Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2024 – 06:11 PM EST

PDB ID	:	8SIQ
Title	:	Crystal structure of SARS-CoV-2 spike receptor-binding domain in complex with broadly neutralizing antibodies CC25.36 and CV38-142 Fab
Authors	:	Liu, H.; Wilson, I.A.
Deposited on	:	2023-04-16
Resolution	:	2.50 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at *validation@mail.wwpdb.org*
A user guide is available at
https://www.wwpdb.org/validation/2017/XrayValidationReportHelp
with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at
http://www.wwpdb.org/validation/2017/FAQs#types.

The following versions of software and data (see references ⓘ) were used in the production of this report:

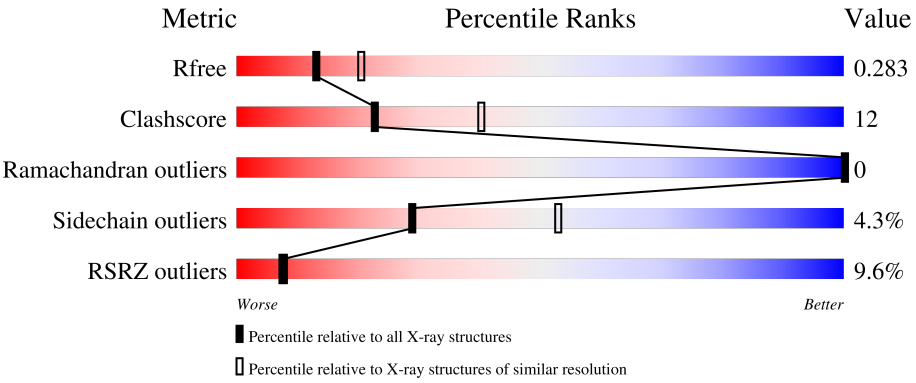
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

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 2.50 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	4661 (2.50-2.50)
Clashscore	141614	5346 (2.50-2.50)
Ramachandran outliers	138981	5231 (2.50-2.50)
Sidechain outliers	138945	5233 (2.50-2.50)
RSRZ outliers	127900	4559 (2.50-2.50)

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	205	7% 66% 29% .
2	H	230	13% 68% 27% .
3	L	217	24% 61% 33% . .
4	M	226	81% 18% .
5	N	217	% 74% 25%

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Mol	Chain	Length	Quality of chain
6	B	4	

2 Entry composition (i)

There are 6 unique types of molecules in this entry. The entry contains 7963 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 Spike protein S1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	196	Total	C	N	O	S	0	0	0
			1530	979	255	288	8			

There are 7 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	531	GLY	-	expression tag	UNP P0DTC2
A	532	HIS	-	expression tag	UNP P0DTC2
A	533	HIS	-	expression tag	UNP P0DTC2
A	534	HIS	-	expression tag	UNP P0DTC2
A	535	HIS	-	expression tag	UNP P0DTC2
A	536	HIS	-	expression tag	UNP P0DTC2
A	537	HIS	-	expression tag	UNP P0DTC2

- Molecule 2 is a protein called CC25.36 Fab heavy chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	H	220	Total	C	N	O	S	0	0	0
			1591	1003	272	309	7			

- Molecule 3 is a protein called CC25.36 Fab light chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	L	210	Total	C	N	O	S	0	0	0
			1474	921	246	303	4			

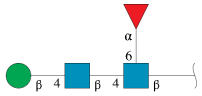
- Molecule 4 is a protein called CV38-142 Fab heavy chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	M	222	Total	C	N	O	S	0	0	0
			1665	1058	273	326	8			

- Molecule 5 is a protein called CV38-142 Fab light chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
5	N	216	1654	1031	278	339	6	0	0	0

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



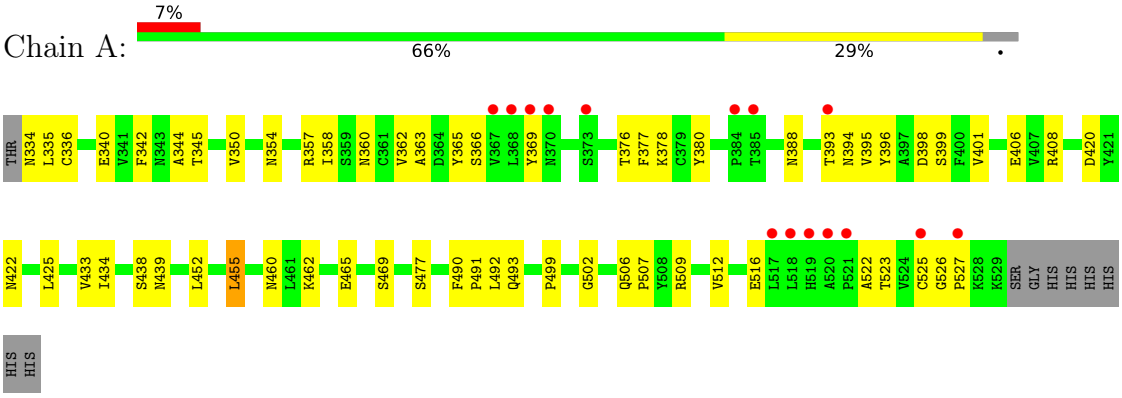
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
			Total	C	N	O			
6	B	4	49	28	2	19	0	0	0

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.

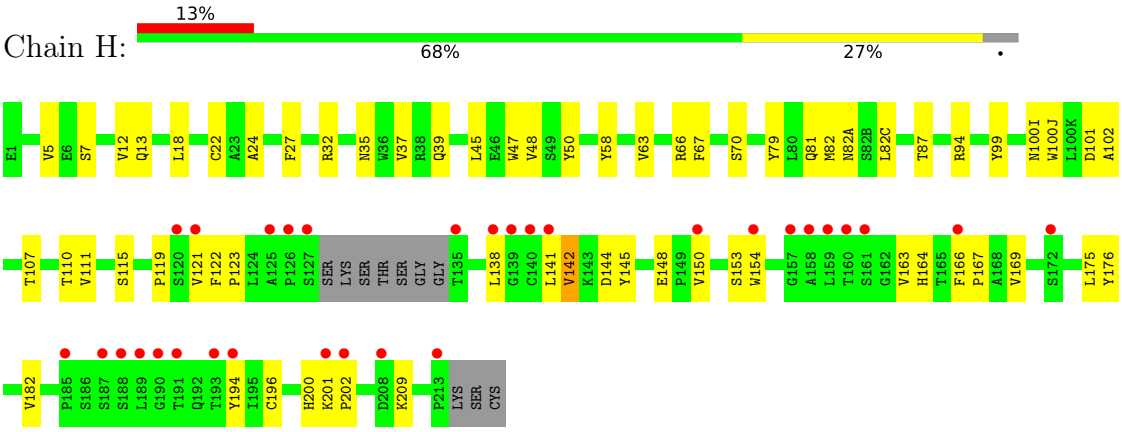
• Molecule 1: Spike protein S1

Chain A:



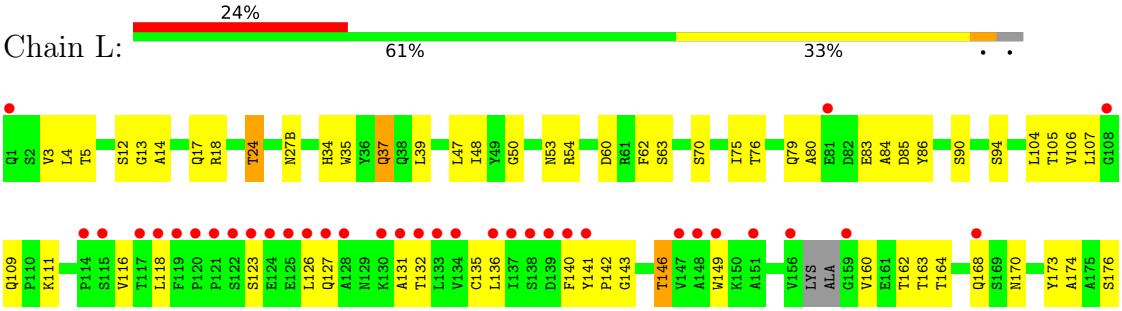
• Molecule 2: CC25.36 Fab heavy chain

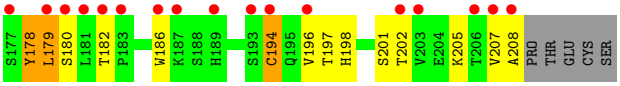
Chain H:



• Molecule 3: CC25.36 Fab light chain

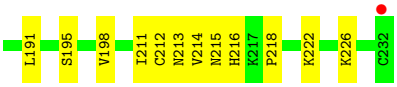
Chain L:





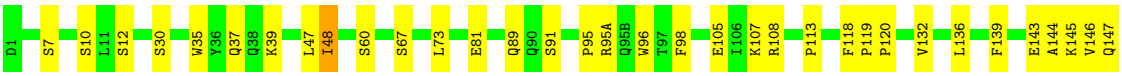
• Molecule 4: CV38-142 Fab heavy chain

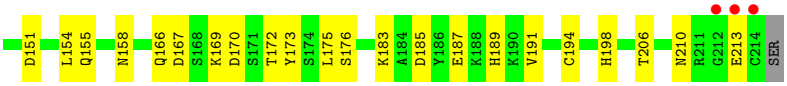
Chain M:



• Molecule 5: CV38-142 Fab light chain

Chain N:





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

Chain B:

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	60.40Å 77.03Å 266.44Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	38.52 – 2.50 38.52 – 2.50	Depositor EDS
% Data completeness (in resolution range)	77.8 (38.52-2.50) 77.7 (38.52-2.50)	Depositor EDS
R_{merge}	0.16	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.86 (at 2.51Å)	Xtriage
Refinement program	PHENIX (1.19.2_4158: ???)	Depositor
R, R_{free}	0.247 , 0.287 0.244 , 0.283	Depositor DCC
R_{free} test set	1635 reflections (4.77%)	wwPDB-VP
Wilson B-factor (Å^2)	41.3	Xtriage
Anisotropy	0.050	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.29 , 34.5	EDS
L-test for twinning[2]	$< \|L\| > = 0.46$, $< L^2 > = 0.29$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.89	EDS
Total number of atoms	7963	wwPDB-VP
Average B, all atoms (Å^2)	50.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.39% 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, 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	0.27	0/1573	0.51	0/2142
2	H	0.27	0/1631	0.53	0/2228
3	L	0.39	1/1510 (0.1%)	0.63	3/2074 (0.1%)
4	M	0.26	0/1709	0.50	0/2326
5	N	0.26	0/1690	0.52	0/2297
All	All	0.29	1/8113 (0.0%)	0.54	3/11067 (0.0%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	L	142	PRO	CG-CD	-8.44	1.22	1.50

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	L	142	PRO	N-CD-CG	-7.06	92.60	103.20
3	L	142	PRO	CA-CB-CG	-5.76	93.06	104.00
3	L	179	LEU	CB-CG-CD1	5.16	119.78	111.00

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	1530	0	1422	37	0
2	H	1591	0	1448	44	0
3	L	1474	0	1337	50	0
4	M	1665	0	1621	26	0
5	N	1654	0	1590	32	1
6	B	49	0	43	1	0
All	All	7963	0	7461	178	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 12.

All (178) 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:L:80:ALA:HA	3:L:106:VAL:HG21	1.49	0.94
3:L:14:ALA:N	3:L:17:GLN:OE1	2.16	0.77
1:A:439:ASN:HD21	1:A:499:PRO:HA	1.47	0.77
1:A:455:LEU:HD11	1:A:493:GLN:HB2	1.65	0.77
5:N:155:GLN:HB3	5:N:158:ASN:HD21	1.49	0.76
1:A:360:ASN:H	1:A:523:THR:HB	1.51	0.75
2:H:18:LEU:HD22	2:H:82(C):LEU:HD11	1.66	0.75
2:H:200:HIS:HD2	2:H:202:PRO:HD2	1.53	0.73
1:A:406:GLU:HA	3:L:53:ASN:HD21	1.54	0.72
4:M:211:ILE:HG12	4:M:226:LYS:HG2	1.73	0.70
4:M:60:SER:HA	5:N:95(A):ARG:HA	1.75	0.68
5:N:147:GLN:HG3	5:N:154:LEU:HD21	1.74	0.68
2:H:87:THR:HG23	2:H:110:THR:HA	1.78	0.66
2:H:48:VAL:HG13	2:H:63:VAL:HG11	1.77	0.66
5:N:183:LYS:HG3	5:N:187:GLU:OE2	1.95	0.66
3:L:132:THR:HA	3:L:180:SER:CB	2.28	0.63
3:L:135:CYS:HB2	3:L:149:TRP:CZ2	2.35	0.62
3:L:83:GLU:OE2	3:L:105:THR:HG22	2.00	0.62
2:H:18:LEU:HD23	2:H:82:MET:HB2	1.80	0.62
2:H:121:VAL:HG22	2:H:142:VAL:HG12	1.82	0.62
2:H:200:HIS:CD2	2:H:202:PRO:HD2	2.35	0.61
3:L:186:TRP:CH2	3:L:208:ALA:HA	2.35	0.61
2:H:144:ASP:HA	2:H:175:LEU:HB3	1.83	0.61
1:A:366:SER:HA	1:A:369:TYR:CE1	2.36	0.60
1:A:357:ARG:HG3	1:A:396:TYR:CE1	2.37	0.58
2:H:5:VAL:O	2:H:22:CYS:HA	2.03	0.58
1:A:420:ASP:HB3	1:A:460:ASN:OD1	2.03	0.58
5:N:170:ASP:OD2	5:N:172:THR:N	2.36	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:N:35:TRP:HB2	5:N:48:ILE:HB	1.85	0.58
2:H:119:PRO:HD3	2:H:200:HIS:ND1	2.19	0.58
1:A:433:VAL:HG22	1:A:512:VAL:HG22	1.86	0.57
5:N:166:GLN:HG3	5:N:173:TYR:CZ	2.40	0.56
2:H:82:MET:HB3	2:H:82(C):LEU:HD21	1.87	0.56
1:A:363:ALA:O	1:A:527:PRO:HD3	2.05	0.56
1:A:388:ASN:O	1:A:526:GLY:HA3	2.05	0.55
1:A:342:PHE:HB2	6:B:1:NAG:H82	1.89	0.55
1:A:376:THR:O	1:A:434:ILE:HA	2.07	0.55
2:H:123:PRO:HD3	2:H:209:LYS:HE2	1.89	0.54
3:L:12:SER:HB2	3:L:107:LEU:HD21	1.89	0.54
4:M:179:VAL:HG22	4:M:198:VAL:HB	1.90	0.54
3:L:35:TRP:HB2	3:L:48:ILE:HB	1.90	0.53
5:N:136:LEU:HD13	5:N:175:LEU:HD22	1.91	0.53
5:N:170:ASP:OD2	5:N:170:ASP:C	2.47	0.52
1:A:394:ASN:OD1	1:A:516:GLU:HB2	2.09	0.52
4:M:132:THR:HG22	4:M:163:PRO:HD3	1.91	0.52
3:L:106:VAL:O	3:L:141:TYR:OH	2.28	0.51
1:A:376:THR:HG23	1:A:378:LYS:HE2	1.93	0.51
2:H:35:ASN:CG	2:H:100(I):ASN:HD21	2.13	0.51
4:M:168:VAL:HG22	4:M:214:VAL:HG22	1.92	0.51
5:N:120:PRO:HG3	5:N:132:VAL:HG22	1.92	0.51
5:N:155:GLN:HB3	5:N:158:ASN:ND2	2.22	0.51
3:L:179:LEU:HD13	3:L:180:SER:N	2.26	0.51
1:A:490:PHE:CD1	1:A:491:PRO:HD2	2.46	0.50
3:L:163:THR:HG22	3:L:164:THR:O	2.11	0.50
4:M:53:GLY:HA2	4:M:73:LYS:HD2	1.93	0.50
4:M:48:MET:HE1	4:M:80:LEU:HD21	1.93	0.50
3:L:140:PHE:HB2	3:L:198:HIS:CD2	2.46	0.50
2:H:66:ARG:HB3	2:H:82(A):ASN:O	2.12	0.50
3:L:168:GLN:HB2	3:L:170:ASN:OD1	2.12	0.50
1:A:350:VAL:HG22	1:A:422:ASN:HB3	1.92	0.50
4:M:12:LYS:O	4:M:111:VAL:HA	2.11	0.50
3:L:14:ALA:HA	3:L:107:LEU:HB2	1.94	0.49
4:M:170:TRP:CH2	4:M:212:CYS:HB3	2.48	0.49
4:M:20:ILE:HD11	4:M:80:LEU:HD23	1.96	0.48
2:H:163:VAL:HA	2:H:182:VAL:HA	1.95	0.48
4:M:175:LEU:HD21	4:M:198:VAL:HG21	1.95	0.48
2:H:138:LEU:HD11	2:H:194:TYR:CD2	2.49	0.48
5:N:144:ALA:C	5:N:145:LYS:HD2	2.34	0.48
3:L:13:GLY:O	3:L:106:VAL:HA	2.14	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:37:VAL:HG22	2:H:47:TRP:HA	1.96	0.47
2:H:35:ASN:OD1	2:H:100(I):ASN:ND2	2.42	0.47
3:L:37:GLN:HB2	3:L:86:TYR:CE2	2.49	0.47
3:L:83:GLU:HG3	3:L:104:LEU:O	2.14	0.47
4:M:154:LEU:HG	4:M:198:VAL:HG13	1.95	0.47
4:M:87:THR:HG23	4:M:110:THR:HA	1.96	0.47
1:A:354:ASN:O	1:A:398:ASP:HA	2.13	0.47
2:H:50:TYR:CD1	2:H:58:TYR:HD2	2.32	0.47
4:M:100(C):TRP:CG	5:N:96:TRP:HZ2	2.33	0.47
4:M:178:GLY:O	4:M:198:VAL:HA	2.14	0.47
5:N:35:TRP:CE2	5:N:73:LEU:HB2	2.49	0.47
5:N:108:ARG:HD2	5:N:170:ASP:O	2.15	0.47
5:N:151:ASP:OD1	5:N:189:HIS:HB3	2.15	0.47
3:L:18:ARG:HG3	3:L:76:THR:HG22	1.95	0.47
4:M:215:ASN:ND2	4:M:222:LYS:HG3	2.29	0.47
2:H:67:PHE:CE2	2:H:82:MET:HG2	2.49	0.47
2:H:94:ARG:HB3	2:H:102:ALA:HB3	1.97	0.47
4:M:20:ILE:O	4:M:79:TYR:HA	2.14	0.47
4:M:101:ASP:OD1	4:M:101:ASP:N	2.48	0.47
1:A:462:LYS:HE3	1:A:465:GLU:OE2	2.14	0.47
2:H:24:ALA:HB1	2:H:27:PHE:CE1	2.50	0.47
3:L:123:SER:HA	3:L:126:LEU:HB2	1.97	0.47
1:A:462:LYS:HE3	1:A:465:GLU:CD	2.35	0.46
2:H:12:VAL:O	2:H:111:VAL:HA	2.15	0.46
4:M:100(C):TRP:HB2	5:N:91:SER:HB2	1.97	0.46
5:N:167:ASP:OD1	5:N:169:LYS:N	2.43	0.46
3:L:186:TRP:HH2	3:L:208:ALA:HA	1.78	0.46
5:N:143:GLU:O	5:N:198:HIS:HD2	1.98	0.46
3:L:196:VAL:O	3:L:202:THR:HA	2.16	0.46
5:N:105:GLU:OE1	5:N:173:TYR:OH	2.33	0.46
1:A:393:THR:HA	1:A:522:ALA:HA	1.98	0.46
3:L:107:LEU:HD23	3:L:107:LEU:HA	1.73	0.46
5:N:210:ASN:HB2	5:N:213:GLU:HB2	1.98	0.46
3:L:176:SER:HB2	3:L:178:TYR:CE1	2.50	0.46
4:M:216:HIS:CD2	4:M:218:PRO:HD2	2.51	0.46
2:H:70:SER:OG	2:H:79:TYR:HB2	2.16	0.45
2:H:39:GLN:HB2	2:H:45:LEU:HD23	1.97	0.45
2:H:67:PHE:CZ	2:H:82:MET:HG2	2.52	0.45
1:A:401:VAL:HG22	1:A:509:ARG:HG2	1.97	0.45
2:H:32:ARG:HG3	2:H:94:ARG:HD2	1.98	0.45
2:H:122:PHE:O	2:H:141:LEU:HB3	2.16	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:L:160:VAL:HA	3:L:179:LEU:CD2	2.47	0.45
5:N:37:GLN:HB2	5:N:47:LEU:HD11	1.99	0.45
1:A:358:ILE:HB	1:A:395:VAL:HB	1.98	0.45
3:L:116:VAL:O	3:L:205:LYS:HG3	2.16	0.45
2:H:13:GLN:HE21	2:H:13:GLN:HB3	1.59	0.45
3:L:37:GLN:HB3	3:L:47:LEU:HG	1.98	0.45
5:N:147:GLN:CG	5:N:154:LEU:HD21	2.46	0.45
3:L:163:THR:HB	3:L:176:SER:O	2.17	0.44
3:L:5:THR:HB	3:L:24:THR:OG1	2.17	0.44
1:A:365:TYR:CD2	1:A:365:TYR:N	2.85	0.44
1:A:425:LEU:HD21	1:A:512:VAL:HG11	2.00	0.44
2:H:119:PRO:HA	2:H:145:TYR:HB3	1.98	0.44
2:H:167:PRO:HB2	3:L:163:THR:HG21	1.99	0.44
1:A:380:TYR:CE2	2:H:99:TYR:HB3	2.52	0.44
1:A:438:SER:HB3	1:A:509:ARG:HG3	2.00	0.44
2:H:67:PHE:HA	2:H:81:GLN:O	2.18	0.44
3:L:140:PHE:CE1	3:L:174:ALA:HA	2.53	0.44
2:H:169:VAL:O	2:H:176:TYR:HA	2.18	0.43
2:H:94:ARG:NH2	2:H:101:ASP:OD2	2.42	0.43
3:L:79:GLN:O	3:L:106:VAL:HG11	2.18	0.43
3:L:143:GLY:HA3	3:L:173:TYR:CG	2.54	0.43
2:H:201:LYS:HB3	2:H:202:PRO:HD3	2.00	0.43
1:A:334:ASN:N	1:A:334:ASN:OD1	2.52	0.43
3:L:116:VAL:HA	3:L:136:LEU:O	2.18	0.43
3:L:3:VAL:HG12	3:L:27(B):ASN:ND2	2.33	0.43
5:N:118:PHE:HA	5:N:119:PRO:HD3	1.90	0.43
5:N:194:CYS:O	5:N:206:THR:HA	2.19	0.42
1:A:439:ASN:HA	1:A:507:PRO:HG2	2.01	0.42
1:A:340:GLU:O	1:A:344:ALA:HB2	2.19	0.42
3:L:54:ARG:NE	3:L:62:PHE:O	2.46	0.42
4:M:13:LYS:HB2	4:M:16:GLU:OE1	2.20	0.42
3:L:4:LEU:HD11	3:L:90:SER:HB3	2.01	0.42
3:L:146:THR:O	3:L:196:VAL:HA	2.19	0.42
4:M:160:ASP:HA	4:M:191:LEU:HB3	2.01	0.42
2:H:18:LEU:CD2	2:H:82(C):LEU:HD11	2.44	0.42
3:L:123:SER:O	3:L:127:GLN:N	2.37	0.42
1:A:406:GLU:HA	3:L:53:ASN:ND2	2.28	0.42
2:H:50:TYR:HD1	2:H:58:TYR:HD2	1.67	0.42
2:H:154:TRP:CZ3	2:H:196:CYS:HB3	2.55	0.42
3:L:62:PHE:CD1	3:L:75:ILE:HG12	2.54	0.42
3:L:118:LEU:HD12	3:L:194:CYS:HB3	2.02	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:N:191:VAL:HG22	5:N:210:ASN:OD1	2.19	0.42
2:H:166:PHE:CE2	3:L:136:LEU:HD13	2.55	0.41
1:A:408:ARG:HG3	2:H:100(J):TRP:CH2	2.55	0.41
4:M:82(C):LEU:HD23	4:M:82(C):LEU:HA	1.91	0.41
5:N:151:ASP:OD1	5:N:189:HIS:CD2	2.74	0.41
3:L:197:THR:HA	3:L:201:SER:O	2.21	0.41
1:A:335:LEU:HA	1:A:362:VAL:O	2.21	0.41
1:A:452:LEU:HD23	1:A:492:LEU:HB3	2.01	0.41
2:H:148:GLU:OE1	2:H:150:VAL:HG22	2.21	0.41
2:H:154:TRP:CH2	2:H:196:CYS:HB3	2.56	0.41
3:L:179:LEU:HD22	3:L:179:LEU:HA	1.53	0.41
3:L:39:LEU:HD12	3:L:84:ALA:HB2	2.02	0.41
3:L:131:ALA:HB3	3:L:182:THR:HA	2.02	0.41
5:N:39:LYS:NZ	5:N:81:GLU:O	2.40	0.41
3:L:34:HIS:HD2	3:L:50:GLY:H	1.69	0.41
3:L:207:VAL:O	3:L:208:ALA:HB2	2.20	0.41
4:M:170:TRP:CZ3	4:M:212:CYS:HB3	2.56	0.41
1:A:345:THR:HA	4:M:98:VAL:HG22	2.03	0.41
1:A:502:GLY:O	1:A:506:GLN:HG3	2.20	0.41
2:H:121:VAL:HA	2:H:141:LEU:O	2.21	0.41
4:M:182:PHE:CE2	5:N:176:SER:HB3	2.56	0.41
3:L:34:HIS:CD2	3:L:50:GLY:H	2.40	0.40
5:N:89:GLN:HB2	5:N:98:PHE:CD2	2.56	0.40
5:N:95:PRO:HA	5:N:96:TRP:CD2	2.56	0.40
5:N:113:PRO:HA	5:N:139:PHE:HB3	2.03	0.40
1:A:336:CYS:SG	1:A:363:ALA:HB2	2.61	0.40
1:A:425:LEU:HD23	1:A:425:LEU:HA	1.91	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)
5:N:60:SER:OG	5:N:185:ASP:OD2[3_455]	2.19	0.01

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	194/205 (95%)	191 (98%)	3 (2%)	0	100	100
2	H	216/230 (94%)	216 (100%)	0	0	100	100
3	L	206/217 (95%)	200 (97%)	6 (3%)	0	100	100
4	M	218/226 (96%)	217 (100%)	1 (0%)	0	100	100
5	N	214/217 (99%)	210 (98%)	4 (2%)	0	100	100
All	All	1048/1095 (96%)	1034 (99%)	14 (1%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains (i)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	162/177 (92%)	156 (96%)	6 (4%)	34	60
2	H	159/194 (82%)	153 (96%)	6 (4%)	33	58
3	L	150/180 (83%)	137 (91%)	13 (9%)	10	20
4	M	186/190 (98%)	183 (98%)	3 (2%)	62	84
5	N	189/192 (98%)	181 (96%)	8 (4%)	30	54
All	All	846/933 (91%)	810 (96%)	36 (4%)	29	53

All (36) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	377	PHE
1	A	399	SER
1	A	455	LEU
1	A	469	SER
1	A	477	SER
1	A	525	CYS

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Mol	Chain	Res	Type
2	H	7	SER
2	H	107	THR
2	H	115	SER
2	H	142	VAL
2	H	153	SER
2	H	164	HIS
3	L	24	THR
3	L	37	GLN
3	L	60	ASP
3	L	63	SER
3	L	70	SER
3	L	85	ASP
3	L	94	SER
3	L	109	GLN
3	L	111	LYS
3	L	146	THR
3	L	162	THR
3	L	178	TYR
3	L	194	CYS
4	M	25	SER
4	M	195	SER
4	M	213	ASN
5	N	7	SER
5	N	10	SER
5	N	12	SER
5	N	30	SER
5	N	48	ILE
5	N	67	SER
5	N	107	LYS
5	N	146	VAL

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

Mol	Chain	Res	Type
1	A	334	ASN
1	A	450	ASN
2	H	13	GLN
2	H	81	GLN
3	L	34	HIS
3	L	53	ASN
3	L	168	GLN
4	M	3	GLN

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Mol	Chain	Res	Type
4	M	215	ASN
4	M	220	ASN
5	N	155	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)

4 monosaccharides are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
6	NAG	B	1	1,6	14,14,15	0.33	0	17,19,21	0.59	0
6	NAG	B	2	6	14,14,15	0.30	0	17,19,21	0.44	0
6	BMA	B	3	6	11,11,12	0.65	0	15,15,17	0.69	0
6	FUC	B	4	6	10,10,11	0.74	0	14,14,16	1.03	2 (14%)

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	1	1,6	-	0/6/23/26	0/1/1/1
6	NAG	B	2	6	-	0/6/23/26	0/1/1/1
6	BMA	B	3	6	-	0/2/19/22	0/1/1/1
6	FUC	B	4	6	-	-	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})
6	B	4	FUC	O5-C5-C4	2.34	113.72	109.52
6	B	4	FUC	C1-O5-C5	2.17	117.69	112.78

There are no chirality outliers.

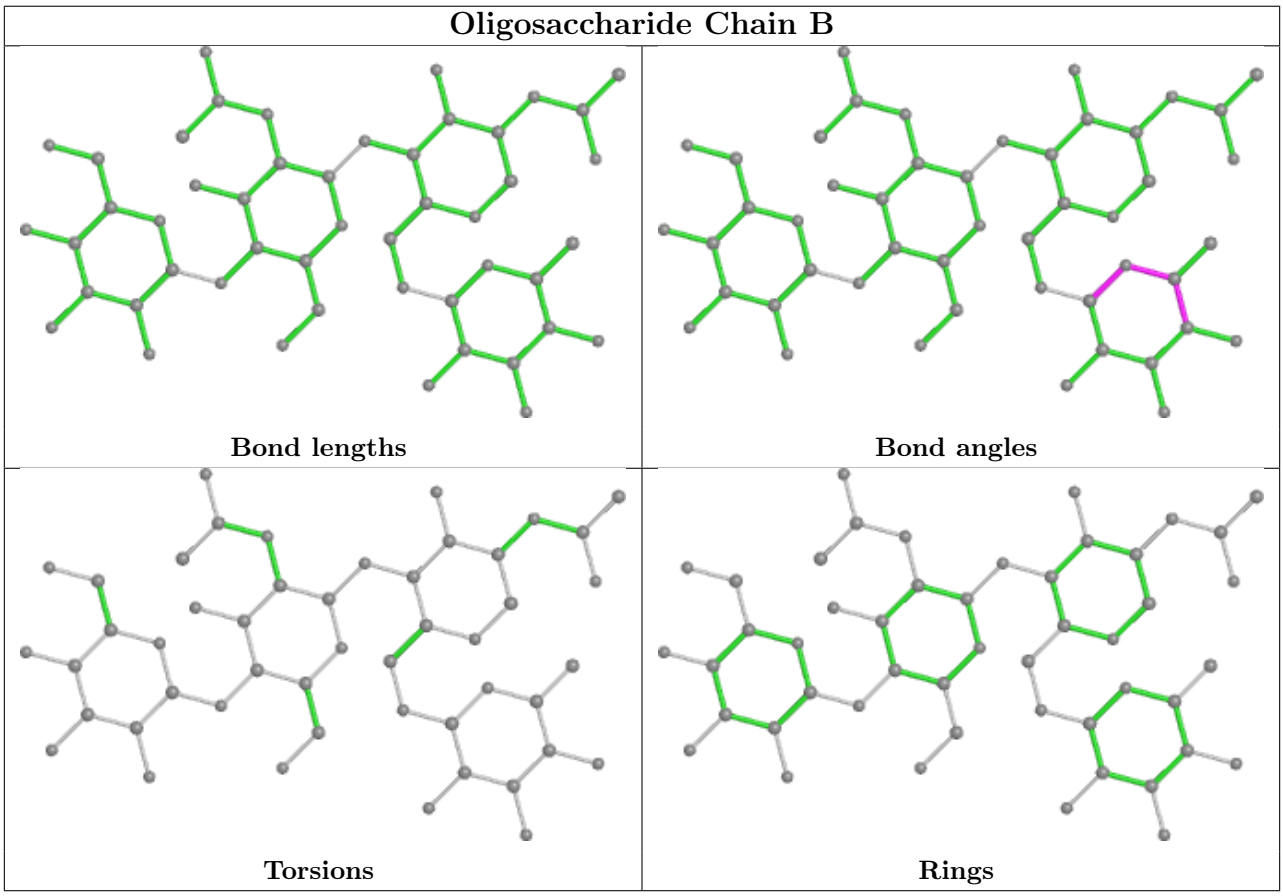
There are no torsion outliers.

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	B	1	NAG	1	0

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



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	196/205 (95%)	0.37	15 (7%) 13 13	25, 34, 99, 189	0
2	H	220/230 (95%)	0.67	31 (14%) 2 2	24, 39, 108, 177	0
3	L	210/217 (96%)	1.10	52 (24%) 0 0	24, 60, 118, 182	0
4	M	222/226 (98%)	-0.06	1 (0%) 91 91	27, 43, 61, 90	0
5	N	216/217 (99%)	0.09	3 (1%) 75 77	28, 44, 62, 206	0
All	All	1064/1095 (97%)	0.43	102 (9%) 8 7	24, 44, 103, 206	0

All (102) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
5	N	212	GLY	12.6
3	L	180	SER	8.8
3	L	194	CYS	8.8
2	H	188	SER	8.2
1	A	519	HIS	7.1
3	L	149	TRP	6.5
1	A	527	PRO	6.2
3	L	130	LYS	6.1
2	H	126	PRO	6.1
2	H	135	THR	5.5
2	H	202	PRO	5.4
2	H	141	LEU	5.3
3	L	207	VAL	5.3
3	L	1	GLN	5.1
5	N	213	GLU	4.9
3	L	133	LEU	4.9
1	A	520	ALA	4.7
3	L	186	TRP	4.6
2	H	127	SER	4.5
3	L	120	PRO	4.5

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Mol	Chain	Res	Type	RSRZ
2	H	140	CYS	4.4
3	L	156	VAL	4.4
2	H	190	GLY	4.4
2	H	121	VAL	4.4
3	L	117	THR	4.3
4	M	232	CYS	4.3
2	H	185	PRO	4.1
2	H	138	LEU	4.1
3	L	128	ALA	4.0
1	A	518	LEU	3.9
2	H	189	LEU	3.9
3	L	132	THR	3.8
2	H	157	GLY	3.6
2	H	159	LEU	3.6
3	L	108	GLY	3.6
1	A	367	VAL	3.6
3	L	123	SER	3.6
3	L	193	SER	3.5
3	L	134	VAL	3.5
1	A	521	PRO	3.4
3	L	147	VAL	3.4
3	L	183	PRO	3.4
3	L	81	GLU	3.4
2	H	158	ALA	3.4
3	L	206	THR	3.3
3	L	148	ALA	3.3
3	L	119	PHE	3.2
1	A	384	PRO	3.2
3	L	189	HIS	3.2
1	A	368	LEU	3.1
1	A	517	LEU	3.1
3	L	131	ALA	3.1
3	L	126	LEU	3.0
3	L	196	VAL	3.0
2	H	187	SER	3.0
3	L	202	THR	3.0
3	L	124	GLU	3.0
2	H	120	SER	3.0
2	H	150	VAL	2.9
3	L	208	ALA	2.9
2	H	160	THR	2.9
3	L	121	PRO	2.8

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Mol	Chain	Res	Type	RSRZ
3	L	137	ILE	2.8
2	H	194	TYR	2.8
3	L	141	TYR	2.8
2	H	161	SER	2.7
3	L	114	PRO	2.7
3	L	127	GLN	2.7
3	L	139	ASP	2.7
3	L	122	SER	2.6
2	H	213	PRO	2.6
2	H	139	GLY	2.6
3	L	125	GLU	2.6
3	L	187	LYS	2.6
2	H	166	PHE	2.5
3	L	118	LEU	2.5
3	L	138	SER	2.5
2	H	201	LYS	2.5
2	H	193	THR	2.4
2	H	154	TRP	2.4
2	H	125	ALA	2.4
3	L	182	THR	2.4
3	L	203	VAL	2.4
3	L	168	GLN	2.4
1	A	370	ASN	2.3
2	H	191	THR	2.3
3	L	136	LEU	2.3
3	L	115	SER	2.3
1	A	369	TYR	2.3
1	A	373	SER	2.3
1	A	385	THR	2.3
5	N	214	CYS	2.2
3	L	181	LEU	2.2
3	L	151	ALA	2.2
2	H	172	SER	2.2
1	A	525	CYS	2.1
3	L	179	LEU	2.1
3	L	140	PHE	2.1
3	L	159	GLY	2.0
3	L	177	SER	2.0
1	A	393	THR	2.0
2	H	208	ASP	2.0

6.2 Non-standard residues in protein, DNA, RNA chains (i)

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

6.3 Carbohydrates (i)

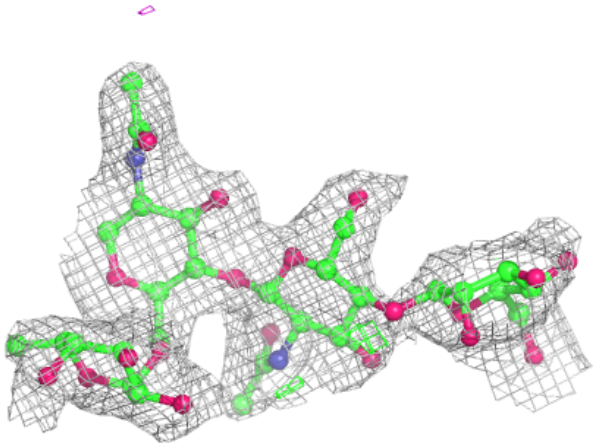
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9'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

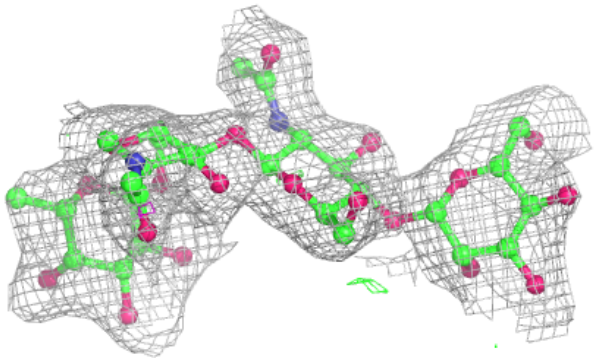
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
6	BMA	B	3	11/12	0.78	0.20	59,68,76,77	0
6	NAG	B	2	14/15	0.88	0.17	34,44,57,76	0
6	NAG	B	1	14/15	0.93	0.12	24,36,47,50	0
6	FUC	B	4	10/11	0.95	0.09	31,40,42,42	0

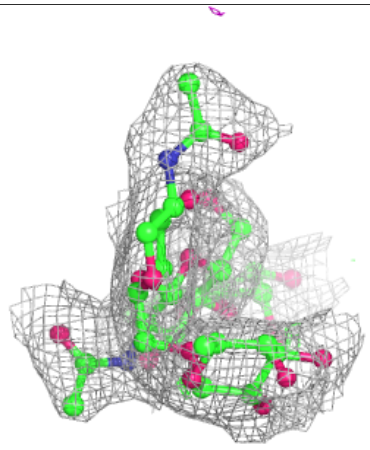
The following is a graphical depiction of the model fit to experimental electron density for oligosaccharide. Each fit is shown from different orientation to approximate a three-dimensional view.

Electron density around Chain B:

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







6.4 Ligands

There are no ligands in this entry.

6.5 Other polymers

There are no such residues in this entry.