Full wwPDB X-ray Structure Validation Report (i)

Nov 22, 2023 – 07:35 PM JST

PDB ID	:	7XSW
Title	:	Structure of SARS-CoV-2 antibody S309 with GX/P2V/2017 RBD
Authors	:	Jia, Y.F.; Chai, Y.; Wang, Q.H.; Gao, G.F.
Deposited on	:	2022-05-15
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:

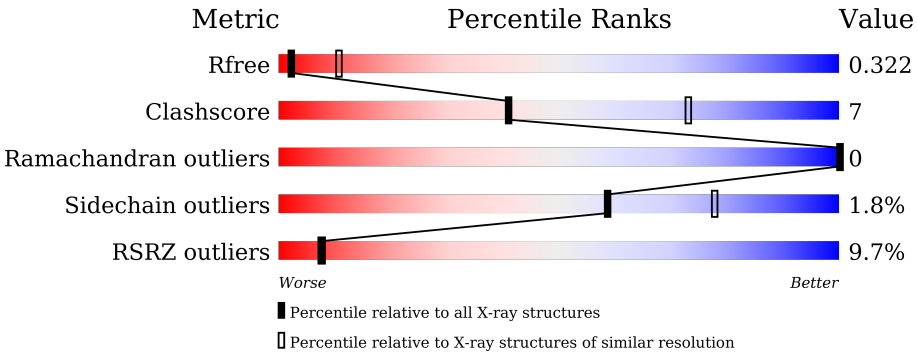
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, 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 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}	130704	1149 (3.34-3.26)
Clashscore	141614	1205 (3.34-3.26)
Ramachandran outliers	138981	1183 (3.34-3.26)
Sidechain outliers	138945	1182 (3.34-3.26)
RSRZ outliers	127900	1115 (3.34-3.26)

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	237	7% 81% 15% .
1	H	237	11% 80% 13% 7%
2	B	215	6% 85% 14% .
2	L	215	2% 80% 20% .
3	C	215	14% 68% 18% 13%
3	R	215	14% 66% 20% 13%

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Mol	Chain	Length	Quality of chain
4	D	3	33% 33% 33%

2 Entry composition (i)

There are 4 unique types of molecules in this entry. The entry contains 9593 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 S309 Heavy Chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	H	220	Total	C	N	O	S	0	0	0
			1654	1043	278	325	8			
1	A	228	Total	C	N	O	S	0	0	0
			1717	1081	292	337	7			

- Molecule 2 is a protein called S309 Lambda Chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	L	213	Total	C	N	O	S	0	0	0
			1624	1011	277	332	4			
2	B	213	Total	C	N	O	S	0	0	0
			1624	1011	277	332	4			

- Molecule 3 is a protein called Spike protein S1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	R	186	Total	C	N	O	S	0	0	0
			1458	935	243	272	8			
3	C	186	Total	C	N	O	S	0	0	0
			1478	950	244	276	8			

There are 12 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
R	528	HIS	-	expression tag	UNP A0A6G6A2Q2
R	529	HIS	-	expression tag	UNP A0A6G6A2Q2
R	530	HIS	-	expression tag	UNP A0A6G6A2Q2
R	531	HIS	-	expression tag	UNP A0A6G6A2Q2
R	532	HIS	-	expression tag	UNP A0A6G6A2Q2
R	533	HIS	-	expression tag	UNP A0A6G6A2Q2
C	528	HIS	-	expression tag	UNP A0A6G6A2Q2
C	529	HIS	-	expression tag	UNP A0A6G6A2Q2

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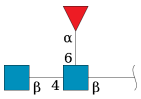
Chain	Residue	Modelled	Actual	Comment	Reference
C	530	HIS	-	expression tag	UNP A0A6G6A2Q2
C	531	HIS	-	expression tag	UNP A0A6G6A2Q2
C	532	HIS	-	expression tag	UNP A0A6G6A2Q2
C	533	HIS	-	expression tag	UNP A0A6G6A2Q2

- 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.

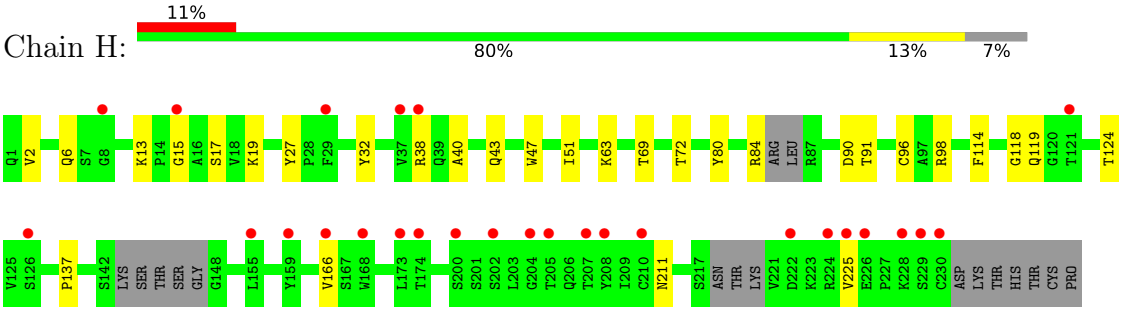


Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
			Total	C	N	O			
4	D	3	38	22	2	14	0	0	0

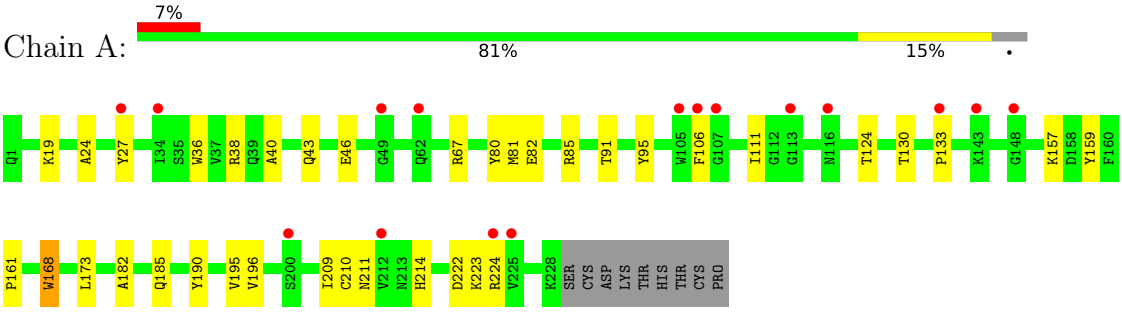
3 Residue-property plots (i)

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.

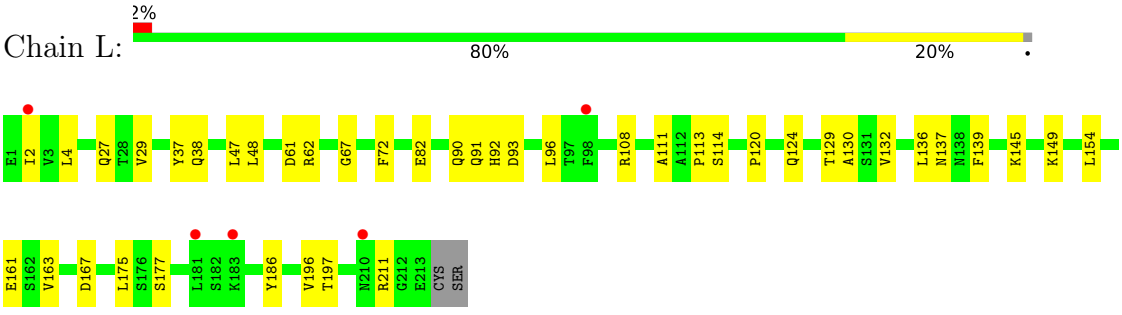
• Molecule 1: S309 Heavy Chain



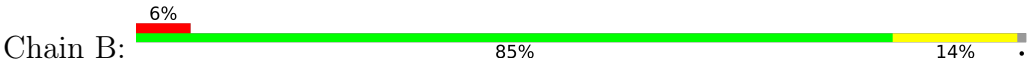
• Molecule 1: S309 Heavy Chain

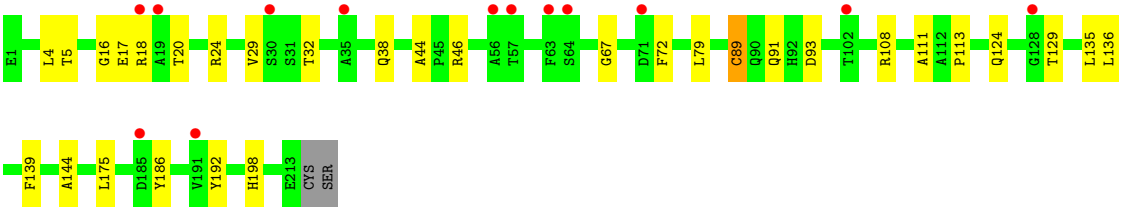


• Molecule 2: S309 Lambda Chain

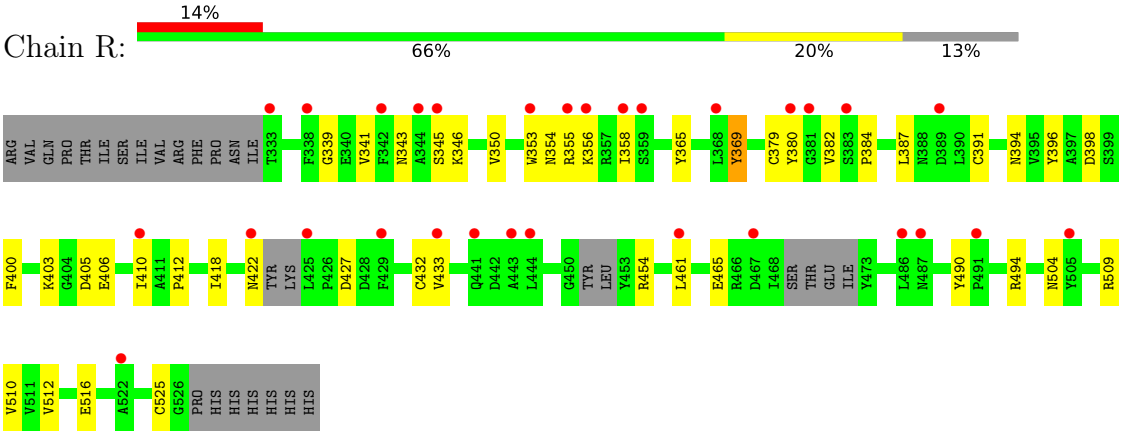


• Molecule 2: S309 Lambda Chain

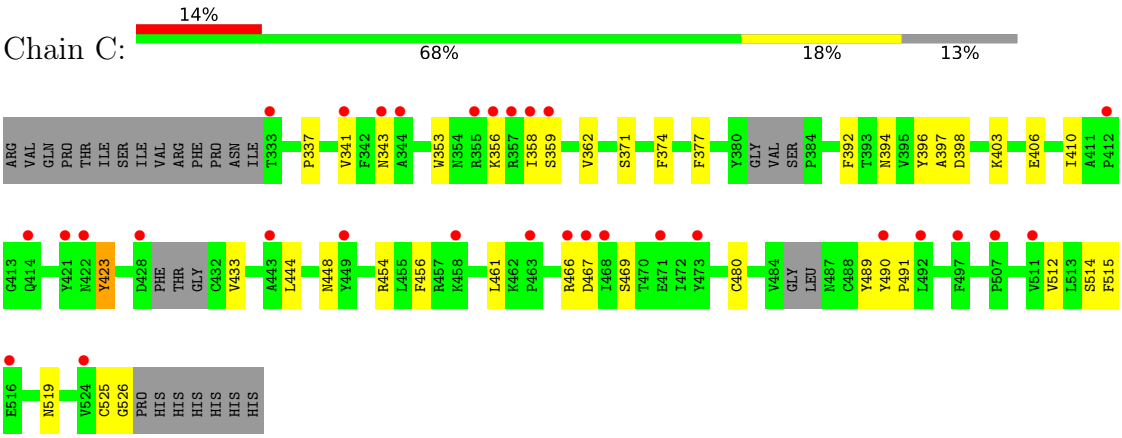




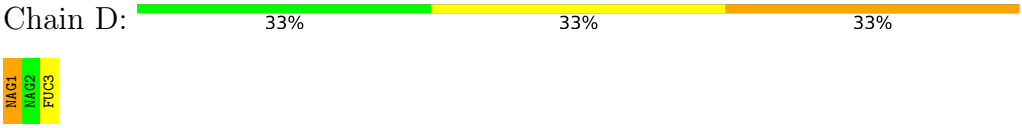
• Molecule 3: Spike protein S1



• Molecule 3: Spike protein S1



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



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α, β, γ	54.64Å 73.60Å 105.61Å 110.53° 92.08° 97.05°	Depositor
Resolution (Å)	48.54 – 3.30 48.54 – 3.30	Depositor EDS
% Data completeness (in resolution range)	94.9 (48.54-3.30) 94.9 (48.54-3.30)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.19 (at 3.33Å)	Xtriage
Refinement program	PHENIX 1.19.2_4158	Depositor
R, R_{free}	0.277 , 0.322 0.277 , 0.322	Depositor DCC
R_{free} test set	1999 reflections (9.21%)	wwPDB-VP
Wilson B-factor (Å^2)	77.6	Xtriage
Anisotropy	0.226	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.30 , 32.7	EDS
L-test for twinning[2]	$< \|L\| > = 0.40$, $< L^2 > = 0.23$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.85	EDS
Total number of atoms	9593	wwPDB-VP
Average B, all atoms (Å^2)	75.0	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

5.1 Standard geometry

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	0.25	0/1760	0.48	0/2398
1	H	0.24	0/1694	0.48	0/2306
2	B	0.26	0/1657	0.50	0/2250
2	L	0.25	0/1657	0.50	0/2250
3	C	0.26	0/1516	0.51	0/2058
3	R	0.25	0/1495	0.49	0/2030
All	All	0.25	0/9779	0.49	0/13292

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	1717	0	1673	26	0
1	H	1654	0	1597	21	0
2	B	1624	0	1582	17	0
2	L	1624	0	1582	29	0
3	C	1478	0	1412	21	0
3	R	1458	0	1389	27	0
4	D	38	0	34	1	0
All	All	9593	0	9269	133	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 (133) 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:C:403:LYS:HB2	3:C:406:GLU:HG3	1.63	0.81
3:R:379:CYS:HB3	3:R:432:CYS:HA	1.65	0.79
3:C:398:ASP:HB2	3:C:512:VAL:HB	1.66	0.77
2:B:17:GLU:O	2:B:18:ARG:HG3	1.86	0.76
2:L:113:PRO:HB3	2:L:139:PHE:HB3	1.66	0.76
2:L:136:LEU:HB2	2:L:175:LEU:HB3	1.68	0.75
3:R:461:LEU:HD22	3:R:465:GLU:HB3	1.69	0.73
2:B:113:PRO:HB3	2:B:139:PHE:HB3	1.69	0.73
3:C:362:VAL:HG13	3:C:526:GLY:HA2	1.69	0.73
3:R:405:ASP:HB3	3:R:504:ASN:HB2	1.71	0.70
1:A:157:LYS:NZ	1:A:185:GLN:OE1	2.24	0.70
3:R:353:TRP:HB3	3:R:400:PHE:HB3	1.75	0.69
1:A:19:LYS:HD2	1:A:82:GLU:HB2	1.75	0.69
3:C:356:LYS:HB3	3:C:397:ALA:HB3	1.75	0.68
3:R:403:LYS:HB2	3:R:406:GLU:HG3	1.76	0.66
1:A:209:ILE:HG12	1:A:224:ARG:HG2	1.79	0.65
1:H:38:ARG:HH22	1:H:63:LYS:HE3	1.63	0.64
2:L:114:SER:HB2	2:L:137:ASN:HB3	1.81	0.62
3:R:422:ASN:HD21	3:R:454:ARG:H	1.45	0.62
3:C:410:ILE:HG23	3:C:423:TYR:HE2	1.64	0.62
1:A:168:TRP:CZ3	1:A:210:CYS:HB2	2.35	0.62
3:C:359:SER:OG	3:C:394:ASN:ND2	2.33	0.61
2:L:92:HIS:HB3	2:L:96:LEU:HD13	1.82	0.61
1:A:168:TRP:HE1	1:A:196:VAL:HB	1.64	0.61
2:L:136:LEU:HD11	2:L:196:VAL:HG11	1.83	0.61
1:H:19:LYS:HE3	1:H:80:TYR:HB3	1.82	0.60
1:A:133:PRO:HB3	1:A:159:TYR:HB3	1.84	0.60
1:H:51:ILE:HD13	1:H:72:THR:HG23	1.83	0.59
3:C:433:VAL:HG22	3:C:512:VAL:HG22	1.83	0.59
3:R:345:SER:O	3:R:509:ARG:NH2	2.37	0.58
3:C:454:ARG:NH1	3:C:467:ASP:O	2.34	0.58
3:R:394:ASN:ND2	3:R:516:GLU:OE2	2.38	0.57
2:B:67:GLY:HA3	2:B:72:PHE:HA	1.85	0.57
1:A:211:ASN:ND2	1:A:222:ASP:OD1	2.36	0.57
2:B:17:GLU:O	2:B:18:ARG:CG	2.53	0.56
2:B:186:TYR:O	2:B:192:TYR:OH	2.23	0.56
3:C:444:LEU:HD12	3:C:448:ASN:HB2	1.88	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:111:ILE:HG12	2:B:32:THR:HB	1.86	0.56
3:R:350:VAL:HA	3:R:400:PHE:HB2	1.88	0.55
3:R:380:TYR:OH	3:R:427:ASP:O	2.22	0.55
2:L:62:ARG:NH2	2:L:82:GLU:OE2	2.40	0.55
2:B:38:GLN:O	2:B:46:ARG:N	2.39	0.54
1:A:67:ARG:HG2	1:A:85:ARG:HH22	1.72	0.54
2:L:61:ASP:OD2	1:A:130:THR:OG1	2.20	0.54
3:C:396:TYR:HB2	3:C:514:SER:HB3	1.88	0.54
1:H:47:TRP:CD1	2:L:96:LEU:HD23	2.43	0.54
2:L:2:ILE:HG12	2:L:27:GLN:HB2	1.90	0.54
3:C:456:PHE:HD2	3:C:491:PRO:HA	1.73	0.54
3:R:369:TYR:HE2	3:R:384:PRO:HB2	1.73	0.53
1:A:36:TRP:CE2	1:A:81:MET:HB2	2.43	0.53
4:D:1:NAG:H83	4:D:1:NAG:H3	1.88	0.53
2:L:29:VAL:HG23	2:L:93:ASP:HB2	1.92	0.52
1:H:6:GLN:H	1:H:119:GLN:HE22	1.56	0.52
1:H:32:TYR:HD2	1:H:98:ARG:HD2	1.74	0.52
3:R:410:ILE:HG21	3:R:510:VAL:HG11	1.91	0.52
1:H:2:VAL:HG21	1:H:27:TYR:HD1	1.74	0.52
3:C:341:VAL:HG22	3:C:356:LYS:HD3	1.92	0.52
2:L:67:GLY:HA3	2:L:72:PHE:HA	1.92	0.51
2:B:108:ARG:HH22	2:B:111:ALA:HB3	1.77	0.50
3:R:398:ASP:HB2	3:R:512:VAL:HB	1.94	0.50
1:A:40:ALA:HB3	1:A:43:GLN:HG3	1.93	0.50
3:R:341:VAL:HG22	3:R:356:LYS:HD3	1.95	0.49
3:R:382:VAL:HG21	3:R:387:LEU:HD13	1.95	0.49
1:A:38:ARG:O	1:A:46:GLU:N	2.41	0.49
3:R:369:TYR:CE2	3:R:384:PRO:HB2	2.47	0.49
2:L:145:LYS:HB3	2:L:197:THR:HB	1.95	0.49
2:L:161:GLU:HA	2:L:177:SER:HA	1.95	0.49
1:H:69:THR:OG1	1:H:84:ARG:NH1	2.46	0.49
1:H:40:ALA:HB3	1:H:43:GLN:HG3	1.96	0.48
3:C:353:TRP:CD1	3:C:466:ARG:HG3	2.48	0.48
1:H:38:ARG:NH1	1:H:90:ASP:OD1	2.47	0.48
1:H:47:TRP:CE3	2:L:96:LEU:HB3	2.49	0.47
1:A:91:THR:HG23	1:A:124:THR:HA	1.95	0.47
1:A:168:TRP:NE1	1:A:196:VAL:HB	2.28	0.47
1:H:91:THR:HG23	1:H:124:THR:HA	1.95	0.47
2:B:5:THR:HB	2:B:24:ARG:HB3	1.97	0.47
3:C:337:PRO:HD2	3:C:358:ILE:HG23	1.95	0.47
3:R:353:TRP:HZ3	3:R:355:ARG:HB2	1.79	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:L:163:VAL:HG22	2:L:175:LEU:HD13	1.96	0.47
1:H:96:CYS:O	1:H:118:GLY:N	2.39	0.47
2:L:108:ARG:HH21	2:L:111:ALA:HB2	1.80	0.46
2:L:113:PRO:HB2	2:L:136:LEU:HD12	1.97	0.46
1:A:24:ALA:HB1	1:A:27:TYR:CE1	2.50	0.46
1:A:24:ALA:HB1	1:A:27:TYR:HE1	1.81	0.46
3:R:433:VAL:HG22	3:R:512:VAL:HG22	1.96	0.46
3:R:350:VAL:HG21	3:R:418:ILE:HD12	1.96	0.46
2:L:4:LEU:HD21	2:L:91:GLN:HG2	1.98	0.45
1:A:168:TRP:HB2	1:A:173:LEU:HB3	1.97	0.45
3:R:339:GLY:O	3:R:343:ASN:HB2	2.17	0.45
2:B:4:LEU:HD13	2:B:89:CYS:SG	2.56	0.45
1:A:195:VAL:HG11	2:B:135:LEU:HD22	1.99	0.45
1:A:210:CYS:SG	1:A:223:LYS:HB3	2.56	0.45
1:A:173:LEU:HD21	1:A:196:VAL:HG21	1.99	0.45
2:B:16:GLY:H	2:B:79:LEU:HB2	1.80	0.45
3:R:365:TYR:CD2	3:R:387:LEU:HG	2.52	0.45
2:L:29:VAL:HG21	2:L:91:GLN:HB2	1.99	0.44
1:H:17:SER:OG	1:H:84:ARG:HA	2.16	0.44
2:L:37:TYR:HE1	2:L:90:GLN:HB3	1.81	0.44
2:L:120:PRO:HD3	2:L:132:VAL:HG22	1.99	0.44
3:C:454:ARG:NH2	3:C:469:SER:O	2.51	0.44
3:R:380:TYR:HE1	3:R:412:PRO:HG3	1.82	0.44
2:L:124:GLN:HG2	2:L:129:THR:O	2.18	0.43
3:R:355:ARG:HE	3:R:396:TYR:HB3	1.83	0.43
1:A:182:ALA:HB1	1:A:190:TYR:HB3	2.01	0.43
1:H:2:VAL:HG21	1:H:27:TYR:CD1	2.53	0.43
2:B:124:GLN:HG2	2:B:129:THR:O	2.19	0.42
3:C:392:PHE:CD2	3:C:515:PHE:HB3	2.55	0.42
1:H:6:GLN:H	1:H:119:GLN:NE2	2.18	0.42
2:L:91:GLN:O	2:L:96:LEU:HD12	2.20	0.42
1:H:114:PHE:O	2:L:47:LEU:HB2	2.20	0.42
1:H:166:VAL:HA	1:H:211:ASN:O	2.20	0.42
2:L:38:GLN:HB2	2:L:48:LEU:HD11	2.00	0.42
2:B:144:ALA:HB2	2:B:198:HIS:HD2	1.84	0.42
3:C:371:SER:HB3	3:C:374:PHE:CE2	2.55	0.42
1:H:47:TRP:CG	2:L:96:LEU:HD23	2.55	0.42
1:A:161:PRO:O	1:A:214:HIS:NE2	2.42	0.41
3:C:353:TRP:CE3	3:C:398:ASP:HB3	2.55	0.41
1:H:137:PRO:HB2	1:H:225:VAL:HG13	2.03	0.41
2:L:149:LYS:HE2	2:L:154:LEU:HD11	2.01	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:95:TYR:HE2	2:B:44:ALA:HA	1.85	0.41
1:H:13:LYS:O	1:H:15:GLY:N	2.47	0.41
2:L:120:PRO:HG3	2:L:130:ALA:HB1	2.03	0.41
3:R:341:VAL:HG21	3:R:358:ILE:HD11	2.03	0.41
1:A:106:PHE:CD2	3:C:356:LYS:HE2	2.56	0.41
2:B:29:VAL:HG21	2:B:91:GLN:HB2	2.02	0.41
2:B:136:LEU:HD13	2:B:175:LEU:HD22	2.02	0.41
3:C:461:LEU:HD23	3:C:461:LEU:HA	1.90	0.41
3:R:461:LEU:HA	3:R:461:LEU:HD23	1.86	0.40
2:L:186:TYR:CE2	2:L:211:ARG:HD3	2.57	0.40
1:A:19:LYS:HE3	1:A:80:TYR:HB3	2.03	0.40
3:R:346:LYS:HD2	3:R:346:LYS:HA	1.79	0.40
3:R:380:TYR:CE1	3:R:412:PRO:HG3	2.57	0.40
3:C:353:TRP:HE3	3:C:398:ASP:HB3	1.86	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	226/237 (95%)	219 (97%)	7 (3%)	0	100	100
1	H	212/237 (90%)	206 (97%)	6 (3%)	0	100	100
2	B	211/215 (98%)	201 (95%)	10 (5%)	0	100	100
2	L	211/215 (98%)	205 (97%)	6 (3%)	0	100	100
3	C	178/215 (83%)	169 (95%)	9 (5%)	0	100	100
3	R	178/215 (83%)	170 (96%)	8 (4%)	0	100	100
All	All	1216/1334 (91%)	1170 (96%)	46 (4%)	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	190/199 (96%)	189 (100%)	1 (0%)	88 93
1	H	183/199 (92%)	183 (100%)	0	100 100
2	B	184/186 (99%)	181 (98%)	3 (2%)	62 79
2	L	184/186 (99%)	183 (100%)	1 (0%)	88 93
3	C	162/188 (86%)	154 (95%)	8 (5%)	25 56
3	R	159/188 (85%)	153 (96%)	6 (4%)	33 62
All	All	1062/1146 (93%)	1043 (98%)	19 (2%)	59 78

All (19) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	L	167	ASP
3	R	354	ASN
3	R	369	TYR
3	R	391	CYS
3	R	490	TYR
3	R	494	ARG
3	R	525	CYS
1	A	168	TRP
2	B	20	THR
2	B	89	CYS
2	B	93	ASP
3	C	343	ASN
3	C	377	PHE
3	C	423	TYR
3	C	480	CYS
3	C	489	TYR
3	C	490	TYR
3	C	519	ASN
3	C	525	CYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (4) such sidechains are listed below:

Mol	Chain	Res	Type
1	H	55	ASN
1	H	57	ASN
3	R	422	ASN
1	A	213	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)

3 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	D	1	4,3	14,14,15	0.46	0	17,19,21	1.41	2 (11%)
4	NAG	D	2	4	14,14,15	0.25	0	17,19,21	0.41	0
4	FUC	D	3	4	10,10,11	1.31	1 (10%)	14,14,16	1.31	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
4	NAG	D	1	4,3	-	5/6/23/26	0/1/1/1
4	NAG	D	2	4	-	0/6/23/26	0/1/1/1
4	FUC	D	3	4	-	-	0/1/1/1

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	D	3	FUC	C1-C2	3.40	1.60	1.52

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	D	1	NAG	C2-N2-C7	4.39	129.15	122.90
4	D	3	FUC	O2-C2-C1	3.02	115.33	109.15
4	D	3	FUC	C1-C2-C3	2.57	112.83	109.67
4	D	1	NAG	C1-C2-N2	2.15	114.16	110.49

There are no chirality outliers.

All (5) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	D	1	NAG	O5-C5-C6-O6
4	D	1	NAG	C4-C5-C6-O6
4	D	1	NAG	C8-C7-N2-C2
4	D	1	NAG	O7-C7-N2-C2
4	D	1	NAG	C3-C2-N2-C7

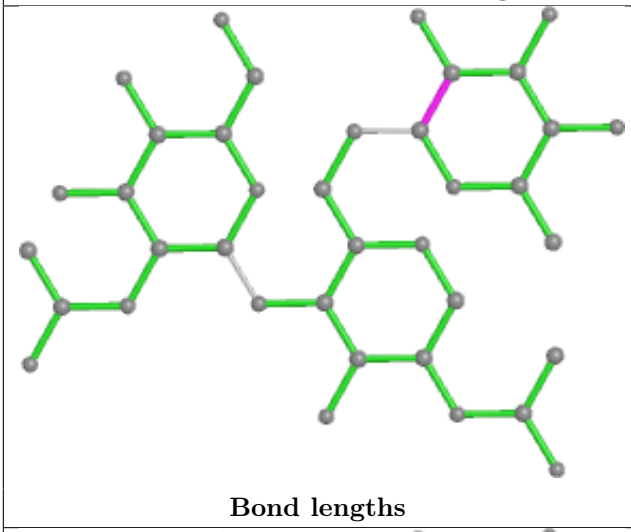
There are no ring outliers.

1 monomer is involved in 1 short contact:

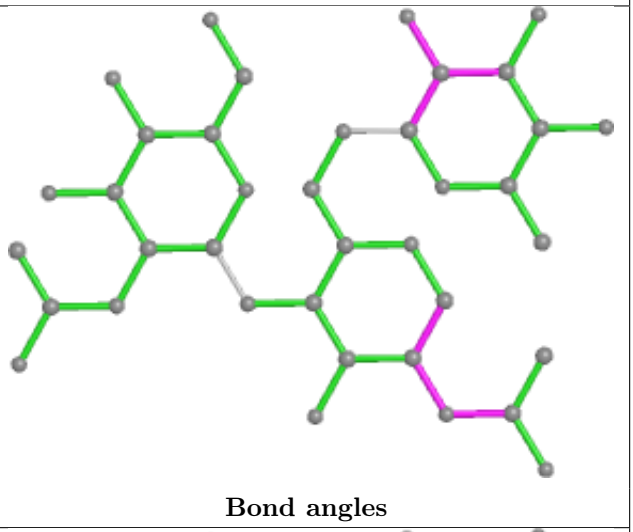
Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	D	1	NAG	1	0

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

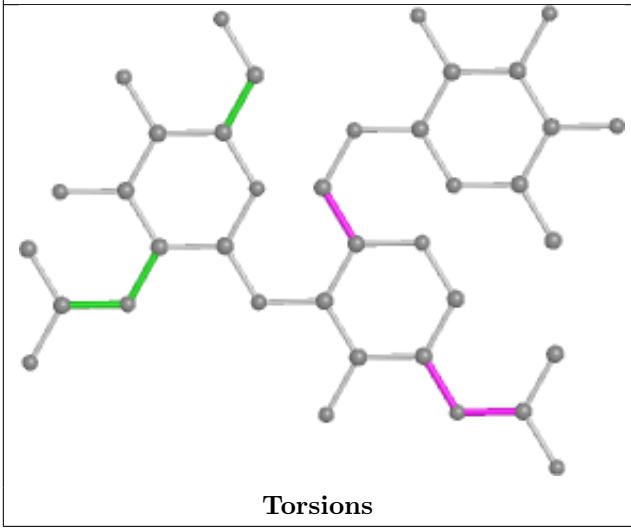
Oligosaccharide Chain D



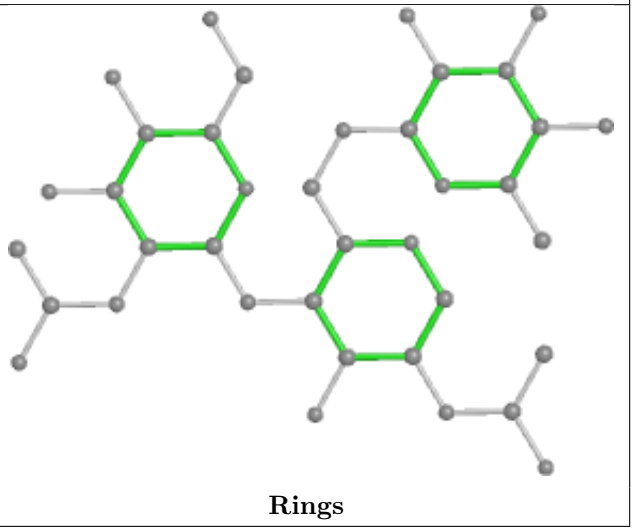
Bond lengths



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	228/237 (96%)	0.47	16 (7%) 16 16	44, 72, 99, 118	0
1	H	220/237 (92%)	0.68	27 (12%) 4 3	53, 84, 112, 122	0
2	B	213/215 (99%)	0.49	13 (6%) 21 20	46, 65, 91, 106	0
2	L	213/215 (99%)	0.46	5 (2%) 60 59	36, 63, 89, 95	0
3	C	186/215 (86%)	0.99	30 (16%) 1 2	63, 89, 113, 124	0
3	R	186/215 (86%)	0.84	30 (16%) 1 2	48, 76, 100, 119	0
All	All	1246/1334 (93%)	0.64	121 (9%) 7 8	36, 74, 105, 124	0

All (121) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	106	PHE	5.0
2	L	181	LEU	4.7
2	B	64	SER	4.7
1	H	205	THR	4.6
1	A	225	VAL	4.6
1	H	8	GLY	4.6
3	C	333	THR	4.4
3	R	486	LEU	4.4
2	B	19	ALA	4.3
3	R	425	LEU	4.3
3	C	343	ASN	3.9
1	H	208	TYR	3.8
3	R	358	ILE	3.8
3	C	357	ARG	3.8
3	C	492	LEU	3.8
1	H	121	THR	3.8
1	H	229	SER	3.7
1	H	222	ASP	3.7
3	R	333	THR	3.6

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Mol	Chain	Res	Type	RSRZ
3	R	491	PRO	3.6
2	L	210	ASN	3.6
3	R	443	ALA	3.5
3	R	422	ASN	3.5
1	H	38	ARG	3.4
3	R	355	ARG	3.4
3	R	345	SER	3.4
3	C	471	GLU	3.4
3	C	463	PRO	3.4
3	R	522	ALA	3.3
1	A	200	SER	3.3
3	C	359	SER	3.3
3	R	380	TYR	3.2
2	B	30	SER	3.2
2	B	191	VAL	3.2
3	C	458	LYS	3.2
3	C	356	LYS	3.2
3	R	338	PHE	3.2
2	B	71	ASP	3.2
1	H	166	VAL	3.1
2	L	183	LYS	3.1
1	H	207	THR	3.0
3	R	441	GLN	3.0
1	H	37	VAL	3.0
1	H	155	LEU	3.0
1	H	200	SER	3.0
1	A	224	ARG	2.9
1	H	159	TYR	2.9
1	A	107	GLY	2.9
3	R	359	SER	2.9
1	H	173	LEU	2.9
2	B	57	THR	2.9
3	C	449	TYR	2.9
2	B	35	ALA	2.9
3	C	507	PRO	2.9
1	A	143	LYS	2.8
3	C	473	TYR	2.8
1	A	49	GLY	2.8
2	B	56	ALA	2.7
1	H	230	CYS	2.7
3	C	466	ARG	2.7
1	H	126	SER	2.7

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Mol	Chain	Res	Type	RSRZ
1	A	116	ASN	2.7
3	C	516	GLU	2.6
1	H	15	GLY	2.6
3	R	381	GLY	2.6
3	R	344	ALA	2.6
3	C	414	GLN	2.6
2	B	102	THR	2.6
3	C	344	ALA	2.6
3	C	421	TYR	2.5
1	H	226	GLU	2.5
3	C	490	TYR	2.5
3	C	468	ILE	2.5
2	B	128	GLY	2.5
3	C	443	ALA	2.5
3	R	368	LEU	2.5
3	C	511	VAL	2.5
3	C	358	ILE	2.5
3	C	341	VAL	2.5
3	R	487	ASN	2.4
1	A	34	ILE	2.4
2	L	2	ILE	2.4
3	R	467	ASP	2.4
1	H	210	CYS	2.4
3	R	342	PHE	2.4
3	C	467	ASP	2.4
3	C	355	ARG	2.3
3	R	410	ILE	2.3
1	H	174	THR	2.3
1	H	224	ARG	2.3
1	A	105	TRP	2.3
1	H	168	TRP	2.3
3	R	505	TYR	2.3
3	R	444	LEU	2.2
1	A	133	PRO	2.2
3	R	383	SER	2.2
1	A	27	TYR	2.2
3	R	356	LYS	2.2
1	H	204	GLY	2.2
3	R	389	ASP	2.2
2	B	63	PHE	2.1
3	R	429	PHE	2.1
3	C	422	ASN	2.1

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Mol	Chain	Res	Type	RSRZ
1	A	62	GLN	2.1
1	H	202	SER	2.1
2	B	18	ARG	2.1
2	B	185	ASP	2.1
1	A	212	VAL	2.1
3	C	524	VAL	2.1
1	A	113	GLY	2.1
3	R	433	VAL	2.1
3	C	497	PHE	2.0
2	L	98	PHE	2.0
3	R	353	TRP	2.0
1	H	225	VAL	2.0
3	C	412	PRO	2.0
1	H	29	PHE	2.0
3	C	428	ASP	2.0
1	H	228	LYS	2.0
3	R	461	LEU	2.0
1	A	148	GLY	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)

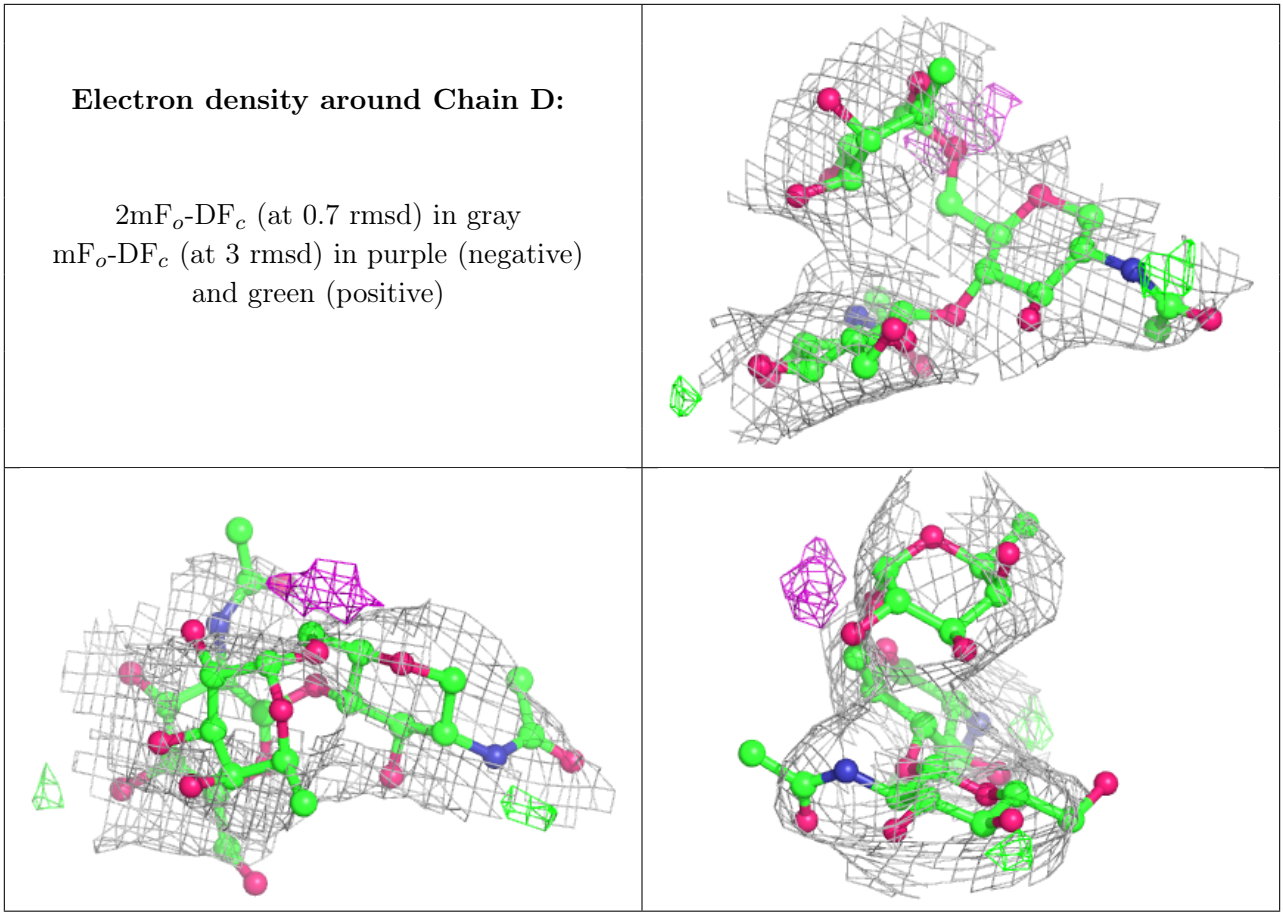
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' 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
4	NAG	D	1	14/15	0.84	0.21	63,76,81,88	0
4	FUC	D	3	10/11	0.84	0.26	73,77,81,82	0
4	NAG	D	2	14/15	0.87	0.22	64,74,83,87	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 D:

$2mF_o$-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.