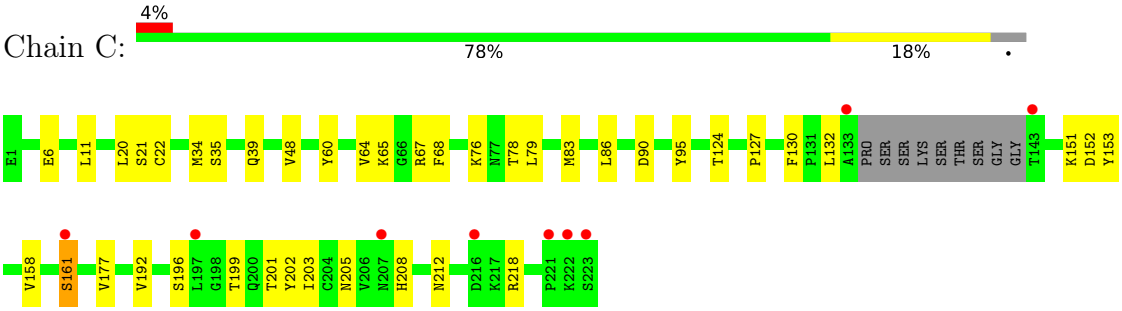


• Molecule 2: SD12 heavy chain



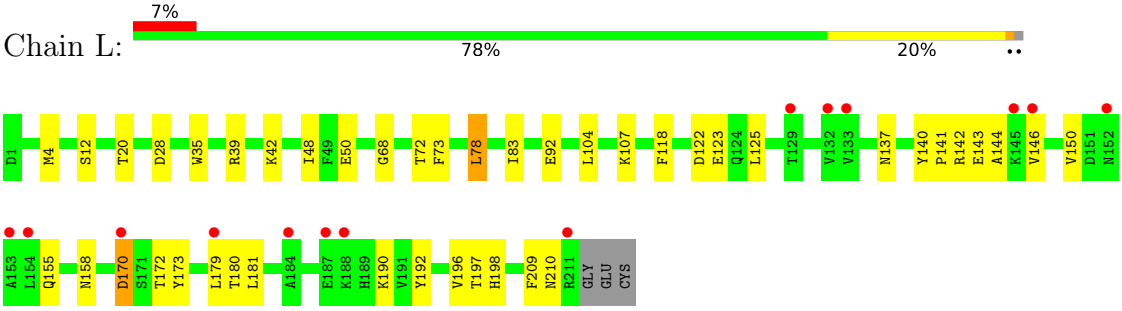
• Molecule 2: SD12 heavy chain

Chain C:



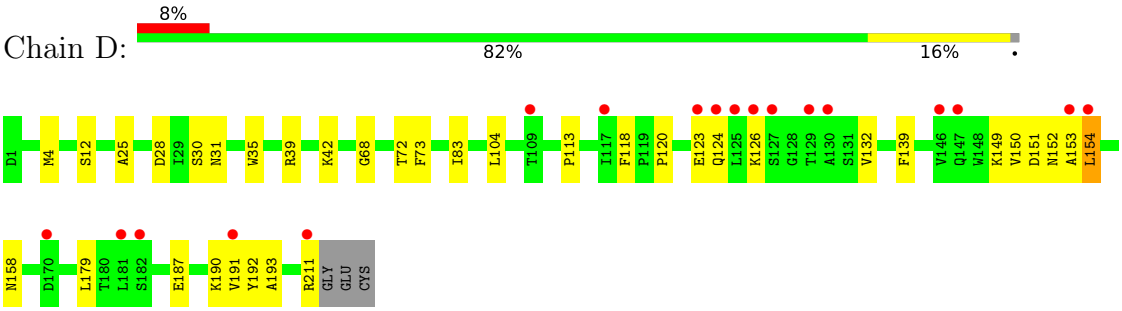
• Molecule 3: SD12 light chain

Chain L:



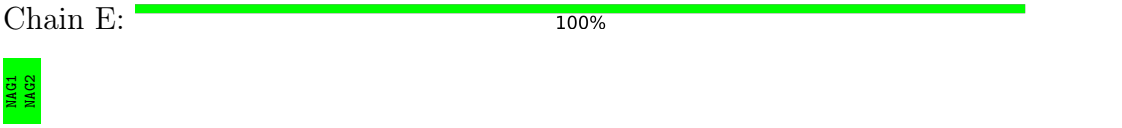
• Molecule 3: SD12 light chain

Chain D:



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

Chain E:



• Molecule 5: beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain F:

• Molecule 5: beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain G:

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	96.06Å 82.34Å 125.29Å 90.00° 104.31° 90.00°	Depositor
Resolution (Å)	45.92 – 2.40 45.92 – 2.40	Depositor EDS
% Data completeness (in resolution range)	89.6 (45.92-2.40) 89.8 (45.92-2.40)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.09 (at 2.39Å)	Xtriage
Refinement program	PHENIX 1.19.2_4158	Depositor
R, R_{free}	0.225 , 0.255 0.225 , 0.255	Depositor DCC
R_{free} test set	3746 reflections (5.05%)	wwPDB-VP
Wilson B-factor (Å^2)	37.8	Xtriage
Anisotropy	0.180	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.34 , 45.0	EDS
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.92	EDS
Total number of atoms	11809	wwPDB-VP
Average B, all atoms (Å^2)	47.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.02% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

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

5 Model quality

5.1 Standard geometry

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

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\#\|Z\| > 5$	RMSZ	$\#\|Z\| > 5$
1	A	0.15	0/2543	0.39	0/3430
1	B	0.18	0/2468	0.39	0/3326
2	C	0.16	0/1634	0.37	0/2221
2	H	0.15	0/1634	0.38	0/2221
3	D	0.23	0/1670	0.41	0/2269
3	L	0.15	0/1673	0.36	0/2272
All	All	0.17	0/11622	0.38	0/15739

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

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	2475	0	2349	24	0
1	B	2406	0	2306	37	0
2	C	1598	0	1556	23	0
2	H	1598	0	1556	23	0
3	D	1636	0	1576	26	0
3	L	1639	0	1585	27	0
4	E	28	0	25	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
5	F	39	0	34	0	0
5	G	39	0	34	0	0
6	B	14	0	13	0	0
7	A	82	0	0	4	0
7	B	51	0	0	1	0
7	C	45	0	0	1	0
7	D	43	0	0	0	0
7	H	70	0	0	2	0
7	L	46	0	0	0	0
All	All	11809	0	11034	156	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 7.

All (156) 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:D:149:LYS:HB2	3:D:193:ALA:HB3	1.48	0.96
1:B:282:ARG:HG3	1:B:305:ARG:HG3	1.59	0.83
3:D:190:LYS:HA	3:D:211:ARG:HG2	1.71	0.73
2:H:67:ARG:NH2	2:H:90:ASP:OD2	2.21	0.72
1:B:120:VAL:HA	1:B:335:MET:HE1	1.72	0.72
3:D:187:GLU:OE1	3:D:211:ARG:NH1	2.23	0.72
1:B:62:LEU:HD21	1:B:130:PHE:HB2	1.72	0.72
1:B:303:LYS:N	7:B:502:HOH:O	2.22	0.71
1:B:89:SER:OG	1:B:178:ASP:OD2	2.09	0.71
2:H:83:MET:HE1	2:H:117:VAL:HG21	1.74	0.68
2:C:48:VAL:HG13	2:C:64:VAL:HG21	1.76	0.68
1:B:205:ASP:O	1:B:339:HIS:N	2.28	0.66
3:D:39:ARG:HE	3:D:42:LYS:HZ2	1.44	0.65
3:D:39:ARG:HH21	3:D:42:LYS:HZ1	1.42	0.65
2:C:201:THR:HG23	2:C:218:ARG:CZ	2.27	0.65
1:B:202:GLU:O	1:B:242:ARG:NH2	2.30	0.64
3:L:144:ALA:HB2	3:L:198:HIS:HD2	1.61	0.64
1:B:199:SER:OG	1:B:240:ILE:O	2.15	0.63
1:B:254:SER:HB2	1:B:276:LYS:HD3	1.80	0.62
2:H:197:LEU:HD13	2:H:221:PRO:HG3	1.80	0.62
2:C:67:ARG:NH2	2:C:90:ASP:OD2	2.32	0.62
3:D:152:ASN:ND2	3:D:152:ASN:O	2.33	0.62
2:H:212:ASN:ND2	7:H:302:HOH:O	2.32	0.61
2:H:127:PRO:HB3	2:H:153:TYR:HB3	1.83	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:L:78:LEU:HD21	3:L:104:LEU:HD21	1.83	0.61
1:A:195:LEU:HB3	1:A:239:ILE:HD13	1.81	0.60
1:A:286:GLN:O	1:A:290:VAL:HG23	2.01	0.59
3:D:149:LYS:CB	3:D:193:ALA:HB3	2.29	0.59
3:L:146:VAL:HG22	3:L:196:VAL:HG22	1.83	0.59
1:A:250:GLN:N	1:A:250:GLN:OE1	2.36	0.58
2:H:67:ARG:HH22	2:H:90:ASP:CG	2.13	0.57
1:A:203:PHE:CZ	1:A:242:ARG:HG2	2.39	0.57
1:A:246:THR:HG22	1:A:317:VAL:HG22	1.87	0.56
1:B:88:ASN:HB3	1:B:91:SER:OG	2.05	0.56
1:A:310[A]:HIS:CE1	7:A:401:HOH:O	2.59	0.55
2:C:6:GLU:OE2	2:C:95:TYR:HA	2.06	0.55
2:H:67:ARG:HD3	7:H:335:HOH:O	2.07	0.55
1:A:88:ASN:HB3	1:A:91:SER:HB3	1.87	0.55
1:B:21:ASP:O	1:B:23:GLY:N	2.40	0.55
1:A:323:ARG:HH11	1:A:323:ARG:HG2	1.72	0.55
3:L:83:ILE:HD12	3:L:104:LEU:O	2.08	0.54
2:C:22:CYS:HB3	2:C:79:LEU:HB3	1.89	0.54
1:B:61:TRP:CE2	1:B:65:HIS:HD2	2.26	0.54
1:A:65:HIS:HB3	1:A:112:LYS:HD2	1.89	0.54
1:B:231:MET:HE3	1:B:241:MET:SD	2.48	0.54
2:H:207:ASN:ND2	2:H:209:LYS:HE3	2.23	0.53
3:D:151:ASP:HA	3:D:191:VAL:HB	1.90	0.53
2:H:196:SER:HB2	2:H:202:TYR:HE2	1.73	0.53
2:H:220:GLU:HB2	2:H:221:PRO:HD2	1.91	0.52
3:L:142:ARG:HD2	3:L:173:TYR:CE1	2.46	0.51
3:D:83:ILE:HD12	3:D:104:LEU:O	2.11	0.51
3:L:150:VAL:HB	3:L:155:GLN:HE21	1.75	0.51
3:L:39:ARG:HB2	3:L:42:LYS:HD3	1.93	0.50
3:D:150:VAL:HG13	3:D:192:TYR:CE1	2.47	0.50
1:A:261:LYS:HB2	1:A:264:THR:HB	1.93	0.49
3:D:30:SER:OG	3:D:31:ASN:N	2.43	0.49
3:L:180:THR:O	3:L:181:LEU:HD23	2.13	0.49
1:B:231:MET:CE	1:B:317:VAL:HG11	2.42	0.49
2:C:192:VAL:HG11	2:C:202:TYR:CZ	2.48	0.49
2:H:203:ILE:HG12	2:H:218:ARG:HG2	1.95	0.48
3:D:149:LYS:CE	3:D:154:LEU:HG	2.43	0.48
1:B:260:TYR:CE1	1:B:305:ARG:HB3	2.49	0.48
2:H:132:LEU:HB3	3:L:118:PHE:CD2	2.49	0.48
2:C:203:ILE:HG13	2:C:218:ARG:HG2	1.96	0.48
3:L:35:TRP:CE2	3:L:73:PHE:HB2	2.49	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:261:LYS:NZ	1:A:302:ALA:O	2.47	0.47
2:C:127:PRO:HB3	2:C:153:TYR:HB3	1.96	0.47
1:A:217:CYS:C	1:A:219:GLY:H	2.21	0.47
3:L:158:ASN:OD1	3:L:158:ASN:N	2.45	0.47
2:C:67:ARG:HH22	2:C:90:ASP:CG	2.21	0.47
3:L:122:ASP:HA	3:L:125:LEU:HD12	1.97	0.47
1:A:254:SER:HB2	1:A:276:LYS:HD3	1.96	0.47
3:L:28:ASP:OD1	3:L:68:GLY:HA2	2.15	0.47
3:L:190:LYS:HE2	3:L:210:ASN:HB3	1.96	0.47
1:A:45:TYR:O	1:A:49:ILE:HG12	2.15	0.46
3:D:39:ARG:HG2	3:D:39:ARG:HH11	1.80	0.46
1:A:89:SER:OG	1:A:178:ASP:OD2	2.33	0.46
1:B:195:LEU:HB3	1:B:239:ILE:HD13	1.97	0.46
2:C:196:SER:HA	2:C:199:THR:HG23	1.98	0.46
2:H:34:MET:HB3	2:H:79:LEU:HD22	1.97	0.46
3:D:113:PRO:HB3	3:D:139:PHE:HB3	1.98	0.46
1:A:153:SER:OG	1:A:155:GLU:HG2	2.16	0.46
3:L:20:THR:HG23	3:L:72:THR:HG23	1.98	0.46
1:B:35:LYS:HD2	1:B:69:GLN:HE21	1.81	0.46
1:B:207:CYS:HB2	1:B:337:THR:OG1	2.16	0.45
2:C:39:GLN:NE2	7:C:301:HOH:O	2.39	0.45
3:D:158:ASN:HD21	3:D:179:LEU:HD11	1.82	0.45
2:C:151:LYS:NZ	2:C:152:ASP:OD2	2.41	0.45
3:D:4:MET:HE1	3:D:25:ALA:HB2	1.99	0.45
3:D:158:ASN:ND2	3:D:179:LEU:HD11	2.30	0.45
1:A:218:GLU:N	7:A:405:HOH:O	2.49	0.45
1:B:237:HIS:ND1	1:B:238:LYS:O	2.50	0.45
1:B:231:MET:O	1:B:231:MET:HG3	2.17	0.44
1:B:203:PHE:CE1	1:B:240:ILE:HG13	2.52	0.44
2:H:217:LYS:NZ	3:L:123:GLU:OE1	2.48	0.44
3:L:179:LEU:HD11	3:L:181:LEU:HD21	1.99	0.44
1:B:123:PRO:HB2	1:B:125:TYR:CE1	2.52	0.44
1:B:123:PRO:HB3	1:B:174:LEU:HD21	2.00	0.43
2:C:83:MET:HB3	2:C:86:LEU:HD21	1.99	0.43
2:H:176:ALA:HA	2:H:186:LEU:HB3	2.00	0.43
2:C:132:LEU:HB3	3:D:118:PHE:CD1	2.52	0.43
3:L:150:VAL:HG22	3:L:192:TYR:CD1	2.53	0.43
1:B:131:PHE:HA	1:B:174:LEU:O	2.18	0.43
2:H:91:THR:HG23	2:H:118:THR:HA	2.00	0.43
3:D:120:PRO:HD3	3:D:132:VAL:HG22	2.01	0.43
2:H:99:ASP:HA	2:H:107:PHE:O	2.18	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:28:ASP:OD1	3:D:68:GLY:HA2	2.19	0.43
1:B:184:MET:HE1	1:B:233:VAL:C	2.44	0.43
1:B:191:THR:HG23	1:B:322:MET:SD	2.59	0.43
1:B:218:GLU:O	1:B:218:GLU:HG2	2.19	0.43
1:A:217:CYS:O	1:A:218:GLU:HB2	2.18	0.43
1:A:323:ARG:HG2	1:A:323:ARG:NH1	2.33	0.43
2:H:211:SER:OG	2:H:213:THR:OG1	2.17	0.43
1:B:261:LYS:HB2	1:B:264:THR:HB	2.00	0.43
2:C:196:SER:HA	2:C:199:THR:CG2	2.49	0.43
1:B:206:ILE:HG23	1:B:336:ALA:HB1	2.01	0.42
1:B:120:VAL:O	1:B:125:TYR:OH	2.34	0.42
3:L:107:LYS:HA	3:L:140:TYR:OH	2.19	0.42
1:B:217:CYS:O	1:B:218:GLU:HB3	2.18	0.42
3:L:140:TYR:CG	3:L:141:PRO:HA	2.55	0.42
1:B:131:PHE:HB3	1:B:174:LEU:HB3	2.01	0.42
3:D:35:TRP:CE2	3:D:73:PHE:HB2	2.55	0.42
3:L:209:PHE:CD1	3:L:209:PHE:C	2.98	0.42
1:B:231:MET:HE1	1:B:317:VAL:CG1	2.49	0.42
3:D:149:LYS:HE3	3:D:154:LEU:HG	2.02	0.42
1:B:72:VAL:HG21	1:B:173:VAL:HG23	2.01	0.41
1:B:316:VAL:HG21	1:B:323:ARG:NH2	2.34	0.41
2:C:60:TYR:HB2	2:C:65:LYS:HG3	2.02	0.41
2:C:86:LEU:HD23	2:C:86:LEU:HA	1.90	0.41
2:C:158:VAL:HG12	2:C:208:HIS:HB2	2.01	0.41
1:A:300:SER:O	1:A:301:GLU:O	2.37	0.41
1:A:325:ARG:HB2	1:A:325:ARG:HH11	1.85	0.41
2:C:34:MET:HE3	2:C:34:MET:HB3	1.80	0.41
3:D:39:ARG:HE	3:D:42:LYS:NZ	2.15	0.41
3:L:170:ASP:HB3	3:L:172:THR:HG23	2.02	0.41
2:C:161:SER:HB3	2:C:205:ASN:OD1	2.20	0.41
3:D:153:ALA:O	3:D:154:LEU:HB2	2.21	0.41
1:A:21:ASP:O	1:A:23:GLY:N	2.54	0.41
2:H:193:PRO:O	2:H:195:SER:N	2.48	0.41
1:B:32:HIS:HB2	1:B:167:LEU:HD22	2.03	0.41
1:B:248:TRP:CH2	1:B:315:VAL:HB	2.56	0.41
2:C:68:PHE:CZ	2:C:83:MET:HG2	2.56	0.41
2:C:130:PHE:CE2	3:D:124:GLN:HG3	2.55	0.41
3:D:123:GLU:O	3:D:126:LYS:HG2	2.20	0.41
2:H:6:GLU:OE2	2:H:95:TYR:HA	2.21	0.41
3:L:4:MET:HE3	3:L:4:MET:HB3	1.77	0.41
1:A:310[A]:HIS:ND1	7:A:401:HOH:O	2.37	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:L:107:LYS:HE3	3:L:107:LYS:HB2	1.80	0.41
3:L:142:ARG:HG2	3:L:142:ARG:NH1	2.36	0.41
2:C:76:LYS:O	2:C:78:THR:HG23	2.21	0.40
1:A:131:PHE:HA	1:A:174:LEU:O	2.21	0.40
7:A:414:HOH:O	3:L:50:GLU:HG3	2.20	0.40
2:H:13:GLN:H	2:H:13:GLN:HG2	1.59	0.40
2:H:193:PRO:C	2:H:195:SER:H	2.29	0.40
2:H:97:ALA:HA	2:H:110:ASP:O	2.21	0.40
3:L:141:PRO:HB2	3:L:143:GLU:OE1	2.21	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	320/325 (98%)	302 (94%)	16 (5%)	2 (1%)	22	33
1	B	308/325 (95%)	294 (96%)	13 (4%)	1 (0%)	37	51
2	C	210/223 (94%)	207 (99%)	3 (1%)	0	100	100
2	H	210/223 (94%)	202 (96%)	7 (3%)	1 (0%)	25	38
3	D	209/214 (98%)	198 (95%)	10 (5%)	1 (0%)	25	38
3	L	209/214 (98%)	201 (96%)	8 (4%)	0	100	100
All	All	1466/1524 (96%)	1404 (96%)	57 (4%)	5 (0%)	37	51

All (5) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	301	GLU
1	B	22	SER
1	A	22	SER

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Mol	Chain	Res	Type
2	H	222	LYS
3	D	154	LEU

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	274/279 (98%)	269 (98%)	5 (2%)	54 73
1	B	268/279 (96%)	266 (99%)	2 (1%)	81 91
2	C	179/186 (96%)	171 (96%)	8 (4%)	23 40
2	H	179/186 (96%)	175 (98%)	4 (2%)	47 67
3	D	187/190 (98%)	185 (99%)	2 (1%)	70 84
3	L	188/190 (99%)	181 (96%)	7 (4%)	29 48
All	All	1275/1310 (97%)	1247 (98%)	28 (2%)	47 67

All (28) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	81	VAL
1	A	91	SER
1	A	103	ASP
1	A	205	ASP
1	A	253	SER
2	H	13	GLN
2	H	78	THR
2	H	87	ARG
2	H	121	SER
3	L	12	SER
3	L	48	ILE
3	L	78	LEU
3	L	92	GLU
3	L	137	ASN
3	L	170	ASP
3	L	197	THR

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Mol	Chain	Res	Type
1	B	152	GLU
1	B	258	VAL
2	C	11	LEU
2	C	20	LEU
2	C	21	SER
2	C	35	SER
2	C	124	THR
2	C	161	SER
2	C	177	VAL
2	C	212	ASN
3	D	12	SER
3	D	72	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (11) such sidechains are listed below:

Mol	Chain	Res	Type
2	H	82	GLN
2	H	207	ASN
3	L	53	ASN
3	L	79	GLN
1	B	65	HIS
1	B	69	GLN
1	B	88	ASN
1	B	235	HIS
2	C	39	GLN
3	D	3	GLN
3	D	38	GLN

5.3.3 RNA

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains

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

5.5 Carbohydrates

8 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	E	1	1,4	14,14,15	0.21	0	17,19,21	0.53	0
4	NAG	E	2	4	14,14,15	0.22	0	17,19,21	0.40	0
5	NAG	F	1	1,5	14,14,15	0.28	0	17,19,21	0.41	0
5	NAG	F	2	5	14,14,15	0.31	0	17,19,21	0.47	0
5	BMA	F	3	5	11,11,12	0.81	0	15,15,17	1.00	1 (6%)
5	NAG	G	1	1,5	14,14,15	0.24	0	17,19,21	0.40	0
5	NAG	G	2	5	14,14,15	0.36	0	17,19,21	0.38	0
5	BMA	G	3	5	11,11,12	0.39	0	15,15,17	0.85	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	E	1	1,4	-	0/6/23/26	0/1/1/1
4	NAG	E	2	4	-	0/6/23/26	0/1/1/1
5	NAG	F	1	1,5	-	0/6/23/26	0/1/1/1
5	NAG	F	2	5	-	0/6/23/26	0/1/1/1
5	BMA	F	3	5	-	2/2/19/22	0/1/1/1
5	NAG	G	1	1,5	-	0/6/23/26	0/1/1/1
5	NAG	G	2	5	-	0/6/23/26	0/1/1/1
5	BMA	G	3	5	-	0/2/19/22	0/1/1/1

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
5	F	3	BMA	C1-O5-C5	2.26	115.25	112.19
5	G	3	BMA	C1-O5-C5	2.10	115.03	112.19

There are no chirality outliers.

All (2) torsion outliers are listed below:

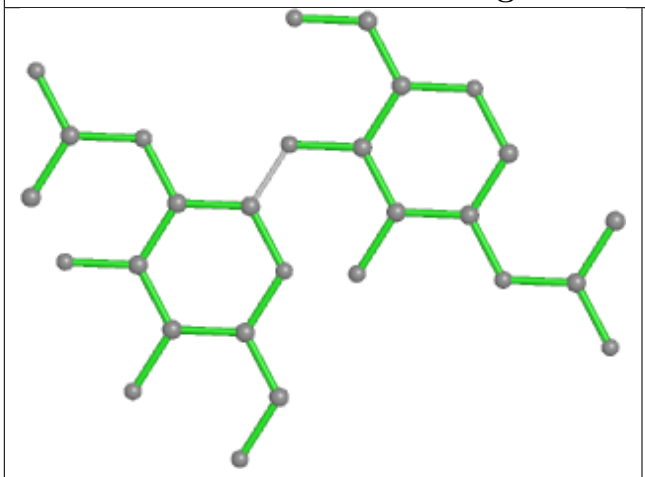
Mol	Chain	Res	Type	Atoms
5	F	3	BMA	O5-C5-C6-O6
5	F	3	BMA	C4-C5-C6-O6

There are no ring outliers.

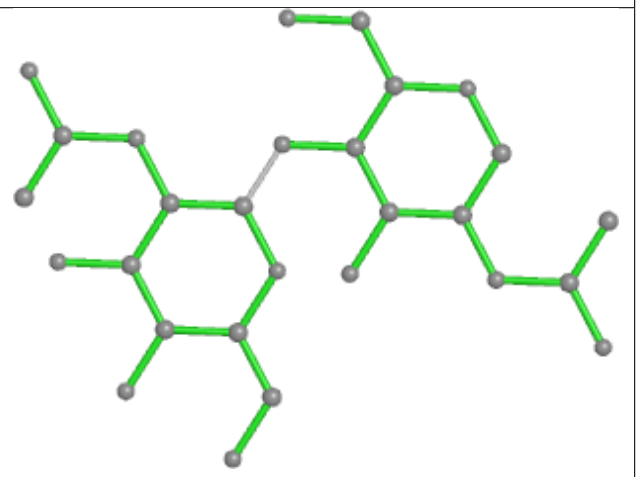
No monomer is involved in short contacts.

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

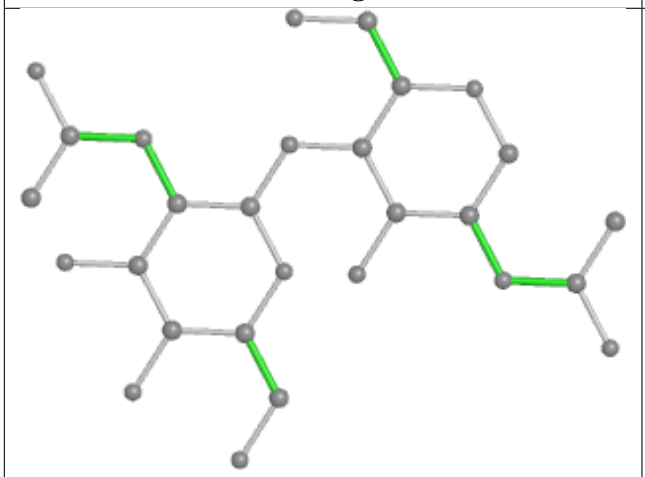
Oligosaccharide Chain E



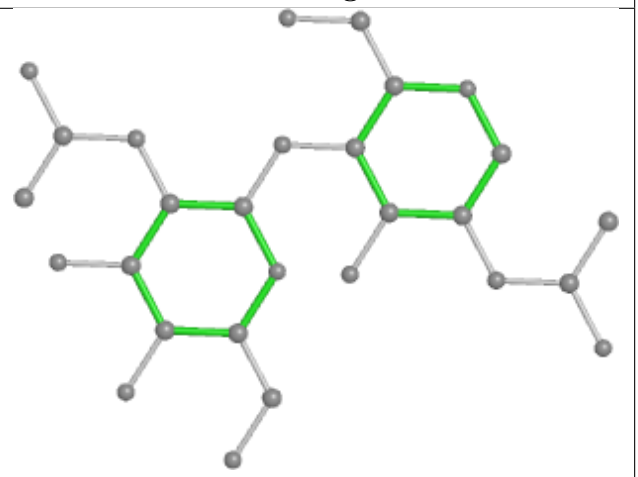
Bond lengths



Bond angles

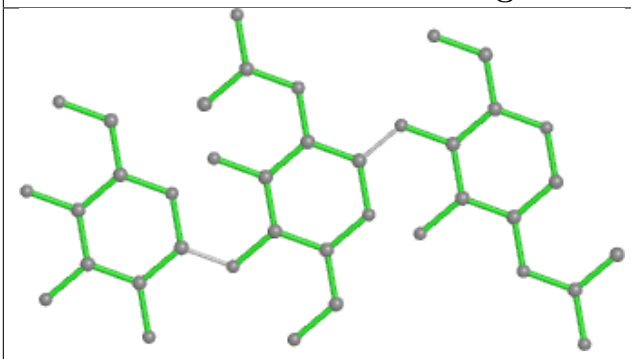


Torsions

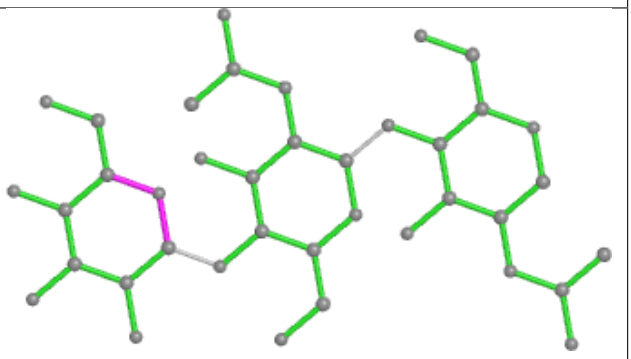


Rings

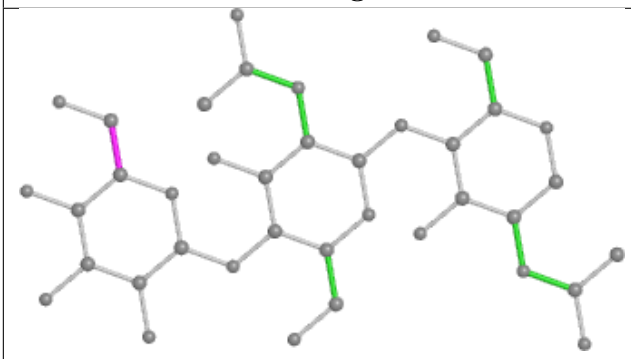
Oligosaccharide Chain F



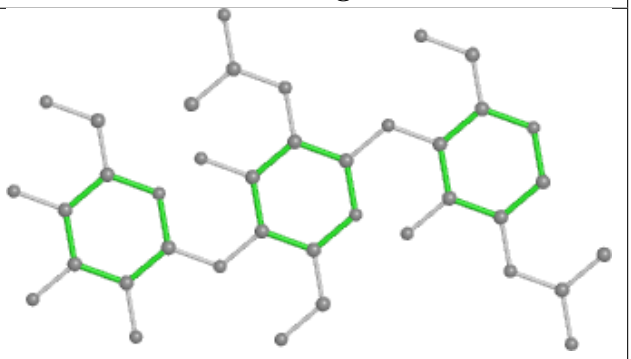
Bond lengths



Bond angles

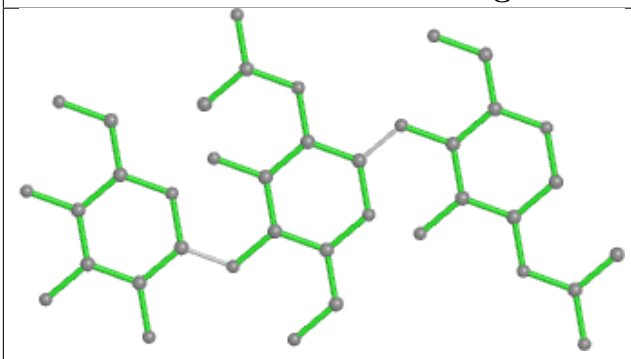


Torsions

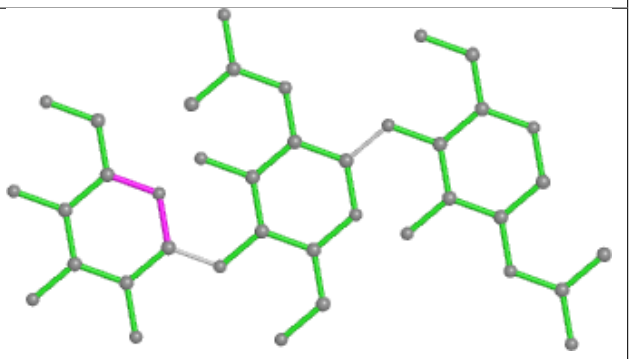


Rings

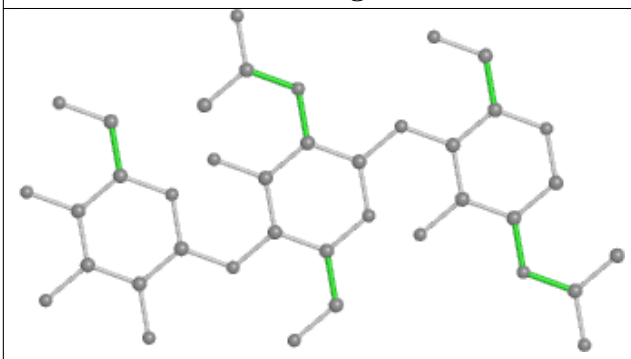
Oligosaccharide Chain G



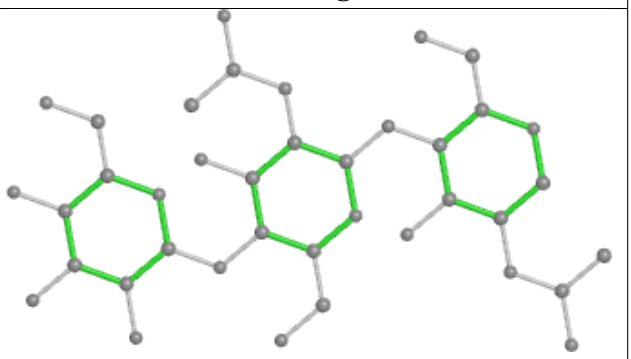
Bond lengths



Bond angles



Torsions



Rings

5.6 Ligand geometry (i)

1 ligand 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	$\#\|Z\| > 2$
6	NAG	B	401	1	14,14,15	0.26	0	17,19,21	0.38	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
6	NAG	B	401	1	-	0/6/23/26	0/1/1/1

There are no bond length outliers.

There are no bond angle outliers.

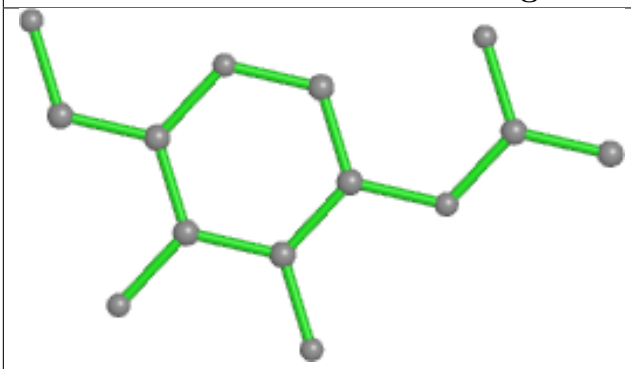
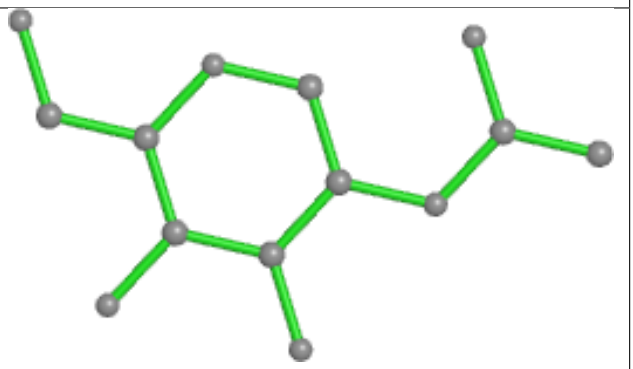
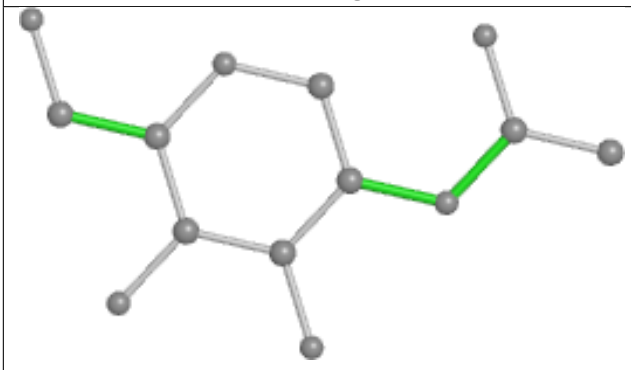
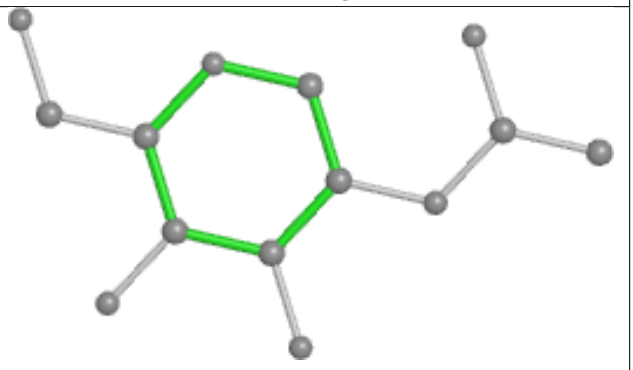
There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less then 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

Ligand NAG B 401	
 Bond lengths	 Bond angles
 Torsions	 Rings

5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

In the following table, the column labelled '#RSRZ> 2' contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95^{th} percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled 'Q< 0.9' lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2			OWAB(Å^2)	Q<0.9
1	A	321/325 (98%)	0.32	21 (6%)	26	24	27, 44, 85, 153	1 (0%)
1	B	312/325 (96%)	0.58	24 (7%)	21	19	32, 50, 77, 129	0
2	C	214/223 (95%)	0.28	9 (4%)	41	38	27, 41, 77, 124	0
2	H	214/223 (95%)	0.23	15 (7%)	24	22	21, 38, 77, 104	0
3	D	211/214 (98%)	0.43	18 (8%)	18	17	26, 42, 76, 93	0
3	L	211/214 (98%)	0.29	14 (6%)	26	23	21, 36, 80, 91	0
All	All	1483/1524 (97%)	0.37	101 (6%)	25	22	21, 43, 79, 153	1 (0%)

All (101) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	219	GLY	5.5
1	B	340	HIS	5.4
1	A	299	THR	5.3
2	H	133	ALA	5.1
2	C	197	LEU	4.6
1	A	295	HIS	4.6
1	A	341	HIS	4.6
2	H	197	LEU	4.5
2	C	223	SER	4.5
2	H	221	PRO	4.4
1	B	282	ARG	4.3
1	B	338	LEU	4.3
3	D	125	LEU	4.3
2	H	222	LYS	4.2
1	B	341	HIS	4.2
2	H	223	SER	4.1
1	B	261	LYS	4.0
1	B	339	HIS	4.0
1	B	303	LYS	4.0

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Mol	Chain	Res	Type	RSRZ
1	A	300	SER	3.8
3	D	129	THR	3.8
3	D	154	LEU	3.8
1	A	297	GLU	3.6
3	D	191	VAL	3.6
3	L	188	LYS	3.6
3	L	154	LEU	3.6
2	H	198	GLY	3.5
1	B	41	HIS	3.5
2	C	222	LYS	3.5
3	L	145	LYS	3.4
2	C	133	ALA	3.4
3	L	129	THR	3.4
2	H	196	SER	3.3
2	C	207	ASN	3.3
1	B	183	LEU	3.2
2	H	199	THR	3.2
2	C	221	PRO	3.2
1	B	260	TYR	3.2
1	A	301	GLU	3.1
1	A	302	ALA	3.1
1	B	285	MET	3.1
1	B	283	GLY	3.1
1	A	340	HIS	3.0
3	L	153	ALA	3.0
3	D	127	SER	2.9
3	D	130	ALA	2.9
2	C	143	THR	2.8
1	A	298	GLU	2.8
1	B	244	HIS	2.8
1	A	303	LYS	2.7
1	A	220	GLU	2.7
1	B	336	ALA	2.7
1	B	310	HIS	2.6
3	L	170	ASP	2.6
3	D	109	THR	2.6
3	D	123	GLU	2.6
2	H	195	SER	2.6
1	B	317	VAL	2.5
3	L	133	VAL	2.5
1	A	216	GLN	2.5
1	A	260	TYR	2.5

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Mol	Chain	Res	Type	RSRZ
2	H	143	THR	2.5
1	B	262	GLU	2.5
1	A	262	GLU	2.5
1	A	263	GLY	2.5
1	A	294	GLU	2.5
3	D	126	LYS	2.5
3	D	153	ALA	2.4
3	L	179	LEU	2.4
3	D	124	GLN	2.4
1	A	282	ARG	2.4
3	L	184	ALA	2.4
3	D	181	LEU	2.3
3	D	170	ASP	2.3
1	B	253	SER	2.3
1	B	242	ARG	2.3
2	C	161	SER	2.3
1	B	251	GLU	2.3
3	L	146	VAL	2.3
1	A	338	LEU	2.2
3	L	211	ARG	2.2
2	C	216	ASP	2.2
2	H	129	VAL	2.2
1	B	263	GLY	2.2
3	D	211	ARG	2.2
2	H	193	PRO	2.1
1	A	285	MET	2.1
1	B	252	SER	2.1
3	L	152	ASN	2.1
2	H	131	PRO	2.1
3	D	146	VAL	2.1
2	H	201	THR	2.1
1	A	155	GLU	2.1
2	H	219	VAL	2.0
3	L	132	VAL	2.0
1	A	264	THR	2.0
1	B	220	GLU	2.0
3	L	187	GLU	2.0
3	D	147	GLN	2.0
3	D	182	SER	2.0
3	D	117	ILE	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)

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6.4 Ligands (i)

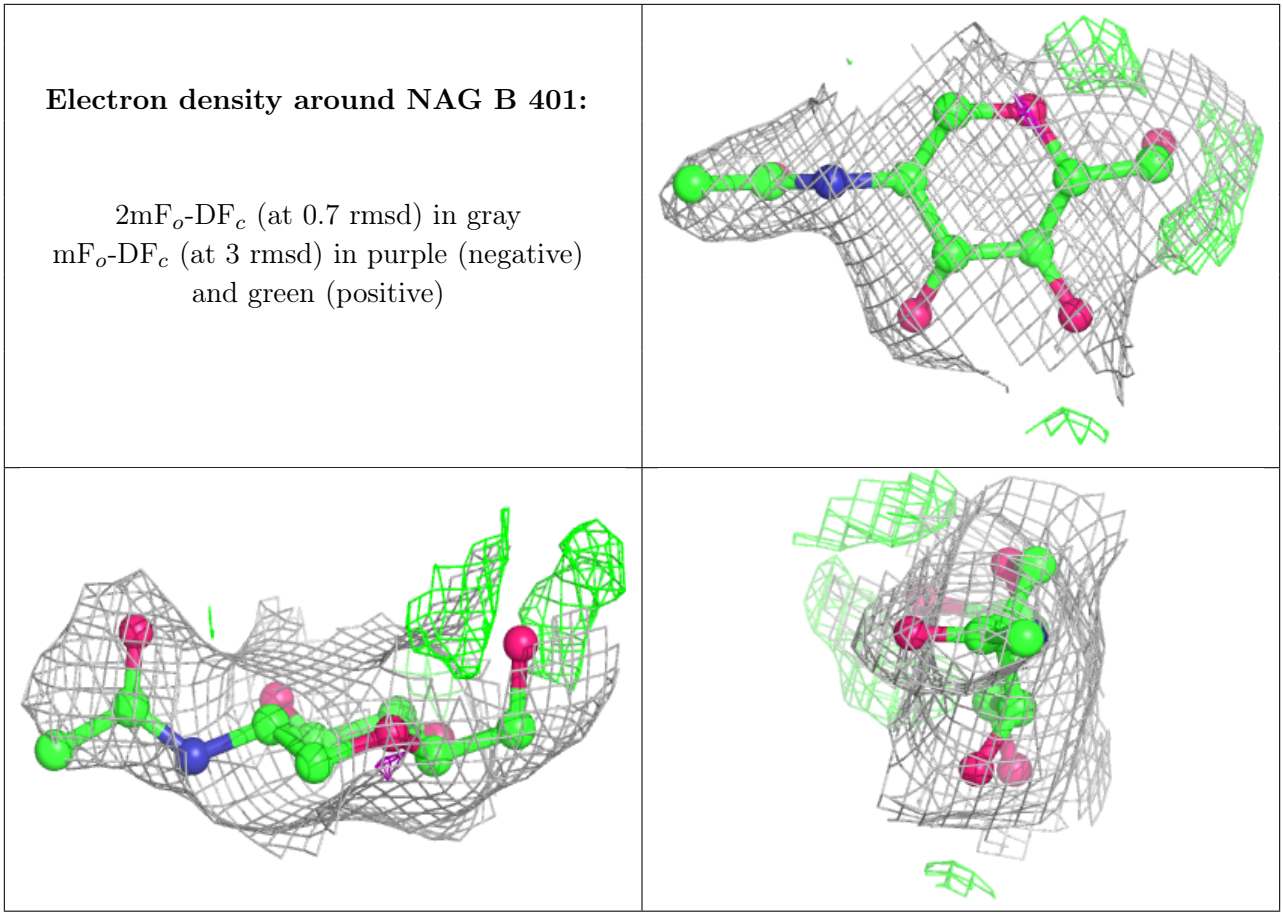
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' 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
6	NAG	B	401	14/15	0.74	0.15	47,52,55,57	0

The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation to approximate a three-dimensional view.

Electron density around NAG B 401:

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



6.5 Other polymers

There are no such residues in this entry.