



wwPDB X-ray Structure Validation Summary Report ⓘ

Mar 5, 2026 – 06:48 PM UTC

PDB ID : 8B3B / pdb_00008b3b
Title : Structure of metacyclic VSG (mVSG) 531 from Trypanosoma brucei
Authors : Chandra, M.; Stebbins, C.E.
Deposited on : 2022-09-16
Resolution : 1.95 Å(reported)

This is a wwPDB X-ray Structure Validation Summary 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

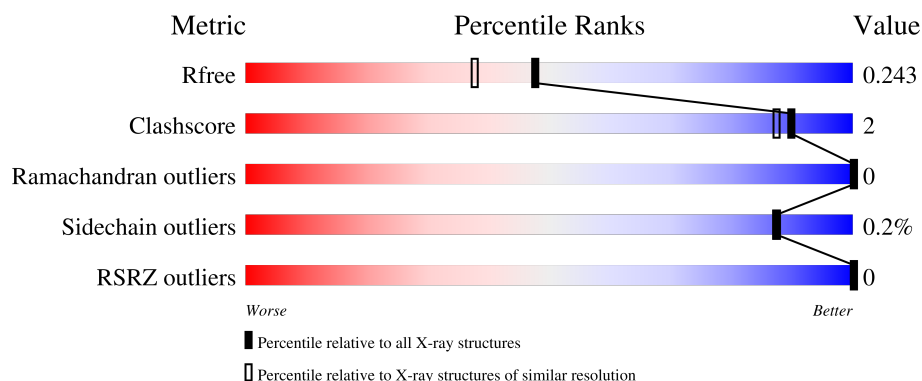
1 Overall quality at a glance ⓘ

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.95 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.



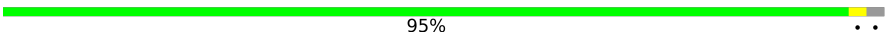
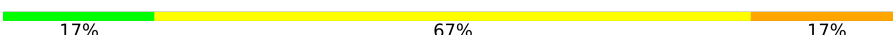
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	1452 (1.94-1.94)
Clashscore	190562	1494 (1.94-1.94)
Ramachandran outliers	187476	1479 (1.94-1.94)
Sidechain outliers	187428	1479 (1.94-1.94)
RSRZ outliers	180081	1453 (1.94-1.94)

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	371	94%
1	C	371	91% 6%
2	D	372	93%
2	G	372	95%
2	H	372	93%

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Mol	Chain	Length	Quality of chain
3	B	370	
3	E	370	
3	F	370	
4	I	6	
4	J	6	

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	I	1	-	-	X	-

2 Entry composition [i](#)

There are 8 unique types of molecules in this entry. The entry contains 43346 atoms, of which 20655 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 531.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	362	Total	C	H	N	O	S	0	0	0
			5243	1639	2616	464	516	8			
1	C	360	Total	C	H	N	O	S	0	0	0
			5224	1633	2608	462	513	8			

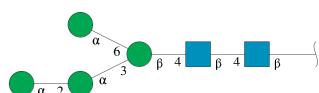
- Molecule 2 is a protein called Variant surface glycoprotein 531.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
2	D	361	Total	C	H	N	O	S	0	0	0
			5200	1632	2590	460	510	8			
2	G	363	Total	C	H	N	O	S	0	0	0
			5230	1639	2599	463	521	8			
2	H	362	Total	C	H	N	O	S	0	0	0
			5210	1634	2596	463	509	8			

- Molecule 3 is a protein called Variant surface glycoprotein 531.

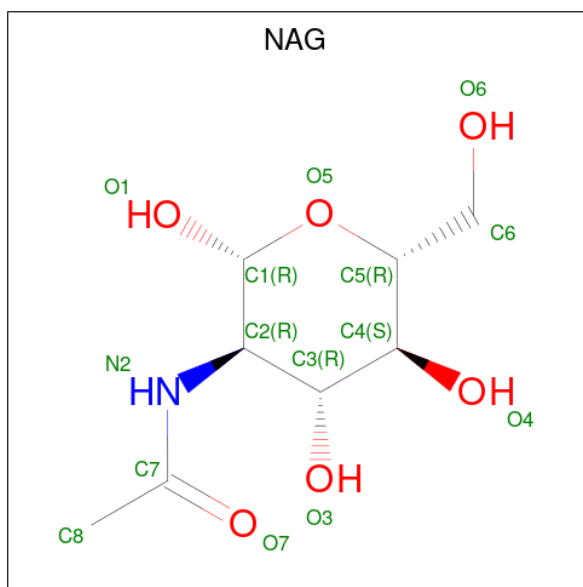
Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
3	B	360	Total	C	H	N	O	S	0	0	0
			5207	1630	2594	463	512	8			
3	E	361	Total	C	H	N	O	S	0	0	0
			5159	1621	2562	456	512	8			
3	F	337	Total	C	H	N	O	S	0	0	0
			4916	1543	2448	430	487	8			

- Molecule 4 is an oligosaccharide called alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-3)-[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
4	I	6	Total	C	H	N	O	0	0	0
			86	40	14	2	30			
4	J	6	Total	C	N	O		0	0	0
			72	40	2	30				

- Molecule 5 is 2-acetamido-2-deoxy-beta-D-glucopyranose (CCD ID: NAG) (formula: $C_8H_{15}NO_6$).



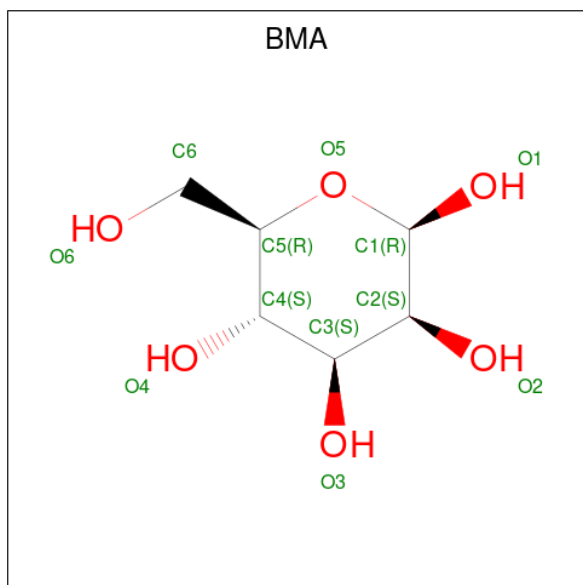
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
5	C	1	Total	C	N	O		0	0
			14	8	1	5			
5	C	1	Total	C	N	O		0	0
			14	8	1	5			
5	D	1	Total	C	N	O		0	0
			14	8	1	5			
5	D	1	Total	C	N	O		0	0
			14	8	1	5			
5	B	1	Total	C	N	O		0	0
			14	8	1	5			
5	B	1	Total	C	N	O		0	0
			14	8	1	5			
5	E	1	Total	C	N	O		0	0
			14	8	1	5			
5	E	1	Total	C	N	O		0	0
			14	8	1	5			
5	F	1	Total	C	N	O		0	0
			14	8	1	5			

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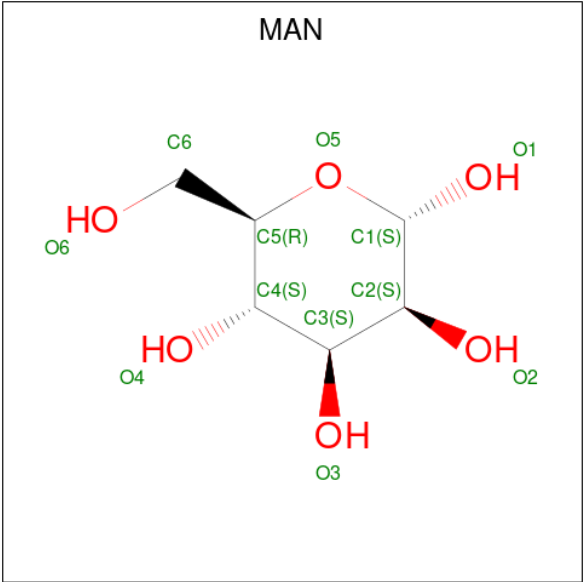
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
5	F	1	Total	C	N	O	0	0
			14	8	1	5		
5	H	1	Total	C	H	N	O	0
			28	8	14	1	5	
5	H	1	Total	C	H	N	O	0
			28	8	14	1	5	

- Molecule 6 is beta-D-mannopyranose (CCD ID: BMA) (formula: $C_6H_{12}O_6$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
6	C	1	Total	C	O	0	0
			11	6	5		
6	D	1	Total	C	O	0	0
			11	6	5		
6	B	1	Total	C	O	0	0
			11	6	5		
6	F	1	Total	C	O	0	0
			11	6	5		
6	H	1	Total	C	O	0	0
			11	6	5		

- Molecule 7 is alpha-D-mannopyranose (CCD ID: MAN) (formula: $C_6H_{12}O_6$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
7	C	1	Total	C	O	0	0
			11	6	5		
7	C	1	Total	C	O	0	0
			11	6	5		
7	C	1	Total	C	O	0	0
			11	6	5		
7	C	1	Total	C	O	0	0
			11	6	5		
7	D	1	Total	C	O	0	0
			11	6	5		
7	D	1	Total	C	O	0	0
			11	6	5		
7	D	1	Total	C	O	0	0
			11	6	5		
7	B	1	Total	C	O	0	0
			11	6	5		
7	B	1	Total	C	O	0	0
			11	6	5		
7	B	1	Total	C	O	0	0
			11	6	5		
7	E	1	Total	C	O	0	0
			11	6	5		
7	E	1	Total	C	O	0	0
			11	6	5		
7	E	1	Total	C	O	0	0
			11	6	5		
7	E	1	Total	C	O	0	0
			11	6	5		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
7	F	1	Total	C	O	0	0
			11	6	5		
7	F	1	Total	C	O	0	0
			11	6	5		
7	H	1	Total	C	O	0	0
			11	6	5		
7	H	1	Total	C	O	0	0
			11	6	5		
7	H	1	Total	C	O	0	0
			11	6	5		

- Molecule 8 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
8	A	204	Total	O	0	0
			204	204		
8	C	251	Total	O	0	0
			251	251		
8	D	209	Total	O	0	0
			209	209		
8	B	168	Total	O	0	0
			168	168		
8	G	137	Total	O	0	0
			137	137		
8	E	129	Total	O	0	0
			129	129		
8	F	109	Total	O	0	0
			109	109		
8	H	132	Total	O	0	0
			132	132		

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 531

Chain A:  94%

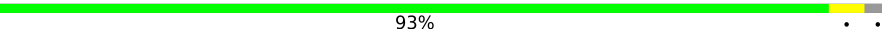


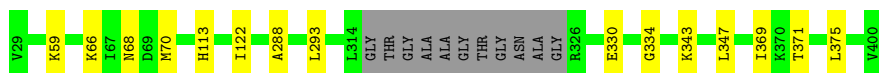
- Molecule 1: Variant surface glycoprotein 531

Chain C:  91% 6%

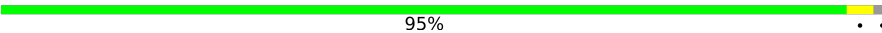


- Molecule 2: Variant surface glycoprotein 531

Chain D:  93%

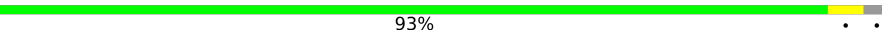


- Molecule 2: Variant surface glycoprotein 531

Chain G:  95%



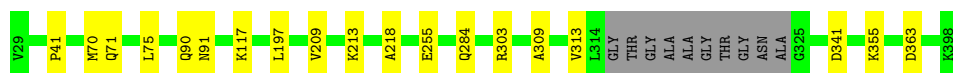
- Molecule 2: Variant surface glycoprotein 531

Chain H:  93%



- Molecule 3: Variant surface glycoprotein 531

Chain B:  92% 5%



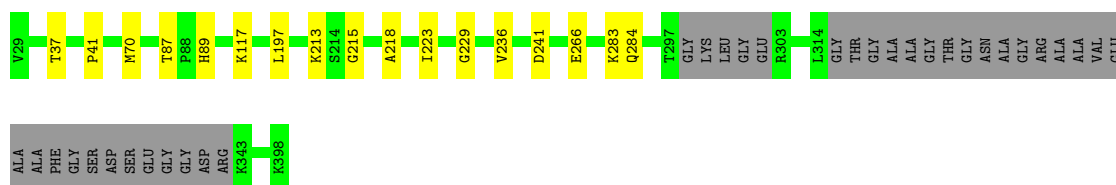
- Molecule 3: Variant surface glycoprotein 531

Chain E: 95%



- Molecule 3: Variant surface glycoprotein 531

Chain F: 86% 5% 9%



- Molecule 4: alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-6)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain I: 17% 67% 17%



- Molecule 4: alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-6)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain J: 17% 50% 33%



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	50.11Å 170.88Å 163.65Å 90.00° 90.71° 90.00°	Depositor
Resolution (Å)	59.09 – 1.95 59.09 – 1.95	Depositor EDS
% Data completeness (in resolution range)	97.7 (59.09-1.95) 97.7 (59.09-1.95)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.44 (at 1.95Å)	Xtriage
Refinement program	PHENIX 1.19-4092-0000	Depositor
R, R_{free}	0.200 , 0.238 0.212 , 0.243	Depositor DCC
R_{free} test set	9616 reflections (4.81%)	wwPDB-VP
Wilson B-factor (Å ²)	34.6	Xtriage
Anisotropy	0.504	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.35 , 33.5	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	0.013 for -h,-l,-k 0.009 for -h,l,k 0.095 for h,-k,-l	Xtriage
F_o, F_c correlation	0.97	EDS
Total number of atoms	43346	wwPDB-VP
Average B, all atoms (Å ²)	51.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.33% 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 [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: BMA, 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	0.22	0/2660	0.40	0/3593
1	C	0.23	1/2649 (0.0%)	0.43	0/3579
2	D	0.19	0/2643	0.39	0/3573
2	G	0.40	2/2663 (0.1%)	0.45	1/3596 (0.0%)
2	H	0.54	0/2646	0.91	3/3576 (0.1%)
3	B	0.18	0/2646	0.39	0/3576
3	E	0.24	1/2629 (0.0%)	0.42	0/3553
3	F	0.20	0/2499	0.38	0/3378
All	All	0.30	4/21035 (0.0%)	0.50	4/28424 (0.0%)

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
2	D	0	1
2	G	0	1
All	All	0	2

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	G	272	ALA	C-N	-14.70	1.15	1.33
2	G	273	GLU	C-O	-6.12	1.17	1.24
3	E	107	GLY	C-O	-6.09	1.16	1.23
1	C	375	LEU	C-O	-5.79	1.17	1.24

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	H	341	ASP	CA-CB-CG	5.49	118.09	112.60
2	H	366	LEU	CA-C-N	5.16	126.59	120.14
2	H	366	LEU	C-N-CA	5.16	126.59	120.14
2	G	273	GLU	O-C-N	-5.13	116.79	122.07

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	D	293	LEU	Peptide
2	G	273	GLU	Mainchain

5.2 Too-close contacts [i](#)

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	2627	2616	2614	14	0
1	C	2616	2608	2606	12	1
2	D	2610	2590	2589	9	0
2	G	2631	2599	2610	7	0
2	H	2614	2596	2601	12	0
3	B	2613	2594	2592	10	0
3	E	2597	2562	2559	6	0
3	F	2468	2448	2455	12	0
4	I	72	14	61	7	0
4	J	72	0	61	2	0
5	B	28	0	24	1	0
5	C	28	0	24	2	0
5	D	28	0	24	1	0
5	E	28	0	24	2	0
5	F	28	0	24	1	0
5	H	28	28	24	6	0
6	B	11	0	8	0	0
6	C	11	0	8	0	0
6	D	11	0	8	0	0
6	F	11	0	8	0	0
6	H	11	0	8	0	0
7	B	33	0	29	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
7	C	44	0	38	0	0
7	D	33	0	29	0	1
7	E	44	0	37	0	0
7	F	22	0	20	0	0
7	H	33	0	29	0	0
8	A	204	0	0	2	0
8	B	168	0	0	0	0
8	C	251	0	0	0	0
8	D	209	0	0	0	0
8	E	129	0	0	1	0
8	F	109	0	0	1	0
8	G	137	0	0	1	0
8	H	132	0	0	0	0
All	All	22691	20655	21114	78	1

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 2.

The worst 5 of 78 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:295:ASN:HD21	4:I:1:NAG:C1	1.03	1.64
2:H:295:ASN:HD21	5:H:501:NAG:C1	1.03	1.56
2:H:295:ASN:ND2	5:H:501:NAG:C1	1.72	1.51
1:A:295:ASN:ND2	4:I:1:NAG:C1	1.72	1.39
1:A:295:ASN:HD21	4:I:1:NAG:C2	1.70	1.05

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:336:ASP:OD1	7:D:506:MAN:O6[1_655]	1.99	0.21

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	358/371 (96%)	347 (97%)	11 (3%)	0	100	100
1	C	356/371 (96%)	344 (97%)	12 (3%)	0	100	100
2	D	357/372 (96%)	346 (97%)	11 (3%)	0	100	100
2	G	359/372 (96%)	349 (97%)	10 (3%)	0	100	100
2	H	356/372 (96%)	341 (96%)	15 (4%)	0	100	100
3	B	356/370 (96%)	344 (97%)	12 (3%)	0	100	100
3	E	357/370 (96%)	347 (97%)	10 (3%)	0	100	100
3	F	331/370 (90%)	321 (97%)	10 (3%)	0	100	100
All	All	2830/2968 (95%)	2739 (97%)	91 (3%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains ⓘ

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	256/270 (95%)	255 (100%)	1 (0%)	84	84
1	C	256/270 (95%)	254 (99%)	2 (1%)	73	71
2	D	252/271 (93%)	251 (100%)	1 (0%)	84	84
2	G	257/271 (95%)	257 (100%)	0	100	100
2	H	252/271 (93%)	251 (100%)	1 (0%)	84	84
3	B	254/270 (94%)	254 (100%)	0	100	100
3	E	249/270 (92%)	249 (100%)	0	100	100
3	F	245/270 (91%)	245 (100%)	0	100	100
All	All	2021/2163 (93%)	2016 (100%)	5 (0%)	87	87

All (5) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	342	ARG
1	C	375	LEU
1	C	397	LEU
2	D	113	HIS
2	H	29	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 21 such sidechains are listed below:

Mol	Chain	Res	Type
3	E	71	GLN
3	F	90	GLN
2	H	295	ASN
2	H	71	GLN
3	F	84	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 ⓘ

12 monosaccharides are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
4	NAG	I	1	4	14,14,15	0.43	0	17,19,21	1.78	5 (29%)
4	NAG	I	2	4	14,14,15	0.76	0	17,19,21	1.15	2 (11%)
4	BMA	I	3	4	11,11,12	0.57	0	15,15,17	1.69	1 (6%)
4	MAN	I	4	4	11,11,12	0.48	0	15,15,17	1.68	2 (13%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
4	MAN	I	5	4	11,11,12	0.38	0	15,15,17	0.64	0
4	MAN	I	6	4	11,11,12	0.43	0	15,15,17	1.38	3 (20%)
4	NAG	J	1	2,4	14,14,15	0.50	0	17,19,21	1.34	2 (11%)
4	NAG	J	2	4	14,14,15	0.59	0	17,19,21	1.48	1 (5%)
4	BMA	J	3	4	11,11,12	0.37	0	15,15,17	1.29	1 (6%)
4	MAN	J	4	4	11,11,12	0.49	0	15,15,17	1.42	3 (20%)
4	MAN	J	5	4	11,11,12	0.33	0	15,15,17	0.84	1 (6%)
4	MAN	J	6	4	11,11,12	0.49	0	15,15,17	0.87	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
4	NAG	I	1	4	-	0/6/23/26	0/1/1/1
4	NAG	I	2	4	-	2/6/23/26	0/1/1/1
4	BMA	I	3	4	-	0/2/19/22	0/1/1/1
4	MAN	I	4	4	-	0/2/19/22	0/1/1/1
4	MAN	I	5	4	-	0/2/19/22	0/1/1/1
4	MAN	I	6	4	-	0/2/19/22	0/1/1/1
4	NAG	J	1	2,4	-	0/6/23/26	0/1/1/1
4	NAG	J	2	4	-	0/6/23/26	0/1/1/1
4	BMA	J	3	4	-	0/2/19/22	0/1/1/1
4	MAN	J	4	4	-	0/2/19/22	0/1/1/1
4	MAN	J	5	4	-	0/2/19/22	0/1/1/1
4	MAN	J	6	4	-	0/2/19/22	0/1/1/1

There are no bond length outliers.

The worst 5 of 21 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	I	3	BMA	C1-O5-C5	5.49	119.55	112.19
4	J	2	NAG	C1-O5-C5	4.98	118.86	112.19
4	I	1	NAG	C1-O5-C5	4.18	117.79	112.19
4	J	3	BMA	C1-O5-C5	4.07	117.64	112.19
4	J	1	NAG	C1-O5-C5	3.93	117.45	112.19

There are no chirality outliers.

All (2) torsion outliers are listed below:

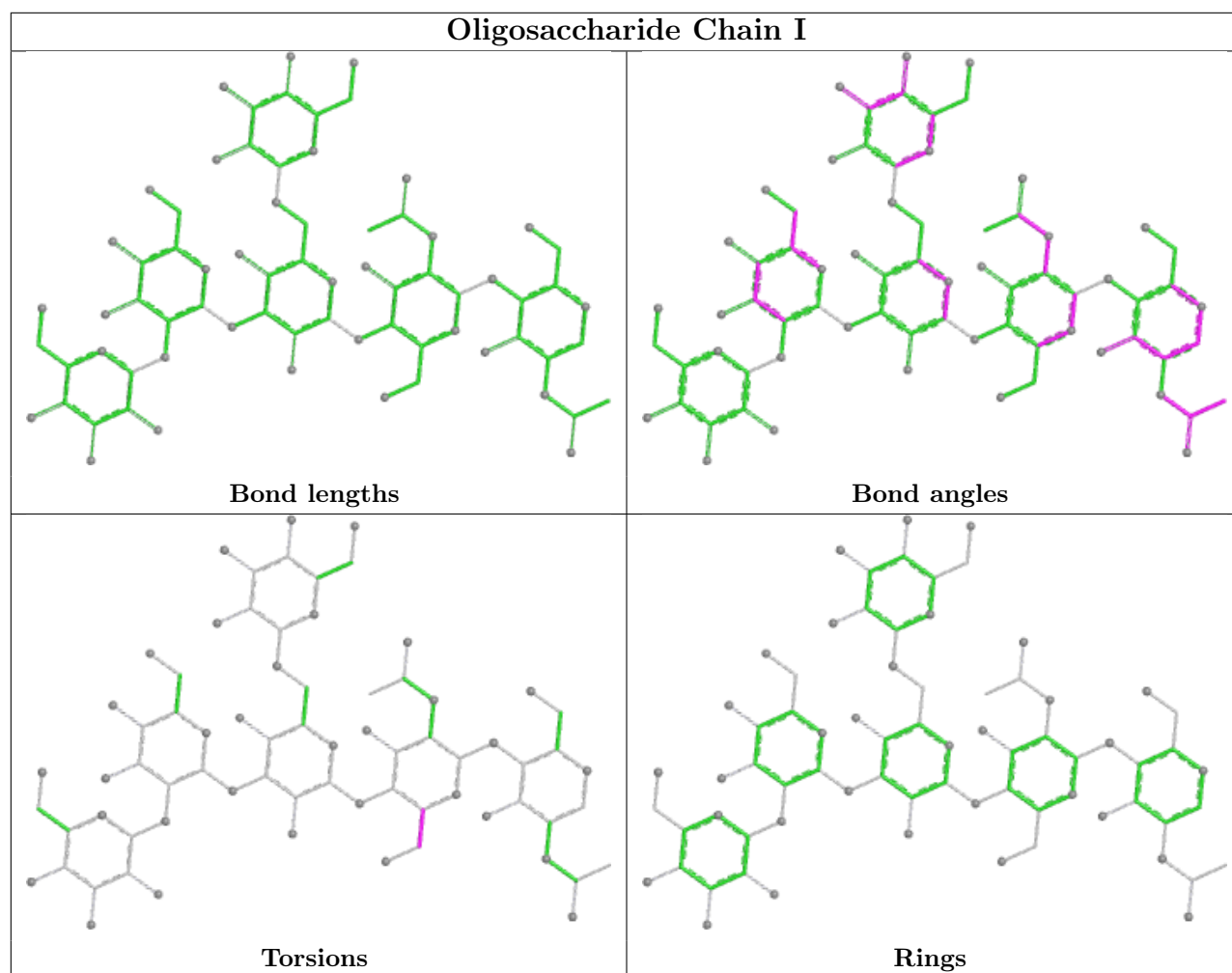
Mol	Chain	Res	Type	Atoms
4	I	2	NAG	C4-C5-C6-O6
4	I	2	NAG	O5-C5-C6-O6

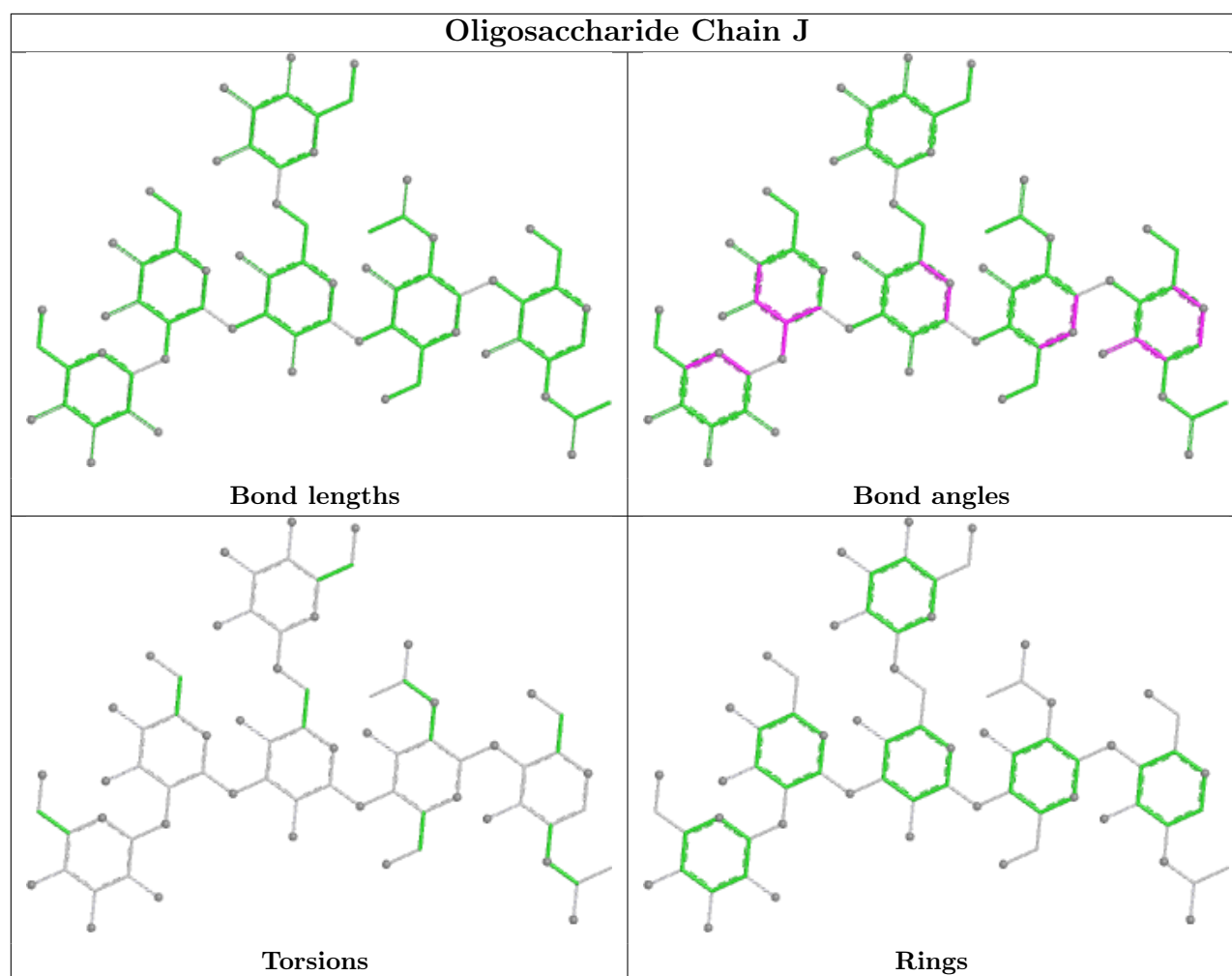
There are no ring outliers.

3 monomers are involved in 9 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	I	1	NAG	7	0
4	J	1	NAG	1	0
4	J	2	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](#)

36 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
7	MAN	C	403	7,6	11,11,12	0.54	0	15,15,17	1.67	5 (33%)
5	NAG	C	401	5,6	14,14,15	0.70	0	17,19,21	1.38	2 (11%)
5	NAG	B	402	5,6	14,14,15	0.73	0	17,19,21	1.47	2 (11%)
5	NAG	D	502	5,6	14,14,15	0.63	0	17,19,21	1.52	1 (5%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
7	MAN	H	506	6	11,11,12	0.39	0	15,15,17	0.66	0
7	MAN	E	403	5,7	11,11,12	0.52	0	15,15,17	1.52	2 (13%)
7	MAN	B	405	6	11,11,12	0.38	0	15,15,17	0.73	0
7	MAN	C	406	6	11,11,12	0.71	0	15,15,17	1.22	2 (13%)
7	MAN	H	504	7,6	11,11,12	0.48	0	15,15,17	1.10	1 (6%)
5	NAG	F	401	5,3	14,14,15	0.48	0	17,19,21	1.50	2 (11%)
7	MAN	F	404	6	11,11,12	0.26	0	15,15,17	0.89	0
5	NAG	E	401	5,3	14,14,15	0.63	0	17,19,21	1.60	2 (11%)
5	NAG	D	501	5,2	14,14,15	0.43	0	17,19,21	1.60	3 (17%)
7	MAN	H	505	7	11,11,12	0.40	0	15,15,17	0.69	0
6	BMA	B	403	5,7	11,11,12	0.44	0	15,15,17	1.56	1 (6%)
7	MAN	D	506	6	11,11,12	0.47	0	15,15,17	0.73	0
7	MAN	E	406	7	11,11,12	0.47	0	15,15,17	0.82	0
6	BMA	F	403	5,7	11,11,12	0.30	0	15,15,17	1.24	1 (6%)
7	MAN	C	405	7	11,11,12	0.18	0	15,15,17	0.79	0
7	MAN	D	505	7	11,11,12	0.28	0	15,15,17	0.71	0
6	BMA	C	402	5,7	11,11,12	0.54	0	15,15,17	1.34	1 (6%)
5	NAG	H	502	5,6	14,14,15	0.61	0	17,19,21	1.72	3 (17%)
7	MAN	C	404	7	11,11,12	0.51	0	15,15,17	0.92	0
5	NAG	H	501	5	14,14,15	0.46	0	17,19,21	1.69	3 (17%)
7	MAN	D	504	7,6	11,11,12	0.49	0	15,15,17	1.55	2 (13%)
5	NAG	F	402	5,6	14,14,15	0.58	0	17,19,21	1.61	2 (11%)
7	MAN	E	405	7	11,11,12	0.35	0	15,15,17	0.88	0
6	BMA	D	503	5,7	11,11,12	0.43	0	15,15,17	1.64	1 (6%)
5	NAG	E	402	5,7	14,14,15	0.84	0	17,19,21	2.51	5 (29%)
5	NAG	B	401	5,3	14,14,15	0.55	0	17,19,21	1.15	2 (11%)
7	MAN	E	404	7	11,11,12	0.31	0	15,15,17	1.24	2 (13%)
5	NAG	C	400	5,1	14,14,15	0.51	0	17,19,21	1.27	2 (11%)
7	MAN	B	404	7,6	11,11,12	0.36	0	15,15,17	1.45	3 (20%)
7	MAN	F	405	6	11,11,12	0.31	0	15,15,17	0.83	0
6	BMA	H	503	5,7	11,11,12	0.42	0	15,15,17	1.30	1 (6%)
7	MAN	B	406	7	11,11,12	0.33	0	15,15,17	0.96	1 (6%)

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	MAN	C	403	7,6	-	0/2/19/22	0/1/1/1
5	NAG	C	401	5,6	-	0/6/23/26	0/1/1/1
5	NAG	B	402	5,6	-	0/6/23/26	0/1/1/1
5	NAG	D	502	5,6	-	0/6/23/26	0/1/1/1
7	MAN	H	506	6	-	2/2/19/22	0/1/1/1
7	MAN	E	403	5,7	-	0/2/19/22	0/1/1/1
7	MAN	B	405	6	-	0/2/19/22	0/1/1/1
7	MAN	C	406	6	-	0/2/19/22	0/1/1/1
7	MAN	H	504	7,6	-	0/2/19/22	0/1/1/1
5	NAG	F	401	5,3	-	0/6/23/26	0/1/1/1
7	MAN	F	404	6	-	2/2/19/22	0/1/1/1
5	NAG	E	401	5,3	-	0/6/23/26	0/1/1/1
5	NAG	D	501	5,2	-	0/6/23/26	0/1/1/1
7	MAN	H	505	7	-	0/2/19/22	0/1/1/1
6	BMA	B	403	5,7	-	0/2/19/22	0/1/1/1
7	MAN	D	506	6	-	0/2/19/22	0/1/1/1
7	MAN	E	406	7	-	0/2/19/22	0/1/1/1
6	BMA	F	403	5,7	-	0/2/19/22	0/1/1/1
7	MAN	C	405	7	-	2/2/19/22	0/1/1/1
7	MAN	D	505	7	-	0/2/19/22	0/1/1/1
6	BMA	C	402	5,7	-	0/2/19/22	0/1/1/1
5	NAG	H	502	5,6	-	2/6/23/26	0/1/1/1
7	MAN	C	404	7	-	1/2/19/22	0/1/1/1
5	NAG	H	501	5	-	0/6/23/26	0/1/1/1
7	MAN	D	504	7,6	-	0/2/19/22	0/1/1/1
5	NAG	F	402	5,6	-	2/6/23/26	0/1/1/1
7	MAN	E	405	7	-	0/2/19/22	0/1/1/1
6	BMA	D	503	5,7	-	0/2/19/22	0/1/1/1
5	NAG	E	402	5,7	-	2/6/23/26	0/1/1/1
5	NAG	B	401	5,3	-	0/6/23/26	0/1/1/1
7	MAN	E	404	7	-	0/2/19/22	0/1/1/1
5	NAG	C	400	5,1	-	0/6/23/26	0/1/1/1
7	MAN	B	404	7,6	-	0/2/19/22	0/1/1/1
7	MAN	F	405	6	-	2/2/19/22	0/1/1/1
6	BMA	H	503	5,7	-	0/2/19/22	0/1/1/1
7	MAN	B	406	7	-	0/2/19/22	0/1/1/1

There are no bond length outliers.

The worst 5 of 52 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	E	402	NAG	O4-C4-C3	-6.11	95.98	110.38
5	E	402	NAG	C1-O5-C5	5.60	119.69	112.19
6	D	503	BMA	C1-O5-C5	5.41	119.43	112.19
6	B	403	BMA	C1-O5-C5	5.20	119.15	112.19
5	F	402	NAG	C1-O5-C5	5.16	119.09	112.19

There are no chirality outliers.

5 of 15 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
7	C	405	MAN	O5-C5-C6-O6
7	H	506	MAN	O5-C5-C6-O6
7	H	506	MAN	C4-C5-C6-O6
7	C	405	MAN	C4-C5-C6-O6
5	E	402	NAG	C4-C5-C6-O6

There are no ring outliers.

9 monomers are involved in 14 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	C	401	NAG	1	0
5	F	401	NAG	1	0
5	E	401	NAG	1	0
5	D	501	NAG	1	0
7	D	506	MAN	0	1
5	H	501	NAG	6	0
5	E	402	NAG	1	0
5	B	401	NAG	1	0
5	C	400	NAG	1	0

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
2	G	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	G	272:ALA	C	273:GLU	N	1.15

6 Fit of model and data [i](#)

6.1 Protein, DNA and RNA chains [i](#)

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	362/371 (97%)	-1.12	0 100 100	28, 42, 71, 94	0
1	C	360/371 (97%)	-1.16	0 100 100	25, 40, 67, 104	0
2	D	361/372 (97%)	-1.09	0 100 100	26, 42, 74, 97	0
2	G	363/372 (97%)	-0.96	0 100 100	30, 54, 75, 118	0
2	H	362/372 (97%)	-0.93	0 100 100	30, 57, 77, 97	0
3	B	360/370 (97%)	-1.10	0 100 100	30, 48, 74, 119	0
3	E	361/370 (97%)	-0.96	0 100 100	33, 56, 80, 113	0
3	F	337/370 (91%)	-0.89	0 100 100	30, 61, 83, 108	0
All	All	2866/2968 (96%)	-1.03	0 100 100	25, 51, 77, 119	0

There are no RSRZ outliers to report.

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.

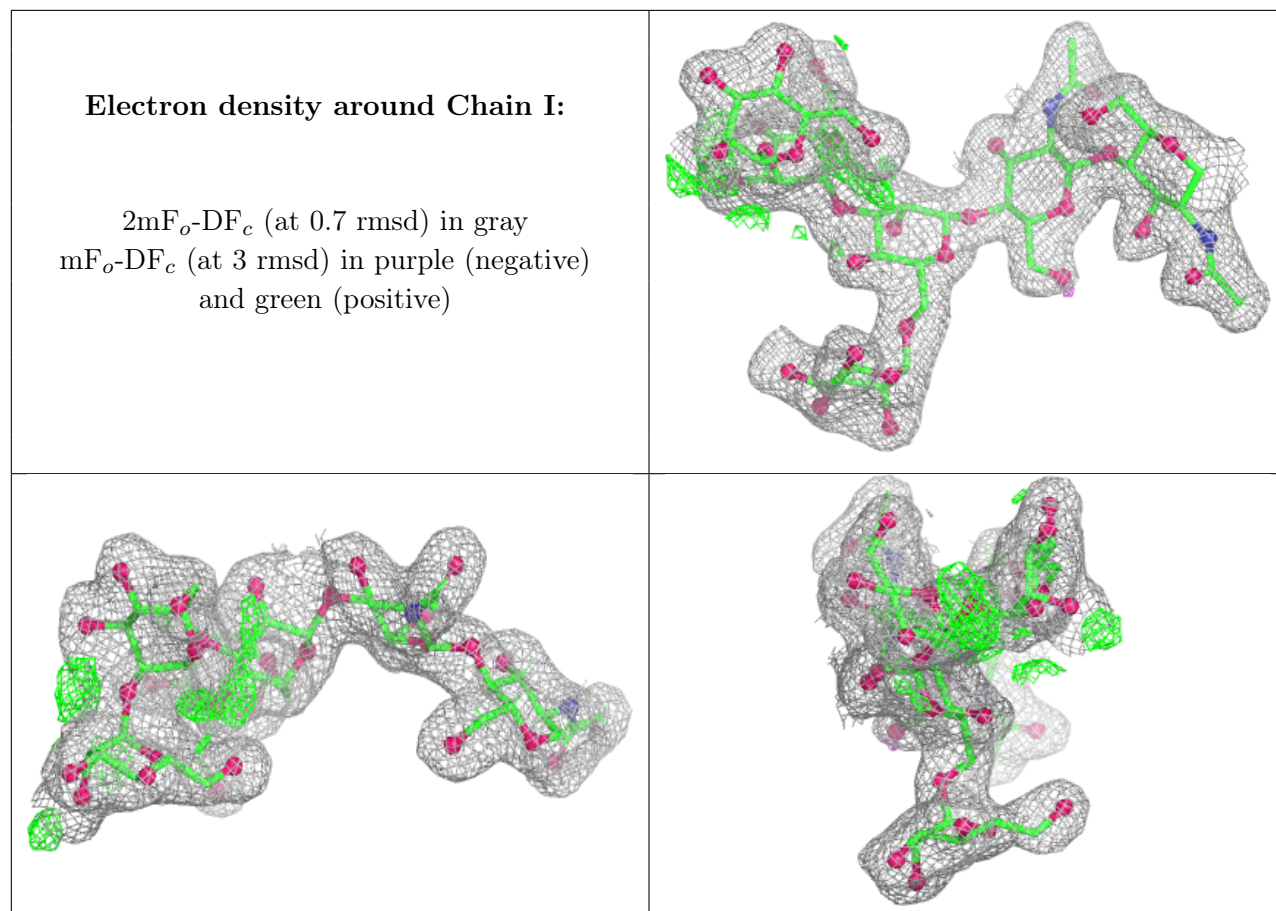
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
4	MAN	J	5	11/12	0.97	0.04	30,30,30,30	0
4	MAN	J	6	11/12	0.97	0.04	30,30,30,30	0
4	MAN	I	6	11/12	0.98	0.05	30,30,30,30	0

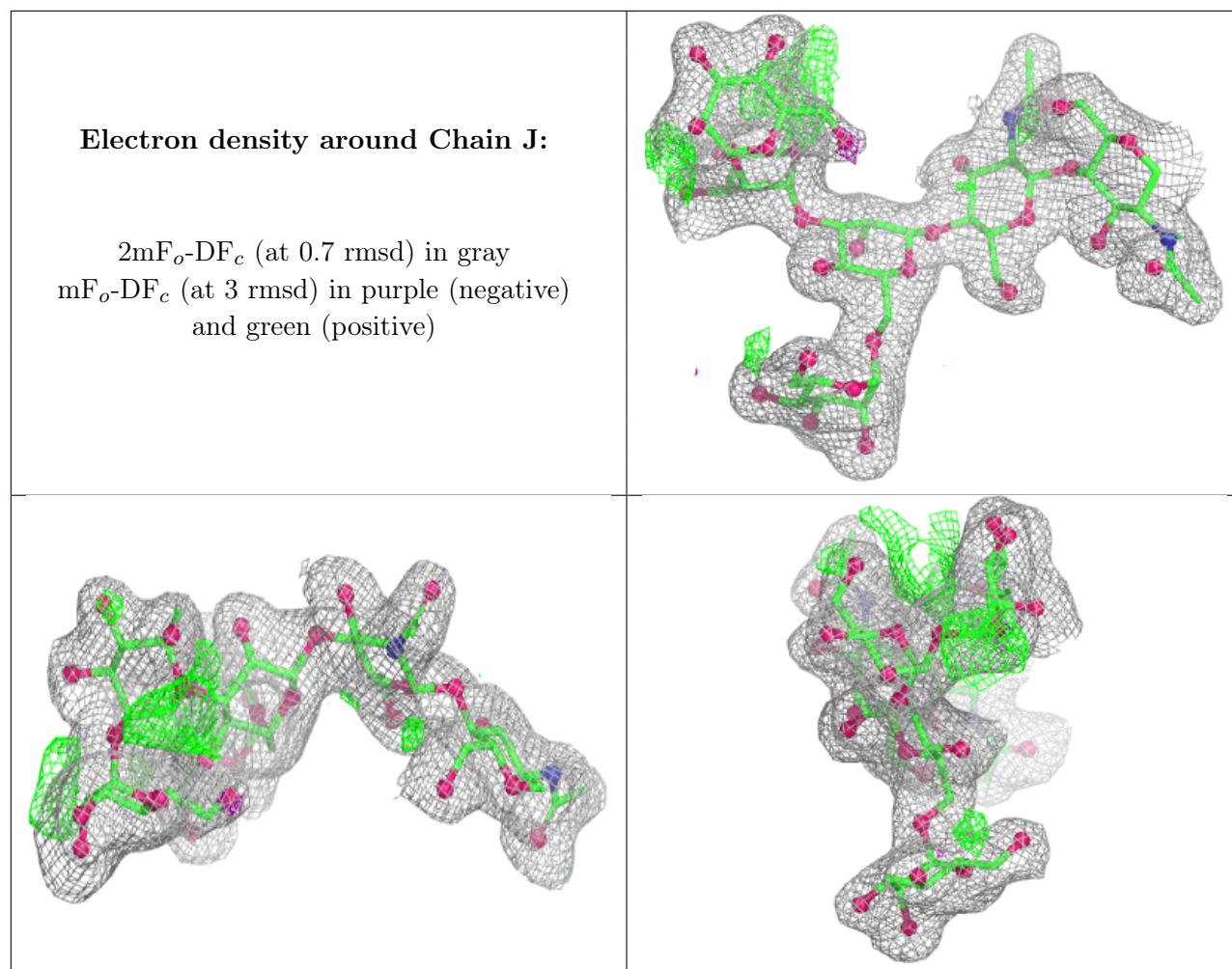
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
4	MAN	J	4	11/12	0.98	0.03	30,30,30,30	0
4	BMA	I	3	11/12	0.98	0.04	30,30,30,30	0
4	MAN	I	5	11/12	0.98	0.03	30,30,30,30	0
4	NAG	J	1	14/15	0.99	0.03	30,30,30,30	0
4	NAG	J	2	14/15	0.99	0.03	30,30,30,30	0
4	BMA	J	3	11/12	0.99	0.03	30,30,30,30	0
4	MAN	I	4	11/12	0.99	0.03	30,30,30,30	0
4	NAG	I	2	14/15	0.99	0.04	30,30,30,30	0
4	NAG	I	1	14/15	0.99	0.02	32,38,44,46	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
7	MAN	C	405	11/12	0.94	0.06	30,30,30,30	0
6	BMA	F	403	11/12	0.96	0.04	30,30,30,30	0
7	MAN	B	406	11/12	0.96	0.04	30,30,30,30	0
7	MAN	F	404	11/12	0.96	0.04	30,30,30,30	0
7	MAN	B	404	11/12	0.97	0.03	30,30,30,30	0
7	MAN	E	405	11/12	0.97	0.04	30,30,30,30	0
7	MAN	E	406	11/12	0.97	0.04	30,30,30,30	0
7	MAN	B	405	11/12	0.97	0.04	30,30,30,30	0
7	MAN	F	405	11/12	0.97	0.04	30,30,30,30	0
7	MAN	H	505	11/12	0.97	0.04	30,30,30,30	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
6	BMA	B	403	11/12	0.98	0.03	30,30,30,30	0
5	NAG	E	402	14/15	0.98	0.04	30,30,30,30	0
7	MAN	C	403	11/12	0.98	0.03	30,30,30,30	0
7	MAN	E	403	11/12	0.98	0.03	30,30,30,30	0
7	MAN	E	404	11/12	0.98	0.03	30,30,30,30	0
7	MAN	C	404	11/12	0.98	0.03	30,30,30,30	0
5	NAG	F	402	14/15	0.98	0.04	30,30,30,30	0
7	MAN	D	504	11/12	0.98	0.03	30,30,30,30	0
7	MAN	D	505	11/12	0.98	0.03	30,30,30,30	0
7	MAN	H	504	11/12	0.98	0.03	30,30,30,30	0
7	MAN	D	506	11/12	0.98	0.03	30,30,30,30	0
7	MAN	H	506	11/12	0.98	0.03	30,30,30,30	0
5	NAG	F	401	14/15	0.99	0.03	30,30,30,30	0
5	NAG	C	401	14/15	0.99	0.02	30,30,30,30	0
5	NAG	H	501	14/15	0.99	0.03	37,48,60,60	0
5	NAG	H	502	14/15	0.99	0.03	42,51,68,73	0
6	BMA	C	402	11/12	0.99	0.02	30,30,30,30	0
6	BMA	D	503	11/12	0.99	0.03	30,30,30,30	0
5	NAG	D	501	14/15	0.99	0.03	30,30,30,30	0
5	NAG	D	502	14/15	0.99	0.03	30,30,30,30	0
6	BMA	H	503	11/12	0.99	0.03	30,30,30,30	0
5	NAG	B	401	14/15	0.99	0.03	30,30,30,30	0
5	NAG	B	402	14/15	0.99	0.03	30,30,30,30	0
5	NAG	E	401	14/15	0.99	0.03	30,30,30,30	0
7	MAN	C	406	11/12	0.99	0.03	30,30,30,30	0
5	NAG	C	400	14/15	0.99	0.02	30,30,30,30	0

6.5 Other polymers [i](#)

There are no such residues in this entry.