Full wwPDB X-ray Structure Validation Report ⓘ

Dec 2, 2021 – 11:10 am GMT

PDB ID	:	7A3T
Title	:	Crystal structure of dengue 3 virus envelope glycoprotein in complex with the Fab fragment of the broadly neutralizing human antibody EDE1 C8
Authors	:	Sharma, A.; Vaney, M.C.; Guardado-Calvo, P.; Duquerroy, S.; Rouvinski, A.; Rey, F.A.
Deposited on	:	2020-08-18
Resolution	:	2.65 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 following versions of software and data (see references ⓘ) were used in the production of this report:

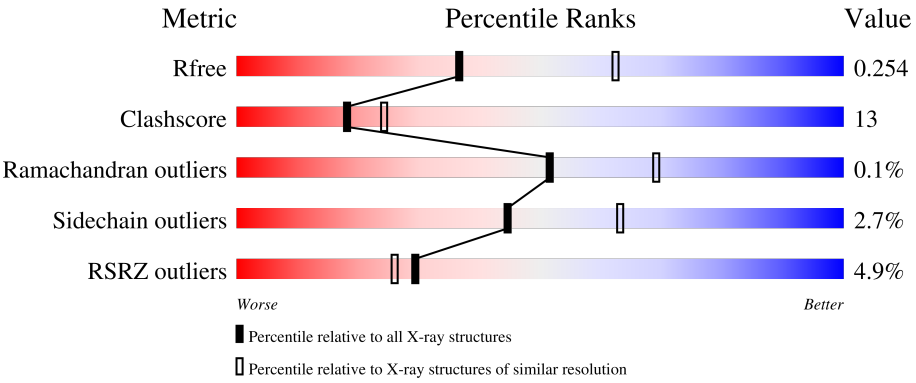
MolProbity	:	4.02b-467
Mogul	:	1.8.4 (270009), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.23.2
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0267
CCP4	:	7.1.010 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.23.2

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 2.65 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	1332 (2.68-2.64)
Clashscore	141614	1374 (2.68-2.64)
Ramachandran outliers	138981	1349 (2.68-2.64)
Sidechain outliers	138945	1349 (2.68-2.64)
RSRZ outliers	127900	1318 (2.68-2.64)

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	428	4% 67% 21% · 10%
2	H	272	6% 54% 26% · 19%
3	L	217	4% 79% 18% ··
4	B	5	60% 40%

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard

residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
4	NAG	B	2	-	-	-	X
6	GOL	A	503	-	-	-	X

2 Entry composition (i)

There are 7 unique types of molecules in this entry. The entry contains 6403 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 Core protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	384	2949	1856	509	561	23	0	0	0

There are 37 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	107	CYS	LEU	engineered mutation	UNP A0A481XTQ0
A	311	CYS	SER	engineered mutation	UNP A0A481XTQ0
A	394	LEU	-	expression tag	UNP A0A481XTQ0
A	395	VAL	-	expression tag	UNP A0A481XTQ0
A	396	PRO	-	expression tag	UNP A0A481XTQ0
A	397	ARG	-	expression tag	UNP A0A481XTQ0
A	398	GLY	-	expression tag	UNP A0A481XTQ0
A	399	SER	-	expression tag	UNP A0A481XTQ0
A	400	SER	-	expression tag	UNP A0A481XTQ0
A	401	ALA	-	expression tag	UNP A0A481XTQ0
A	402	TRP	-	expression tag	UNP A0A481XTQ0
A	403	SER	-	expression tag	UNP A0A481XTQ0
A	404	HIS	-	expression tag	UNP A0A481XTQ0
A	405	PRO	-	expression tag	UNP A0A481XTQ0
A	406	GLN	-	expression tag	UNP A0A481XTQ0
A	407	PHE	-	expression tag	UNP A0A481XTQ0
A	408	GLU	-	expression tag	UNP A0A481XTQ0
A	409	LYS	-	expression tag	UNP A0A481XTQ0
A	410	GLY	-	expression tag	UNP A0A481XTQ0
A	411	GLY	-	expression tag	UNP A0A481XTQ0
A	412	SER	-	expression tag	UNP A0A481XTQ0
A	413	GLY	-	expression tag	UNP A0A481XTQ0
A	414	GLY	-	expression tag	UNP A0A481XTQ0
A	415	GLY	-	expression tag	UNP A0A481XTQ0
A	416	SER	-	expression tag	UNP A0A481XTQ0
A	417	GLY	-	expression tag	UNP A0A481XTQ0
A	418	GLY	-	expression tag	UNP A0A481XTQ0

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
A	419	SER	-	expression tag	UNP A0A481XTQ0
A	420	ALA	-	expression tag	UNP A0A481XTQ0
A	421	TRP	-	expression tag	UNP A0A481XTQ0
A	422	SER	-	expression tag	UNP A0A481XTQ0
A	423	HIS	-	expression tag	UNP A0A481XTQ0
A	424	PRO	-	expression tag	UNP A0A481XTQ0
A	425	GLN	-	expression tag	UNP A0A481XTQ0
A	426	PHE	-	expression tag	UNP A0A481XTQ0
A	427	GLU	-	expression tag	UNP A0A481XTQ0
A	428	LYS	-	expression tag	UNP A0A481XTQ0

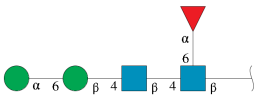
- Molecule 2 is a protein called EDE1 C8 antibody Fab fragment.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	H	219	Total	C	N	O	S	0	1	0
			1653	1047	269	329	8			

- Molecule 3 is a protein called EDE1 C8 antibody Fab fragment.

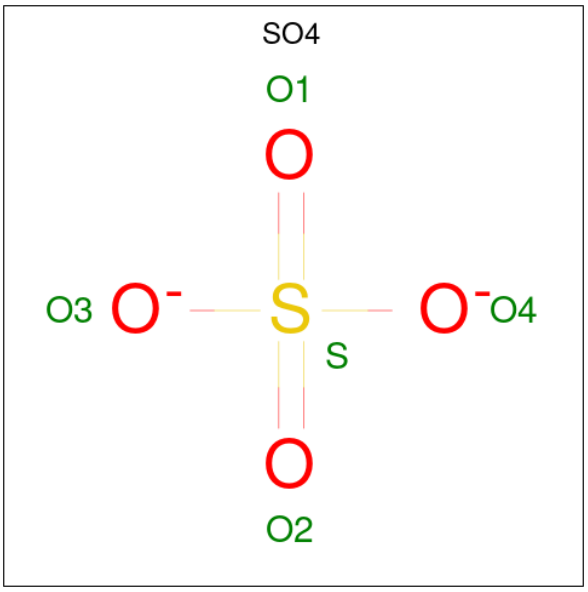
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	L	215	Total	C	N	O	S	0	2	0
			1689	1061	288	336	4			

- Molecule 4 is an oligosaccharide called alpha-D-mannopyranose-(1-6)-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.



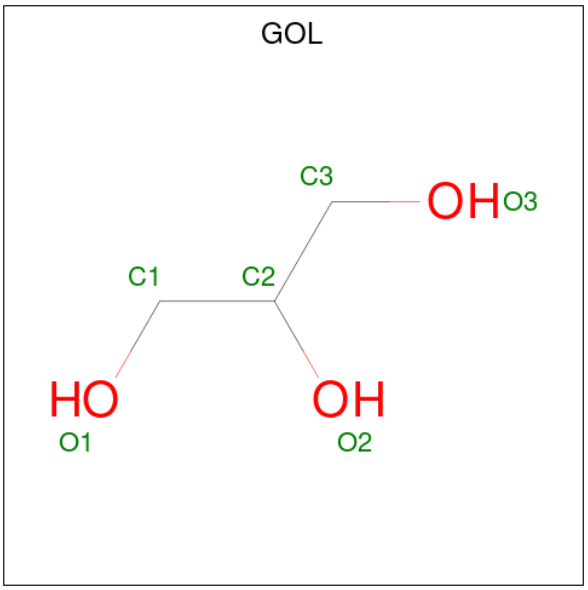
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
4	B	5	Total	C	N	O	0	0	0
			60	34	2	24			

- Molecule 5 is SULFATE ION (three-letter code: SO4) (formula: O_4S).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	1	Total O S 5 4 1	0	0
5	A	1	Total O S 5 4 1	0	0
5	H	1	Total O S 5 4 1	0	0
5	H	1	Total O S 5 4 1	0	0

- Molecule 6 is GLYCEROL (three-letter code: GOL) (formula: $C_3H_8O_3$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	A	1	Total C O 6 3 3	0	0
6	A	1	Total C O 6 3 3	0	0
6	A	1	Total C O 6 3 3	0	0
6	L	1	Total C O 6 3 3	0	0

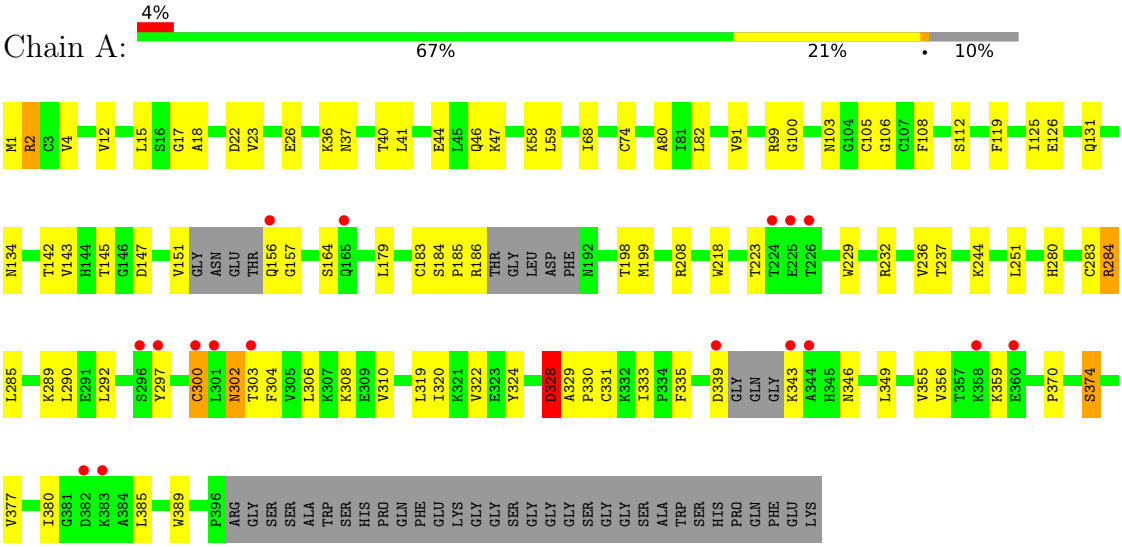
- Molecule 7 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
7	A	2	Total O 2 2	0	0
7	H	1	Total O 1 1	0	0
7	L	5	Total O 5 5	0	0

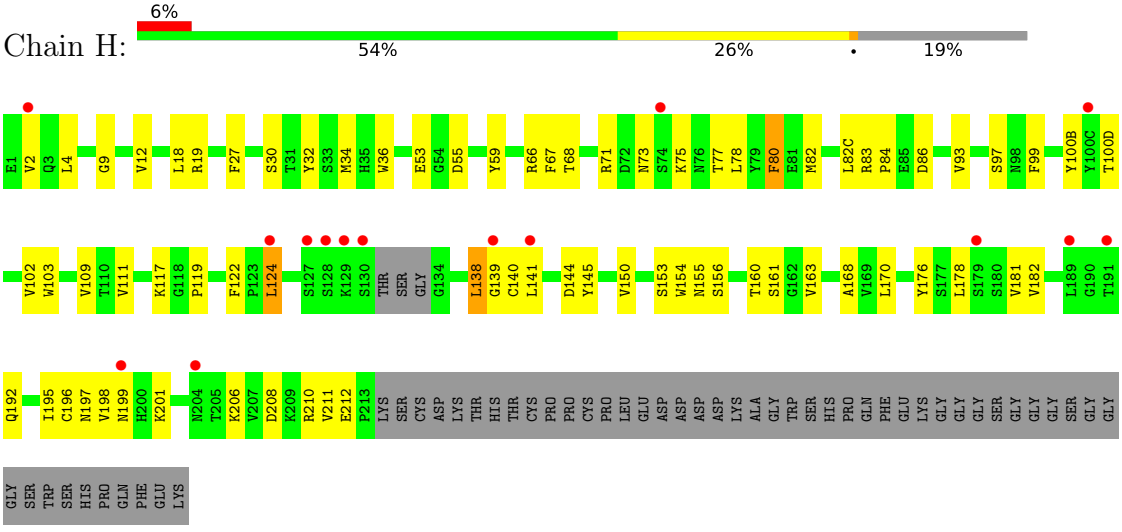
3 Residue-property plots (i)

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density (RSRZ > 2). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

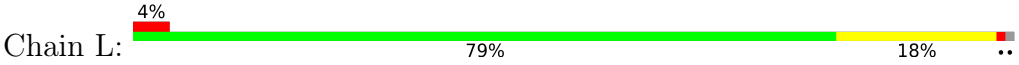
• Molecule 1: Core protein

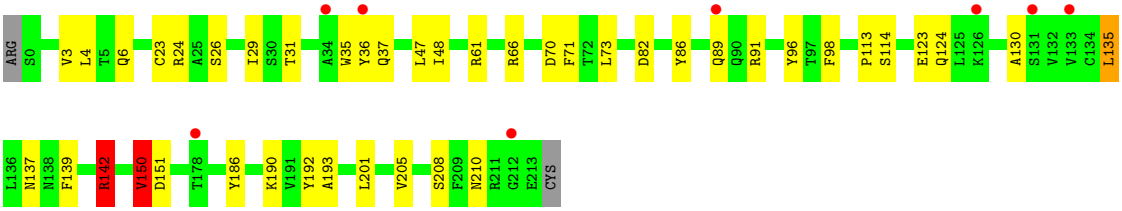


• Molecule 2: EDE1 C8 antibody Fab fragment



• Molecule 3: EDE1 C8 antibody Fab fragment





• Molecule 4: alpha-D-mannopyranose-(1-6)-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 31 2 1	Depositor
Cell constants a, b, c, α, β, γ	110.31Å 110.31Å 217.34Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	29.53 – 2.65 29.53 – 2.66	Depositor EDS
% Data completeness (in resolution range)	74.0 (29.53-2.65) 74.0 (29.53-2.66)	Depositor EDS
R_{merge}	0.32	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.21 (at 2.64Å)	Xtriage
Refinement program	PHENIX 1.17.1_3660	Depositor
R, R_{free}	0.207 , 0.254 0.207 , 0.254	Depositor DCC
R_{free} test set	2029 reflections (6.11%)	wwPDB-VP
Wilson B-factor (Å^2)	66.3	Xtriage
Anisotropy	0.080	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	(Not available) , (Not available)	EDS
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.32$	Xtriage
Estimated twinning fraction	0.026 for -h,-k,l	Xtriage
F_o,F_c correlation	0.93	EDS
Total number of atoms	6403	wwPDB-VP
Average B, all atoms (Å^2)	70.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.40% 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: SO4, FUC, BMA, GOL, NAG, MAN

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	0.35	0/3002	0.63	3/4063 (0.1%)
2	H	0.36	0/1698	0.61	1/2312 (0.0%)
3	L	0.36	0/1732	0.66	4/2356 (0.2%)
All	All	0.35	0/6432	0.63	8/8731 (0.1%)

There are no bond length outliers.

All (8) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	105	CYS	CA-CB-SG	-7.45	100.59	114.00
3	L	150	VAL	C-N-CA	-6.90	104.45	121.70
2	H	124	LEU	CA-CB-CG	5.98	129.06	115.30
1	A	328	ASP	N-CA-C	-5.98	94.86	111.00
3	L	142[A]	ARG	NE-CZ-NH1	5.86	123.23	120.30
3	L	142[B]	ARG	NE-CZ-NH1	5.86	123.23	120.30
3	L	29	ILE	C-N-CA	5.77	136.12	121.70
1	A	74	CYS	CA-CB-SG	-5.61	103.89	114.00

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	2949	0	2940	75	0
2	H	1653	0	1591	58	0
3	L	1689	0	1643	42	0
4	B	60	0	52	1	0
5	A	10	0	0	1	0
5	H	10	0	0	0	0
6	A	18	0	24	1	0
6	L	6	0	8	0	0
7	A	2	0	0	0	0
7	H	1	0	0	0	0
7	L	5	0	0	0	0
All	All	6403	0	6258	169	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 13.

All (169) 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:131:GLN:HE21	1:A:134:ASN:HB3	1.24	1.01
3:L:150:VAL:HG13	3:L:151:ASP:H	1.23	1.00
3:L:142[A]:ARG:HH11	3:L:142[A]:ARG:HG3	1.30	0.95
3:L:150:VAL:CG1	3:L:151:ASP:N	2.38	0.87
3:L:24:ARG:HH21	3:L:70:ASP:HB2	1.40	0.84
3:L:150:VAL:HG13	3:L:151:ASP:N	1.89	0.81
1:A:99:ARG:HA	1:A:103:ASN:HD21	1.46	0.80
2:H:66:ARG:NH2	2:H:86:ASP:OD2	2.15	0.80
3:L:61:ARG:NH1	3:L:82:ASP:OD2	2.14	0.79
1:A:179:LEU:HD11	1:A:285:LEU:HB3	1.64	0.79
3:L:150:VAL:CG1	3:L:151:ASP:H	1.94	0.77
2:H:163:VAL:HG12	2:H:182:VAL:HB	1.64	0.77
3:L:150:VAL:O	3:L:151:ASP:C	2.17	0.76
2:H:84:PRO:HA	2:H:111:VAL:HG23	1.69	0.74
2:H:201:LYS:HZ1	2:H:206:LYS:HE2	1.53	0.73
3:L:36:TYR:OH	3:L:91:ARG:NH2	2.21	0.73
1:A:4:VAL:HG11	1:A:319:LEU:HD22	1.69	0.72
1:A:328:ASP:OD2	1:A:328:ASP:N	2.11	0.71
1:A:12:VAL:HG11	1:A:23:VAL:HG12	1.73	0.71
2:H:181:VAL:HG21	3:L:135:LEU:HD13	1.72	0.70
1:A:164:SER:HA	1:A:185:PRO:HG2	1.74	0.70
3:L:37:GLN:HB2	3:L:47:LEU:HD11	1.74	0.69
1:A:91:VAL:HG11	1:A:236:VAL:HG21	1.75	0.69

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:339:ASP:HB3	1:A:343:LYS:HB2	1.77	0.67
1:A:22:ASP:HA	1:A:284:ARG:HB3	1.77	0.66
2:H:12:VAL:HG11	2:H:82(C):LEU:HD12	1.78	0.66
1:A:26:GLU:HG2	1:A:280:HIS:ND1	2.10	0.66
1:A:292:LEU:H	1:A:292:LEU:HD12	1.60	0.65
2:H:139:GLY:O	2:H:211:VAL:HG21	1.96	0.65
2:H:12:VAL:HB	2:H:111:VAL:HG12	1.80	0.64
1:A:300:CYS:SG	1:A:324:TYR:CZ	2.92	0.63
1:A:183:CYS:HA	1:A:283:CYS:HA	1.81	0.62
2:H:119:PRO:HB3	2:H:145:TYR:HB3	1.81	0.62
1:A:1:MET:HB3	1:A:151:VAL:HG11	1.82	0.61
2:H:124:LEU:CD1	2:H:181:VAL:HG22	2.30	0.61
2:H:139:GLY:HA2	2:H:154:TRP:CH2	2.36	0.61
2:H:9:GLY:HA2	2:H:109:VAL:HG12	1.83	0.61
3:L:150:VAL:O	3:L:151:ASP:O	2.18	0.60
3:L:193:ALA:HB2	3:L:208:SER:HB3	1.84	0.60
1:A:142:THR:HG22	1:A:157:GLY:HA3	1.84	0.60
2:H:181:VAL:HG21	3:L:135:LEU:CD1	2.31	0.59
1:A:339:ASP:HB3	1:A:343:LYS:CB	2.33	0.59
1:A:297:TYR:HD1	1:A:355:VAL:HG21	1.68	0.58
2:H:32:TYR:O	2:H:71:ARG:NH2	2.34	0.58
2:H:170:LEU:HD12	2:H:176:TYR:CZ	2.38	0.58
2:H:82:MET:HB3	2:H:82(C):LEU:HD21	1.85	0.58
1:A:46:GLN:HG2	1:A:47:LYS:HG2	1.86	0.58
2:H:154:TRP:CH2	2:H:196:CYS:HB3	2.39	0.58
2:H:160:THR:O	2:H:163:VAL:HG22	2.05	0.57
3:L:123[A]:GLU:OE1	3:L:123[A]:GLU:N	2.35	0.57
3:L:123[B]:GLU:OE1	3:L:123[B]:GLU:N	2.35	0.57
1:A:1:MET:HE1	1:A:319:LEU:HD11	1.88	0.55
1:A:308:LYS:HE2	3:L:31:THR:CG2	2.37	0.55
2:H:82(C):LEU:HB3	2:H:111:VAL:HG11	1.89	0.55
1:A:308:LYS:HE2	3:L:31:THR:HG21	1.89	0.54
2:H:124:LEU:HD11	2:H:181:VAL:HG22	1.90	0.54
1:A:335:PHE:CE1	1:A:349:LEU:HD21	2.43	0.53
2:H:4:LEU:HD11	2:H:102:VAL:HG13	1.91	0.53
2:H:124:LEU:HG	2:H:139:GLY:C	2.30	0.52
2:H:2:VAL:HG13	2:H:27:PHE:CD1	2.44	0.52
3:L:113:PRO:HB3	3:L:139:PHE:HB3	1.91	0.52
2:H:97:SER:OG	2:H:100(B):TYR:O	2.14	0.52
1:A:37:ASN:C	1:A:292:LEU:HD11	2.29	0.51
1:A:184:SER:O	1:A:186:ARG:N	2.44	0.51

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:156:SER:HA	2:H:197:ASN:HD21	1.76	0.51
2:H:18:LEU:HD12	2:H:19:ARG:H	1.75	0.51
1:A:306:LEU:HD23	1:A:306:LEU:H	1.75	0.51
2:H:83:ARG:O	2:H:111:VAL:HG21	2.10	0.51
3:L:142[A]:ARG:HG3	3:L:142[A]:ARG:NH1	2.09	0.51
2:H:71:ARG:HD3	2:H:73:ASN:OD1	2.12	0.50
2:H:156:SER:HA	2:H:197:ASN:ND2	2.26	0.50
2:H:124:LEU:HG	2:H:140:CYS:N	2.26	0.50
1:A:297:TYR:CD1	1:A:355:VAL:HG21	2.46	0.50
3:L:6:GLN:NE2	3:L:86:TYR:O	2.41	0.50
3:L:190:LYS:HE2	3:L:210:ASN:OD1	2.12	0.50
1:A:145:THR:HG21	1:A:147:ASP:HB2	1.94	0.49
2:H:34[B]:MET:HG2	2:H:71:ARG:NH2	2.28	0.49
2:H:117:LYS:HD3	2:H:144:ASP:O	2.12	0.49
3:L:61:ARG:HH12	3:L:82:ASP:CG	2.15	0.49
3:L:186:TYR:O	3:L:192:TYR:OH	2.30	0.49
1:A:329:ALA:HB3	1:A:330:PRO:HD3	1.95	0.48
1:A:68:ILE:N	6:A:504:GOL:O1	2.46	0.48
1:A:119:PHE:CD2	1:A:232:ARG:HG2	2.49	0.48
2:H:75:LYS:O	2:H:77:THR:HG23	2.13	0.48
2:H:124:LEU:HB2	2:H:139:GLY:N	2.29	0.48
1:A:370:PRO:HG2	1:A:374:SER:HB2	1.96	0.48
2:H:93:VAL:HG22	2:H:103:TRP:CD2	2.49	0.47
1:A:310:VAL:HG12	1:A:320:ILE:HG12	1.95	0.47
2:H:196:CYS:O	2:H:208:ASP:HA	2.14	0.47
2:H:53:GLU:HB2	2:H:55:ASP:OD1	2.14	0.47
1:A:289:LYS:HD3	1:A:289:LYS:O	2.14	0.47
2:H:155:ASN:HA	2:H:195:ILE:HG13	1.96	0.47
1:A:145:THR:HG23	1:A:147:ASP:H	1.79	0.47
1:A:2:ARG:HH21	1:A:44:GLU:CD	2.18	0.47
1:A:100:GLY:HA3	1:A:108:PHE:CE1	2.50	0.46
1:A:330:PRO:HA	1:A:356:VAL:O	2.15	0.46
2:H:67:PHE:HD2	2:H:80:PHE:CZ	2.33	0.46
3:L:3:VAL:HG22	3:L:26:SER:HB2	1.98	0.46
1:A:302:ASN:HB3	1:A:324:TYR:CE2	2.50	0.46
2:H:59:TYR:CE1	2:H:68:THR:HA	2.50	0.46
3:L:124:GLN:OE1	3:L:130:ALA:HA	2.16	0.46
1:A:15:LEU:O	1:A:18:ALA:N	2.49	0.46
3:L:3:VAL:H	3:L:26:SER:HB3	1.80	0.46
1:A:125:ILE:HG21	1:A:199:MET:HE2	1.96	0.46
1:A:302:ASN:ND2	1:A:303:THR:H	2.13	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:237:THR:HG23	1:A:251:LEU:HD21	1.98	0.46
1:A:377:VAL:HA	1:A:385:LEU:O	2.16	0.46
3:L:89:GLN:HB2	3:L:98:PHE:CD1	2.51	0.45
1:A:59:LEU:HD22	1:A:218:TRP:HB3	1.97	0.45
3:L:35:TRP:HD1	3:L:48:ILE:HD11	1.82	0.45
1:A:1:MET:HG2	1:A:145:THR:O	2.16	0.45
1:A:304:PHE:CE2	1:A:324:TYR:HB2	2.52	0.45
3:L:201:LEU:HD13	3:L:205:VAL:HG13	1.98	0.45
1:A:179:LEU:HB2	1:A:290:LEU:HD11	1.98	0.45
1:A:333:ILE:HG12	1:A:356:VAL:HG23	1.99	0.45
2:H:36:TRP:CE2	2:H:80:PHE:HB2	2.51	0.45
2:H:67:PHE:CD1	2:H:67:PHE:N	2.85	0.45
3:L:150:VAL:HG12	3:L:151:ASP:N	2.26	0.45
2:H:170:LEU:HD12	2:H:176:TYR:CE2	2.53	0.44
3:L:89:GLN:HB2	3:L:98:PHE:CE1	2.51	0.44
1:A:223:THR:O	1:A:223:THR:HG22	2.17	0.44
1:A:2:ARG:HD3	1:A:142:THR:HG21	1.98	0.44
1:A:331:CYS:O	1:A:355:VAL:HG23	2.16	0.44
1:A:80:ALA:H	1:A:112:SER:HB3	1.82	0.44
1:A:335:PHE:CD1	1:A:349:LEU:HD21	2.52	0.44
1:A:292:LEU:HD12	1:A:292:LEU:N	2.29	0.44
1:A:306:LEU:H	1:A:306:LEU:CD2	2.31	0.44
3:L:114:SER:HB2	3:L:137:ASN:HB3	2.00	0.44
2:H:100(D):THR:O	3:L:91:ARG:NH1	2.46	0.44
4:B:3:BMA:C5	4:B:4:MAN:H2	2.47	0.44
1:A:320:ILE:HG22	1:A:322:VAL:HG13	1.99	0.44
2:H:153:SER:OG	2:H:197:ASN:HB2	2.18	0.44
1:A:126:GLU:HB2	1:A:198:THR:CG2	2.48	0.43
1:A:229:TRP:O	1:A:232:ARG:HG3	2.18	0.43
2:H:12:VAL:O	2:H:111:VAL:HA	2.18	0.43
1:A:58:LYS:C	1:A:59:LEU:HD23	2.39	0.43
2:H:67:PHE:CD2	2:H:82:MET:HG2	2.53	0.43
1:A:40:THR:O	1:A:41:LEU:HD23	2.18	0.43
2:H:150:VAL:HG11	2:H:198:VAL:HG13	2.01	0.43
1:A:17:GLY:H	1:A:36:LYS:HZ1	1.67	0.43
1:A:82:LEU:HD23	1:A:82:LEU:HA	1.77	0.43
1:A:310:VAL:HG23	1:A:389:TRP:HZ3	1.84	0.43
2:H:199:ASN:HD21	2:H:201:LYS:NZ	2.16	0.43
3:L:24:ARG:NH2	3:L:70:ASP:HB2	2.19	0.43
1:A:1:MET:CB	1:A:151:VAL:HG11	2.48	0.42
1:A:329:ALA:CB	1:A:330:PRO:HD3	2.49	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:210:ARG:HH21	2:H:212:GLU:CD	2.22	0.42
2:H:34[B]:MET:HB3	2:H:78:LEU:HD22	2.00	0.42
2:H:122:PHE:CE2	3:L:124:GLN:HG3	2.54	0.42
3:L:4:LEU:HB3	3:L:23:CYS:SG	2.59	0.42
1:A:17:GLY:H	1:A:36:LYS:NZ	2.17	0.42
3:L:66:ARG:HG3	3:L:71:PHE:CE2	2.55	0.42
2:H:138:LEU:N	2:H:138:LEU:HD23	2.34	0.42
1:A:12:VAL:HG11	1:A:23:VAL:CG1	2.46	0.42
1:A:179:LEU:HD21	1:A:285:LEU:HD12	2.00	0.42
1:A:106:GLY:N	5:A:501:SO4:O3	2.53	0.42
1:A:310:VAL:CG1	1:A:320:ILE:HG12	2.50	0.41
1:A:380:ILE:HA	1:A:380:ILE:HD12	1.80	0.41
3:L:35:TRP:CD1	3:L:48:ILE:HD11	2.56	0.41
3:L:91:ARG:HA	3:L:96:TYR:CD1	2.56	0.41
1:A:131:GLN:H	1:A:131:GLN:CD	2.25	0.41
1:A:143:VAL:O	1:A:145:THR:N	2.54	0.41
2:H:141:LEU:HD12	2:H:178:LEU:O	2.21	0.41
2:H:168:ALA:HA	2:H:178:LEU:HB3	2.03	0.41
2:H:181:VAL:HG11	3:L:135:LEU:HD13	2.03	0.41
1:A:292:LEU:H	1:A:292:LEU:CD1	2.33	0.40
2:H:4:LEU:HD12	2:H:102:VAL:HG22	2.02	0.40
3:L:35:TRP:CD2	3:L:73:LEU:HB2	2.56	0.40
2:H:67:PHE:N	2:H:67:PHE:HD1	2.19	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	376/428 (88%)	358 (95%)	18 (5%)	0	100	100
2	H	216/272 (79%)	207 (96%)	9 (4%)	0	100	100

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
3	L	215/217 (99%)	205 (95%)	9 (4%)	1 (0%)	29 43
All	All	807/917 (88%)	770 (95%)	36 (4%)	1 (0%)	51 69

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
3	L	150	VAL

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	323/355 (91%)	312 (97%)	11 (3%)	37 53
2	H	186/226 (82%)	180 (97%)	6 (3%)	39 56
3	L	190/190 (100%)	187 (98%)	3 (2%)	62 78
All	All	699/771 (91%)	679 (97%)	20 (3%)	44 60

All (20) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	2	ARG
1	A	156	GLN
1	A	208	ARG
1	A	244	LYS
1	A	284	ARG
1	A	300	CYS
1	A	302	ASN
1	A	328	ASP
1	A	346	ASN
1	A	359	LYS
1	A	374	SER
2	H	30	SER
2	H	80	PHE
2	H	99	PHE

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
2	H	138	LEU
2	H	161	SER
2	H	192	GLN
3	L	135	LEU
3	L	142[A]	ARG
3	L	142[B]	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (1) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	346	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.

There are no bond length outliers.

There are no bond angle outliers.

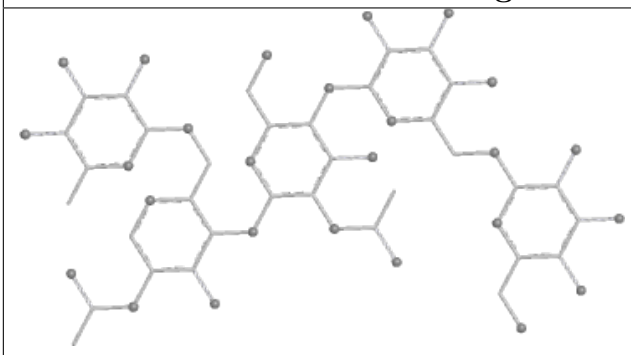
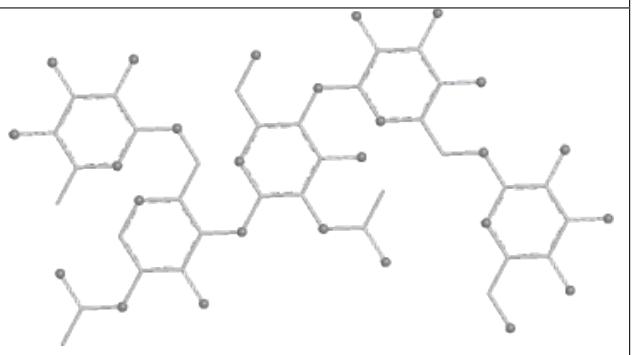
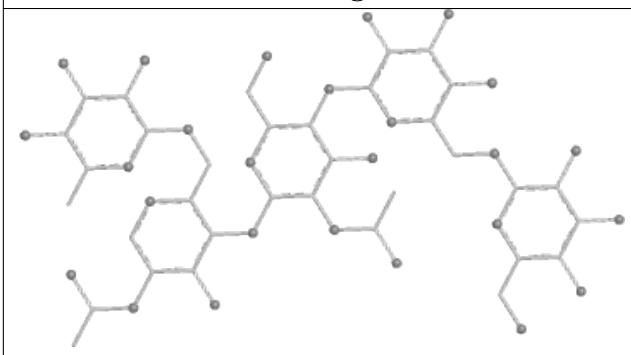
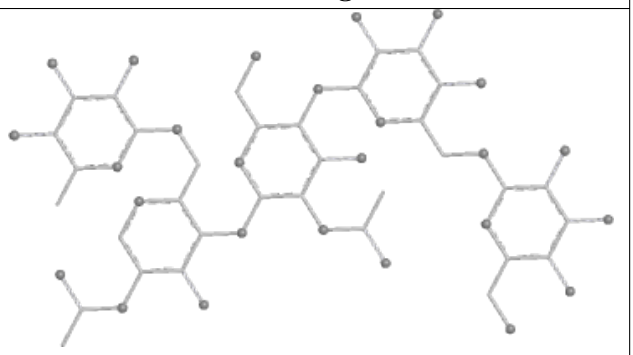
There are no chirality outliers.

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 oligosaccharide.

Oligosaccharide Chain B	
	
Bond lengths	Bond angles
	
Torsions	Rings

5.6 Ligand geometry

8 ligands are modelled in this entry.

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.

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	384/428 (89%)	0.17	17 (4%)	34	31	50, 75, 115, 139	0
2	H	219/272 (80%)	0.36	15 (6%)	17	14	40, 64, 102, 118	0
3	L	215/217 (99%)	-0.01	8 (3%)	41	38	37, 57, 81, 107	0
All	All	818/917 (89%)	0.18	40 (4%)	29	26	37, 66, 107, 139	0

All (40) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	H	130	SER	5.7
2	H	189	LEU	4.4
1	A	339	ASP	4.4
2	H	128	SER	4.3
1	A	224	THR	3.6
2	H	129	LYS	3.5
1	A	383	LYS	3.5
1	A	382	ASP	3.3
1	A	344	ALA	3.1
1	A	300	CYS	3.0
1	A	225	GLU	2.9
1	A	360	GLU	2.9
1	A	297	TYR	2.9
2	H	204	ASN	2.8
3	L	36	TYR	2.7
3	L	212	GLY	2.7
1	A	296	SER	2.6
2	H	179	SER	2.6
3	L	126	LYS	2.5
1	A	303	THR	2.5
3	L	178	THR	2.5
2	H	139	GLY	2.5
2	H	124	LEU	2.5

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	A	301	LEU	2.4
1	A	226	THR	2.4
2	H	127	SER	2.4
2	H	141	LEU	2.4
3	L	133	VAL	2.4
2	H	100(C)	TYR	2.3
2	H	199	ASN	2.2
1	A	358	LYS	2.1
3	L	131	SER	2.1
1	A	343	LYS	2.1
3	L	34	ALA	2.1
2	H	191	THR	2.1
2	H	74	SER	2.1
1	A	156	GLN	2.1
3	L	89	GLN	2.0
1	A	165	GLN	2.0
2	H	2	VAL	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)

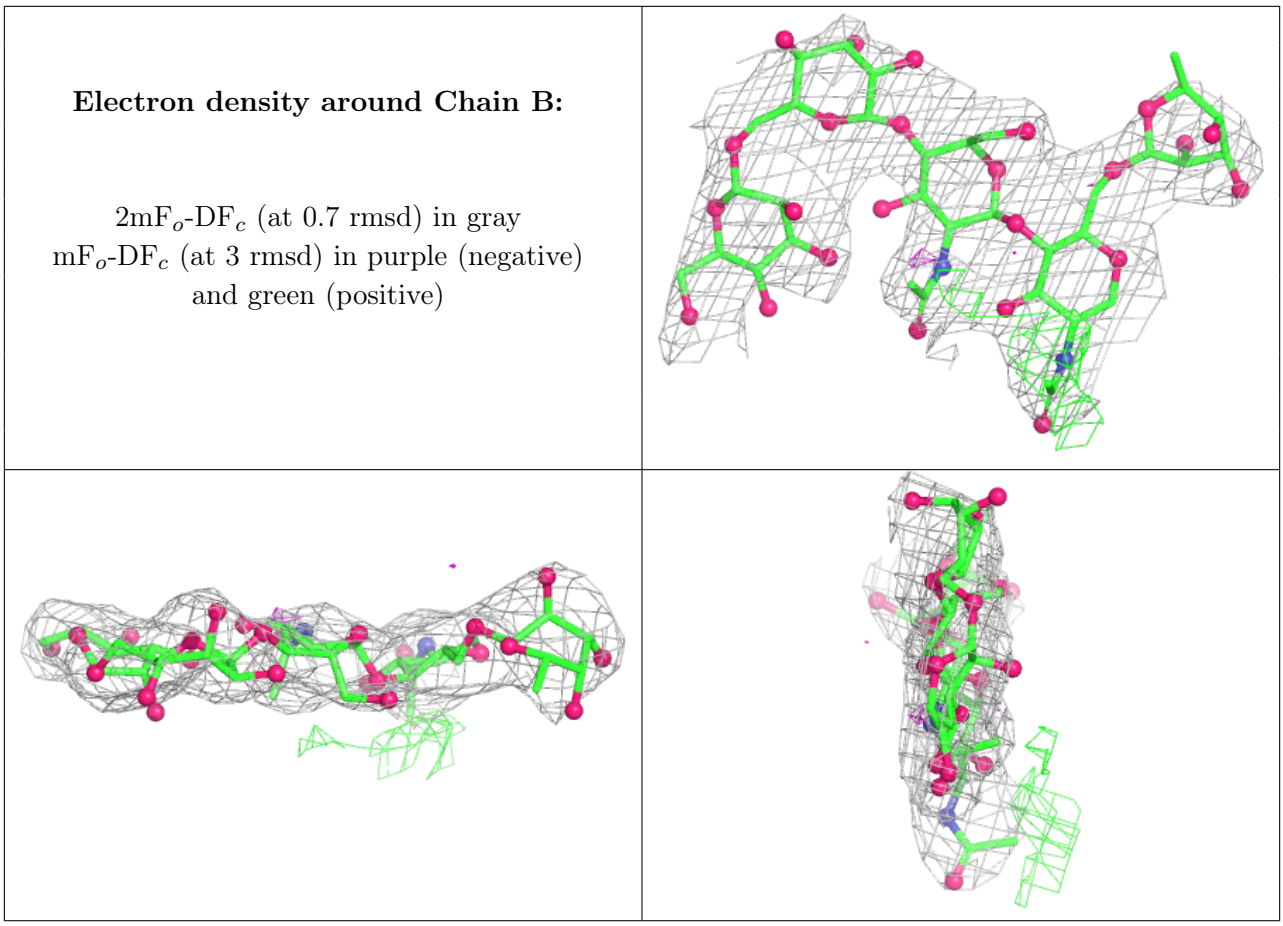
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' 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	B	2	14/15	0.71	0.41	90,124,138,138	0
4	MAN	B	4	11/12	0.81	0.37	91,116,130,134	0
4	FUC	B	5	10/11	0.82	0.31	104,110,131,144	0
4	NAG	B	1	14/15	0.85	0.20	78,94,113,128	0
4	BMA	B	3	11/12	0.85	0.38	116,122,133,133	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

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	GOL	A	503	6/6	0.65	0.48	86,91,96,99	0
5	SO4	A	502	5/5	0.87	0.21	91,99,120,121	0
6	GOL	L	301	6/6	0.87	0.32	60,74,75,81	0
5	SO4	H	302	5/5	0.89	0.26	96,105,111,132	0
6	GOL	A	505	6/6	0.90	0.27	72,80,80,81	0
6	GOL	A	504	6/6	0.91	0.23	53,68,75,97	0
5	SO4	H	301	5/5	0.93	0.20	96,108,110,130	0
5	SO4	A	501	5/5	0.96	0.24	82,101,103,106	0

6.5 Other polymers

There are no such residues in this entry.