



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 11:23 AM UTC

PDB ID : 6Z8G / pdb_00006z8g
Title : Crystal structure of VSG13 soaked in 0.5 M used to phase VSG13 to solve the structure.
Authors : Stebbins, C.E.; Hempelmann, A.; Van Straaten, M.; Zeelen, J.
Deposited on : 2020-06-02
Resolution : 1.56 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

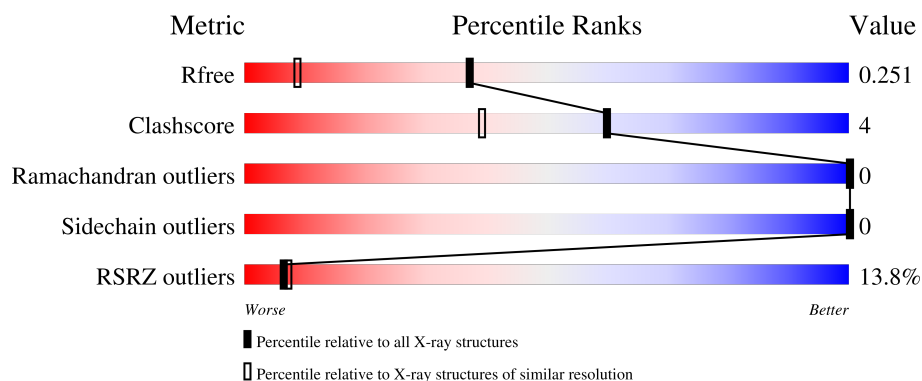
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.56 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	2145 (1.56-1.56)
Clashscore	190562	2189 (1.56-1.56)
Ramachandran outliers	187476	2153 (1.56-1.56)
Sidechain outliers	187428	2150 (1.56-1.56)
RSRZ outliers	180081	2146 (1.56-1.56)

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	
1	B	499	
2	C	4	
2	D	4	

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
3	BR	A	506	-	-	X	-
3	BR	B	505	-	-	X	-
3	BR	B	506	-	-	X	-

2 Entry composition [i](#)

There are 5 unique types of molecules in this entry. The entry contains 5799 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 Variant surface glycoprotein MITat 1.13.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	346	Total	C	N	O	S	0	0	0
			2576	1593	459	514	10			
1	B	349	Total	C	N	O	S	0	0	0
			2566	1590	452	514	10			

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



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
2	C	4	Total	C	N	O	0	0	0
			50	28	2	20			
2	D	4	Total	C	N	O	0	0	0
			50	28	2	20			

- Molecule 3 is BROMIDE ION (CCD ID: BR) (formula: Br).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	6	Total	Br	0	0
			6	6		
3	B	17	Total	Br	0	0
			17	17		

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



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

- Molecule 5 is water.

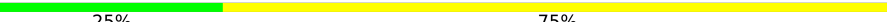
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	230	Total	O	0	0
			230	230		
5	B	299	Total	O	0	0
			299	299		

- Molecule 2: alpha-D-mannopyranose-(1-6)-beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain C:  75% 25%

MAG1
MAG2
BMA3
MAN4

- Molecule 2: alpha-D-mannopyranose-(1-6)-beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain D:  25% 75%

MAG1
MAG2
BMA3
MAN4

4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	74.15Å 68.41Å 157.76Å 90.00° 92.17° 90.00°	Depositor
Resolution (Å)	52.55 – 1.56 52.55 – 1.56	Depositor EDS
% Data completeness (in resolution range)	95.7 (52.55-1.56) 88.8 (52.55-1.56)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	0.89 (at 1.56Å)	Xtriage
Refinement program	PHENIX 1.15.2_3472	Depositor
R, R_{free}	0.226 , 0.233 (Not available) , 0.251	Depositor DCC
R_{free} test set	1997 reflections (1.78%)	wwPDB-VP
Wilson B-factor (Å ²)	16.7	Xtriage
Anisotropy	0.572	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.35 , 50.4	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	0.016 for -h,-k,l	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	5799	wwPDB-VP
Average B, all atoms (Å ²)	32.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.11% 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: BMA, MAN, SO4, BR, NAG

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	0.42	0/2612	0.56	0/3539
1	B	0.43	0/2603	0.55	0/3536
All	All	0.43	0/5215	0.55	0/7075

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	2576	0	2543	21	0
1	B	2566	0	2515	31	0
2	C	50	0	43	0	0
2	D	50	0	43	0	0
3	A	6	0	0	3	0
3	B	17	0	0	7	0
4	B	5	0	0	0	0
5	A	230	0	0	2	0
5	B	299	0	0	0	0
All	All	5799	0	5144	45	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 4.

All (45) 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:B:505:BR:BR	3:B:506:BR:BR	3.06	0.84
1:B:353:ASP:OD2	1:B:355:PRO:HD2	1.83	0.79
1:B:139:GLU:HG2	1:B:221:HIS:CD2	2.26	0.70
1:A:125:THR:HG21	1:B:125:THR:OG1	1.92	0.69
1:A:326:ASN:OD1	3:A:506:BR:BR	2.66	0.69
1:B:207:GLN:NE2	3:B:506:BR:BR	2.84	0.66
1:A:125:THR:OG1	1:B:125:THR:HG21	1.95	0.65
1:A:291:ARG:NH2	3:A:506:BR:BR	2.84	0.65
1:B:140:PHE:C	3:B:505:BR:BR	2.95	0.65
1:A:45:LEU:HB2	1:A:116:ILE:HD13	1.84	0.58
1:B:353:ASP:OD2	1:B:355:PRO:CD	2.52	0.57
1:B:353:ASP:OD2	1:B:355:PRO:HG2	2.05	0.57
1:B:139:GLU:CG	1:B:221:HIS:CD2	2.90	0.55
1:B:207:GLN:HG2	1:B:221:HIS:CG	2.42	0.54
1:A:124:ASN:ND2	1:B:118:GLU:OE2	2.40	0.54
1:B:353:ASP:HB3	1:B:356:GLY:O	2.08	0.54
1:A:216:VAL:HG12	1:B:145:LEU:HB3	1.91	0.53
1:A:216:VAL:HG23	1:A:220:THR:HG21	1.92	0.51
1:B:353:ASP:OD2	1:B:355:PRO:CG	2.59	0.50
1:B:138:ILE:HD11	1:B:152:PHE:CE2	2.47	0.49
1:A:180:GLU:H	1:A:180:GLU:CD	2.21	0.48
1:A:137:LYS:CB	1:A:154:ALA:HB3	2.43	0.48
1:B:277:SER:HB2	3:B:502:BR:BR	2.68	0.48
1:B:246:LYS:O	1:B:247:ARG:NH1	2.40	0.47
1:B:205:VAL:HA	1:B:219:ASN:HD22	1.80	0.46
1:B:207:GLN:HG2	1:B:221:HIS:ND1	2.32	0.45
1:A:216:VAL:CG1	1:B:145:LEU:HB3	2.46	0.45
1:B:106:ARG:HD3	3:B:515:BR:BR	2.71	0.45
1:B:161:HIS:CE1	1:B:163:ALA:HB3	2.51	0.45
1:B:291:ARG:HH12	1:B:332:GLU:HA	1.82	0.45
1:A:154:ALA:HA	5:A:617:HOH:O	2.19	0.43
1:A:224:LEU:HD12	1:B:224:LEU:HD12	2.01	0.43
1:A:190:LYS:HA	1:A:257:LEU:HD12	2.00	0.42
1:A:216:VAL:HG12	1:B:145:LEU:O	2.19	0.42
1:A:93:ASP:OD1	1:B:369:PRO:HB3	2.19	0.42
1:B:133:LEU:HA	1:B:133:LEU:HD23	1.78	0.42
1:B:77:VAL:HB	1:B:78:PRO:HD2	2.01	0.42
1:A:106:ARG:HD3	3:B:516:BR:BR	2.75	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:83:LYS:HE2	3:A:502:BR:BR	2.75	0.41
1:B:192:ILE:HG23	1:B:228:PHE:HB3	2.02	0.41
1:A:76:ALA:HB1	1:A:80:MET:HB3	2.02	0.41
1:A:79:THR:HG23	5:A:734:HOH:O	2.21	0.40
1:B:191:LEU:N	3:B:511:BR:BR	3.02	0.40
1:B:217:GLU:H	1:B:220:THR:HG1	1.69	0.40
1:A:351:LYS:HD2	1:A:365:LEU:HD21	2.03	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	337/499 (68%)	328 (97%)	9 (3%)	0	100	100
1	B	342/499 (68%)	338 (99%)	4 (1%)	0	100	100
All	All	679/998 (68%)	666 (98%)	13 (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	270/404 (67%)	270 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	B	268/404 (66%)	268 (100%)	0	100	100
All	All	538/808 (67%)	538 (100%)	0	100	100

There are no protein residues with a non-rotameric sidechain to report.

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (5) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	161	HIS
1	A	219	ASN
1	A	245	ASN
1	A	370	GLN
1	B	219	ASN

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 ⓘ

8 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	NAG	C	1	2,1	14,14,15	0.44	0	17,19,21	0.56	0
2	NAG	C	2	2	14,14,15	0.28	0	17,19,21	0.49	0
2	BMA	C	3	2	11,11,12	0.95	0	15,15,17	0.73	0
2	MAN	C	4	2	11,11,12	0.65	0	15,15,17	1.29	2 (13%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	NAG	D	1	2,1	14,14,15	0.58	1 (7%)	17,19,21	0.41	0
2	NAG	D	2	2	14,14,15	0.36	0	17,19,21	0.82	0
2	BMA	D	3	2	11,11,12	1.08	0	15,15,17	0.94	1 (6%)
2	MAN	D	4	2	11,11,12	0.77	0	15,15,17	0.92	2 (13%)

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	NAG	C	1	2,1	-	0/6/23/26	0/1/1/1
2	NAG	C	2	2	-	2/6/23/26	0/1/1/1
2	BMA	C	3	2	-	0/2/19/22	0/1/1/1
2	MAN	C	4	2	-	0/2/19/22	0/1/1/1
2	NAG	D	1	2,1	-	0/6/23/26	0/1/1/1
2	NAG	D	2	2	-	0/6/23/26	0/1/1/1
2	BMA	D	3	2	-	0/2/19/22	0/1/1/1
2	MAN	D	4	2	-	0/2/19/22	0/1/1/1

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	1	NAG	C1-C2	2.00	1.55	1.52

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	4	MAN	C1-O5-C5	3.33	116.64	112.19
2	C	4	MAN	O2-C2-C3	-2.94	104.06	110.15
2	D	3	BMA	O2-C2-C3	-2.83	104.30	110.15
2	D	4	MAN	C1-O5-C5	2.14	115.06	112.19
2	D	4	MAN	O2-C2-C3	-2.01	106.00	110.15

There are no chirality outliers.

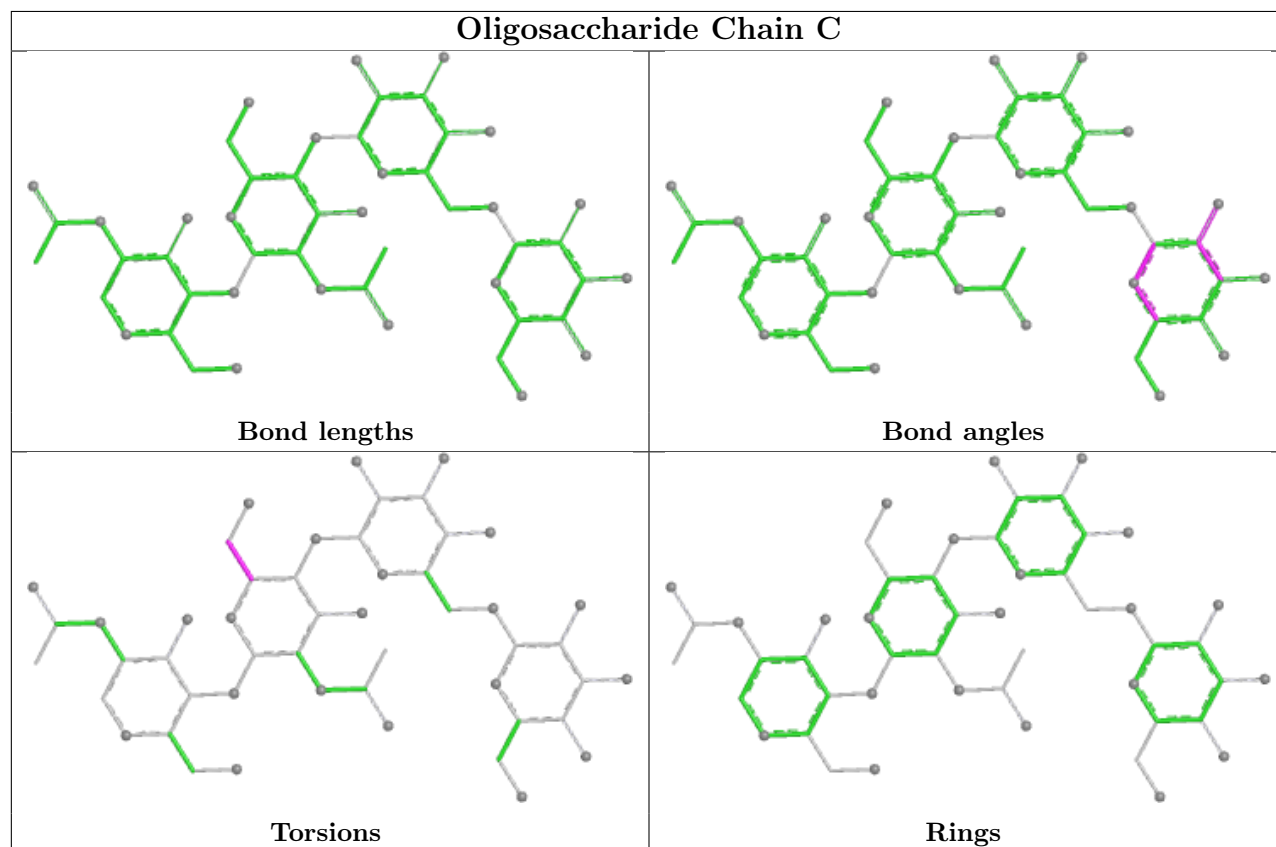
All (2) torsion outliers are listed below:

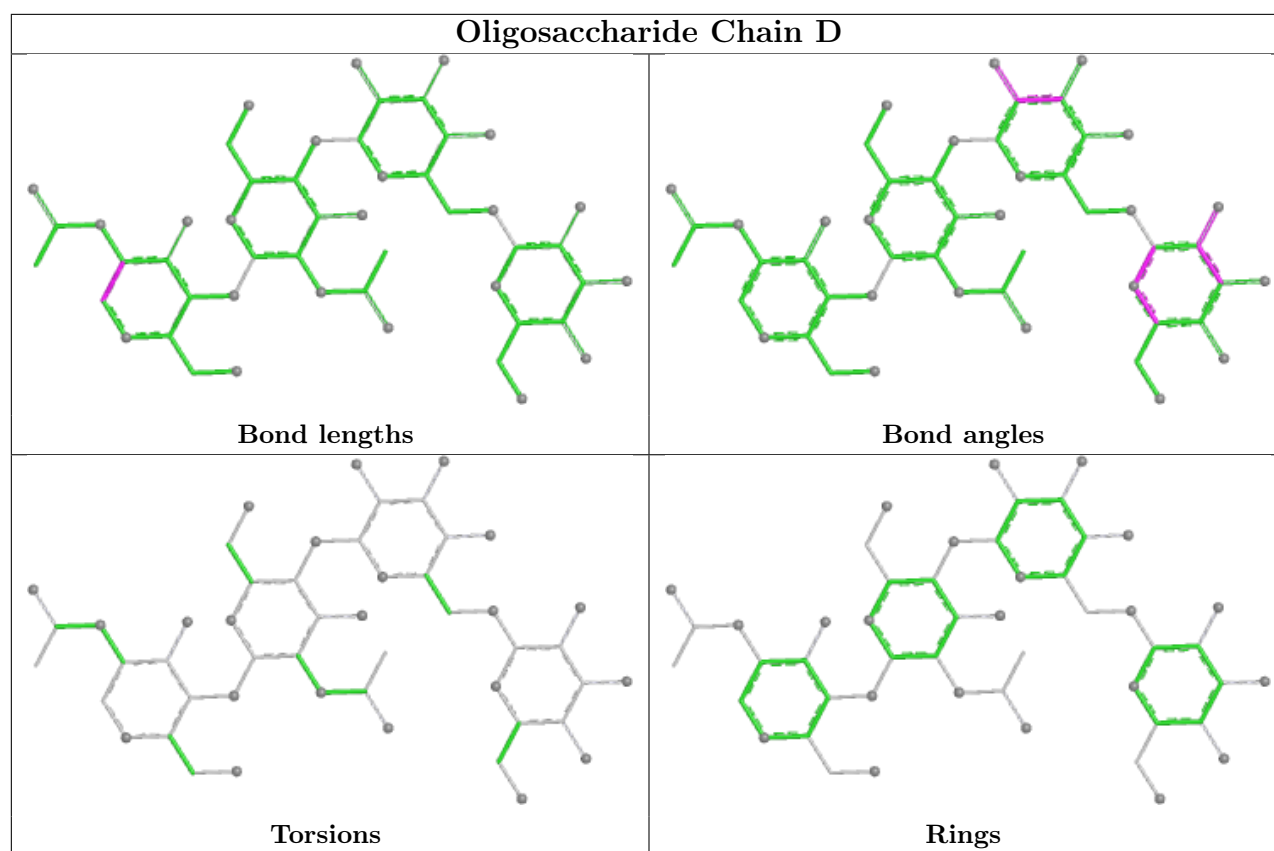
Mol	Chain	Res	Type	Atoms
2	C	2	NAG	O5-C5-C6-O6
2	C	2	NAG	C4-C5-C6-O6

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.





5.6 Ligand geometry [i](#)

Of 24 ligands modelled in this entry, 23 are monoatomic - leaving 1 for Mogul analysis.

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	SO4	B	501	-	4,4,4	0.29	0	6,6,6	0.42	0

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 [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	346/499 (69%)	1.01	56 (16%) 4 5	19, 32, 58, 76	0
1	B	349/499 (69%)	0.67	40 (11%) 9 11	17, 26, 51, 73	0
All	All	695/998 (69%)	0.84	96 (13%) 6 7	17, 29, 56, 76	0

All (96) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	205	VAL	6.4
1	B	138	ILE	5.9
1	B	150	THR	5.8
1	A	204	GLY	5.8
1	B	143	THR	5.6
1	B	148	THR	5.4
1	B	147	LEU	5.1
1	A	211	CYS	5.1
1	A	202	ALA	5.1
1	A	214	THR	5.1
1	A	168	ALA	4.5
1	A	216	VAL	4.2
1	A	239	TRP	4.1
1	A	201	CYS	4.0
1	A	203	SER	4.0
1	A	177	ILE	3.9
1	B	145	LEU	3.9
1	A	238	THR	3.9
1	A	237	ALA	3.9
1	B	144	ASP	3.8
1	A	31	CYS	3.8
1	B	152	PHE	3.7
1	A	215	ALA	3.7
1	A	209	SER	3.6

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Mol	Chain	Res	Type	RSRZ
1	A	29	ALA	3.6
1	A	28	ASN	3.6
1	A	381	GLN	3.5
1	A	184	ASN	3.5
1	A	236	SER	3.5
1	B	218	ALA	3.5
1	A	124	ASN	3.4
1	B	140	PHE	3.3
1	A	241	ALA	3.3
1	A	313	GLU	3.3
1	A	218	ALA	3.1
1	A	167	ASN	3.1
1	B	204	GLY	3.1
1	A	220	THR	3.1
1	A	183	GLU	3.1
1	B	151	LYS	3.0
1	A	155	THR	3.0
1	B	139	GLU	3.0
1	A	154	ALA	2.9
1	B	146	ARG	2.9
1	A	243	THR	2.9
1	A	242	ALA	2.9
1	A	244	ASN	2.8
1	B	206	GLY	2.8
1	A	240	ASN	2.8
1	B	219	ASN	2.7
1	B	175	VAL	2.7
1	A	186	PRO	2.7
1	A	222	LEU	2.6
1	A	169	ASP	2.6
1	B	384	THR	2.6
1	B	149	LYS	2.6
1	A	142	GLY	2.6
1	A	383	ILE	2.5
1	B	74	LEU	2.5
1	B	167	ASN	2.5
1	B	355	PRO	2.5
1	A	145	LEU	2.5
1	B	166	PRO	2.5
1	A	292	ALA	2.4
1	A	172	GLU	2.4
1	B	153	ARG	2.4

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Mol	Chain	Res	Type	RSRZ
1	A	210	SER	2.4
1	A	176	LYS	2.3
1	B	221	HIS	2.3
1	B	31	CYS	2.3
1	A	153	ARG	2.3
1	B	136	ALA	2.3
1	A	199	ALA	2.2
1	B	202	ALA	2.2
1	B	216	VAL	2.2
1	A	197	LEU	2.2
1	A	366	SER	2.2
1	B	41	LEU	2.2
1	A	339	LYS	2.2
1	A	41	LEU	2.1
1	A	248	ALA	2.1
1	A	225	GLY	2.1
1	B	131	ARG	2.1
1	B	203	SER	2.1
1	B	209	SER	2.1
1	B	154	ALA	2.1
1	A	219	ASN	2.1
1	B	177	ILE	2.1
1	B	365	LEU	2.1
1	B	79	THR	2.0
1	B	220	THR	2.0
1	A	221	HIS	2.0
1	A	217	GLU	2.0
1	B	172	GLU	2.0
1	A	245	ASN	2.0
1	A	353	ASP	2.0

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

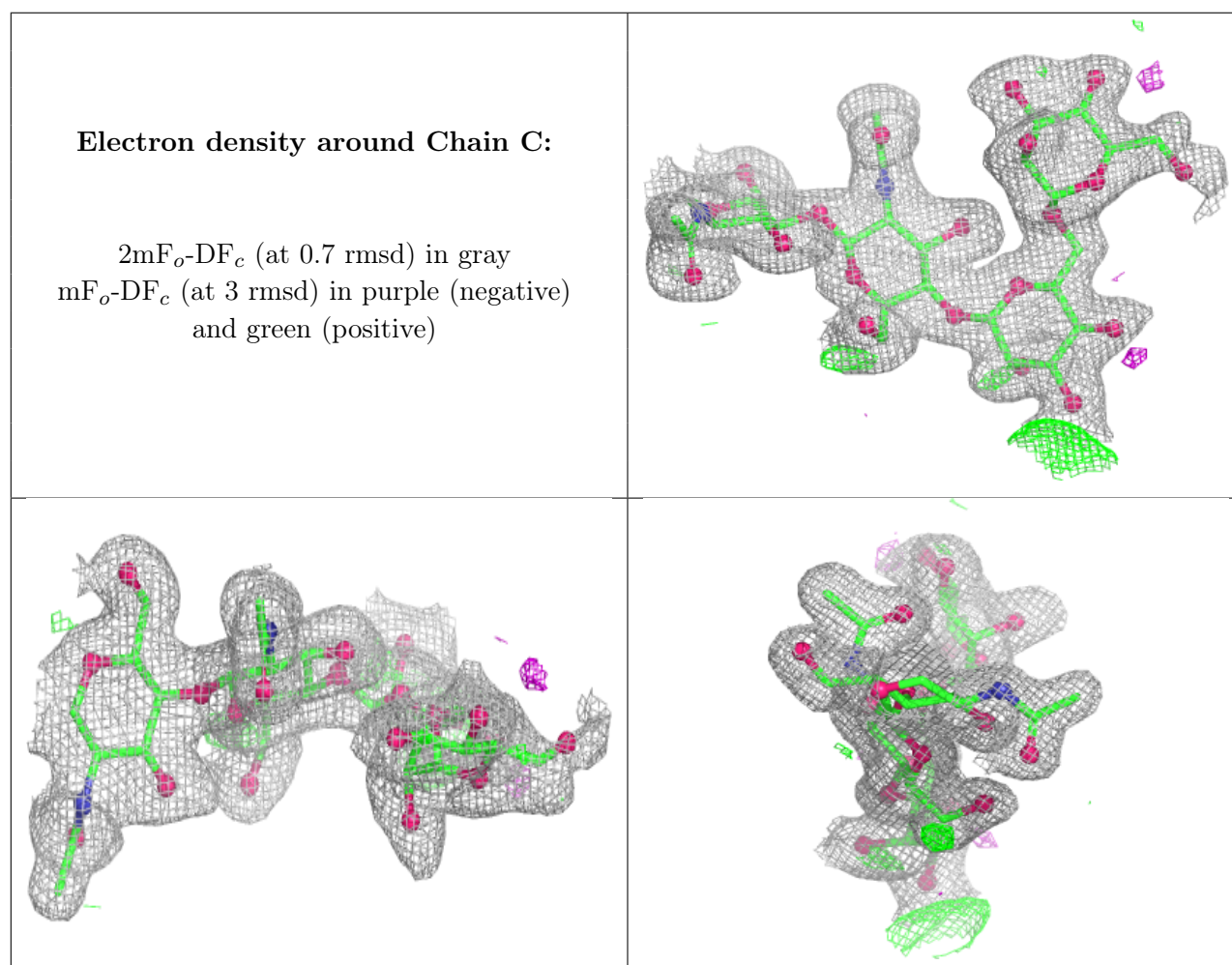
There are no non-standard protein/DNA/RNA residues in this entry.

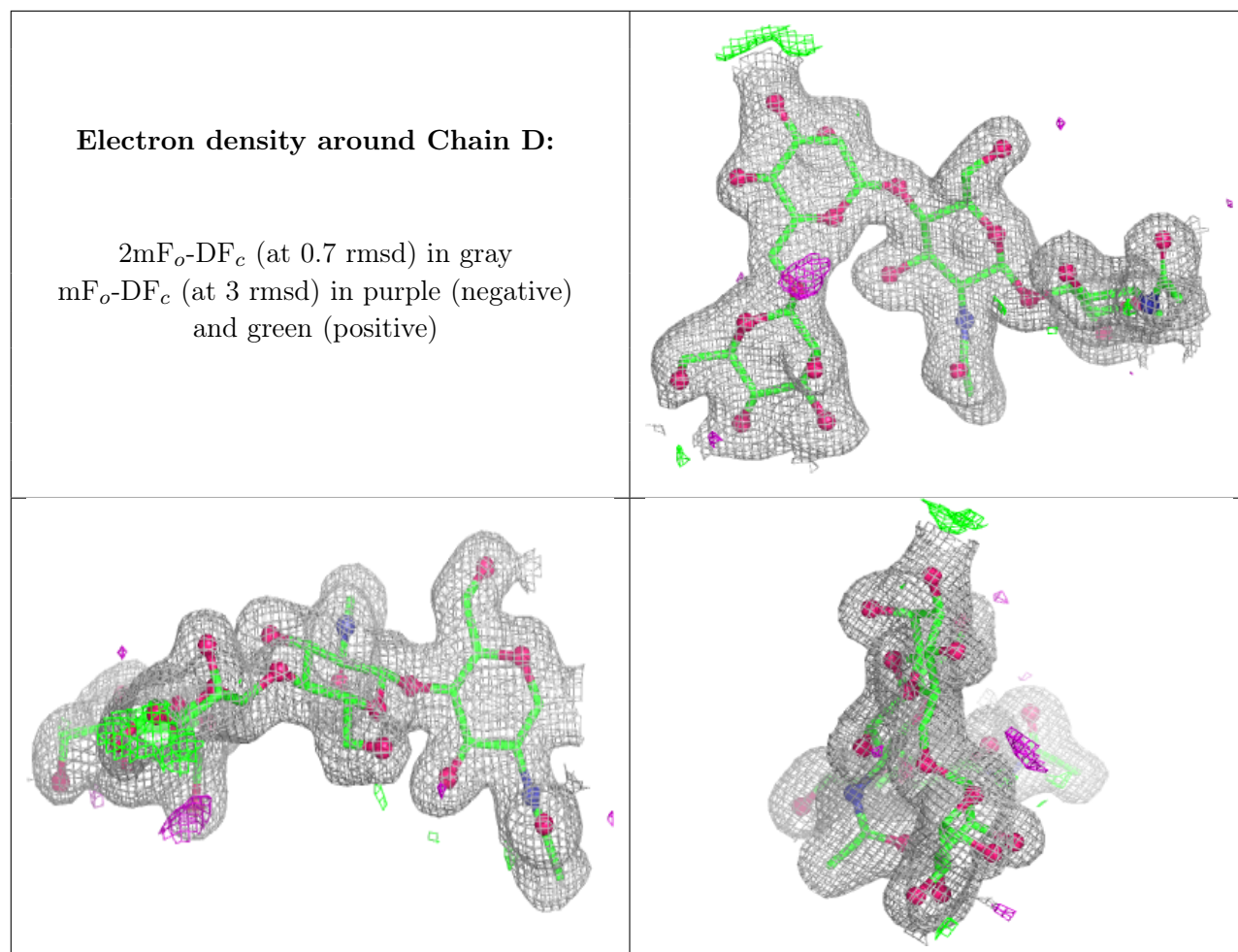
6.3 Carbohydrates [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 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	BMA	C	3	11/12	0.88	0.10	35,41,43,46	0
2	MAN	C	4	11/12	0.88	0.12	31,39,48,57	0
2	NAG	C	2	14/15	0.90	0.10	25,32,38,39	0
2	MAN	D	4	11/12	0.91	0.10	33,37,47,48	0
2	BMA	D	3	11/12	0.93	0.10	32,36,42,47	0
2	NAG	D	2	14/15	0.94	0.08	25,27,33,35	0
2	NAG	D	1	14/15	0.95	0.07	20,22,24,25	0
2	NAG	C	1	14/15	0.96	0.07	25,28,32,32	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($\text{\AA}^2$)	Q<0.9
3	BR	B	504	1/1	0.69	0.25	64,64,64,64	1
3	BR	B	506	1/1	0.76	0.19	113,113,113,113	1
3	BR	A	503	1/1	0.77	0.23	103,103,103,103	1
3	BR	B	503	1/1	0.82	0.21	86,86,86,86	1
3	BR	A	504	1/1	0.85	0.22	81,81,81,81	0
3	BR	A	501	1/1	0.87	0.16	82,82,82,82	0
3	BR	B	505	1/1	0.88	0.17	79,79,79,79	0
3	BR	A	506	1/1	0.89	0.25	89,89,89,89	1
3	BR	A	502	1/1	0.90	0.15	81,81,81,81	0
3	BR	B	509	1/1	0.91	0.17	71,71,71,71	1
3	BR	B	510	1/1	0.91	0.15	45,45,45,45	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
3	BR	B	518	1/1	0.91	0.13	46,46,46,46	1
3	BR	B	514	1/1	0.92	0.16	64,64,64,64	1
3	BR	B	511	1/1	0.93	0.20	68,68,68,68	0
3	BR	B	512	1/1	0.93	0.14	56,56,56,56	1
3	BR	A	505	1/1	0.93	0.19	48,48,48,48	1
3	BR	B	508	1/1	0.93	0.22	70,70,70,70	0
3	BR	B	502	1/1	0.94	0.16	81,81,81,81	0
3	BR	B	515	1/1	0.94	0.17	53,53,53,53	1
3	BR	B	516	1/1	0.94	0.18	57,57,57,57	0
3	BR	B	517	1/1	0.94	0.11	42,42,42,42	1
3	BR	B	513	1/1	0.94	0.19	69,69,69,69	1
4	SO4	B	501	5/5	0.94	0.13	22,36,37,38	0
3	BR	B	507	1/1	0.96	0.12	47,47,47,47	0

6.5 Other polymers [i](#)

There are no such residues in this entry.