Full wwPDB X-ray Structure Validation Report (i)

Dec 14, 2021 – 12:10 pm GMT

PDB ID	:	7PS2
Title	:	Crystal structure of the receptor binding domain of SARS-CoV-2 beta variant spike glycoprotein in complex with Beta-29 and Beta-53 Fabs
Authors	:	Zhou, D.; Ren, J.; Stuart, D.I.
Deposited on	:	2021-09-22
Resolution	:	2.99 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 following versions of software and data (see references (i)) were used in the production of this report:

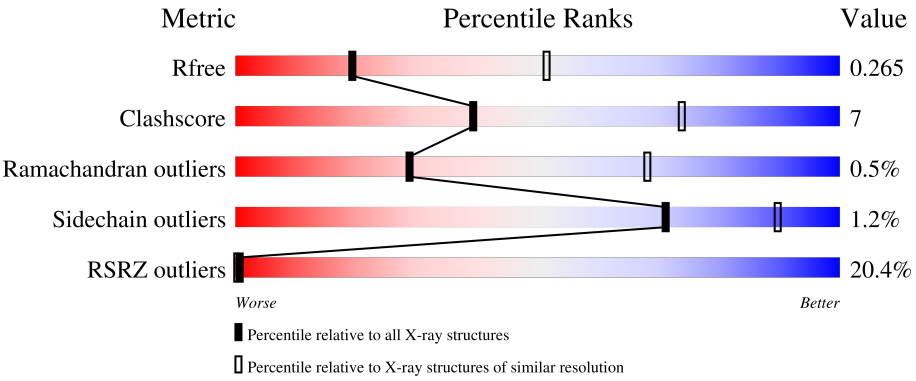
MolProbity	:	4.02b-467
Mogul	:	1.8.4, CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.24
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0267
CCP4	:	7.1.010 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.24

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 2.99 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	2092 (3.00-3.00)
Clashscore	141614	2416 (3.00-3.00)
Ramachandran outliers	138981	2333 (3.00-3.00)
Sidechain outliers	138945	2336 (3.00-3.00)
RSRZ outliers	127900	1990 (3.00-3.00)

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	B	221	16% 84% 15% ·
2	G	210	% 79% 15% 6%
3	A	232	12% 75% 22% ··
4	H	226	29% 77% 19% ·
5	L	215	41% 83% 16%

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Mol	Chain	Length	Quality of chain
6	E	4	50% 50%

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
8	SO4	G	608	-	-	X	-

2 Entry composition (i)

There are 9 unique types of molecules in this entry. The entry contains 8431 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 Beta-29 Fab light chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	B	221	Total	C	N	O	S	0	1	0
			1714	1074	287	348	5			

- Molecule 2 is a protein called Spike protein S1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	G	197	Total	C	N	O	S	0	1	0
			1580	1013	268	291	8			

There are 19 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
G	319	MET	-	initiating methionine	UNP P0DTC2
G	320	GLY	-	expression tag	UNP P0DTC2
G	321	CYS	-	expression tag	UNP P0DTC2
G	322	VAL	-	expression tag	UNP P0DTC2
G	323	ALA	-	expression tag	UNP P0DTC2
G	324	GLU	-	expression tag	UNP P0DTC2
G	325	THR	-	expression tag	UNP P0DTC2
G	326	GLY	-	expression tag	UNP P0DTC2
G	327	HIS	-	expression tag	UNP P0DTC2
G	328	HIS	-	expression tag	UNP P0DTC2
G	329	HIS	-	expression tag	UNP P0DTC2
G	330	HIS	-	expression tag	UNP P0DTC2
G	331	HIS	-	expression tag	UNP P0DTC2
G	332	HIS	-	expression tag	UNP P0DTC2
G	417	ASN	LYS	variant	UNP P0DTC2
G	484	LYS	GLU	variant	UNP P0DTC2
G	501	TYR	ASN	variant	UNP P0DTC2
G	527	LYS	-	expression tag	UNP P0DTC2
G	528	LYS	-	expression tag	UNP P0DTC2

- Molecule 3 is a protein called Beta-29 Fab heavy chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	A	227	Total	C	N	O	S	0	0	0
			1700	1063	294	334	9			

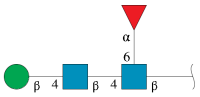
- Molecule 4 is a protein called Beta-53 heavy chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	H	219	Total	C	N	O	S	0	0	0
			1650	1046	276	321	7			

- Molecule 5 is a protein called Beta-53 Fab light chain.

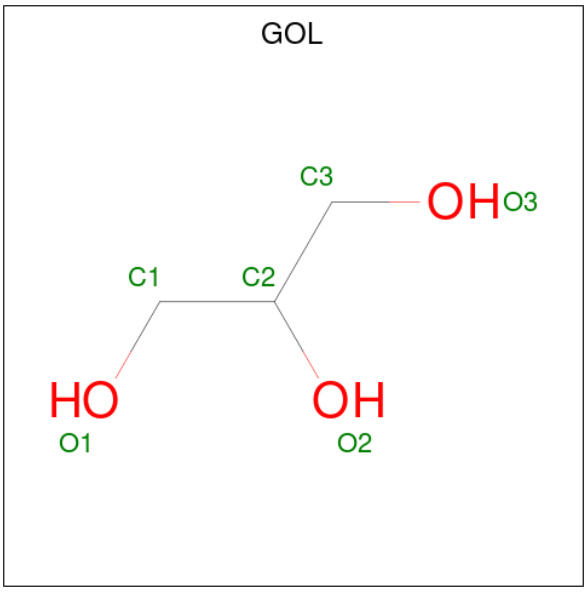
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
5	L	214	Total	C	N	O	S	0	1	0
			1649	1030	280	334	5			

- 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.



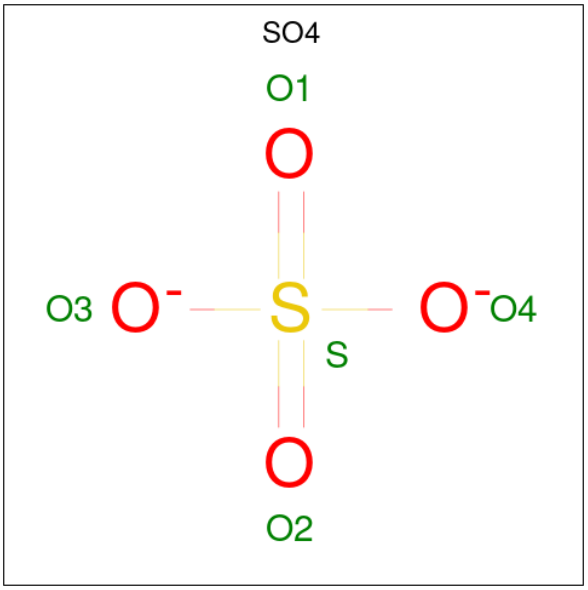
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
6	E	4	Total	C	N	O	0	0	0
			49	28	2	19			

- Molecule 7 is GLYCEROL (three-letter code: GOL) (formula: $C_3H_8O_3$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
7	B	1	Total C O 6 3 3	0	0
7	G	1	Total C O 6 3 3	0	0

- Molecule 8 is SULFATE ION (three-letter code: SO4) (formula: O_4S).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
8	B	1	Total O S 5 4 1	0	0
8	G	1	Total O S 5 4 1	0	0

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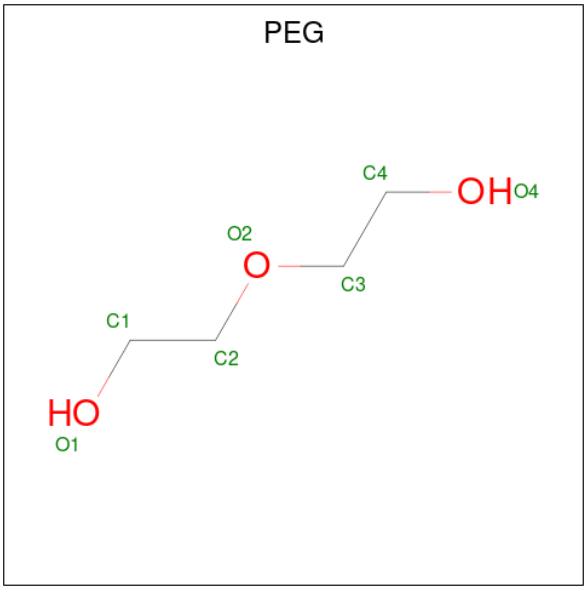
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
8	G	1	Total O S 5 4 1	0	0
8	G	1	Total O S 5 4 1	0	0
8	G	1	Total O S 5 4 1	0	0
8	G	1	Total O S 5 4 1	0	0
8	G	1	Total O S 5 4 1	0	0
8	A	1	Total O S 5 4 1	0	0
8	A	1	Total O S 5 4 1	0	0
8	A	1	Total O S 5 4 1	0	0
8	A	1	Total O S 5 4 1	0	0
8	H	1	Total O S 5 4 1	0	0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

- Molecule 9 is DI(HYDROXYETHYL)ETHER (three-letter code: PEG) (formula: $C_4H_{10}O_3$).

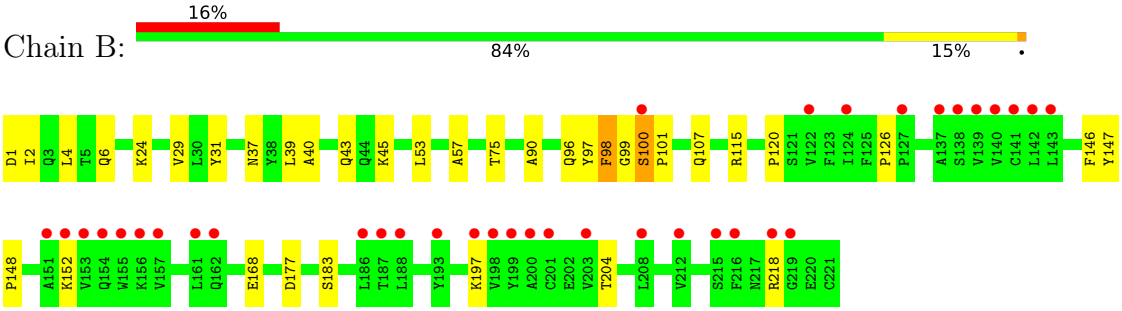


Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
9	G	1	Total C O 7 4 3	0	0

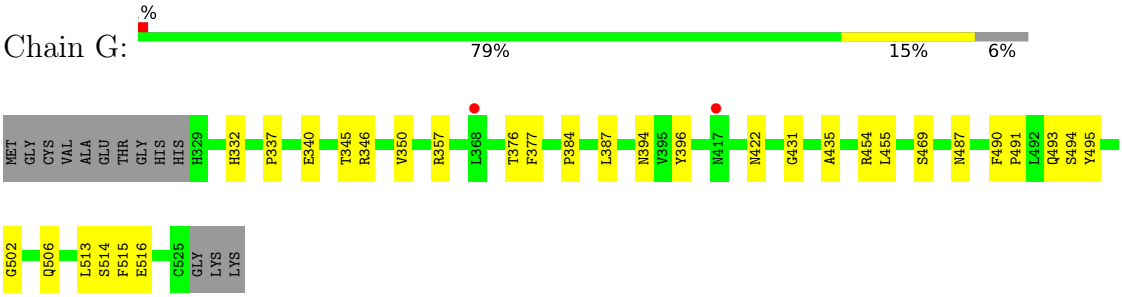
3 Residue-property plots (i)

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.

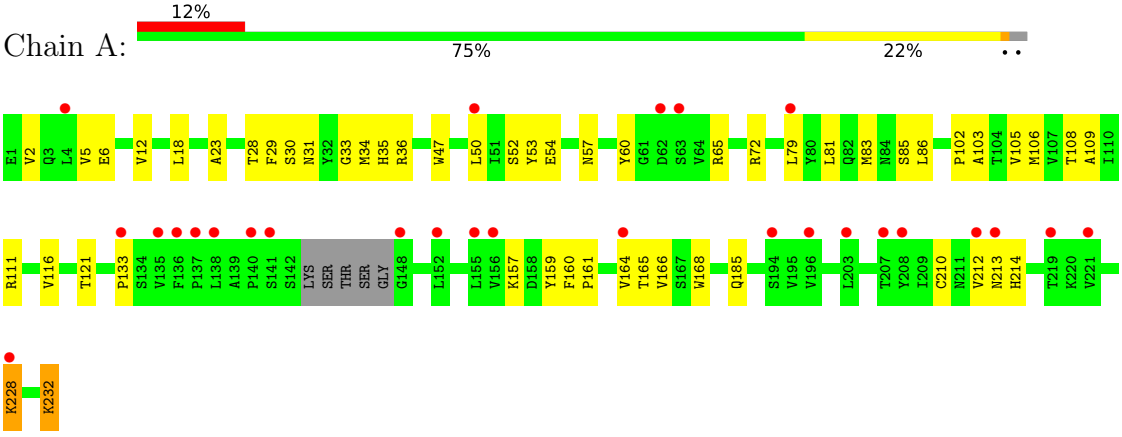
• Molecule 1: Beta-29 Fab light chain



• Molecule 2: Spike protein S1

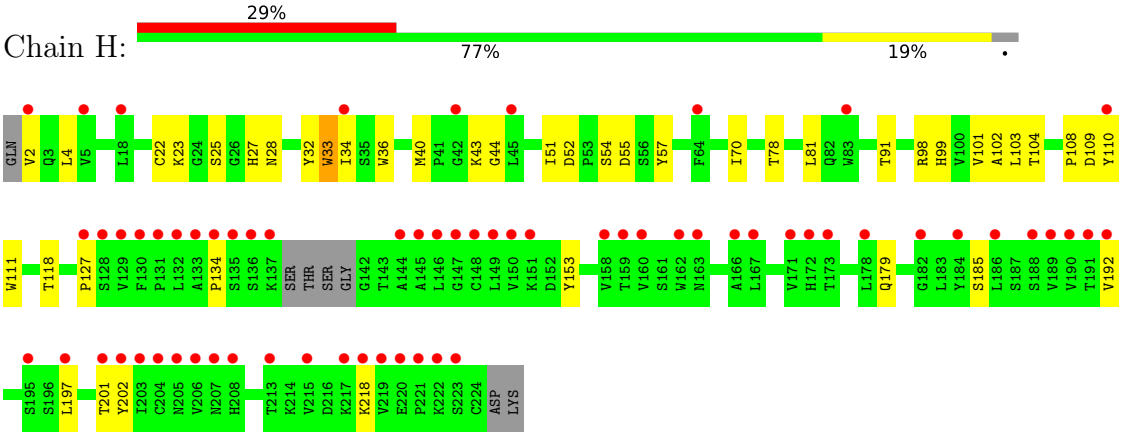


• Molecule 3: Beta-29 Fab heavy chain



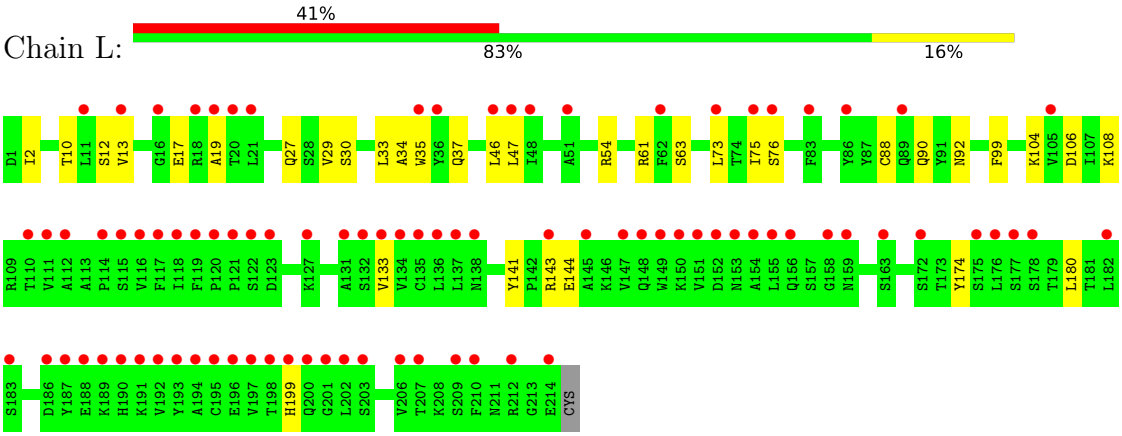
• Molecule 4: Beta-53 heavy chain

Chain H:



• Molecule 5: Beta-53 Fab light chain

Chain L:



• 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 E:

4 Data and refinement statistics (i)

Property	Value	Source
Space group	H 3 2	Depositor
Cell constants a, b, c, α, β, γ	213.40Å 213.40Å 226.79Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	48.33 – 2.99 50.00 – 2.99	Depositor EDS
% Data completeness (in resolution range)	99.8 (48.33-2.99) 99.9 (50.00-2.99)	Depositor EDS
R_{merge}	0.29	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.00 (at 3.01Å)	Xtriage
Refinement program	PHENIX 1.19_4092	Depositor
R, R_{free}	0.233 , 0.266 0.233 , 0.265	Depositor DCC
R_{free} test set	2013 reflections (5.02%)	wwPDB-VP
Wilson B-factor (Å^2)	103.1	Xtriage
Anisotropy	0.263	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	(Not available) , (Not available)	EDS
L-test for twinning[2]	$< \|L\| > = 0.47$, $< L^2 > = 0.30$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.93	EDS
Total number of atoms	8431	wwPDB-VP
Average B, all atoms (Å^2)	147.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.57% 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, NAG, GOL, PEG, BMA, 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	B	0.26	0/1754	0.49	0/2383
2	G	0.26	0/1631	0.49	0/2221
3	A	0.26	0/1736	0.51	0/2360
4	H	0.26	0/1696	0.50	0/2317
5	L	0.25	0/1688	0.49	0/2295
All	All	0.26	0/8505	0.50	0/11576

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand.A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
5	L	0	1

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
5	L	92	ASN	Peptide

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	B	1714	0	1662	23	0
2	G	1580	0	1486	25	0
3	A	1700	0	1673	38	0
4	H	1650	0	1605	31	0
5	L	1649	0	1598	18	0
6	E	49	0	43	1	0
7	B	6	0	8	0	0
7	G	6	0	8	0	0
8	A	20	0	0	1	0
8	B	5	0	0	0	0
8	G	30	0	0	2	0
8	H	10	0	0	0	0
8	L	5	0	0	0	0
9	G	7	0	10	0	0
All	All	8431	0	8093	122	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 (122) 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:A:36:ARG:HG2	3:A:81:LEU:HD22	1.63	0.80
3:A:52:SER:HB3	3:A:57:ASN:HB2	1.65	0.77
5:L:106:ASP:OD2	5:L:174:TYR:OH	2.02	0.77
5:L:12:SER:HB3	5:L:108:LYS:HA	1.73	0.70
1:B:100:SER:HB2	1:B:101:PRO:HD3	1.75	0.69
5:L:13:VAL:HG13	5:L:17:GLU:HB2	1.75	0.68
2:G:455:LEU:HD21	3:A:102:PRO:HG3	1.74	0.68
1:B:197:LYS:HA	1:B:218:ARG:HB3	1.76	0.68
1:B:2:ILE:H	1:B:101:PRO:HG3	1.60	0.66
3:A:52:SER:O	3:A:72:ARG:NH1	2.28	0.66
2:G:357:ARG:NH1	8:G:608:SO4:O1	2.28	0.66
4:H:51:ILE:HD11	4:H:70:ILE:HG13	1.80	0.64
2:G:376:THR:HB	2:G:435:ALA:HB3	1.79	0.64
5:L:143:ARG:O	5:L:143:ARG:NH1	2.30	0.62
2:G:337:PRO:HB2	2:G:340:GLU:HG3	1.81	0.61
3:A:50:LEU:HD11	3:A:103:ALA:HB1	1.81	0.61
1:B:29:VAL:HG13	1:B:98:PHE:HB2	1.83	0.61
1:B:43:GLN:HB2	1:B:53:LEU:HD11	1.83	0.61
3:A:108:THR:HA	3:A:111:ARG:HG2	1.84	0.60
2:G:345:THR:HA	4:H:101:VAL:HG21	1.84	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:L:37:GLN:HB2	5:L:47:LEU:HD11	1.83	0.59
2:G:396:TYR:HB2	2:G:514:SER:HB2	1.85	0.58
2:G:495:TYR:O	3:A:28:THR:OG1	2.18	0.58
5:L:133:VAL:HB	5:L:180:LEU:HB3	1.84	0.58
3:A:2:VAL:HG11	3:A:116:VAL:HG21	1.86	0.57
3:A:6:GLU:HB2	3:A:121:THR:HG23	1.85	0.57
4:H:25:SER:O	4:H:98:ARG:NH2	2.38	0.57
5:L:54:ARG:HH21	5:L:63:SER:HB3	1.67	0.57
2:G:494:SER:O	3:A:31:ASN:ND2	2.38	0.57
4:H:108:PRO:HG2	5:L:46:LEU:HD22	1.85	0.57
3:A:133:PRO:HB3	3:A:159:TYR:HB3	1.87	0.56
5:L:29:VAL:HG11	5:L:90:GLN:HB2	1.88	0.56
4:H:99:HIS:CE1	4:H:108:PRO:HB3	2.41	0.56
4:H:98:ARG:NH1	4:H:109:ASP:OD2	2.38	0.55
3:A:29:PHE:C	3:A:31:ASN:H	2.10	0.55
3:A:105:VAL:HA	3:A:111:ARG:HH11	1.73	0.54
4:H:43:LYS:HG2	4:H:44:GLY:H	1.73	0.53
1:B:100:SER:HB2	1:B:101:PRO:CD	2.38	0.53
2:G:346:ARG:NH2	4:H:57:TYR:HB3	2.23	0.53
3:A:83:MET:HE2	3:A:86:LEU:HD21	1.91	0.53
4:H:22:CYS:SG	4:H:34:ILE:HD11	2.48	0.53
1:B:4:LEU:HD11	1:B:96:GLN:H	1.74	0.53
5:L:33:LEU:HD11	5:L:88:CYS:HB2	1.90	0.52
3:A:12:VAL:HG11	3:A:18:LEU:HB2	1.91	0.52
3:A:35:HIS:CE1	3:A:50:LEU:HD13	2.45	0.52
4:H:98:ARG:HB3	4:H:109:ASP:OD1	2.10	0.52
3:A:33:GLY:HA3	3:A:103:ALA:HB3	1.92	0.51
3:A:54:GLU:OE1	3:A:54:GLU:N	2.37	0.51
5:L:61:ARG:HB2	5:L:76:SER:O	2.11	0.51
3:A:12:VAL:HG21	3:A:86:LEU:HD13	1.92	0.50
3:A:47:TRP:HZ2	3:A:50:LEU:HB2	1.77	0.50
2:G:357:ARG:NH1	8:G:608:SO4:O3	2.45	0.50
5:L:2:ILE:HG23	5:L:27:GLN:HG2	1.92	0.50
2:G:431:GLY:HA2	2:G:515:PHE:CD2	2.46	0.50
3:A:166:VAL:HG22	3:A:212:VAL:HG22	1.94	0.49
2:G:455:LEU:HD22	2:G:493:GLN:OE1	2.12	0.49
4:H:2:VAL:HG12	4:H:110:TYR:HB2	1.95	0.49
2:G:346:ARG:HH22	4:H:55:ASP:HB3	1.77	0.48
4:H:33:TRP:CE3	4:H:33:TRP:HA	2.47	0.48
4:H:40:MET:HB2	4:H:43:LYS:HB2	1.95	0.48
2:G:490:PHE:CD1	2:G:491:PRO:HD2	2.47	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:G:346:ARG:HH21	4:H:52:ASP:HB3	1.78	0.48
4:H:52:ASP:OD1	4:H:54:SER:OG	2.31	0.47
4:H:102:ALA:O	4:H:104:THR:N	2.47	0.47
5:L:10:THR:OG1	5:L:144:GLU:OE2	2.28	0.47
1:B:1:ASP:HA	1:B:101:PRO:HG3	1.96	0.47
4:H:28:ASN:ND2	6:E:1:NAG:O5	2.39	0.47
3:A:157:LYS:NZ	3:A:185:GLN:OE1	2.46	0.47
4:H:127:PRO:HB3	4:H:153:TYR:HB3	1.97	0.47
1:B:40:ALA:HB2	1:B:97:TYR:HE2	1.79	0.47
1:B:152:LYS:HB3	1:B:204:THR:OG1	2.16	0.46
1:B:45:LYS:HG2	1:B:90:ALA:HB2	1.97	0.46
2:G:394:ASN:HB3	2:G:516:GLU:HB2	1.97	0.46
3:A:232:LYS:HD2	3:A:232:LYS:HA	1.42	0.46
1:B:120:PRO:HB3	1:B:146:PHE:HB3	1.98	0.46
4:H:23:LYS:HG2	4:H:78:THR:HG23	1.97	0.45
1:B:31:TYR:HE2	3:A:109:ALA:HB2	1.80	0.45
2:G:350:VAL:HG22	2:G:422:ASN:HB3	1.99	0.45
3:A:29:PHE:O	3:A:31:ASN:N	2.49	0.45
4:H:4:LEU:HA	4:H:23:LYS:O	2.16	0.45
3:A:34:MET:HB3	3:A:79:LEU:HD22	1.98	0.45
3:A:85:SER:O	3:A:85:SER:OG	2.33	0.45
5:L:10:THR:HG22	5:L:104:LYS:HB3	1.98	0.45
1:B:115:ARG:NH1	1:B:177:ASP:O	2.50	0.45
4:H:201:THR:HB	4:H:218:LYS:HE3	1.99	0.44
1:B:2:ILE:N	1:B:101:PRO:HG3	2.28	0.44
2:G:431:GLY:HA2	2:G:515:PHE:HD2	1.82	0.44
2:G:384:PRO:HA	2:G:387:LEU:HG	2.00	0.44
5:L:19:ALA:HB3	5:L:75:ILE:HB	1.99	0.44
1:B:147:TYR:CG	1:B:148:PRO:HA	2.52	0.44
3:A:165:THR:OG1	3:A:213:ASN:HB3	2.18	0.44
3:A:105:VAL:HA	3:A:111:ARG:NH1	2.33	0.43
1:B:37:ASN:HB2	1:B:57:ALA:HB2	2.00	0.43
2:G:487:ASN:HD21	3:A:106:MET:HG3	1.83	0.43
4:H:91:THR:HG23	4:H:118:THR:HA	1.99	0.43
4:H:179:GLN:NE2	4:H:185:SER:OG	2.51	0.43
4:H:4:LEU:HG	4:H:110:TYR:HD2	1.83	0.43
2:G:346:ARG:NH1	4:H:55:ASP:OD2	2.45	0.43
2:G:502:GLY:O	2:G:506:GLN:HG3	2.19	0.42
4:H:4:LEU:HG	4:H:110:TYR:CD2	2.54	0.42
5:L:141:TYR:O	5:L:199:HIS:HE1	2.01	0.42
4:H:33:TRP:HA	4:H:33:TRP:HE3	1.82	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:H:192:VAL:HG11	4:H:202:TYR:CE1	2.55	0.42
1:B:24:LYS:HA	1:B:75:THR:O	2.19	0.42
3:A:60:TYR:OH	8:A:301:SO4:O2	2.30	0.42
1:B:126:PRO:HG2	3:A:228:LYS:NZ	2.35	0.42
1:B:99:GLY:HA2	3:A:111:ARG:NH1	2.35	0.41
3:A:53:TYR:CD1	3:A:102:PRO:HB2	2.55	0.41
4:H:36:TRP:CE2	4:H:81:LEU:HB2	2.54	0.41
2:G:387:LEU:HD23	2:G:387:LEU:HA	1.89	0.41
2:G:454:ARG:NH2	2:G:469:SER:O	2.43	0.41
3:A:160:PHE:HA	3:A:161:PRO:HA	1.88	0.41
3:A:164:VAL:HG12	3:A:214:HIS:HB2	2.02	0.41
5:L:35:TRP:CE2	5:L:73:LEU:HB2	2.56	0.41
4:H:134:PRO:HG3	4:H:197:LEU:HD22	2.02	0.41
1:B:4:LEU:HD11	1:B:96:GLN:N	2.36	0.41
3:A:168:TRP:CH2	3:A:210:CYS:HB3	2.56	0.40
1:B:168:GLU:HA	1:B:183:SER:O	2.21	0.40
2:G:396:TYR:O	2:G:513:LEU:HA	2.21	0.40
1:B:6:GLN:O	1:B:107:GLN:NE2	2.54	0.40
3:A:5:VAL:HG23	3:A:23:ALA:HB3	2.04	0.40
5:L:33:LEU:HG	5:L:34:ALA:N	2.37	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	B	220/221 (100%)	209 (95%)	10 (4%)	1 (0%)	29 68
2	G	196/210 (93%)	183 (93%)	13 (7%)	0	100 100
3	A	223/232 (96%)	204 (92%)	17 (8%)	2 (1%)	17 55
4	H	215/226 (95%)	192 (89%)	22 (10%)	1 (0%)	29 68

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
5	L	213/215 (99%)	199 (93%)	13 (6%)	1 (0%)	29 68
All	All	1067/1104 (97%)	987 (92%)	75 (7%)	5 (0%)	29 68

All (5) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
3	A	30	SER
4	H	103	LEU
1	B	100	SER
3	A	228	LYS
5	L	30	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	B	196/195 (100%)	194 (99%)	2 (1%)	76 91
2	G	172/180 (96%)	170 (99%)	2 (1%)	71 90
3	A	191/195 (98%)	189 (99%)	2 (1%)	76 91
4	H	188/195 (96%)	184 (98%)	4 (2%)	53 82
5	L	186/186 (100%)	185 (100%)	1 (0%)	88 96
All	All	933/951 (98%)	922 (99%)	11 (1%)	71 90

All (11) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	39	LEU
1	B	98	PHE
2	G	332	HIS
2	G	377	PHE
3	A	65	ARG
3	A	232	LYS
4	H	27	HIS

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Mol	Chain	Res	Type
4	H	32	TYR
4	H	33	TRP
4	H	111	TRP
5	L	99	PHE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

5.3.3 RNA

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates

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	E	1	2,6	14,14,15	0.38	0	17,19,21	0.41	0
6	NAG	E	2	6	14,14,15	0.44	0	17,19,21	0.38	0
6	BMA	E	3	6	11,11,12	0.81	0	15,15,17	0.91	0
6	FUC	E	4	6	10,10,11	0.75	0	14,14,16	1.05	1 (7%)

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	E	1	2,6	-	0/6/23/26	0/1/1/1
6	NAG	E	2	6	-	2/6/23/26	0/1/1/1
6	BMA	E	3	6	-	0/2/19/22	0/1/1/1
6	FUC	E	4	6	-	-	0/1/1/1

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
6	E	4	FUC	C1-O5-C5	2.20	117.76	112.78

There are no chirality outliers.

All (2) torsion outliers are listed below:

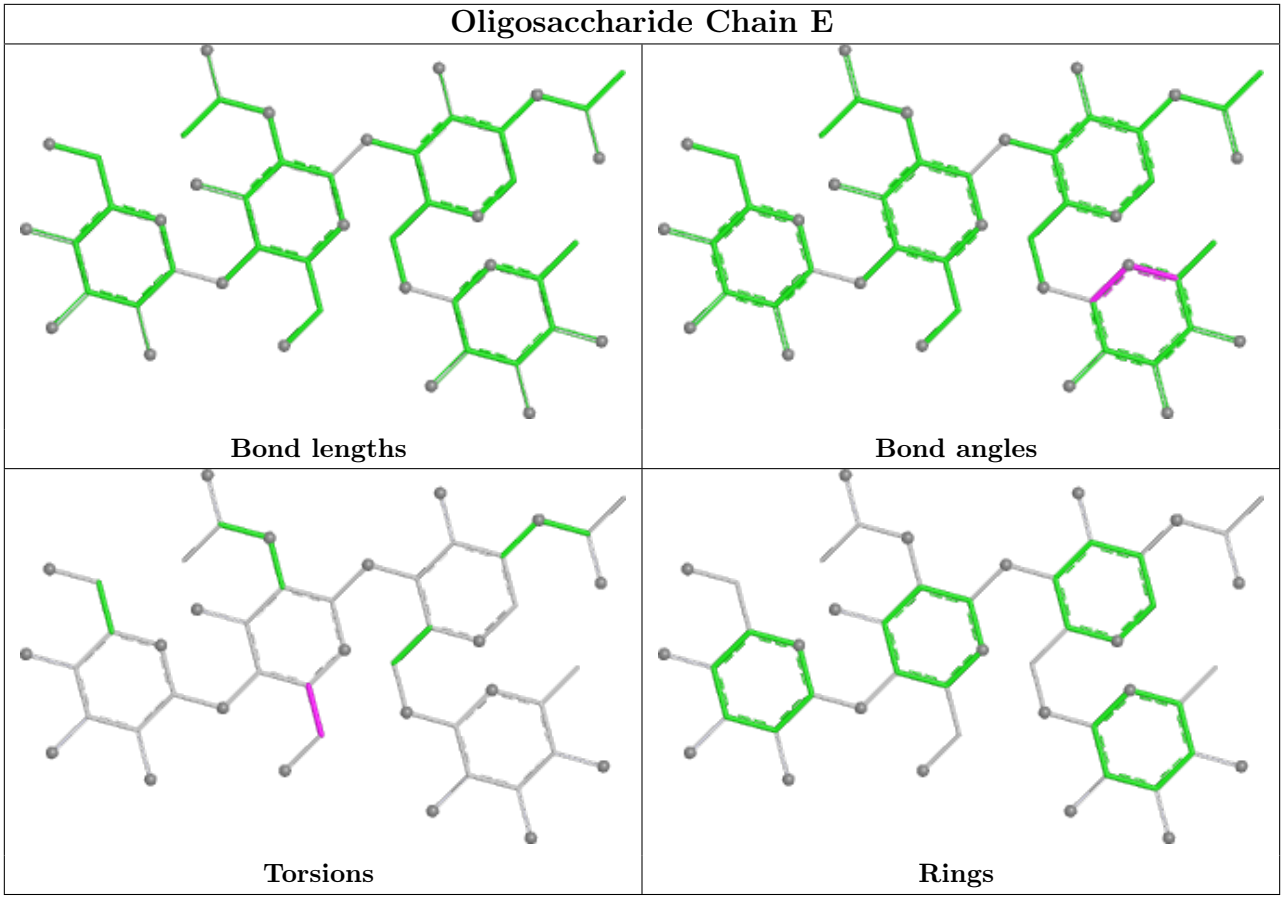
Mol	Chain	Res	Type	Atoms
6	E	2	NAG	O5-C5-C6-O6
6	E	2	NAG	C4-C5-C6-O6

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	E	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 (i)

17 ligands 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	$\#\|Z\| > 2$
8	SO4	G	603	-	4,4,4	0.13	0	6,6,6	0.06	0
8	SO4	A	303	-	4,4,4	0.13	0	6,6,6	0.13	0
8	SO4	G	605	-	4,4,4	0.15	0	6,6,6	0.11	0
9	PEG	G	602	-	6,6,6	0.22	0	5,5,5	0.04	0
8	SO4	H	302	-	4,4,4	0.14	0	6,6,6	0.09	0
8	SO4	G	606	-	4,4,4	0.42	0	6,6,6	0.48	0
8	SO4	A	302	-	4,4,4	0.14	0	6,6,6	0.12	0
8	SO4	L	301	-	4,4,4	0.14	0	6,6,6	0.08	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
8	SO4	B	302	-	4,4,4	0.39	0	6,6,6	0.41	0
8	SO4	H	301	-	4,4,4	0.17	0	6,6,6	0.14	0
7	GOL	B	301	-	5,5,5	0.69	0	5,5,5	1.10	1 (20%)
8	SO4	G	608	-	4,4,4	0.42	0	6,6,6	0.69	0
8	SO4	A	304	-	4,4,4	0.45	0	6,6,6	0.59	0
8	SO4	A	301	-	4,4,4	0.15	0	6,6,6	0.09	0
7	GOL	G	601	-	5,5,5	0.67	0	5,5,5	1.17	0
8	SO4	G	604	-	4,4,4	0.14	0	6,6,6	0.11	0
8	SO4	G	607	-	4,4,4	0.31	0	6,6,6	0.43	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
7	GOL	B	301	-	-	4/4/4/4	-
9	PEG	G	602	-	-	4/4/4/4	-
7	GOL	G	601	-	-	0/4/4/4	-

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
7	B	301	GOL	C3-C2-C1	-2.02	103.87	111.70

There are no chirality outliers.

All (8) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
7	B	301	GOL	C1-C2-C3-O3
9	G	602	PEG	O2-C3-C4-O4
7	B	301	GOL	O1-C1-C2-C3
7	B	301	GOL	O2-C2-C3-O3
7	B	301	GOL	O1-C1-C2-O2
9	G	602	PEG	C4-C3-O2-C2
9	G	602	PEG	O1-C1-C2-O2
9	G	602	PEG	C1-C2-O2-C3

There are no ring outliers.

2 monomers are involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
8	G	608	SO4	2	0
8	A	301	SO4	1	0

5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å^2)	Q<0.9
1	B	221/221 (100%)	0.99	36 (16%) 1 0	81, 136, 198, 248	0
2	G	197/210 (93%)	0.62	2 (1%) 82 59	70, 90, 129, 179	0
3	A	227/232 (97%)	0.82	27 (11%) 4 1	83, 133, 195, 235	0
4	H	219/226 (96%)	2.46	66 (30%) 0 0	88, 144, 302, 366	0
5	L	214/215 (99%)	2.29	89 (41%) 0 0	99, 210, 286, 347	0
All	All	1078/1104 (97%)	1.44	220 (20%) 1 0	70, 132, 270, 366	0

All (220) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
4	H	189	VAL	28.4
4	H	188	SER	24.3
4	H	148	CYS	23.6
4	H	149	LEU	20.1
4	H	158	VAL	17.9
4	H	190	VAL	17.6
5	L	136	LEU	15.4
5	L	137	LEU	14.9
5	L	115	SER	13.7
4	H	191	THR	13.5
4	H	192	VAL	13.4
5	L	120	PRO	13.2
4	H	146	LEU	11.2
4	H	206	VAL	11.2
5	L	176	LEU	10.3
4	H	133	ALA	10.0
5	L	119	PHE	10.0
4	H	129	VAL	10.0
4	H	221	PRO	9.6
4	H	147	GLY	9.3

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Mol	Chain	Res	Type	RSRZ
4	H	144	ALA	9.2
5	L	187	TYR	9.2
4	H	131	PRO	8.7
5	L	121	PRO	8.7
4	H	134	PRO	8.5
4	H	130	PHE	8.4
4	H	213	THR	8.1
4	H	136	SER	8.0
5	L	148	GLN	7.9
5	L	133	VAL	7.8
5	L	145	ALA	7.8
5	L	196	GLU	7.7
4	H	160	VAL	7.7
4	H	163	ASN	7.7
5	L	117	PHE	7.6
3	A	135	VAL	7.4
1	B	200	ALA	7.0
5	L	154	ALA	6.9
4	H	215	VAL	6.9
4	H	150	VAL	6.8
5	L	19	ALA	6.8
4	H	219	VAL	6.7
5	L	209	SER	6.7
4	H	202	TYR	6.5
4	H	171	VAL	6.4
5	L	149	TRP	6.3
5	L	194	ALA	6.3
5	L	123	ASP	6.0
5	L	195	CYS	6.0
1	B	203	VAL	6.0
5	L	193	TYR	6.0
4	H	222	LYS	6.0
5	L	190	HIS	5.9
3	A	155	LEU	5.9
4	H	167	LEU	5.9
4	H	159	THR	5.8
5	L	206	VAL	5.8
4	H	162	TRP	5.7
5	L	153	ASN	5.6
5	L	197	VAL	5.6
5	L	182	LEU	5.6
4	H	203	ILE	5.5

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Mol	Chain	Res	Type	RSRZ
4	H	220	GLU	5.5
5	L	203	SER	5.5
5	L	175	SER	5.4
1	B	156	LYS	5.4
5	L	202	LEU	5.3
5	L	86	TYR	5.3
5	L	189	LYS	5.2
5	L	138	ASN	5.2
5	L	76	SER	5.1
5	L	134	VAL	4.9
3	A	140	PRO	4.8
4	H	137	LYS	4.8
3	A	156	VAL	4.8
1	B	188	LEU	4.8
5	L	20	THR	4.8
4	H	132	LEU	4.7
4	H	208	HIS	4.6
5	L	111	VAL	4.6
4	H	2	VAL	4.5
1	B	139	VAL	4.4
1	B	140	VAL	4.4
1	B	199	TYR	4.3
5	L	18	ARG	4.3
5	L	16	GLY	4.2
1	B	151	ALA	4.2
4	H	166	ALA	4.1
1	B	215	SER	4.1
1	B	216	PHE	4.1
5	L	177	SER	4.1
5	L	199	HIS	4.0
3	A	203	LEU	4.0
5	L	13	VAL	4.0
5	L	112	ALA	3.9
1	B	162	GLN	3.8
4	H	128	SER	3.7
1	B	153	VAL	3.7
3	A	208	TYR	3.7
5	L	143	ARG	3.7
5	L	62	PHE	3.7
5	L	151	VAL	3.6
1	B	138	SER	3.6
1	B	124	ILE	3.6

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Mol	Chain	Res	Type	RSRZ
5	L	147	VAL	3.6
1	B	141	CYS	3.5
1	B	212	VAL	3.5
5	L	83	PHE	3.5
5	L	150	LYS	3.5
1	B	187	THR	3.4
1	B	193	TYR	3.4
5	L	21	LEU	3.4
5	L	186	ASP	3.4
1	B	143	LEU	3.4
1	B	157	VAL	3.4
1	B	142	LEU	3.4
3	A	136	PHE	3.4
5	L	155	LEU	3.3
4	H	204	CYS	3.3
1	B	152	LYS	3.3
4	H	218	LYS	3.3
5	L	212	ARG	3.3
4	H	5	VAL	3.3
3	A	152	LEU	3.3
5	L	188	GLU	3.3
3	A	212	VAL	3.3
1	B	137	ALA	3.2
3	A	196	VAL	3.2
4	H	182	GLY	3.2
4	H	145	ALA	3.2
5	L	36	TYR	3.2
5	L	89	GLN	3.2
3	A	141	SER	3.2
4	H	173	THR	3.1
3	A	221	VAL	3.1
4	H	197	LEU	3.1
5	L	105	VAL	3.1
5	L	201	GLY	3.1
4	H	151	LYS	3.0
5	L	152	ASP	3.0
5	L	131	ALA	3.0
5	L	73	LEU	3.0
5	L	192	VAL	3.0
5	L	214	GLU	3.0
5	L	35	TRP	3.0
1	B	161	LEU	3.0

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Mol	Chain	Res	Type	RSRZ
3	A	164	VAL	3.0
5	L	116	VAL	3.0
5	L	158	GLY	2.9
5	L	172	SER	2.9
5	L	135	CYS	2.9
4	H	83	TRP	2.9
5	L	114	PRO	2.9
5	L	11	LEU	2.9
5	L	198	THR	2.8
5	L	156	GLN	2.8
1	B	201	CYS	2.8
4	H	207	ASN	2.8
5	L	47	LEU	2.8
5	L	75	ILE	2.8
1	B	155	TRP	2.7
5	L	48	ILE	2.7
3	A	137	PRO	2.7
5	L	178	SER	2.7
4	H	217	LYS	2.7
4	H	201	THR	2.6
5	L	127	LYS	2.6
3	A	219	THR	2.6
4	H	18	LEU	2.6
2	G	417[A]	ASN	2.6
4	H	223	SER	2.6
5	L	51	ALA	2.6
3	A	213	ASN	2.6
4	H	42	GLY	2.5
5	L	183	SER	2.5
1	B	154	GLN	2.5
3	A	138	LEU	2.5
4	H	186	LEU	2.5
1	B	218	ARG	2.5
1	B	208	LEU	2.5
3	A	133	PRO	2.5
5	L	163	SER	2.5
4	H	178	LEU	2.5
5	L	122	SER	2.4
5	L	200	GLN	2.4
1	B	186	LEU	2.4
1	B	127	PRO	2.4
4	H	127	PRO	2.4

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Mol	Chain	Res	Type	RSRZ
5	L	118	ILE	2.4
4	H	172	HIS	2.4
2	G	368	LEU	2.3
4	H	135	SER	2.3
5	L	207	THR	2.3
1	B	219	GLY	2.3
3	A	4	LEU	2.3
3	A	148	GLY	2.3
3	A	79	LEU	2.3
3	A	194	SER	2.2
3	A	50	LEU	2.2
3	A	63	SER	2.2
4	H	45	LEU	2.2
4	H	110	TYR	2.2
4	H	34	ILE	2.2
1	B	198	VAL	2.2
5	L	46	LEU	2.2
5	L	191	LYS	2.2
5	L	110	THR	2.2
3	A	62	ASP	2.2
5	L	132	SER	2.2
1	B	122	VAL	2.2
4	H	195	SER	2.1
5	L	159	ASN	2.1
1	B	197	LYS	2.1
3	A	207	THR	2.1
1	B	100	SER	2.1
4	H	184	TYR	2.0
3	A	228	LYS	2.0
4	H	205	ASN	2.0
4	H	64	PHE	2.0
5	L	210	PHE	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,

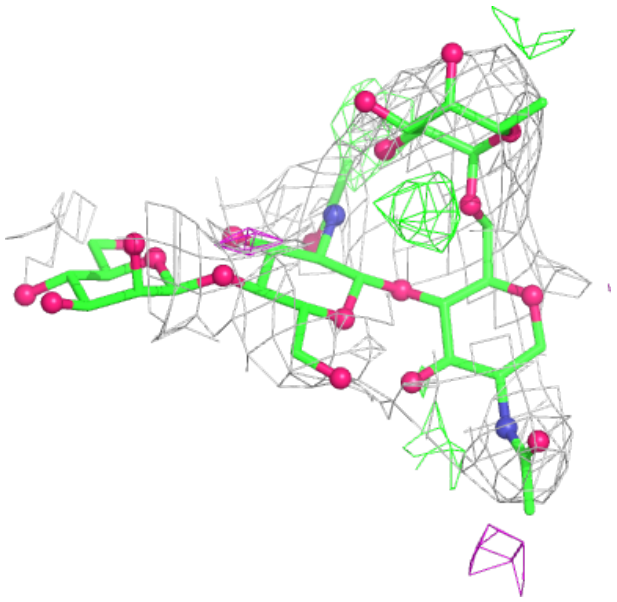
median, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

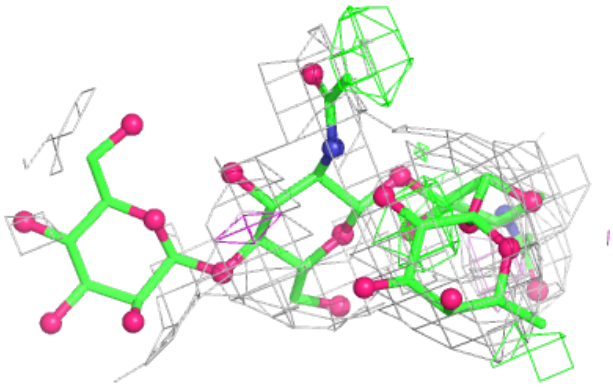
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
6	BMA	E	3	11/12	0.51	0.20	129,156,170,170	0
6	NAG	E	2	14/15	0.77	0.20	149,172,183,186	0
6	NAG	E	1	14/15	0.89	0.22	84,125,139,157	0
6	FUC	E	4	10/11	0.90	0.27	123,157,176,189	0

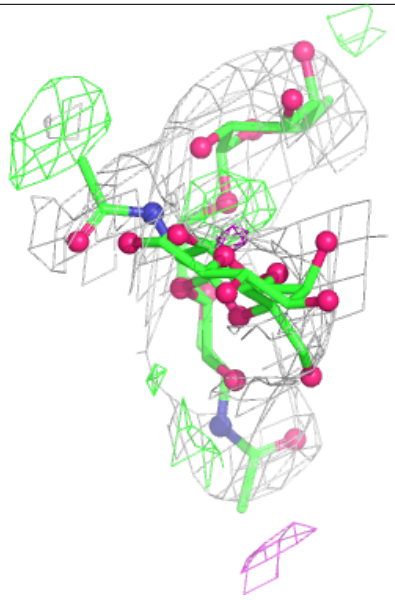
The following is a graphical depiction of the model fit to experimental electron density for oligosaccharide. Each fit is shown from different orientation to approximate a three-dimensional view.

Electron density around Chain E:

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







6.4 Ligands (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
7	GOL	B	301	6/6	0.61	0.35	102,106,109,125	0
8	SO4	A	303	5/5	0.67	0.34	145,158,184,233	0
8	SO4	G	608	5/5	0.71	0.33	144,151,205,283	0
8	SO4	A	304	5/5	0.76	0.24	158,164,174,259	0
8	SO4	G	603	5/5	0.80	0.18	120,121,172,211	0
8	SO4	G	604	5/5	0.82	0.29	123,133,175,221	0
8	SO4	A	301	5/5	0.82	0.45	108,139,161,484	0
8	SO4	G	606	5/5	0.83	0.33	110,119,178,225	0
7	GOL	G	601	6/6	0.84	0.28	89,106,119,124	0
9	PEG	G	602	7/7	0.85	0.25	93,94,112,116	0
8	SO4	G	607	5/5	0.87	0.18	119,137,164,195	0
8	SO4	H	302	5/5	0.87	0.22	152,163,206,272	0
8	SO4	B	302	5/5	0.87	0.22	141,152,173,241	0
8	SO4	A	302	5/5	0.89	0.12	151,168,184,231	0
8	SO4	H	301	5/5	0.92	0.18	100,118,137,141	0
8	SO4	G	605	5/5	0.94	0.11	101,133,153,197	0
8	SO4	L	301	5/5	0.95	0.19	124,147,157,171	0

6.5 Other polymers (i)

There are no such residues in this entry.