



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 28, 2026 – 10:22 PM UTC

PDB ID : 7QU1 / pdb_00007qu1
Title : Machupo virus GP1 glycoprotein in complex with Fab fragment of antibody MAC1
Authors : Ng, W.M.; Sahin, M.; Krumm, S.A.; Seow, J.; Zeltina, A.; Harlos, K.; Paesen, G.; Pinschewer, D.D.; Doores, K.J.; Bowden, T.A.
Deposited on : 2022-01-17
Resolution : 1.91 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

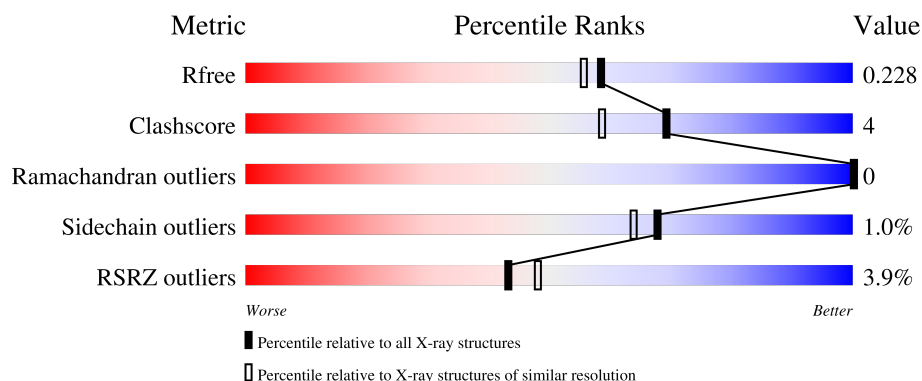
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.91 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	1188 (1.92-1.92)
Clashscore	190562	1209 (1.92-1.92)
Ramachandran outliers	187476	1195 (1.92-1.92)
Sidechain outliers	187428	1195 (1.92-1.92)
RSRZ outliers	180081	1188 (1.92-1.92)

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	234	4% 87% 8% 5%
2	B	217	2% 88% 11% .
3	C	182	5% 79% 5% 16%
4	D	9	56% 44%

2 Entry composition

There are 7 unique types of molecules in this entry. The entry contains 5149 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 Fab MAC1 heavy chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	222	Total	C	N	O	S	0	1	0
			1682	1064	280	331	7			

- Molecule 2 is a protein called Fab MAC1 light chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	215	Total	C	N	O	S	0	1	0
			1683	1042	288	347	6			

- Molecule 3 is a protein called Pre-glycoprotein polyprotein GP complex.

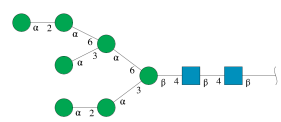
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	C	152	Total	C	N	O	S	0	0	0
			1219	772	204	229	14			

There are 11 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
C	258	GLY	-	expression tag	UNP Q6PXP4
C	259	THR	-	expression tag	UNP Q6PXP4
C	260	GLY	-	expression tag	UNP Q6PXP4
C	261	THR	-	expression tag	UNP Q6PXP4
C	262	LYS	-	expression tag	UNP Q6PXP4
C	263	HIS	-	expression tag	UNP Q6PXP4
C	264	HIS	-	expression tag	UNP Q6PXP4
C	265	HIS	-	expression tag	UNP Q6PXP4
C	266	HIS	-	expression tag	UNP Q6PXP4
C	267	HIS	-	expression tag	UNP Q6PXP4
C	268	HIS	-	expression tag	UNP Q6PXP4

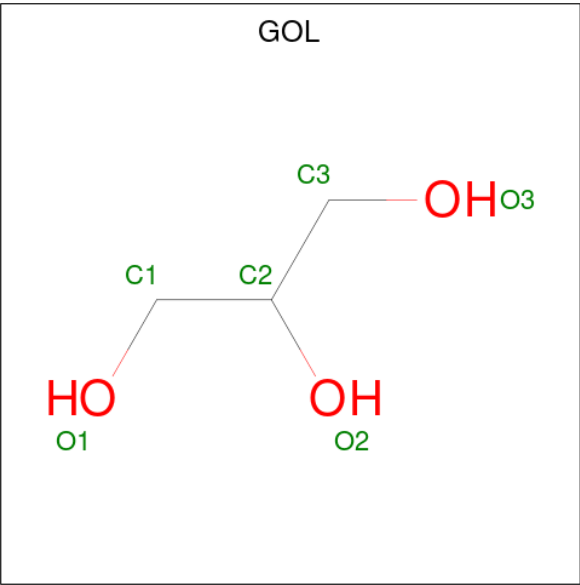
- Molecule 4 is an oligosaccharide called alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-6)-[alpha-D-mannopyranose-(1-3)]alpha-D-mannopyranose-(1-6)-[alpha-D-mannopyr

anose-(1-2)-alpha-D-mannopyranose-(1-3)]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	D	9	Total	C	N	O	0	0	0
			105	58	2	45			

- Molecule 5 is GLYCEROL (CCD ID: GOL) (formula: C₃H₈O₃).



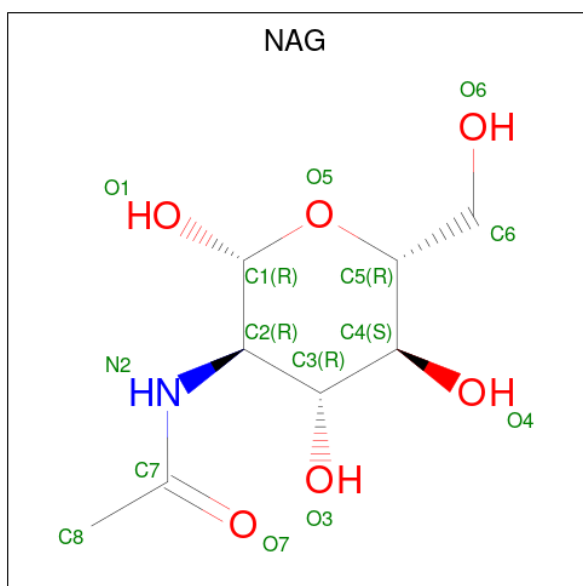
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	A	1	Total	C	O	0	0
			6	3	3		
5	A	1	Total	C	O	0	0
			6	3	3		
5	A	1	Total	C	O	0	0
			6	3	3		
5	A	1	Total	C	O	0	0
			6	3	3		
5	A	1	Total	C	O	0	0
			6	3	3		
5	A	1	Total	C	O	0	0
			6	3	3		
5	B	1	Total	C	O	0	0
			6	3	3		

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

- Molecule 6 is 2-acetamido-2-deoxy-beta-D-glucopyranose (CCD ID: NAG) (formula: $C_8H_{15}NO_6$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
6	C	1	Total	C	N	O	0	0
			14	8	1	5		
6	C	1	Total	C	N	O	0	0
			14	8	1	5		
6	C	1	Total	C	N	O	0	0
			14	8	1	5		

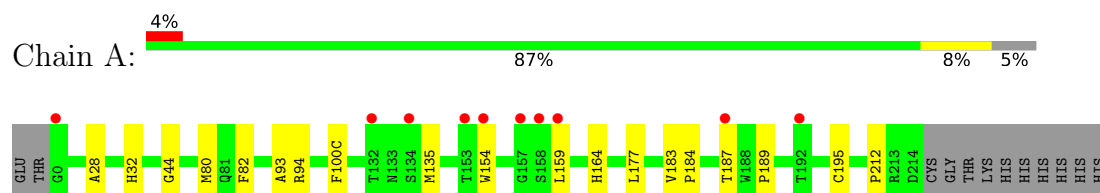
- Molecule 7 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	A	144	Total	O	0	0
			144	144		
7	B	146	Total	O	0	0
			146	146		
7	C	68	Total	O	0	0
			68	68		

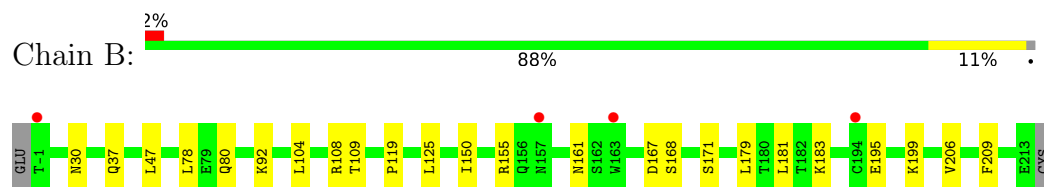
3 Residue-property plots [i](#)

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.

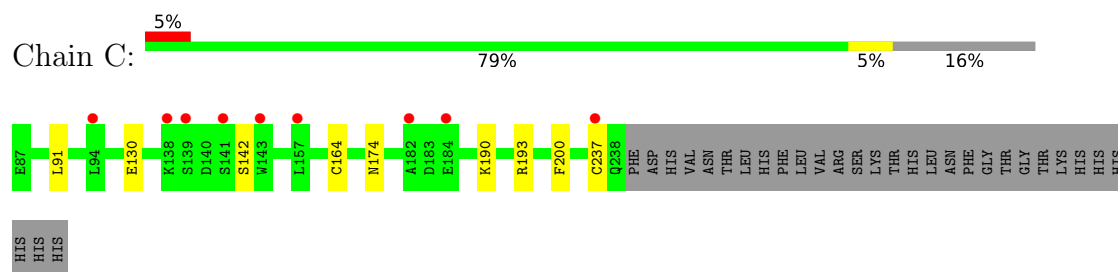
- Molecule 1: Fab MAC1 heavy chain



- Molecule 2: Fab MAC1 light chain



- Molecule 3: Pre-glycoprotein polyprotein GP complex



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



4 Data and refinement statistics

Property	Value	Source
Space group	I 2 2 2	Depositor
Cell constants a, b, c, α , β , γ	91.69Å 100.73Å 164.84Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	50.37 – 1.91 50.37 – 1.91	Depositor EDS
% Data completeness (in resolution range)	99.9 (50.37-1.91) 99.9 (50.37-1.91)	Depositor EDS
R_{merge}	0.12	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.35 (at 1.91Å)	Xtriage
Refinement program	PHENIX 1.19.2_4158	Depositor
R, R_{free}	0.194 , 0.229 0.194 , 0.228	Depositor DCC
R_{free} test set	3022 reflections (5.09%)	wwPDB-VP
Wilson B-factor (Å ²)	35.0	Xtriage
Anisotropy	0.396	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.37 , 48.6	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.34$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	5149	wwPDB-VP
Average B, all atoms (Å ²)	44.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.72% 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: GOL, 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	0.28	0/1731	0.46	0/2360
2	B	0.29	0/1716	0.51	0/2328
3	C	0.23	0/1249	0.41	0/1683
All	All	0.27	0/4696	0.47	0/6371

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 [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	1682	0	1628	11	0
2	B	1683	0	1620	14	0
3	C	1219	0	1160	7	0
4	D	105	0	88	0	0
5	A	36	0	48	3	0
5	B	24	0	32	5	0
6	C	42	0	39	0	0
7	A	144	0	0	0	0
7	B	146	0	0	1	0
7	C	68	0	0	0	0
All	All	5149	0	4615	33	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 (33) 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)
5:B:303:GOL:O2	7:B:401:HOH:O	2.08	0.72
1:A:28:ALA:HB3	5:A:304:GOL:H32	1.78	0.65
2:B:108:ARG:NH1	2:B:109:THR:O	2.31	0.63
1:A:32:HIS:NE2	5:A:304:GOL:H31	2.16	0.60
2:B:30[A]:ASN:OD1	2:B:92:LYS:HE3	2.06	0.55
3:C:130:GLU:H	3:C:130:GLU:CD	2.15	0.53
2:B:195:GLU:HG2	2:B:206:VAL:HG22	1.91	0.52
2:B:167:ASP:HB2	5:B:302:GOL:H11	1.90	0.52
1:A:189:PRO:HB3	1:A:212:PRO:HG3	1.90	0.52
2:B:37:GLN:HB2	2:B:47:LEU:HD11	1.92	0.51
1:A:154:TRP:CZ3	1:A:195:CYS:HB3	2.46	0.51
2:B:161:ASN:H	5:B:304:GOL:H31	1.76	0.50
1:A:184:PRO:HB2	1:A:187:THR:HG23	1.94	0.50
1:A:164:HIS:CE1	5:B:302:GOL:H12	2.47	0.50
1:A:164:HIS:ND1	5:B:302:GOL:H12	2.28	0.48
2:B:150:ILE:HD11	2:B:179:LEU:HD21	1.95	0.48
2:B:78:LEU:HD11	2:B:104:LEU:HD21	1.95	0.47
2:B:108:ARG:HD2	2:B:171:SER:HB2	1.97	0.47
1:A:44:GLY:H	5:A:305:GOL:H11	1.78	0.47
1:A:159:LEU:HD21	1:A:183:VAL:HG11	1.98	0.46
3:C:190:LYS:HE2	3:C:193:ARG:HH21	1.82	0.44
3:C:91:LEU:HB3	3:C:200:PHE:CE2	2.53	0.44
2:B:80:GLN:HG3	2:B:168:SER:O	2.18	0.44
3:C:164:CYS:HA	3:C:174:ASN:O	2.18	0.43
2:B:155:ARG:NH2	2:B:181:LEU:HD22	2.34	0.43
1:A:80:MET:HE3	1:A:82:PHE:CZ	2.54	0.42
2:B:119:PRO:HB3	2:B:209:PHE:CE2	2.55	0.42
3:C:190:LYS:NZ	3:C:193:ARG:HE	2.18	0.42
3:C:190:LYS:HA	3:C:190:LYS:HD3	1.72	0.41
1:A:93:ALA:HB1	1:A:100(C):PHE:HB3	2.03	0.41
3:C:130:GLU:CD	3:C:130:GLU:N	2.79	0.41
2:B:125:LEU:O	2:B:183:LYS:HD2	2.21	0.40
2:B:199:LYS:HE2	2:B:199:LYS:HB2	1.89	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	221/234 (94%)	216 (98%)	5 (2%)	0	100	100
2	B	214/217 (99%)	210 (98%)	4 (2%)	0	100	100
3	C	150/182 (82%)	145 (97%)	5 (3%)	0	100	100
All	All	585/633 (92%)	571 (98%)	14 (2%)	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	186/196 (95%)	183 (98%)	3 (2%)	55	44
2	B	194/195 (100%)	194 (100%)	0	100	100
3	C	137/165 (83%)	135 (98%)	2 (2%)	57	47
All	All	517/556 (93%)	512 (99%)	5 (1%)	68	64

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

Mol	Chain	Res	Type
1	A	94	ARG
1	A	135	MET
1	A	177	LEU
3	C	142	SER
3	C	237	CYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (6) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	39	GLN
2	B	38	GLN
2	B	80	GLN
2	B	189	HIS
3	C	176	GLN
3	C	219	GLN

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 ⓘ

9 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	D	1	3,4	14,14,15	0.37	0	17,19,21	0.51	0
4	NAG	D	2	4	14,14,15	0.44	0	17,19,21	0.43	0
4	BMA	D	3	4	11,11,12	0.76	0	15,15,17	0.71	0
4	MAN	D	4	4	11,11,12	0.80	0	15,15,17	1.06	1 (6%)
4	MAN	D	5	4	11,11,12	0.99	1 (9%)	15,15,17	1.12	1 (6%)
4	MAN	D	6	4	11,11,12	0.77	0	15,15,17	0.91	2 (13%)
4	MAN	D	7	4	11,11,12	0.81	0	15,15,17	0.79	0
4	MAN	D	8	4	11,11,12	0.82	0	15,15,17	0.97	0
4	MAN	D	9	4	11,11,12	0.73	0	15,15,17	0.85	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
4	NAG	D	1	3,4	-	0/6/23/26	0/1/1/1
4	NAG	D	2	4	-	0/6/23/26	0/1/1/1
4	BMA	D	3	4	-	0/2/19/22	0/1/1/1
4	MAN	D	4	4	-	0/2/19/22	0/1/1/1
4	MAN	D	5	4	-	0/2/19/22	0/1/1/1
4	MAN	D	6	4	-	0/2/19/22	0/1/1/1
4	MAN	D	7	4	-	0/2/19/22	0/1/1/1
4	MAN	D	8	4	-	0/2/19/22	0/1/1/1
4	MAN	D	9	4	-	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)
4	D	5	MAN	C2-C3	2.00	1.55	1.52

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	D	5	MAN	C1-O5-C5	3.61	117.02	112.19
4	D	4	MAN	C1-O5-C5	2.93	116.12	112.19
4	D	6	MAN	C1-O5-C5	2.27	115.22	112.19
4	D	6	MAN	O2-C2-C3	-2.18	105.64	110.15
4	D	9	MAN	C1-O5-C5	2.07	114.96	112.19

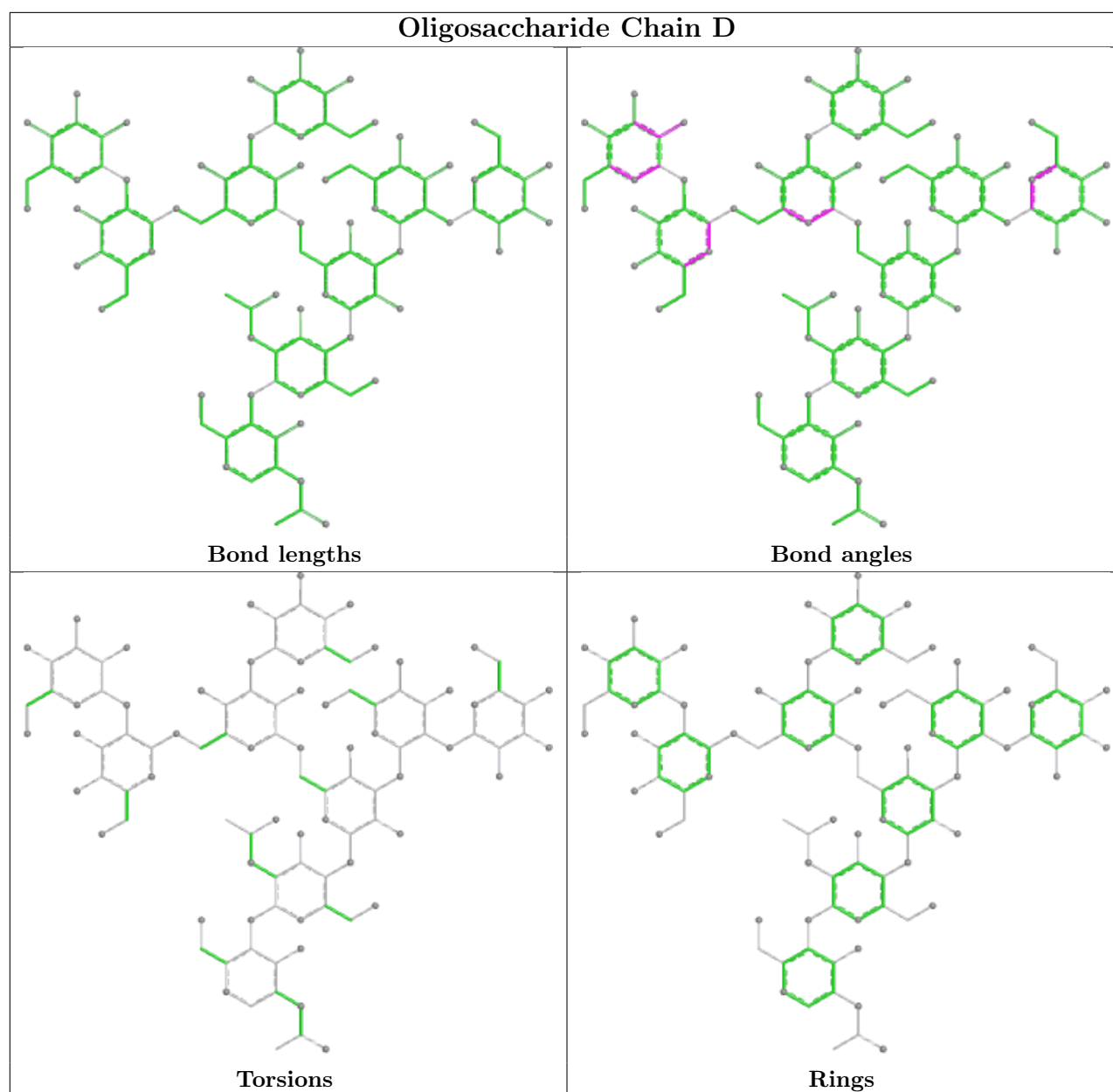
There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for oligosaccharide.



5.6 Ligand geometry [i](#)

13 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
5	GOL	A	306	-	5,5,5	0.92	0	5,5,5	0.96	0
5	GOL	B	304	-	5,5,5	0.99	0	5,5,5	1.00	0
5	GOL	A	301	-	5,5,5	0.98	0	5,5,5	0.98	0
6	NAG	C	303	3	14,14,15	0.34	0	17,19,21	0.52	0
5	GOL	A	304	-	5,5,5	0.77	0	5,5,5	1.06	0
5	GOL	A	302	-	5,5,5	0.92	0	5,5,5	1.15	0
6	NAG	C	302	3	14,14,15	0.36	0	17,19,21	0.69	1 (5%)
5	GOL	B	302	-	5,5,5	1.01	0	5,5,5	0.84	0
5	GOL	A	305	-	5,5,5	1.10	0	5,5,5	0.93	0
5	GOL	B	301	-	5,5,5	1.03	0	5,5,5	0.92	0
5	GOL	B	303	-	5,5,5	0.77	0	5,5,5	0.94	0
5	GOL	A	303	-	5,5,5	0.92	0	5,5,5	1.20	1 (20%)
6	NAG	C	301	3	14,14,15	0.45	0	17,19,21	0.65	1 (5%)

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
5	GOL	A	306	-	-	0/4/4/4	-
5	GOL	B	304	-	-	2/4/4/4	-
5	GOL	A	301	-	-	1/4/4/4	-
6	NAG	C	303	3	-	0/6/23/26	0/1/1/1
5	GOL	A	304	-	-	2/4/4/4	-
5	GOL	A	302	-	-	2/4/4/4	-
6	NAG	C	302	3	-	0/6/23/26	0/1/1/1
5	GOL	B	302	-	-	4/4/4/4	-
5	GOL	A	305	-	-	2/4/4/4	-
5	GOL	B	301	-	-	0/4/4/4	-
5	GOL	B	303	-	-	0/4/4/4	-
5	GOL	A	303	-	-	2/4/4/4	-
6	NAG	C	301	3	-	0/6/23/26	0/1/1/1

There are no bond length outliers.

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	A	303	GOL	C3-C2-C1	-2.29	103.40	111.80
6	C	301	NAG	C1-O5-C5	2.26	115.22	112.19

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	C	302	NAG	C1-O5-C5	2.25	115.20	112.19

There are no chirality outliers.

All (15) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	A	304	GOL	C1-C2-C3-O3
5	B	302	GOL	C1-C2-C3-O3
5	A	302	GOL	O1-C1-C2-C3
5	A	303	GOL	O1-C1-C2-C3
5	A	305	GOL	C1-C2-C3-O3
5	B	302	GOL	O1-C1-C2-C3
5	B	304	GOL	C1-C2-C3-O3
5	A	302	GOL	O1-C1-C2-O2
5	A	305	GOL	O2-C2-C3-O3
5	B	302	GOL	O1-C1-C2-O2
5	B	302	GOL	O2-C2-C3-O3
5	B	304	GOL	O2-C2-C3-O3
5	A	304	GOL	O2-C2-C3-O3
5	A	303	GOL	O1-C1-C2-O2
5	A	301	GOL	O2-C2-C3-O3

There are no ring outliers.

5 monomers are involved in 8 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	B	304	GOL	1	0
5	A	304	GOL	2	0
5	B	302	GOL	3	0
5	A	305	GOL	1	0
5	B	303	GOL	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, 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	222/234 (94%)	0.26	10 (4%) 38 43	17, 40, 72, 112	1 (0%)
2	B	215/217 (99%)	0.13	4 (1%) 66 73	17, 41, 54, 79	1 (0%)
3	C	152/182 (83%)	0.45	9 (5%) 28 32	30, 48, 79, 95	0
All	All	589/633 (93%)	0.26	23 (3%) 43 48	17, 41, 70, 112	2 (0%)

All (23) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	159	LEU	4.3
1	A	0	GLY	3.7
1	A	157	GLY	3.3
2	B	-1	THR	3.3
3	C	139	SER	3.1
3	C	184	GLU	3.0
1	A	158	SER	3.0
3	C	141	SER	3.0
1	A	132	THR	3.0
3	C	157	LEU	2.8
1	A	192	THR	2.6
2	B	194	CYS	2.6
1	A	134	SER	2.5
3	C	237	CYS	2.5
3	C	138	LYS	2.5
1	A	187	THR	2.4
3	C	182	ALA	2.3
2	B	163	TRP	2.3
3	C	94	LEU	2.3
1	A	153	THR	2.3
2	B	157	ASN	2.1
3	C	143	TRP	2.1
1	A	154	TRP	2.1

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

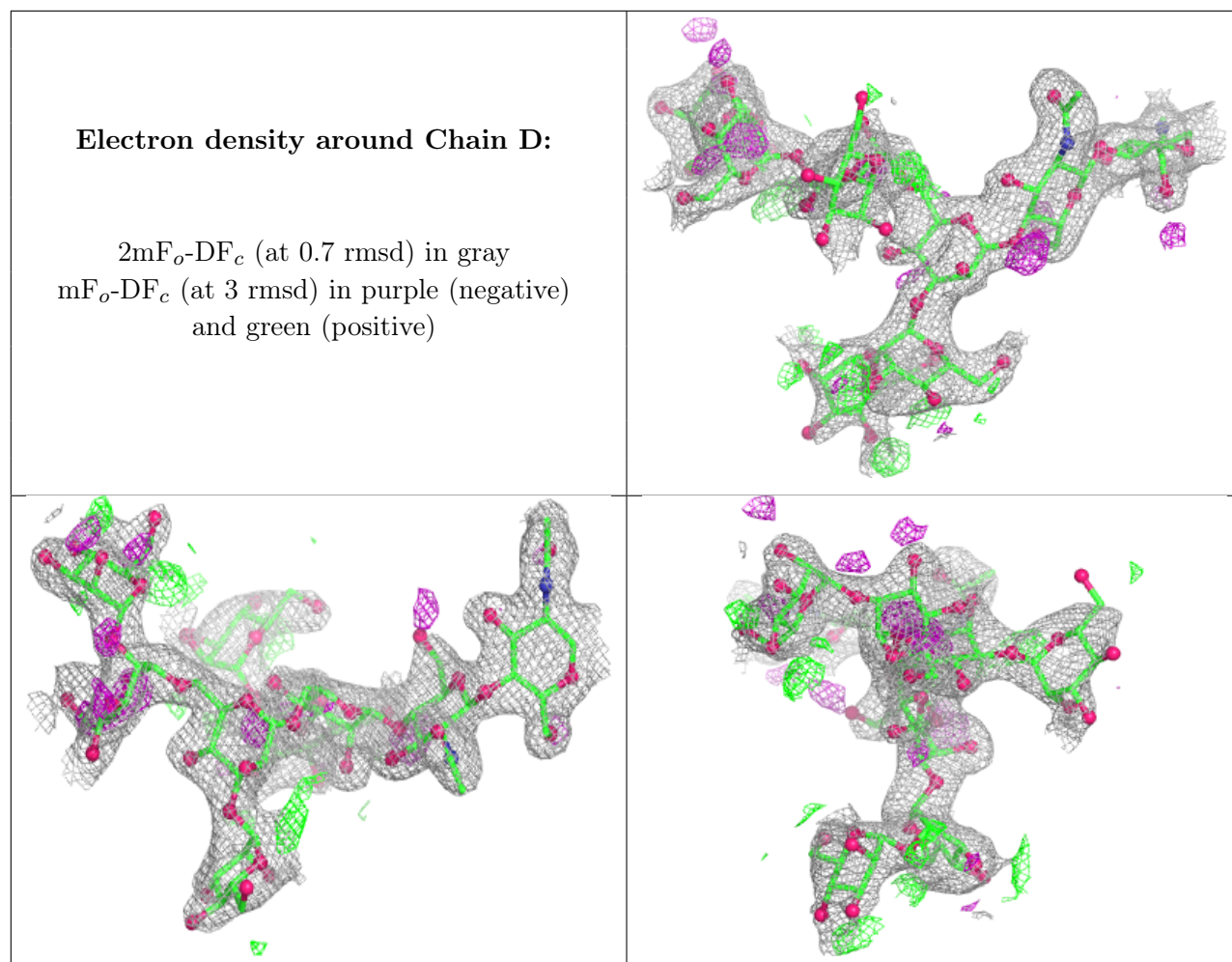
There are no non-standard protein/DNA/RNA residues in this entry.

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
4	MAN	D	9	11/12	0.38	0.17	93,113,121,124	0
4	MAN	D	7	11/12	0.42	0.15	93,103,105,107	0
4	MAN	D	8	11/12	0.75	0.14	60,69,82,90	0
4	MAN	D	4	11/12	0.77	0.11	72,79,87,91	0
4	MAN	D	6	11/12	0.81	0.15	53,64,78,89	0
4	MAN	D	5	11/12	0.81	0.14	58,67,71,72	0
4	BMA	D	3	11/12	0.87	0.10	60,67,71,73	0
4	NAG	D	2	14/15	0.88	0.11	49,55,58,63	0
4	NAG	D	1	14/15	0.93	0.08	42,46,51,51	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
5	GOL	A	302	6/6	0.70	0.15	53,59,69,70	0
5	GOL	A	303	6/6	0.71	0.19	49,60,74,76	0
5	GOL	B	304	6/6	0.71	0.18	63,74,77,78	0
6	NAG	C	303	14/15	0.74	0.15	61,77,86,92	0
5	GOL	A	305	6/6	0.77	0.17	42,57,60,68	0
5	GOL	B	301	6/6	0.77	0.18	42,48,61,65	0
5	GOL	B	303	6/6	0.82	0.15	59,60,66,72	0
5	GOL	B	302	6/6	0.83	0.13	44,54,58,59	0
5	GOL	A	304	6/6	0.85	0.15	54,56,64,67	0
6	NAG	C	302	14/15	0.90	0.09	44,51,57,61	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
5	GOL	A	306	6/6	0.91	0.11	41,58,63,70	0
6	NAG	C	301	14/15	0.91	0.09	59,64,76,79	0
5	GOL	A	301	6/6	0.94	0.09	35,41,44,48	0

6.5 Other polymers [i](#)

There are no such residues in this entry.