



Full wwPDB X-ray Structure Validation Report ⓘ

Aug 7, 2020 – 09:20 AM BST

PDB ID : 5LY9
Title : Structure of MITat 1.1
Authors : Schaefer, C.; Bartossek, T.; Jones, N.; Kuper, J.; Kisker, C.; Engstler, M.
Deposited on : 2016-09-26
Resolution : 1.65 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 following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity : 4.02b-467
Mogul : 1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix) : 1.13
EDS : 2.13.1
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac : 5.8.0158
CCP4 : 7.0.044 (Gargrove)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.13.1

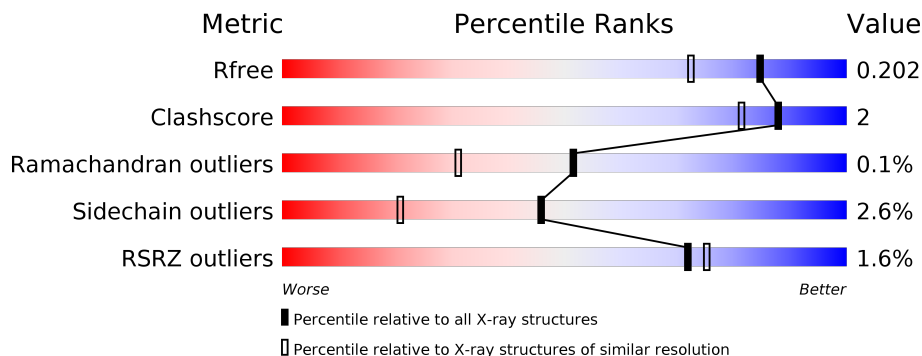
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.65 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	1827 (1.66-1.66)
Clashscore	141614	1931 (1.66-1.66)
Ramachandran outliers	138981	1891 (1.66-1.66)
Sidechain outliers	138945	1891 (1.66-1.66)
RSRZ outliers	127900	1791 (1.66-1.66)

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 on 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	368	<p>96%</p>
1	B	368	<p>92% 6% 2%</p>
2	C	5	<p>40% 60%</p>
3	D	5	<p>80% 20%</p>

2 Entry composition [i](#)

There are 6 unique types of molecules in this entry. The entry contains 6649 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.

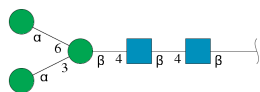
- Molecule 1 is a protein called Variant surface glycoprotein MITAT 1.1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	368	2797	1743	481	560	13	0	5	0
1	B	364	2757	1719	475	549	14	0	5	0

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	31	GLU	LYS	conflict	UNP P26331
A	65	LEU	SER	conflict	UNP P26331
B	31	GLU	LYS	conflict	UNP P26331
B	65	LEU	SER	conflict	UNP P26331

- Molecule 2 is an oligosaccharide called 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.



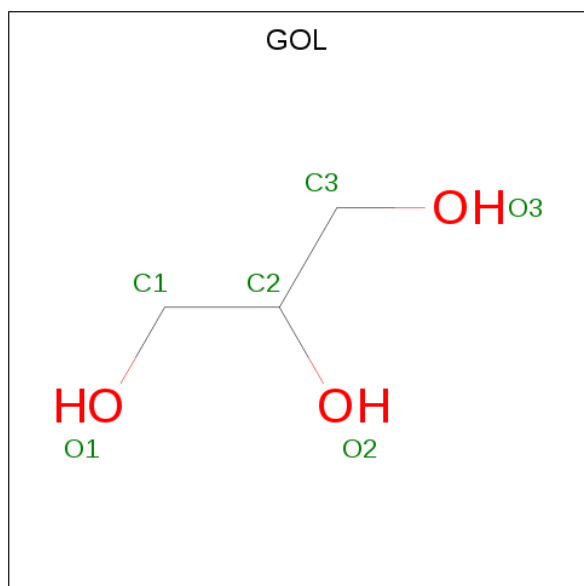
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
			Total	C	N	O			
2	C	5	61	34	2	25	0	0	0

- Molecule 3 is an oligosaccharide called 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.



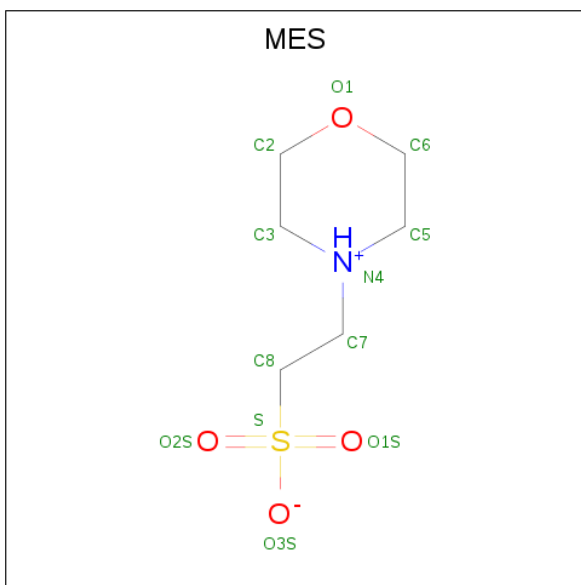
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
			Total	C	N	O			
3	D	5	61	34	2	25	0	0	0

- Molecule 4 is GLYCEROL (three-letter code: GOL) (formula: C₃H₈O₃).



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

- Molecule 5 is 2-(N-MORPHOLINO)-ETHANESULFONIC ACID (three-letter code: MES) (formula: C₆H₁₃NO₄S).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
			Total	C	N	O	S		
5	B	1	12	6	1	4	1	0	0

- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	484	Total	O	0	7
			491	491		
6	B	430	Total	O	0	4
			434	434		

3 Residue-property plots [i](#)

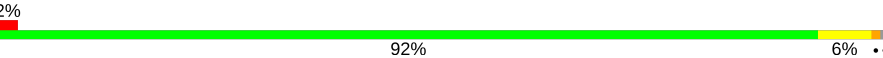
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. 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.

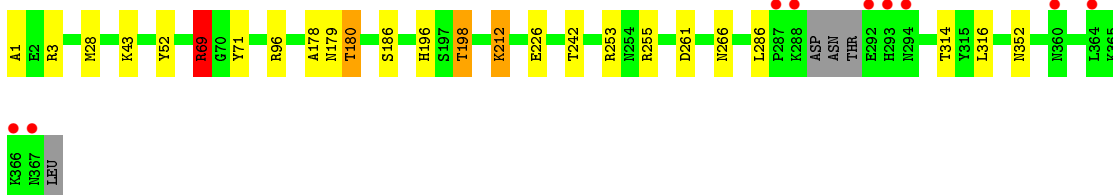
- Molecule 1: Variant surface glycoprotein MITAT 1.1

Chain A: 



- Molecule 1: Variant surface glycoprotein MITAT 1.1

Chain B: 




- Molecule 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

Chain C: 



- Molecule 3: 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

Chain D: 



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	78.51Å 95.04Å 103.75Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	47.52 – 1.65 47.52 – 1.65	Depositor EDS
% Data completeness (in resolution range)	99.6 (47.52-1.65) 99.6 (47.52-1.65)	Depositor EDS
R_{merge}	0.11	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.71 (at 1.65Å)	Xtrriage
Refinement program	REFMAC 5.8.0155	Depositor
R, R_{free}	0.165 , 0.205 0.172 , 0.202	Depositor DCC
R_{free} test set	4696 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å ²)	17.6	Xtrriage
Anisotropy	0.055	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 60.4	EDS
L-test for twinning ²	$\langle L \rangle = 0.47$, $\langle L^2 \rangle = 0.31$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
F_o, F_c correlation	0.97	EDS
Total number of atoms	6649	wwPDB-VP
Average B, all atoms (Å ²)	29.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.16% of the height of the origin peak. No significant pseudotranslation is detected.*

¹ Intensities estimated from amplitudes.

² Theoretical 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, MES, 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	0.98	3/2851 (0.1%)	0.95	7/3863 (0.2%)
1	B	0.99	2/2810 (0.1%)	0.95	4/3806 (0.1%)
All	All	0.98	5/5661 (0.1%)	0.95	11/7669 (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	B	0	1

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	69	ARG	CZ-NH1	6.59	1.41	1.33
1	A	104	SER	CB-OG	5.56	1.49	1.42
1	A	354	GLU	CG-CD	5.33	1.59	1.51
1	B	52	TYR	CG-CD2	-5.05	1.32	1.39
1	A	345	GLU	CD-OE2	5.00	1.31	1.25

All (11) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	141	ASP	CB-CG-OD2	-8.95	110.25	118.30
1	A	141	ASP	CB-CG-OD1	8.34	125.80	118.30
1	A	86[A]	MET	CG-SD-CE	7.08	111.53	100.20
1	A	86[B]	MET	CG-SD-CE	7.08	111.53	100.20
1	A	310	ASP	CB-CG-OD1	6.62	124.25	118.30
1	B	261	ASP	CB-CG-OD2	-6.38	112.56	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	69	ARG	NE-CZ-NH1	6.07	123.34	120.30
1	B	255	ARG	NE-CZ-NH2	-5.89	117.35	120.30
1	A	170	LEU	CB-CG-CD2	5.68	120.66	111.00
1	B	253	ARG	NE-CZ-NH1	-5.58	117.51	120.30
1	B	69	ARG	NE-CZ-NH2	5.05	122.82	120.30

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	B	69	ARG	Sidechain

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	2797	0	2841	7	0
1	B	2757	0	2792	16	0
2	C	61	0	52	0	0
3	D	61	0	52	1	0
4	A	18	0	24	0	0
4	B	18	0	24	0	0
5	B	12	0	13	0	0
6	A	491	0	0	8	0
6	B	434	0	0	7	0
All	All	6649	0	5798	23	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 2.

All (23) 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:71:TYR:CE2	6:A:1101:HOH:O	2.17	0.98
1:B:71:TYR:CE2	6:B:502:HOH:O	2.26	0.88

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:71:TYR:CZ	6:A:1101:HOH:O	2.29	0.84
1:A:266:ASN:OD1	6:A:1101:HOH:O	1.97	0.81
1:B:266:ASN:OD1	6:B:502:HOH:O	1.97	0.80
1:A:143:GLN:OE1	6:A:1102:HOH:O	2.09	0.69
1:B:71:TYR:CZ	6:B:502:HOH:O	2.46	0.68
1:A:71:TYR:OH	6:A:1101:HOH:O	2.01	0.62
1:A:71:TYR:HE2	6:A:1101:HOH:O	1.73	0.56
1:B:1:ALA:HB2	1:B:179:ASN:OD1	2.08	0.53
1:B:1:ALA:HB3	1:B:226:GLU:OE2	2.11	0.50
1:A:212[A]:LYS:NZ	6:A:1105:HOH:O	2.43	0.50
1:B:314:THR:HG23	6:B:647:HOH:O	2.13	0.49
6:A:1269:HOH:O	1:B:43:LYS:HD2	2.15	0.47
1:B:71:TYR:HE2	6:B:502:HOH:O	1.83	0.47
1:B:1:ALA:CB	1:B:226:GLU:OE2	2.63	0.46
1:B:212[A]:LYS:HD2	1:B:212[A]:LYS:HA	1.80	0.46
1:B:196:HIS:CE1	1:B:198:THR:HG23	2.50	0.46
1:B:180:THR:HG21	6:B:827:HOH:O	2.17	0.44
1:B:316:LEU:HD22	3:D:2:NAG:H82	2.00	0.44
1:B:180:THR:CG2	6:B:827:HOH:O	2.65	0.43
1:B:28:MET:HE2	1:B:28:MET:HA	2.02	0.41
1:B:178:ALA:HB3	1:B:180:THR:HG22	2.01	0.41

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	371/368 (101%)	360 (97%)	11 (3%)	0	100	100
1	B	365/368 (99%)	356 (98%)	8 (2%)	1 (0%)	41	22
All	All	736/736 (100%)	716 (97%)	19 (3%)	1 (0%)	51	31

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	186	SER

5.3.2 Protein sidechains [i](#)

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	299/294 (102%)	292 (98%)	7 (2%)	50	25
1	B	292/294 (99%)	282 (97%)	10 (3%)	37	12
All	All	591/588 (100%)	574 (97%)	17 (3%)	46	16

All (17) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	3	ARG
1	A	69	ARG
1	A	96	ARG
1	A	212[A]	LYS
1	A	212[B]	LYS
1	A	352	ASN
1	A	366	LYS
1	B	3	ARG
1	B	69	ARG
1	B	96	ARG
1	B	180	THR
1	B	198	THR
1	B	212[A]	LYS
1	B	212[B]	LYS
1	B	242	THR
1	B	286	LEU
1	B	352	ASN

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

Mol	Chain	Res	Type
1	A	171	GLN
1	A	294	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](#)

10 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	1,2	14,14,15	0.65	0	17,19,21	1.09	1 (5%)
2	NAG	C	2	2	14,14,15	1.01	1 (7%)	17,19,21	1.24	2 (11%)
2	BMA	C	3	2	11,11,12	0.22	0	15,15,17	0.77	0
2	MAN	C	4	2	11,11,12	0.80	0	15,15,17	2.00	5 (33%)
2	MAN	C	5	2	11,11,12	0.34	0	15,15,17	0.78	0
3	NAG	D	1	1,3	14,14,15	0.74	0	17,19,21	1.00	1 (5%)
3	NAG	D	2	3	14,14,15	0.72	0	17,19,21	1.45	3 (17%)
3	BMA	D	3	3	11,11,12	0.34	0	15,15,17	1.89	3 (20%)
3	MAN	D	4	3	11,11,12	0.51	0	15,15,17	1.54	2 (13%)
3	MAN	D	5	3	11,11,12	0.78	0	15,15,17	1.55	3 (20%)

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	1,2	-	0/6/23/26	0/1/1/1
2	NAG	C	2	2	-	0/6/23/26	0/1/1/1
2	BMA	C	3	2	-	0/2/19/22	0/1/1/1
2	MAN	C	4	2	-	2/2/19/22	0/1/1/1
2	MAN	C	5	2	-	0/2/19/22	0/1/1/1
3	NAG	D	1	1,3	-	0/6/23/26	0/1/1/1
3	NAG	D	2	3	-	0/6/23/26	0/1/1/1
3	BMA	D	3	3	-	0/2/19/22	0/1/1/1
3	MAN	D	4	3	-	0/2/19/22	0/1/1/1
3	MAN	D	5	3	-	2/2/19/22	1/1/1/1

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	2	NAG	O4-C4	2.06	1.47	1.43

All (20) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	4	MAN	C1-O5-C5	5.13	119.14	112.19
3	D	3	BMA	C1-O5-C5	4.59	118.41	112.19
3	D	4	MAN	O2-C2-C3	-4.14	101.85	110.14
3	D	3	BMA	C3-C4-C5	3.74	116.91	110.24
3	D	2	NAG	C1-O5-C5	3.52	116.96	112.19
2	C	4	MAN	O3-C3-C2	-2.86	104.52	109.99
2	C	2	NAG	O4-C4-C5	2.81	116.27	109.30
3	D	5	MAN	O5-C5-C6	2.58	111.24	107.20
2	C	4	MAN	C3-C4-C5	2.57	114.82	110.24
2	C	4	MAN	C1-C2-C3	-2.52	106.57	109.67
3	D	2	NAG	O4-C4-C5	2.52	115.56	109.30
3	D	5	MAN	C2-C3-C4	-2.46	106.64	110.89
3	D	3	BMA	O3-C3-C4	-2.39	104.83	110.35
2	C	1	NAG	C4-C3-C2	-2.33	107.60	111.02
3	D	4	MAN	C1-C2-C3	2.25	112.44	109.67
3	D	2	NAG	C6-C5-C4	-2.25	107.74	113.00
3	D	1	NAG	C8-C7-N2	2.23	119.88	116.10
3	D	5	MAN	O2-C2-C1	2.09	113.43	109.15
2	C	2	NAG	C3-C4-C5	-2.03	106.61	110.24
2	C	4	MAN	O5-C5-C6	-2.00	104.07	107.20

There are no chirality outliers.

All (4) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	C	4	MAN	O5-C5-C6-O6
2	C	4	MAN	C4-C5-C6-O6
3	D	5	MAN	C4-C5-C6-O6
3	D	5	MAN	O5-C5-C6-O6

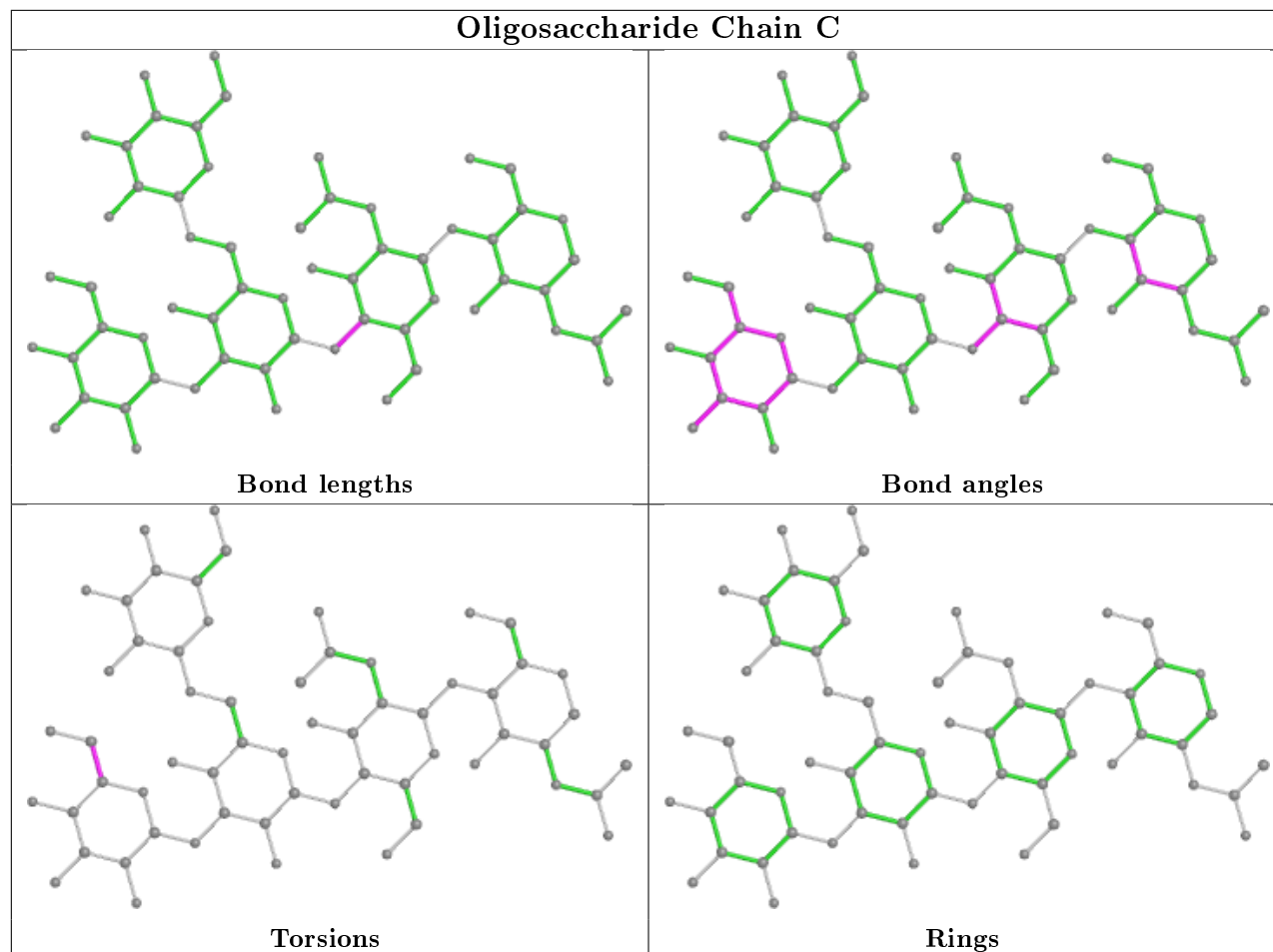
All (1) ring outliers are listed below:

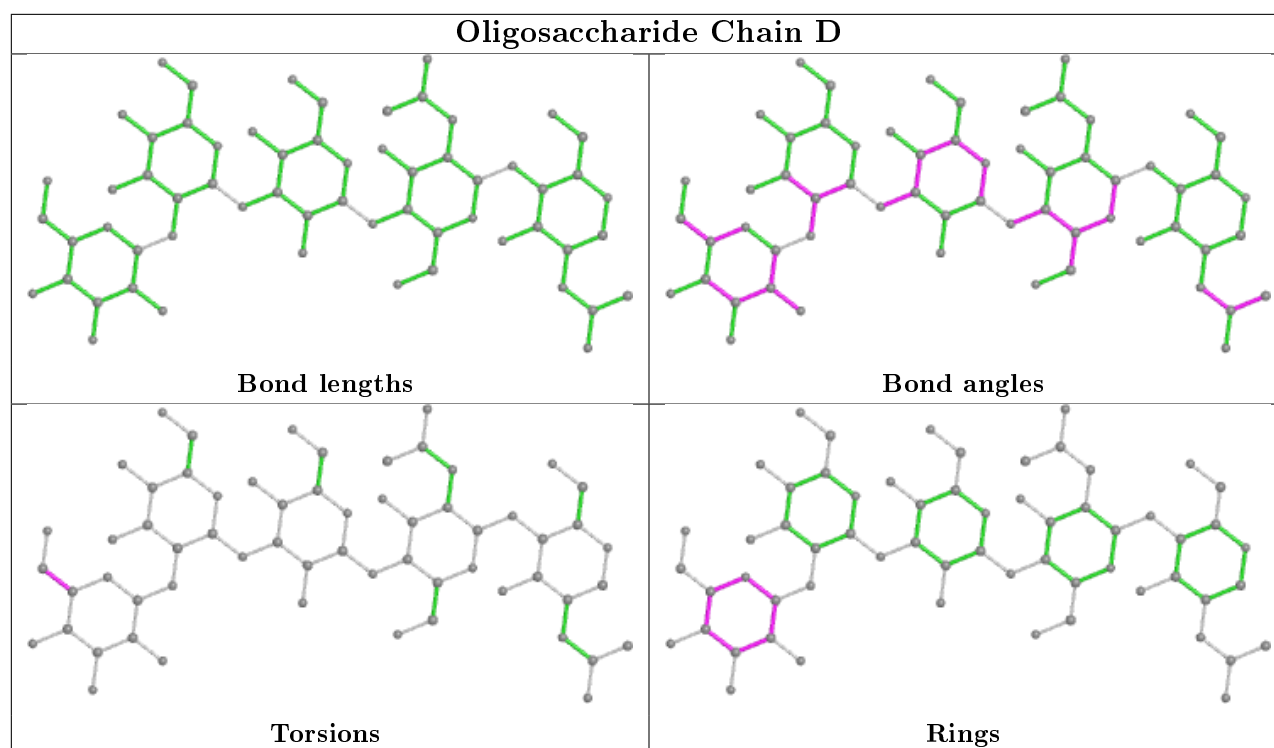
Mol	Chain	Res	Type	Atoms
3	D	5	MAN	C1-C2-C3-C4-C5-O5

1 monomer is involved in 1 short contact:

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

7 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$
4	GOL	B	408	-	5,5,5	0.22	0	5,5,5	0.33	0
4	GOL	B	407	-	5,5,5	0.49	0	5,5,5	0.71	0
4	GOL	A	408	-	5,5,5	0.76	0	5,5,5	1.26	1 (20%)
4	GOL	A	406	-	5,5,5	0.33	0	5,5,5	0.46	0
5	MES	B	409	-	12,12,12	1.72	1 (8%)	14,16,16	2.60	6 (42%)
4	GOL	B	406	-	5,5,5	0.41	0	5,5,5	1.46	1 (20%)
4	GOL	A	407	-	5,5,5	0.44	0	5,5,5	0.34	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	GOL	B	408	-	-	0/4/4/4	-
4	GOL	B	407	-	-	0/4/4/4	-
4	GOL	A	408	-	-	2/4/4/4	-
4	GOL	A	406	-	-	0/4/4/4	-
5	MES	B	409	-	-	2/6/14/14	0/1/1/1
4	GOL	B	406	-	-	3/4/4/4	-
4	GOL	A	407	-	-	0/4/4/4	-

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	B	409	MES	C8-S	-4.97	1.70	1.77

All (8) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	B	409	MES	O3S-S-C8	7.11	117.26	105.77
5	B	409	MES	O3S-S-O1S	-2.97	104.02	111.27
5	B	409	MES	C6-C5-N4	2.94	114.57	110.10
4	B	406	GOL	O1-C1-C2	-2.81	96.72	110.20
5	B	409	MES	C2-C3-N4	2.76	114.29	110.10
5	B	409	MES	O2S-S-C8	2.59	110.03	106.92
4	A	408	GOL	C3-C2-C1	-2.42	102.31	111.70
5	B	409	MES	C7-N4-C5	2.24	116.98	111.23

There are no chirality outliers.

All (7) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	A	408	GOL	C1-C2-C3-O3
4	A	408	GOL	O2-C2-C3-O3
5	B	409	MES	C8-C7-N4-C5
4	B	406	GOL	O1-C1-C2-O2
4	B	406	GOL	O1-C1-C2-C3
4	B	406	GOL	C1-C2-C3-O3
5	B	409	MES	C8-C7-N4-C3

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 [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	368/368 (100%)	-0.31	3 (0%) 86 88	18, 25, 38, 85	0
1	B	364/368 (98%)	-0.24	9 (2%) 57 58	18, 27, 43, 93	0
All	All	732/736 (99%)	-0.27	12 (1%) 72 75	18, 26, 42, 93	0

All (12) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	287	PRO	4.9
1	A	367	ASN	4.3
1	B	367	ASN	3.6
1	A	332	THR	3.6
1	B	293	HIS	3.5
1	B	288	LYS	3.5
1	A	368	LEU	3.3
1	B	364	LEU	2.7
1	B	292	GLU	2.2
1	B	366	LYS	2.2
1	B	360	ASN	2.1
1	B	294	ASN	2.1

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

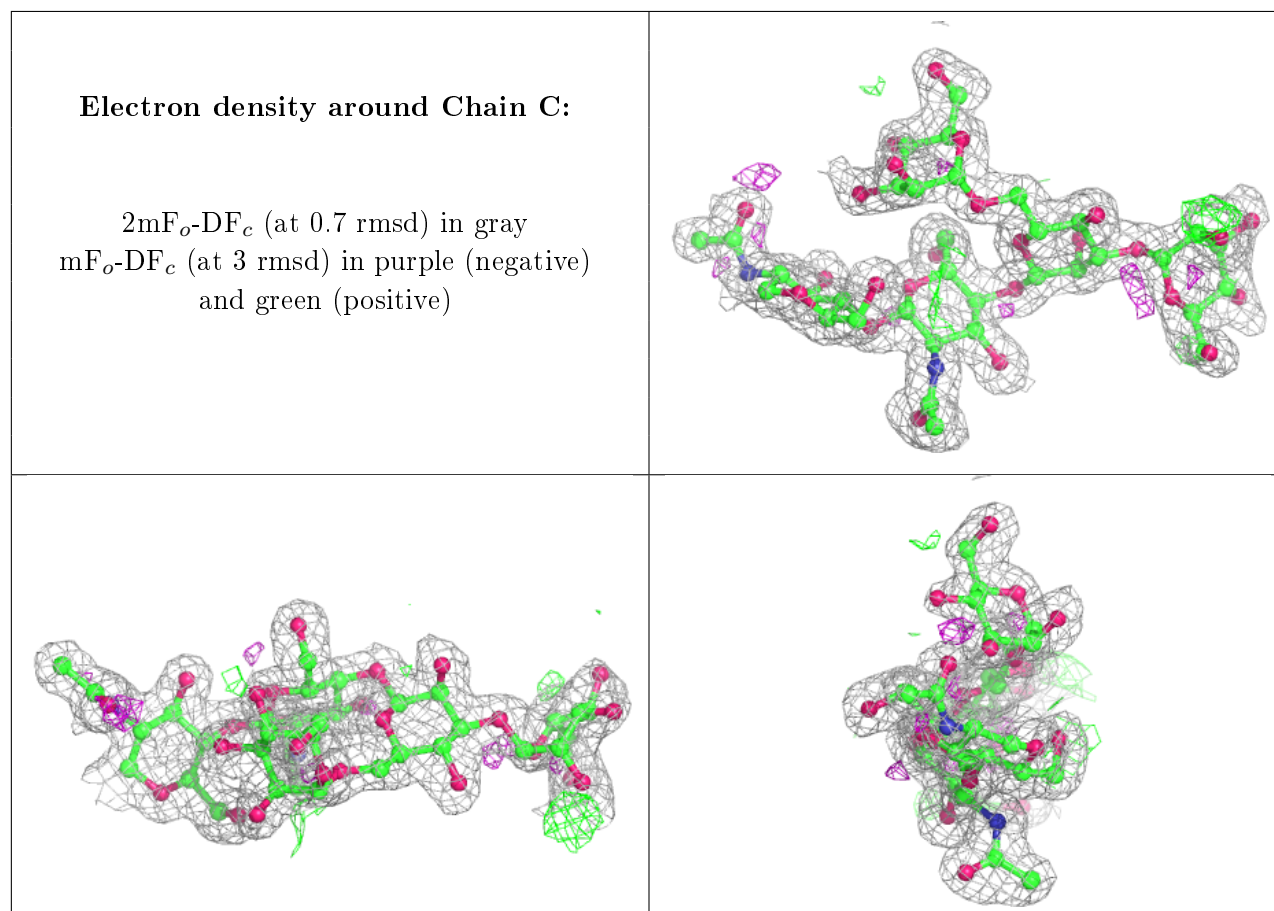
There are no non-standard protein/DNA/RNA residues in this entry.

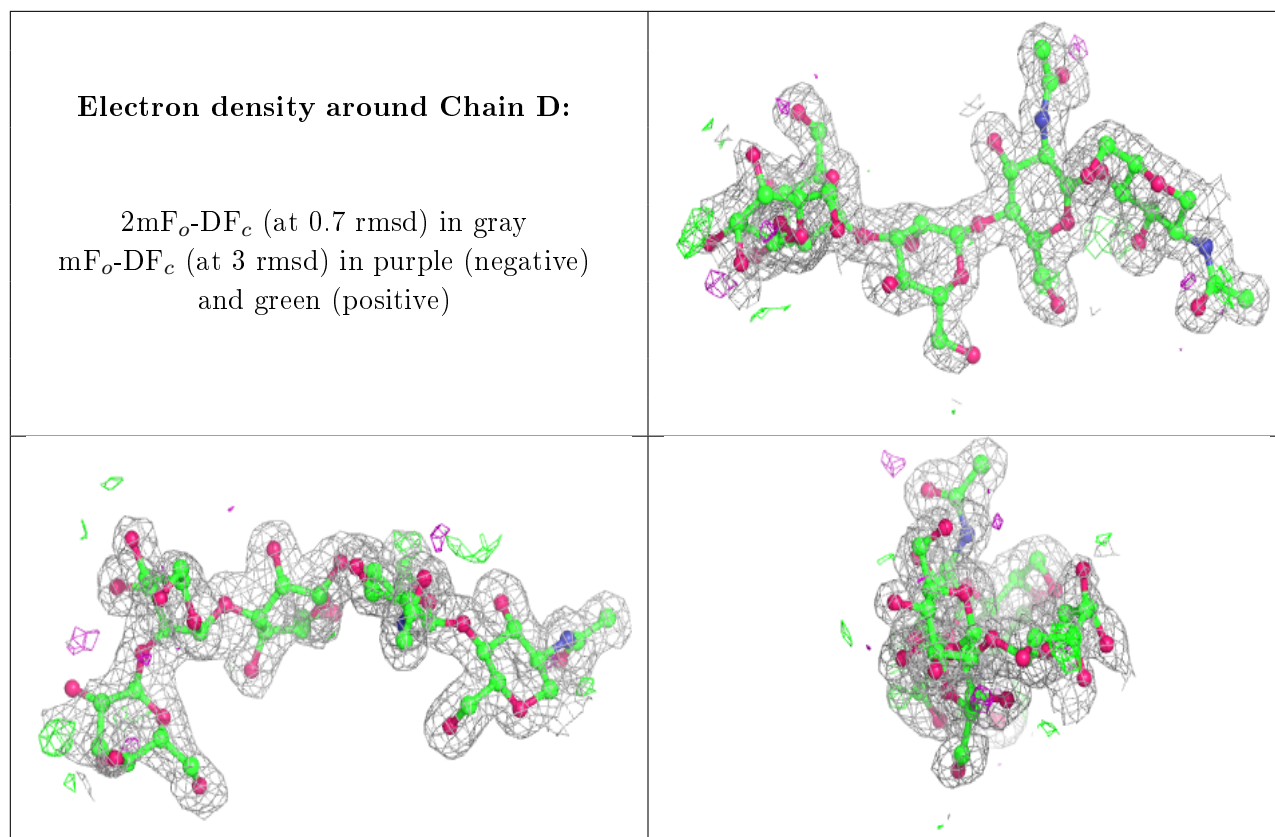
6.3 Carbohydrates [i](#)

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(\AA^2)	Q<0.9
2	MAN	C	4	11/12	0.73	0.18	43,47,57,60	0
3	MAN	D	5	11/12	0.75	0.22	47,59,69,74	0
2	MAN	C	5	11/12	0.82	0.20	43,47,49,57	0
3	MAN	D	4	11/12	0.86	0.18	39,44,46,46	0
3	BMA	D	3	11/12	0.91	0.15	35,41,54,64	0
2	BMA	C	3	11/12	0.92	0.14	35,40,44,44	0
3	NAG	D	2	14/15	0.94	0.08	24,27,32,42	0
2	NAG	C	2	14/15	0.94	0.10	28,29,35,35	0
2	NAG	C	1	14/15	0.96	0.08	24,26,29,29	0
3	NAG	D	1	14/15	0.96	0.07	22,23,24,29	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	GOL	A	408	6/6	0.89	0.12	33,34,36,36	0
4	GOL	B	406	6/6	0.90	0.11	31,36,39,40	0
4	GOL	B	408	6/6	0.91	0.09	30,34,36,37	0
5	MES	B	409	12/12	0.92	0.19	45,53,56,56	0
4	GOL	B	407	6/6	0.95	0.07	29,32,33,36	0
4	GOL	A	406	6/6	0.95	0.09	29,32,34,43	0
4	GOL	A	407	6/6	0.97	0.07	25,29,29,31	0

6.5 Other polymers [i](#)

There are no such residues in this entry.