Full wwPDB X-ray Structure Validation Report (i)

Jun 12, 2025 – 02:03 PM JST

PDB ID	:	9JQU / pdb_00009jqu
Title	:	The crystal structure of SFTSV Gn and SD4 antibody complex
Authors	:	Shi, W.F.; Quan, C.S.; Qi, J.X.
Deposited on	:	2024-09-28
Resolution	:	3.30 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 (1)) were used in the production of this report:

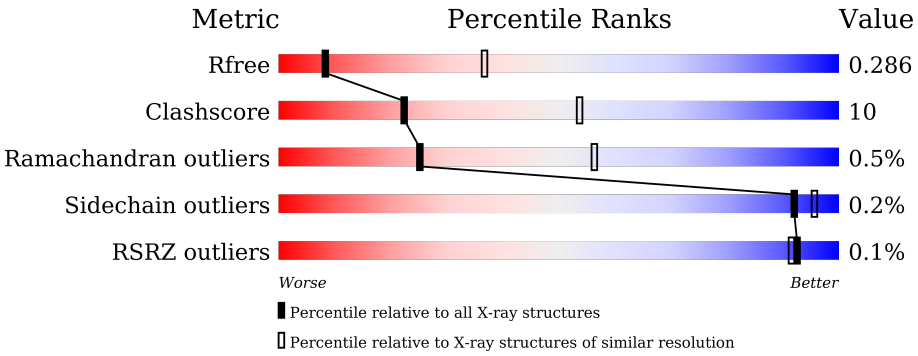
MolProbity	:	4-5-2 with Phenix2.0rc1
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	2.0rc1
EDS	:	3.0
Percentile statistics	:	20231227.v01 (using entries in the PDB archive December 27th 2023)
CCP4	:	9.0.006 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
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 3.30 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	1085 (3.32-3.28)
Clashscore	180529	1128 (3.32-3.28)
Ramachandran outliers	177936	1125 (3.32-3.28)
Sidechain outliers	177891	1124 (3.32-3.28)
RSRZ outliers	164620	1085 (3.32-3.28)

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	71% 27%
2	L	214	82% 16%
3	H	223	70% 25%
4	B	3	100%
5	C	2	50% 50%

2 Entry composition (i)

There are 5 unique types of molecules in this entry. The entry contains 5781 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
			Total	C	N	O	S			
1	A	321	2472	1545	432	469	26	0	0	0

There are 6 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

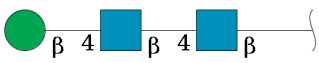
- Molecule 2 is a protein called SD4 light chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
2	L	211	1625	1016	269	334	6	0	0	0

- Molecule 3 is a protein called SD4 heavy chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
3	H	213	1617	1024	273	314	6	0	0	0

- Molecule 4 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
			Total	C	N	O			
4	B	3	39	22	2	15	0	0	0

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

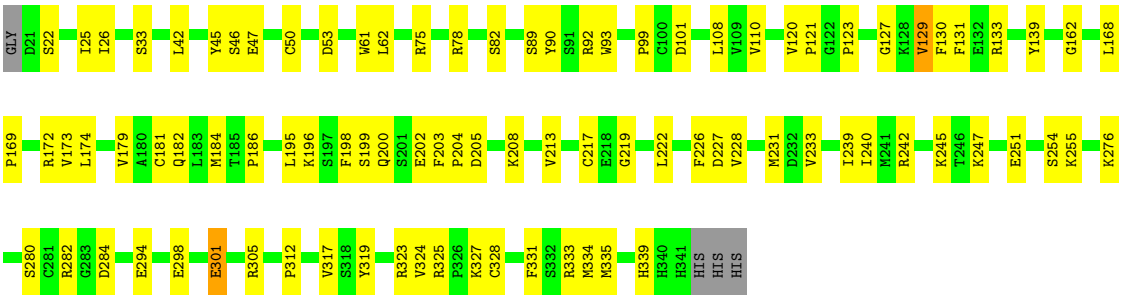
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
			Total	C	N	O			
5	C	2	28	16	2	10	0	0	0

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.

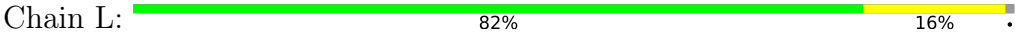
• Molecule 1: Envelopment polyprotein

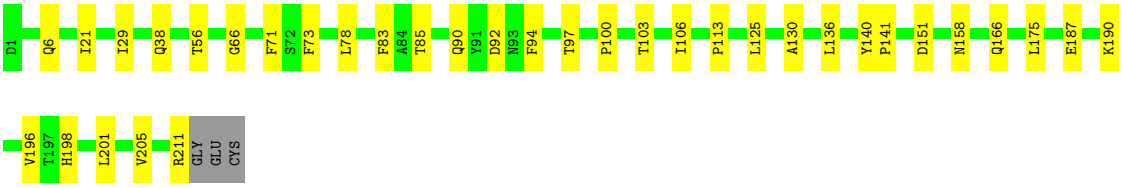
Chain A:



• Molecule 2: SD4 light chain

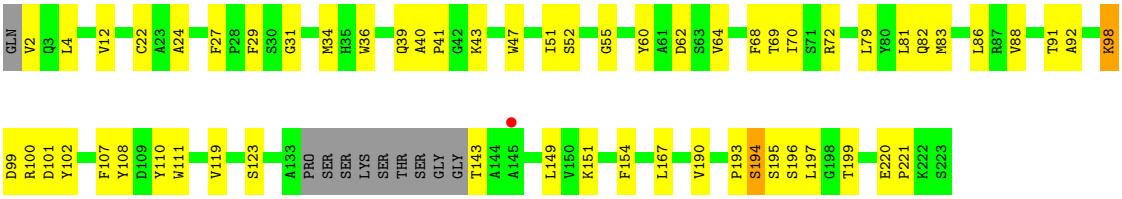
Chain L:





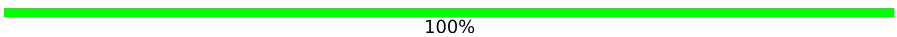
• Molecule 3: SD4 heavy chain

Chain H:



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

Chain B:



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

Chain C:

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	96.86Å 46.36Å 97.32Å 90.00° 113.30° 90.00°	Depositor
Resolution (Å)	32.21 – 3.30 32.21 – 3.30	Depositor EDS
% Data completeness (in resolution range)	95.1 (32.21-3.30) 95.0 (32.21-3.30)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.26 (at 3.32Å)	Xtriage
Refinement program	PHENIX 1.19.2	Depositor
R, R_{free}	0.250 , 0.289 0.248 , 0.286	Depositor DCC
R_{free} test set	620 reflections (5.01%)	wwPDB-VP
Wilson B-factor (Å^2)	84.4	Xtriage
Anisotropy	0.307	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.31 , 32.3	EDS
L-test for twinning[2]	$< \|L\| > = 0.48$, $< L^2 > = 0.30$	Xtriage
Estimated twinning fraction	0.017 for l,-k,h	Xtriage
F_o,F_c correlation	0.89	EDS
Total number of atoms	5781	wwPDB-VP
Average B, all atoms (Å^2)	78.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.77% 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: BMA, NAG

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#$\|Z\|$ >5	RMSZ	#$\|Z\|$ >5
1	A	0.18	0/2536	0.49	1/3419 (0.0%)
2	L	0.15	0/1663	0.38	0/2264
3	H	0.17	0/1657	0.43	0/2254
All	All	0.17	0/5856	0.44	1/7937 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	129	VAL	N-CA-C	-5.62	107.33	112.96

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	2472	0	2353	58	0
2	L	1625	0	1549	23	0
3	H	1617	0	1569	42	0
4	B	39	0	34	0	0
5	C	28	0	25	1	0
All	All	5781	0	5530	118	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 10.

All (118) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:195:LEU:HB3	1:A:239:ILE:HD12	1.40	1.01
3:H:51:ILE:HD11	3:H:55:GLY:HA2	1.66	0.77
1:A:62:LEU:HD11	1:A:130:PHE:HB2	1.66	0.76
3:H:22:CYS:HB3	3:H:79:LEU:HB3	1.70	0.73
1:A:195:LEU:HB3	1:A:239:ILE:CD1	2.19	0.68
3:H:193:PRO:O	3:H:195:SER:N	2.26	0.67
3:H:220:GLU:HB2	3:H:221:PRO:HD2	1.77	0.67
3:H:4:LEU:H	3:H:110:TYR:HE2	1.42	0.67
1:A:245:LYS:HZ1	1:A:247:LYS:HB2	1.60	0.67
2:L:198:HIS:HB3	2:L:201:LEU:HD12	1.78	0.66
3:H:34:MET:HB3	3:H:79:LEU:CD1	2.25	0.66
3:H:34:MET:HB3	3:H:79:LEU:HD11	1.79	0.65
1:A:123:PRO:HB3	1:A:174:LEU:HD21	1.79	0.64
3:H:29:PHE:O	3:H:72:ARG:NH2	2.33	0.61
3:H:167:LEU:HD21	3:H:190:VAL:HG21	1.83	0.60
1:A:205:ASP:OD1	1:A:339:HIS:HB2	2.02	0.60
1:A:89:SER:O	1:A:92:ARG:HG2	2.01	0.59
3:H:149:LEU:HD22	3:H:151:LYS:HB2	1.85	0.59
3:H:143:THR:N	3:H:194:SER:HG	1.99	0.59
3:H:47:TRP:CD1	3:H:108:TYR:HH	2.21	0.58
3:H:41:PRO:HD3	3:H:92:ALA:HA	1.86	0.58
1:A:203:PHE:HA	1:A:242:ARG:HH12	1.70	0.57
1:A:199:SER:OG	1:A:239:ILE:HG13	2.03	0.57
1:A:226:PHE:HB3	1:A:334:MET:O	2.06	0.56
1:A:247:LYS:HB3	1:A:323:ARG:HH22	1.69	0.56
1:A:25:ILE:HB	1:A:53:ASP:OD2	2.05	0.56
3:H:123:SER:O	3:H:154:PHE:HD2	1.88	0.56
2:L:90:GLN:HE21	2:L:97:THR:H	1.54	0.56
1:A:202:GLU:O	1:A:242:ARG:NH1	2.39	0.55
2:L:6:GLN:HG3	2:L:100:PRO:HD2	1.88	0.55
2:L:78:LEU:HD13	2:L:83:PHE:CZ	2.41	0.55
2:L:38:GLN:NE2	3:H:39:GLN:HE22	2.05	0.55
1:A:208:LYS:HG2	1:A:213:VAL:HA	1.89	0.54
1:A:282:ARG:HG2	1:A:305:ARG:HD2	1.89	0.53
1:A:284:ASP:HA	1:A:305:ARG:HH21	1.73	0.53
1:A:45:TYR:CZ	1:A:255:LYS:HG2	2.44	0.53
1:A:231:MET:SD	1:A:317:VAL:HG11	2.49	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:108:LEU:HD12	1:A:139:TYR:CD1	2.44	0.52
3:H:2:VAL:HG12	3:H:27:PHE:HB3	1.90	0.52
1:A:121:PRO:HD3	1:A:335:MET:HE1	1.91	0.52
2:L:125:LEU:HD21	2:L:130:ALA:HB2	1.92	0.52
1:A:184:MET:HE2	1:A:186:PRO:HA	1.91	0.52
3:H:36:TRP:NE1	3:H:81:LEU:HB2	2.23	0.52
1:A:120:VAL:HG11	1:A:333:ARG:HG2	1.92	0.52
3:H:52:SER:O	3:H:72:ARG:NH1	2.44	0.51
1:A:42:LEU:HB3	1:A:47:GLU:HB3	1.94	0.50
1:A:90:TYR:HA	1:A:93:TRP:HE3	1.77	0.50
1:A:99:PRO:HG3	1:A:179:VAL:HG11	1.95	0.49
1:A:131:PHE:HA	1:A:174:LEU:O	2.12	0.49
1:A:203:PHE:CZ	1:A:242:ARG:HG3	2.48	0.49
2:L:85:THR:HG22	2:L:103:THR:HG22	1.94	0.49
1:A:217:CYS:C	1:A:219:GLY:H	2.21	0.48
1:A:182:GLN:N	1:A:327:LYS:O	2.38	0.48
3:H:196:SER:HA	3:H:199:THR:OG1	2.14	0.48
2:L:151:ASP:OD2	2:L:190:LYS:HD2	2.14	0.48
3:H:62:ASP:C	3:H:64:VAL:H	2.20	0.48
2:L:106:ILE:HG22	2:L:166:GLN:CD	2.39	0.48
3:H:88:VAL:O	3:H:91:THR:HG22	2.14	0.47
3:H:12:VAL:O	3:H:119:VAL:HA	2.14	0.47
1:A:78:ARG:NE	1:A:101:ASP:OD2	2.47	0.47
1:A:196:LYS:O	1:A:200:GLN:HG3	2.15	0.47
3:H:27:PHE:CE2	3:H:98:LYS:HG3	2.50	0.47
3:H:220:GLU:HB2	3:H:221:PRO:CD	2.44	0.47
3:H:99:ASP:HA	3:H:107:PHE:O	2.15	0.47
1:A:61:TRP:CD1	1:A:110:VAL:HG13	2.50	0.46
3:H:123:SER:O	3:H:154:PHE:CD2	2.68	0.46
1:A:251:GLU:OE2	1:A:325:ARG:NH2	2.43	0.46
1:A:280:SER:HA	1:A:294:GLU:HB3	1.98	0.46
1:A:129:VAL:HG21	1:A:168:LEU:HD23	1.97	0.46
3:H:69:THR:OG1	3:H:82:GLN:HB3	2.16	0.46
1:A:33:SER:O	3:H:100:ARG:HD3	2.16	0.45
1:A:181:CYS:HA	1:A:328:CYS:HA	1.98	0.45
2:L:158:ASN:OD1	2:L:158:ASN:N	2.44	0.45
3:H:149:LEU:CD2	3:H:151:LYS:HB2	2.45	0.45
1:A:93:TRP:CG	1:A:312:PRO:HD3	2.52	0.45
1:A:133:ARG:NH1	1:A:334:MET:HA	2.31	0.45
3:H:60:TYR:CZ	3:H:70:ILE:HG22	2.52	0.45
1:A:82:SER:OG	1:A:173:VAL:O	2.31	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:198:PHE:HD2	1:A:319:TYR:CZ	2.35	0.45
1:A:231:MET:HE3	1:A:239:ILE:HG21	1.98	0.45
3:H:40:ALA:HB3	3:H:43:LYS:HB2	1.98	0.44
3:H:24:ALA:HB1	3:H:27:PHE:HE1	1.82	0.44
1:A:245:LYS:NZ	1:A:247:LYS:HB2	2.30	0.43
2:L:66:GLY:HA3	2:L:71:PHE:HA	2.00	0.43
2:L:136:LEU:HB2	2:L:175:LEU:HB3	1.99	0.43
2:L:29:ILE:HG23	2:L:92:ASP:HB2	2.01	0.43
3:H:64:VAL:HB	3:H:68:PHE:CG	2.54	0.43
1:A:75:ARG:CZ	2:L:94:PHE:HE1	2.32	0.43
1:A:162:GLY:HA2	3:H:31:GLY:HA2	2.00	0.43
1:A:217:CYS:SG	1:A:339:HIS:CE1	3.12	0.43
2:L:90:GLN:NE2	2:L:97:THR:H	2.16	0.43
2:L:113:PRO:HD2	2:L:201:LEU:HD11	2.01	0.42
2:L:21:ILE:HD12	2:L:73:PHE:CD2	2.54	0.42
3:H:34:MET:HB2	3:H:51:ILE:HG23	2.01	0.42
2:L:187:GLU:O	2:L:211:ARG:NH2	2.53	0.42
3:H:12:VAL:HG11	3:H:86:LEU:HD13	2.00	0.42
2:L:196:VAL:HB	2:L:205:VAL:HB	2.00	0.42
1:A:227:ASP:HB3	1:A:331:PHE:CE2	2.54	0.42
3:H:197:LEU:HD13	3:H:221:PRO:HB3	2.02	0.42
1:A:26:ILE:HD11	1:A:50:CYS:N	2.34	0.42
1:A:222:LEU:HD23	1:A:222:LEU:HA	1.96	0.42
1:A:239:ILE:HD11	1:A:319:TYR:CE2	2.54	0.42
2:L:140:TYR:CD1	2:L:141:PRO:HA	2.55	0.42
1:A:202:GLU:O	1:A:204:PRO:HD3	2.20	0.41
1:A:298:GLU:CD	1:A:301:GLU:HB2	2.45	0.41
2:L:140:TYR:CG	2:L:141:PRO:HA	2.55	0.41
3:H:34:MET:HB3	3:H:79:LEU:HD12	2.02	0.41
1:A:233:VAL:HG12	1:A:324:VAL:HG11	2.03	0.41
1:A:254:SER:HB2	1:A:276:LYS:HD3	2.02	0.41
3:H:101:ASP:OD1	3:H:102:TYR:HD1	2.02	0.41
1:A:226:PHE:CZ	1:A:228:VAL:HB	2.56	0.41
3:H:108:TYR:HD2	3:H:111:TRP:CZ2	2.39	0.41
1:A:228:VAL:HG21	1:A:240:ILE:HB	2.02	0.41
1:A:169:PRO:HB3	3:H:102:TYR:CE2	2.56	0.41
2:L:56:THR:HB	5:C:2:NAG:H61	2.02	0.41
3:H:83:MET:HB3	3:H:86:LEU:HD21	2.03	0.40
1:A:127:GLY:O	1:A:172:ARG:HD2	2.21	0.40
2:L:83:PHE:CZ	2:L:106:ILE:HG13	2.56	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	319/325 (98%)	283 (89%)	33 (10%)	3 (1%)	14 44
2	L	209/214 (98%)	196 (94%)	13 (6%)	0	100 100
3	H	209/223 (94%)	192 (92%)	16 (8%)	1 (0%)	25 56
All	All	737/762 (97%)	671 (91%)	62 (8%)	4 (0%)	25 56

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	46	SER
1	A	301	GLU
3	H	194	SER
1	A	22	SER

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%)	274 (100%)	0	100 100
2	L	187/190 (98%)	187 (100%)	0	100 100
3	H	179/187 (96%)	178 (99%)	1 (1%)	84 90
All	All	640/656 (98%)	639 (100%)	1 (0%)	92 95

All (1) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
3	H	98	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (6) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	80	GLN
2	L	38	GLN
2	L	152	ASN
3	H	3	GLN
3	H	113	GLN
3	H	207	ASN

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)

5 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	B	1	4,1	14,14,15	0.30	0	17,19,21	0.60	0
4	NAG	B	2	4	14,14,15	0.33	0	17,19,21	0.55	0
4	BMA	B	3	4	11,11,12	0.50	0	15,15,17	0.79	0
5	NAG	C	1	5,1	14,14,15	0.65	1 (7%)	17,19,21	0.80	1 (5%)
5	NAG	C	2	5	14,14,15	0.69	1 (7%)	17,19,21	0.47	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	B	1	4,1	-	0/6/23/26	0/1/1/1
4	NAG	B	2	4	-	2/6/23/26	0/1/1/1
4	BMA	B	3	4	-	0/2/19/22	0/1/1/1
5	NAG	C	1	5,1	-	0/6/23/26	0/1/1/1
5	NAG	C	2	5	-	0/6/23/26	0/1/1/1

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	C	2	NAG	O5-C1	2.37	1.47	1.43
5	C	1	NAG	O5-C1	-2.20	1.40	1.43

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
5	C	1	NAG	O4-C4-C5	-2.30	103.59	109.30

There are no chirality outliers.

All (2) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	B	2	NAG	O5-C5-C6-O6
4	B	2	NAG	C3-C2-N2-C7

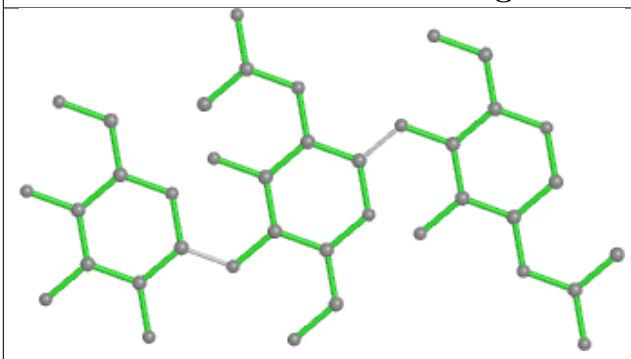
There are no ring outliers.

1 monomer is involved in 1 short contact:

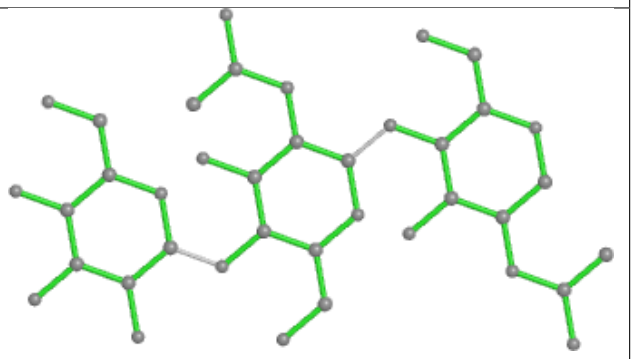
Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	C	2	NAG	1	0

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

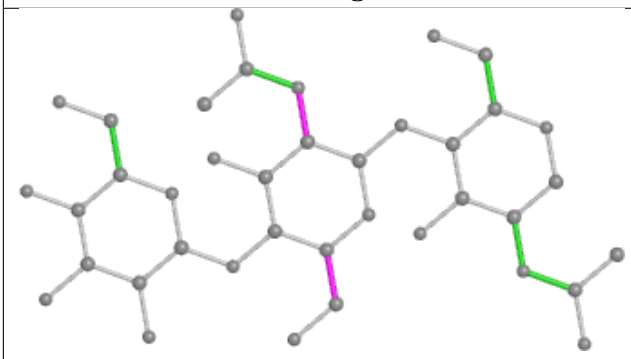
Oligosaccharide Chain B



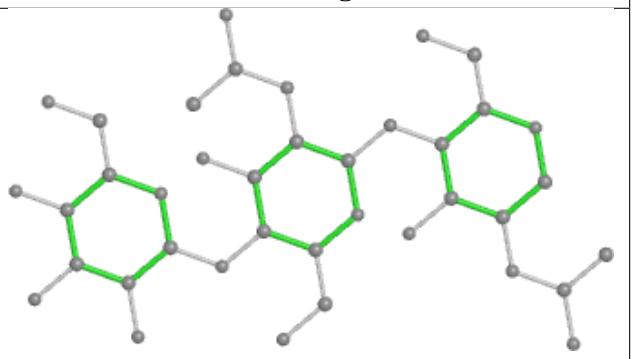
Bond lengths



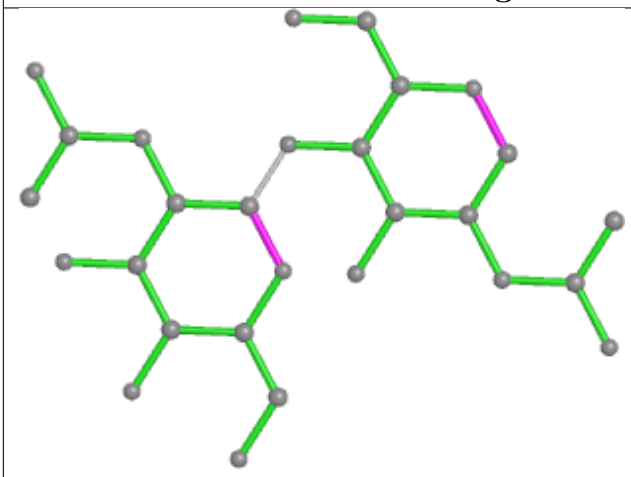
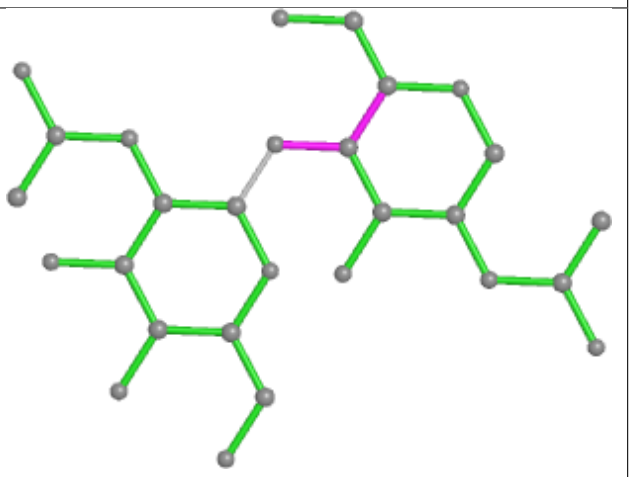
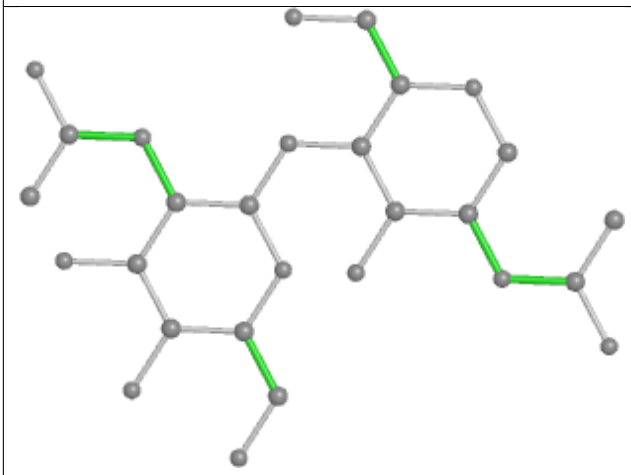
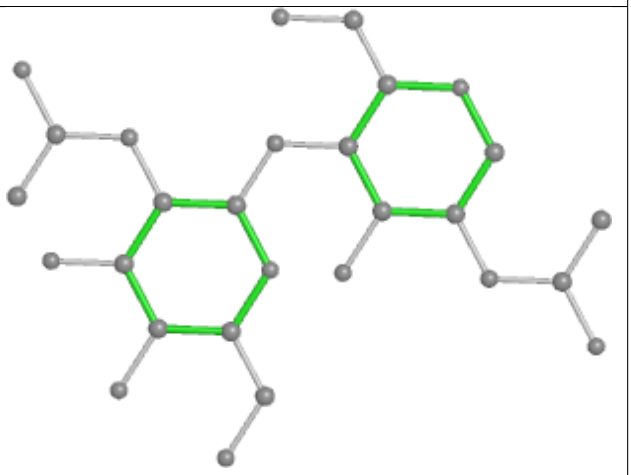
Bond angles



Torsions



Rings

Oligosaccharide Chain C	
 Bond lengths	 Bond angles
 Torsions	 Rings

5.6 Ligand geometry

There are no ligands in this entry.

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2			OWAB(Å^2)	Q<0.9
1	A	321/325 (98%)	-0.19	0	100	100	55, 73, 115, 173	0
2	L	211/214 (98%)	-0.22	0	100	100	60, 76, 92, 115	0
3	H	213/223 (95%)	-0.16	1 (0%)	87	80	61, 77, 96, 112	0
All	All	745/762 (97%)	-0.19	1 (0%)	92	91	55, 75, 102, 173	0

All (1) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
3	H	145	ALA	2.3

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

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

6.3 Carbohydrates

SUGAR-RSR INFOmissingINFO

6.4 Ligands

There are no ligands in this entry.

6.5 Other polymers

There are no such residues in this entry.