



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 05:59 PM UTC

PDB ID : 6Z8H / pdb_00006z8h
Title : Crystal structure of Variant Surface Glycoprotein VSG13
Authors : Stebbins, C.E.; Hempelmann, A.; Van Straaten, M.; Zeelen, J.
Deposited on : 2020-06-02
Resolution : 1.38 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 : 4-5-2 with Phenix2.0
Mogul : 2022.3.0, CSD as543be (2022)
Xtriage (Phenix) : 2.0
EDS : 3.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4 : 9.0.010 (Gargrove)
Density-Fitness : 1.0.12
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

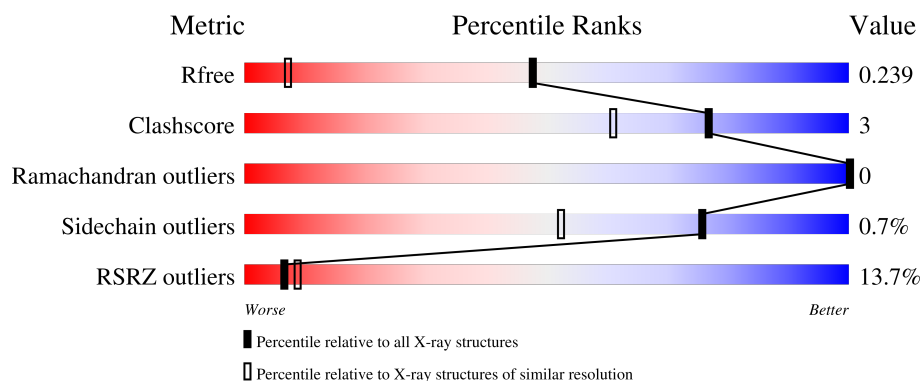
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.38 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}	180053	4403 (1.40-1.36)
Clashscore	190562	4528 (1.40-1.36)
Ramachandran outliers	187476	4459 (1.40-1.36)
Sidechain outliers	187428	4458 (1.40-1.36)
RSRZ outliers	180081	4399 (1.40-1.36)

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 $\leq 5\%$. 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	499	12% 65% 5% 30%
1	B	499	7% 66% . 30%
2	C	2	100%
2	D	2	50% 50%

2 Entry composition

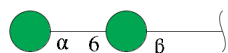
There are 5 unique types of molecules in this entry. The entry contains 11110 atoms, of which 5328 are hydrogens and 0 are deuteriums.

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 Variant surface glycoprotein MITat 1.13.

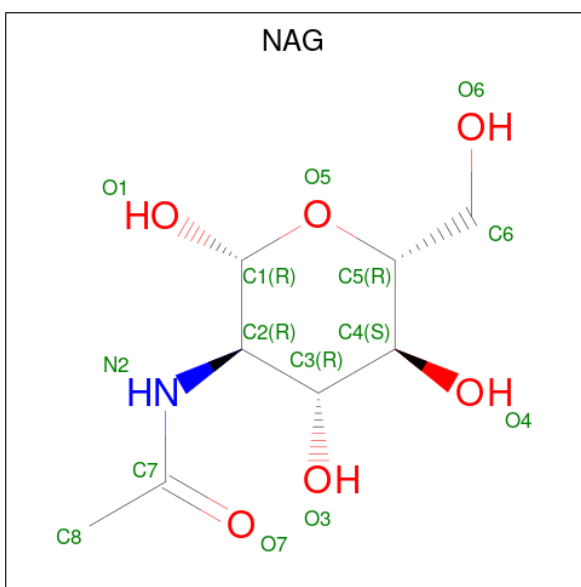
Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	351	Total	C	H	N	O	S	0	0	0
			5236	1622	2610	467	527	10			
1	B	350	Total	C	H	N	O	S	0	0	0
			5252	1626	2622	469	525	10			

- Molecule 2 is an oligosaccharide called alpha-D-mannopyranose-(1-6)-beta-D-mannopyranose.



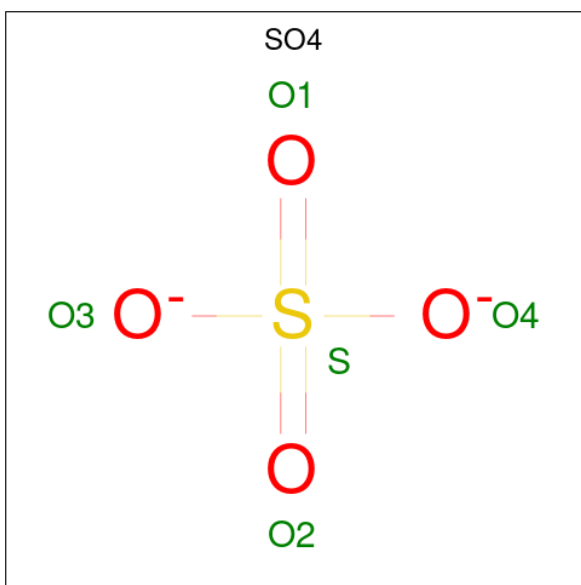
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
2	C	2	Total	C	H	O	0	0	0
			42	12	20	10			
2	D	2	Total	C	H	O	0	0	0
			42	12	20	10			

- Molecule 3 is 2-acetamido-2-deoxy-beta-D-glucopyranose (CCD ID: NAG) (formula: C₈H₁₅NO₆).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	A	1	Total	C	H	N	O	0	0
			28	8	14	1	5		
3	A	1	Total	C	H	N	O	0	0
			28	8	14	1	5		
3	B	1	Total	C	H	N	O	0	0
			28	8	14	1	5		
3	B	1	Total	C	H	N	O	0	0
			28	8	14	1	5		

- Molecule 4 is SULFATE ION (CCD ID: SO4) (formula: O₄S).



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

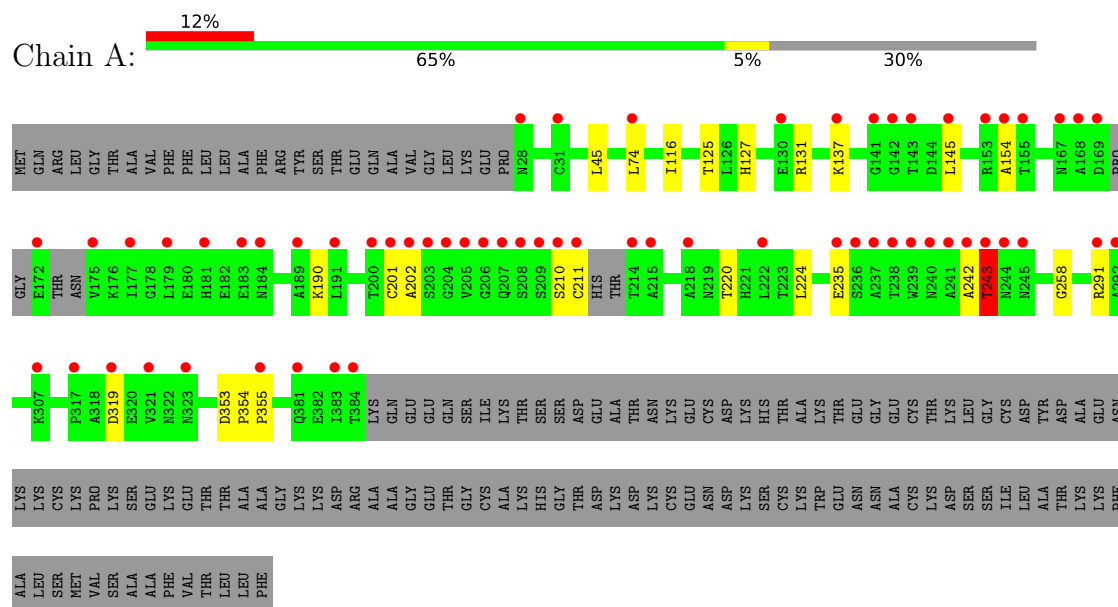
- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	165	Total	O	0	0
			165	165		
5	B	256	Total	O	0	0
			256	256		

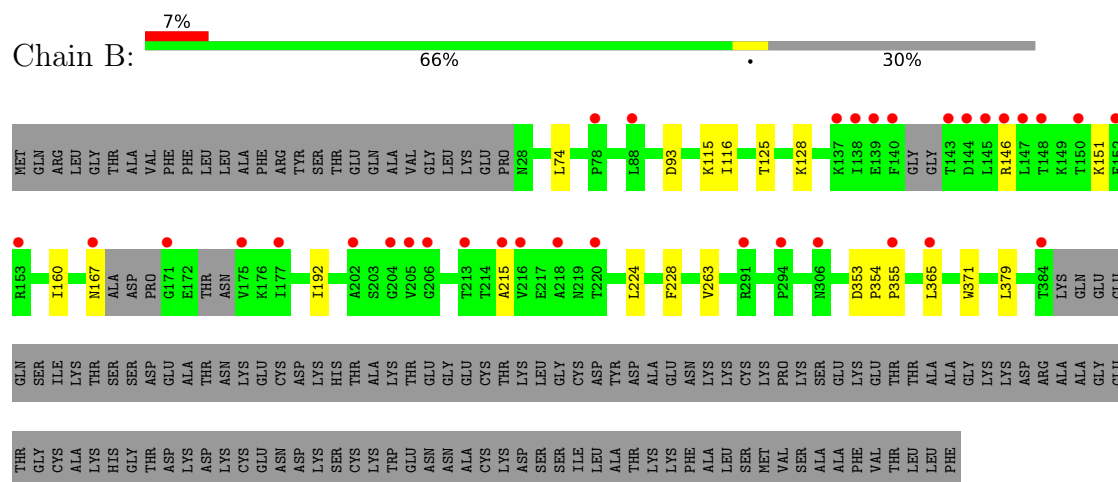
3 Residue-property plots [i](#)

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: Variant surface glycoprotein MITat 1.13



- Molecule 1: Variant surface glycoprotein MITat 1.13



- Molecule 2: alpha-D-mannopyranose-(1-6)-beta-D-mannopyranose



BM11
MAN2

- Molecule 2: alpha-D-mannopyranose-(1-6)-beta-D-mannopyranose

Chain D:

50%

50%

BM11
MAN2

4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	73.72Å 68.34Å 156.90Å 90.00° 92.55° 90.00°	Depositor
Resolution (Å)	48.14 – 1.38 48.14 – 1.38	Depositor EDS
% Data completeness (in resolution range)	97.1 (48.14-1.38) 97.2 (48.14-1.38)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.44 (at 1.38Å)	Xtriage
Refinement program	PHENIX 1.15.2_3472	Depositor
R, R_{free}	0.218 , 0.241 0.218 , 0.239	Depositor DCC
R_{free} test set	1639 reflections (0.63%)	wwPDB-VP
Wilson B-factor (Å ²)	18.5	Xtriage
Anisotropy	0.374	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.40 , 33.9	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	0.009 for -h,-k,l	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	11110	wwPDB-VP
Average B, all atoms (Å ²)	34.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.81% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ 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: MAN, NAG, SO4, BMA

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	0.55	4/2663 (0.2%)	0.66	3/3608 (0.1%)
1	B	0.49	0/2668	0.66	1/3614 (0.0%)
All	All	0.52	4/5331 (0.1%)	0.66	4/7222 (0.1%)

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
1	A	0	1

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	127	HIS	CE1-NE2	-8.85	1.23	1.32
1	A	319	ASP	C-O	-7.31	1.15	1.24
1	A	127	HIS	CG-ND1	-5.92	1.31	1.38
1	A	127	HIS	ND1-CE1	-5.10	1.27	1.32

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	93	ASP	CB-CA-C	5.58	120.34	110.85
1	A	242	ALA	CA-C-N	5.38	129.70	120.72
1	A	242	ALA	C-N-CA	5.38	129.70	120.72
1	A	319	ASP	CA-C-O	-5.13	115.43	120.82

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	243	THR	Mainchain

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	2626	2610	2609	23	0
1	B	2630	2622	2622	13	0
2	C	22	20	19	0	0
2	D	22	20	19	1	0
3	A	28	28	24	0	0
3	B	28	28	24	0	0
4	A	5	0	0	0	0
5	A	165	0	0	1	0
5	B	256	0	0	0	0
All	All	5782	5328	5317	31	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 3.

All (31) 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:125:THR:HG21	1:B:125:THR:OG1	1.84	0.77
1:B:128:LYS:HD3	1:B:160:ILE:HD12	1.73	0.70
1:A:125:THR:OG1	1:B:125:THR:HG21	1.94	0.68
1:A:235:GLU:HG2	5:A:670:HOH:O	1.95	0.66
1:A:211:CYS:H	1:A:243:THR:HG21	1.62	0.65
1:B:353:ASP:OD1	1:B:355:PRO:HD2	1.97	0.65
1:B:365:LEU:O	1:B:371:TRP:NE1	2.33	0.61
1:A:224:LEU:HD12	1:B:224:LEU:HD12	1.84	0.60
1:A:74:LEU:HD12	1:B:379:LEU:HD21	1.84	0.59
1:A:190:LYS:HE3	1:A:258:GLY:O	2.02	0.59
1:A:137:LYS:HB3	1:A:154:ALA:HB3	1.86	0.57
1:A:202:ALA:O	1:A:220:THR:HA	2.05	0.56
1:A:137:LYS:CB	1:A:154:ALA:HB3	2.36	0.56
1:A:353:ASP:OD2	1:A:355:PRO:HD2	2.05	0.55

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:354:PRO:HB2	1:B:355:PRO:HD3	1.90	0.54
1:A:45:LEU:HD13	1:A:116:ILE:HD12	1.90	0.53
1:A:201:CYS:HB3	1:A:243:THR:HG23	1.90	0.53
1:A:201:CYS:O	1:A:243:THR:CG2	2.60	0.49
1:A:354:PRO:HB2	1:A:355:PRO:HD3	1.95	0.48
1:A:131:ARG:HG3	1:A:131:ARG:HH11	1.79	0.48
1:A:210:SER:OG	1:A:243:THR:HB	2.14	0.48
1:A:201:CYS:HB3	1:A:243:THR:CG2	2.46	0.45
1:B:167:ASN:O	2:D:2:MAN:O6	2.33	0.45
1:B:115:LYS:HD3	1:B:263:VAL:HG12	1.99	0.45
1:A:131:ARG:HG3	1:A:131:ARG:NH1	2.31	0.44
1:A:211:CYS:H	1:A:243:THR:CG2	2.30	0.43
1:A:45:LEU:HB2	1:A:116:ILE:HD13	2.00	0.42
1:A:201:CYS:O	1:A:243:THR:HG23	2.20	0.42
1:A:145:LEU:HB2	1:B:215:ALA:HB1	2.03	0.40
1:B:146:ARG:O	1:B:151:LYS:HE3	2.22	0.40
1:B:192:ILE:HG23	1:B:228:PHE:HB3	2.03	0.40

There are no symmetry-related clashes.

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

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	344/499 (69%)	335 (97%)	9 (3%)	0	100	100
1	B	342/499 (68%)	335 (98%)	7 (2%)	0	100	100
All	All	686/998 (69%)	670 (98%)	16 (2%)	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	280/404 (69%)	278 (99%)	2 (1%)	76	52
1	B	282/404 (70%)	280 (99%)	2 (1%)	76	52
All	All	562/808 (70%)	558 (99%)	4 (1%)	76	52

All (4) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	243	THR
1	A	291	ARG
1	B	74	LEU
1	B	116	ILE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (2) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	245	ASN
1	B	219	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](#)

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
2	BMA	C	1	2	11,11,12	2.04	1 (9%)	15,15,17	1.34	3 (20%)
2	MAN	C	2	2	11,11,12	0.88	1 (9%)	15,15,17	1.45	2 (13%)
2	BMA	D	1	2	11,11,12	1.91	1 (9%)	15,15,17	1.02	0
2	MAN	D	2	2	11,11,12	1.19	1 (9%)	15,15,17	2.16	4 (26%)

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
2	BMA	C	1	2	-	0/2/19/22	0/1/1/1
2	MAN	C	2	2	-	2/2/19/22	0/1/1/1
2	BMA	D	1	2	-	0/2/19/22	0/1/1/1
2	MAN	D	2	2	-	2/2/19/22	0/1/1/1

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	1	BMA	O5-C1	-5.49	1.34	1.43
2	C	1	BMA	O5-C1	-5.42	1.34	1.43
2	D	2	MAN	C6-C5	2.41	1.59	1.51
2	C	2	MAN	C2-C3	-2.08	1.49	1.52

All (9) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	2	MAN	C1-O5-C5	6.55	120.96	112.19
2	C	2	MAN	O2-C2-C3	-3.44	103.03	110.15
2	C	2	MAN	C1-O5-C5	3.26	116.55	112.19
2	C	1	BMA	C1-C2-C3	-3.11	105.11	109.64
2	D	2	MAN	O5-C5-C6	-2.63	102.55	107.66
2	D	2	MAN	C1-C2-C3	2.41	113.15	109.64
2	C	1	BMA	O5-C1-C2	2.22	116.08	110.79
2	C	1	BMA	C1-O5-C5	-2.15	109.31	112.19

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	2	MAN	O5-C5-C4	2.04	115.79	110.83

There are no chirality outliers.

All (4) torsion outliers are listed below:

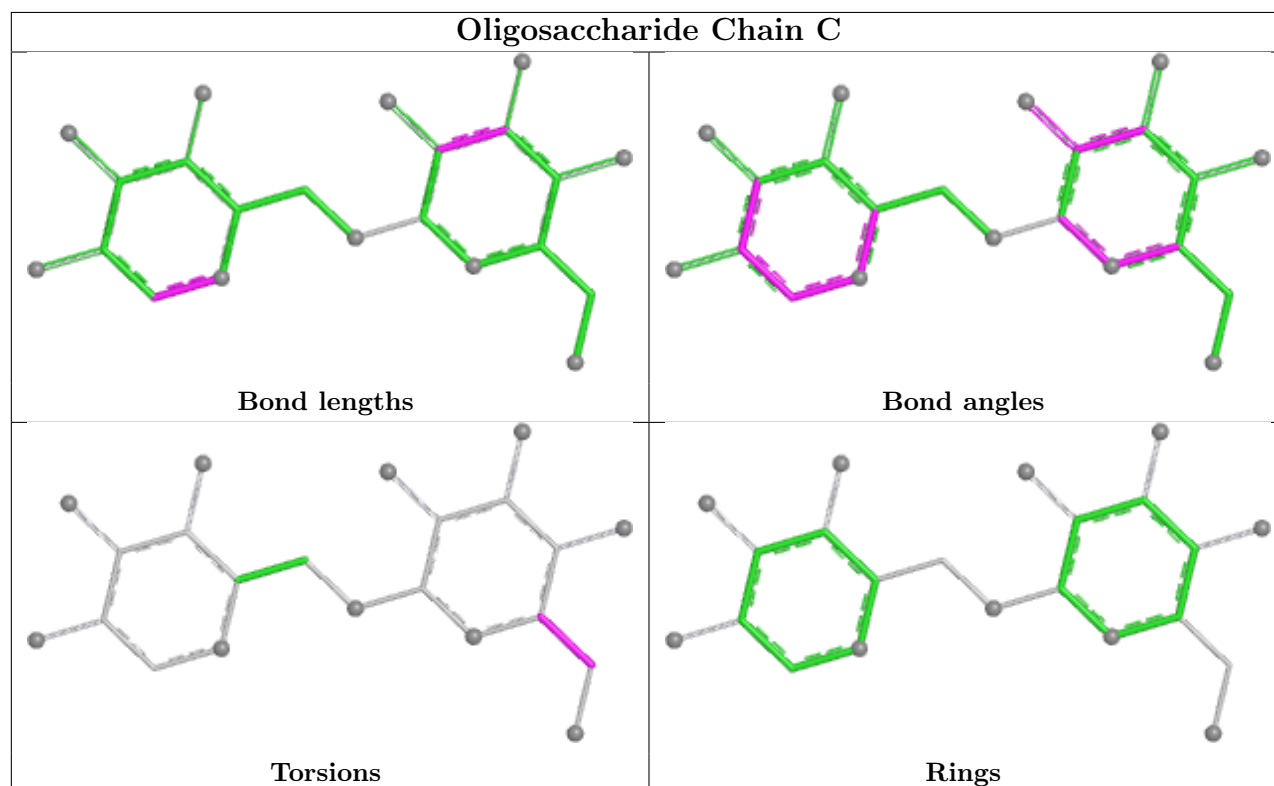
Mol	Chain	Res	Type	Atoms
2	D	2	MAN	O5-C5-C6-O6
2	C	2	MAN	O5-C5-C6-O6
2	D	2	MAN	C4-C5-C6-O6
2	C	2	MAN	C4-C5-C6-O6

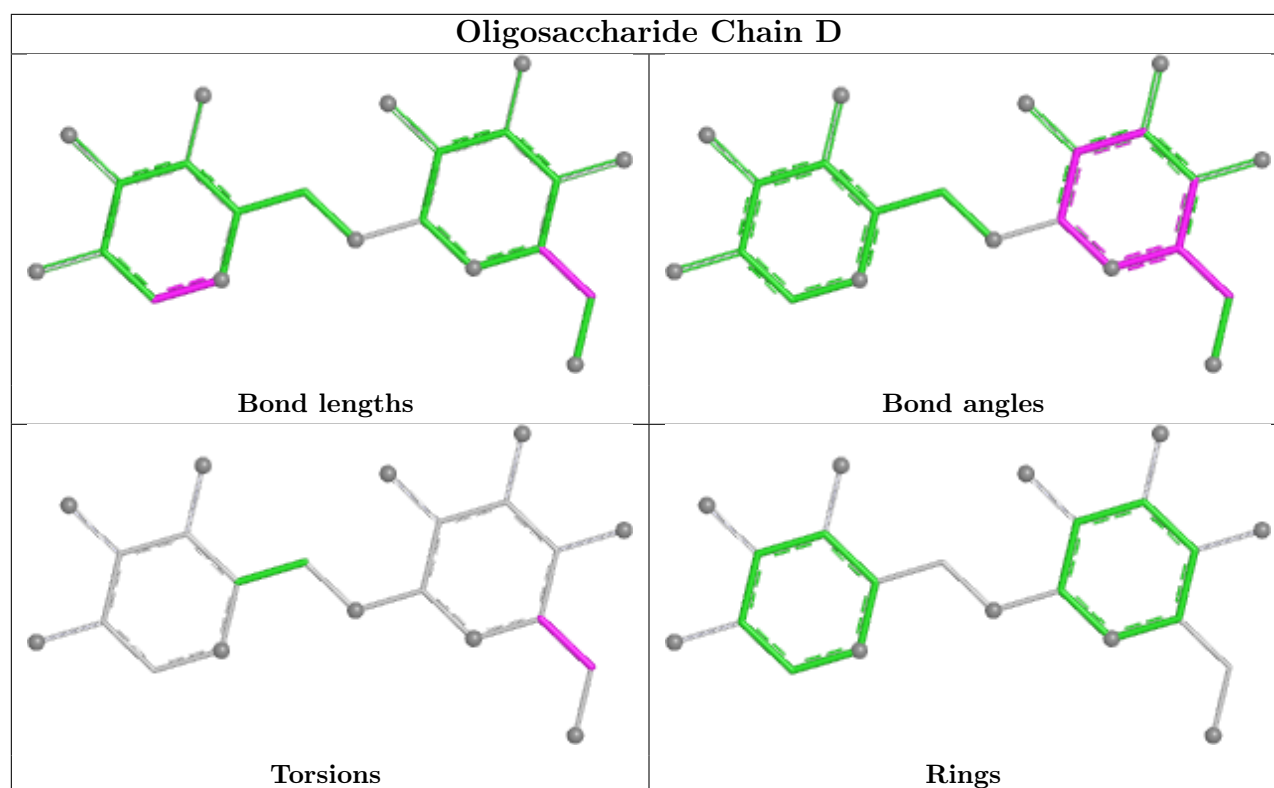
There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	D	2	MAN	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](#)

5 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
3	NAG	B	501	-	14,14,15	1.92	3 (21%)	17,19,21	1.55	4 (23%)
3	NAG	A	501	1	14,14,15	2.29	6 (42%)	17,19,21	1.86	4 (23%)
3	NAG	A	502	-	14,14,15	1.76	3 (21%)	17,19,21	1.54	3 (17%)
4	SO4	A	505	-	4,4,4	0.34	0	6,6,6	0.08	0
3	NAG	B	504	1	14,14,15	1.79	3 (21%)	17,19,21	2.12	6 (35%)

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
3	NAG	A	502	-	-	0/6/23/26	0/1/1/1
3	NAG	B	501	-	-	2/6/23/26	0/1/1/1
3	NAG	B	504	1	-	0/6/23/26	0/1/1/1
3	NAG	A	501	1	-	0/6/23/26	0/1/1/1

All (15) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	501	NAG	C1-C2	5.91	1.60	1.52
3	B	501	NAG	O5-C5	-4.48	1.34	1.43
3	B	504	NAG	C1-C2	4.12	1.58	1.52
3	A	502	NAG	O5-C5	-4.10	1.35	1.43
3	B	504	NAG	O7-C7	-3.48	1.15	1.23
3	B	501	NAG	O5-C1	-3.39	1.38	1.43
3	A	501	NAG	O5-C1	-3.28	1.38	1.43
3	A	502	NAG	O5-C1	-3.17	1.38	1.43
3	A	502	NAG	O7-C7	-2.85	1.16	1.23
3	A	501	NAG	O5-C5	-2.70	1.38	1.43
3	B	501	NAG	O7-C7	-2.64	1.17	1.23
3	A	501	NAG	O7-C7	-2.59	1.17	1.23
3	A	501	NAG	O4-C4	-2.40	1.37	1.43
3	B	504	NAG	O5-C1	-2.06	1.40	1.43
3	A	501	NAG	C3-C2	-2.04	1.48	1.52

All (17) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	501	NAG	O4-C4-C3	-4.77	99.14	110.38
3	B	504	NAG	O4-C4-C3	-4.73	99.23	110.38
3	B	504	NAG	C1-O5-C5	-4.38	106.32	112.19
3	A	501	NAG	O5-C1-C2	-3.93	105.20	111.29
3	B	504	NAG	C8-C7-N2	-3.32	110.61	116.12
3	A	502	NAG	C2-N2-C7	3.20	127.19	122.90
3	B	501	NAG	C2-N2-C7	2.70	126.51	122.90
3	B	501	NAG	C4-C3-C2	-2.69	107.08	111.02
3	B	501	NAG	C1-O5-C5	2.57	115.63	112.19
3	B	504	NAG	O7-C7-N2	2.55	126.49	121.98
3	A	502	NAG	O4-C4-C5	-2.45	103.29	109.32
3	B	504	NAG	O3-C3-C2	-2.42	104.38	109.40
3	A	501	NAG	O7-C7-N2	2.30	126.04	121.98
3	A	502	NAG	O4-C4-C3	2.25	115.67	110.38
3	B	504	NAG	O5-C1-C2	-2.22	107.86	111.29
3	B	501	NAG	O4-C4-C5	-2.21	103.89	109.32

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	501	NAG	C1-O5-C5	-2.20	109.23	112.19

There are no chirality outliers.

All (2) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	B	501	NAG	C4-C5-C6-O6
3	B	501	NAG	O5-C5-C6-O6

There are no ring outliers.

No monomer is involved in short contacts.

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, 95th 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	351/499 (70%)	1.11	62 (17%) 4 5	21, 35, 52, 67	0
1	B	350/499 (70%)	0.59	34 (9%) 13 15	18, 29, 47, 60	0
All	All	701/998 (70%)	0.85	96 (13%) 6 9	18, 33, 49, 67	0

All (96) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	205	VAL	7.7
1	A	202	ALA	5.5
1	A	175	VAL	5.3
1	A	242	ALA	5.3
1	A	237	ALA	5.2
1	A	209	SER	4.9
1	A	241	ALA	4.8
1	B	143	THR	4.8
1	A	211	CYS	4.8
1	B	145	LEU	4.7
1	B	205	VAL	4.7
1	A	240	ASN	4.7
1	A	210	SER	4.5
1	B	171	GLY	4.5
1	A	204	GLY	4.5
1	B	140	PHE	4.4
1	A	383	ILE	4.1
1	A	238	THR	4.1
1	B	148	THR	3.9
1	B	153	ARG	3.9
1	A	239	TRP	3.9
1	A	208	SER	3.8
1	A	31	CYS	3.8
1	A	215	ALA	3.7

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	A	236	SER	3.6
1	A	177	ILE	3.6
1	A	243	THR	3.3
1	B	150	THR	3.3
1	A	168	ALA	3.3
1	A	169	ASP	3.2
1	B	294	PRO	3.2
1	A	206	GLY	3.2
1	A	292	ALA	3.1
1	B	152	PHE	3.1
1	B	206	GLY	3.1
1	A	74	LEU	3.1
1	A	235	GLU	3.0
1	A	214	THR	3.0
1	A	130	GLU	3.0
1	A	218	ALA	3.0
1	A	355	PRO	3.0
1	A	184	ASN	2.9
1	A	201	CYS	2.9
1	A	172	GLU	2.9
1	A	222	LEU	2.8
1	B	144	ASP	2.8
1	A	203	SER	2.8
1	B	355	PRO	2.8
1	A	384	THR	2.8
1	B	147	LEU	2.8
1	B	177	ILE	2.7
1	B	167	ASN	2.7
1	B	215	ALA	2.7
1	A	145	LEU	2.7
1	B	137	LYS	2.6
1	A	167	ASN	2.6
1	B	365	LEU	2.6
1	A	323	ASN	2.6
1	B	216	VAL	2.6
1	A	245	ASN	2.6
1	A	307	LYS	2.5
1	B	220	THR	2.5
1	A	154	ALA	2.5
1	B	88	LEU	2.5
1	A	291	ARG	2.5
1	B	138	ILE	2.5

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	A	155	THR	2.4
1	A	153	ARG	2.4
1	B	291	ARG	2.4
1	A	207	GLN	2.4
1	A	381	GLN	2.4
1	A	321	VAL	2.4
1	B	218	ALA	2.4
1	A	28	ASN	2.4
1	A	142	GLY	2.3
1	A	137	LYS	2.3
1	B	204	GLY	2.3
1	A	183	GLU	2.3
1	A	143	THR	2.3
1	A	200	THR	2.3
1	A	179	LEU	2.3
1	A	191	LEU	2.3
1	B	146	ARG	2.2
1	A	317	PRO	2.2
1	A	181	HIS	2.2
1	B	175	VAL	2.2
1	A	319	ASP	2.2
1	B	384	THR	2.2
1	A	189	ALA	2.1
1	B	202	ALA	2.1
1	B	306	ASN	2.1
1	B	78	PRO	2.1
1	A	244	ASN	2.0
1	B	213	THR	2.0
1	B	139	GLU	2.0
1	A	141	GLY	2.0

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

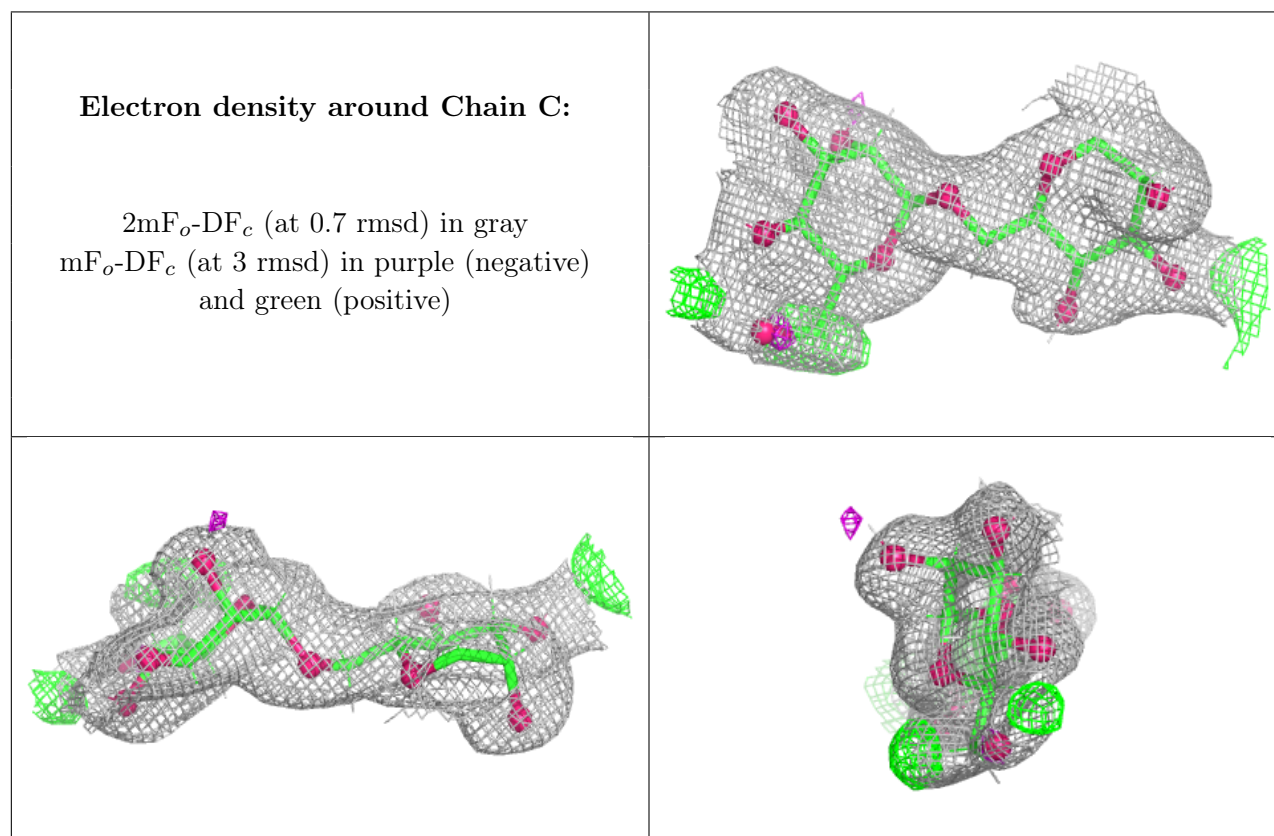
There are no non-standard protein/DNA/RNA residues in this entry.

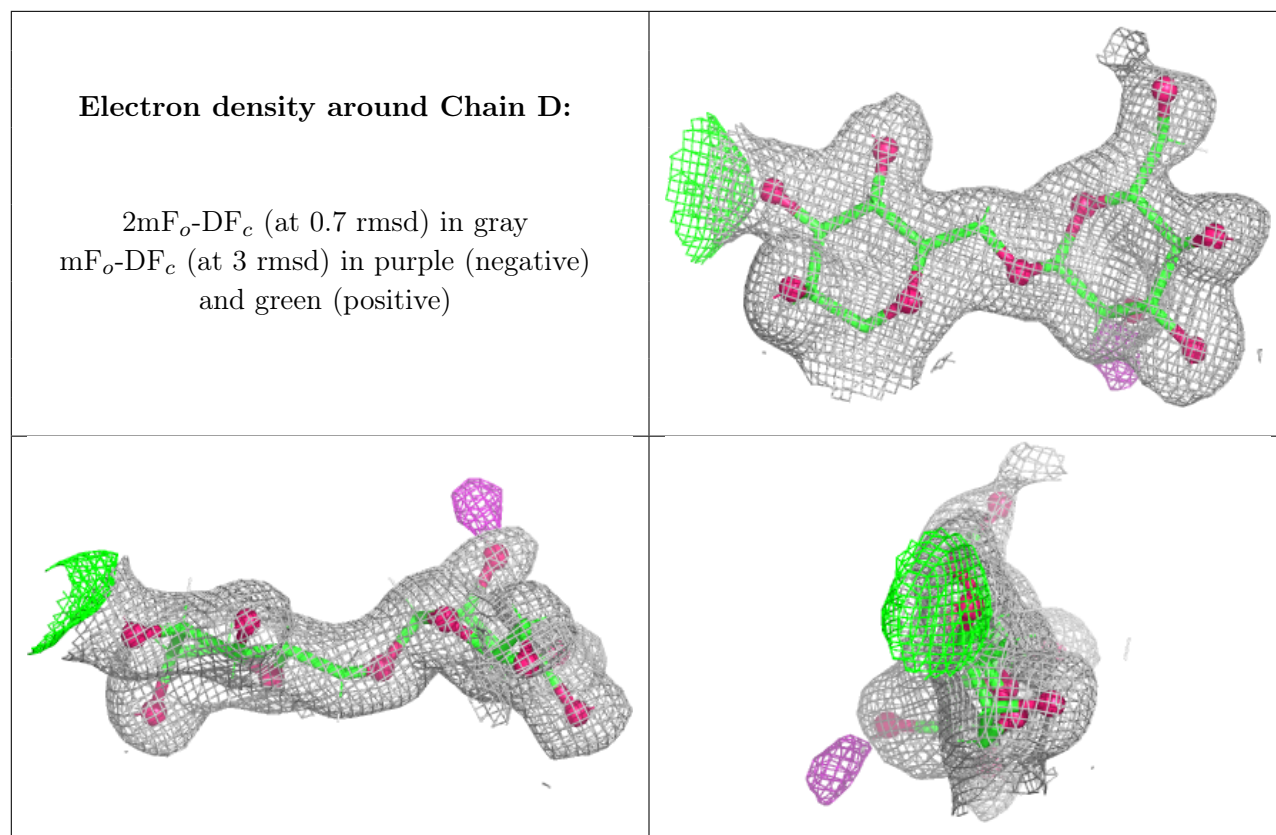
6.3 Carbohydrates

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, 95th 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($\text{\AA}^2$)	Q<0.9
2	MAN	C	2	11/12	0.87	0.12	36,43,47,52	0
2	MAN	D	2	11/12	0.91	0.11	33,39,44,47	0
2	BMA	C	1	11/12	0.93	0.09	34,40,46,48	0
2	BMA	D	1	11/12	0.94	0.08	33,35,42,45	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.





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, 95th 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	SO4	A	505	5/5	0.83	0.20	59,59,60,61	0
3	NAG	B	501	14/15	0.94	0.08	25,32,43,48	0
3	NAG	A	502	14/15	0.94	0.09	27,33,39,42	0
3	NAG	B	504	14/15	0.96	0.06	24,30,37,37	0
3	NAG	A	501	14/15	0.96	0.06	26,30,34,35	0

6.5 Other polymers [i](#)

There are no such residues in this entry.