Full wwPDB X-ray Structure Validation Report (i)

Aug 22, 2020 – 05:43 AM BST

PDB ID	:	4LYQ
Title	:	Crystal Structure of Glycoside Hydrolase Family 5 Mannosidase from Rhizomucor miehei, E202A mutant
Authors	:	Jiang, Z.Q.; Zhou, P.; Yang, S.Q.; Liu, Y.; Yan, Q.J.
Deposited on	:	2013-07-31
Resolution	:	2.00 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 (i) symbol.

The following versions of software and data (see references (1)) were used in the production of this report:

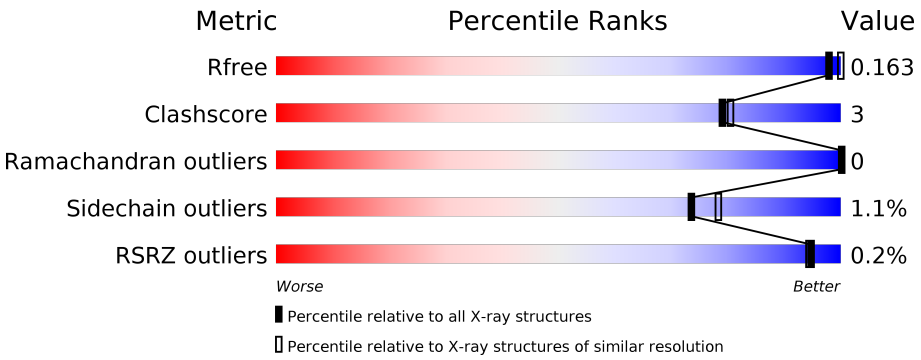
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.13.1
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry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

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 2.00 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	8085 (2.00-2.00)
Clashscore	141614	9178 (2.00-2.00)
Ramachandran outliers	138981	9054 (2.00-2.00)
Sidechain outliers	138945	9053 (2.00-2.00)
RSRZ outliers	127900	7900 (2.00-2.00)

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 <=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	449	85% 7% 8%
2	B	3	67% 33%

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	TRS	A	504	-	X	-	-

2 Entry composition (i)

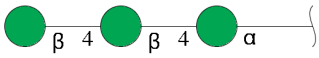
There are 5 unique types of molecules in this entry. The entry contains 3849 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 Exo-beta-1,4-mannosidase.

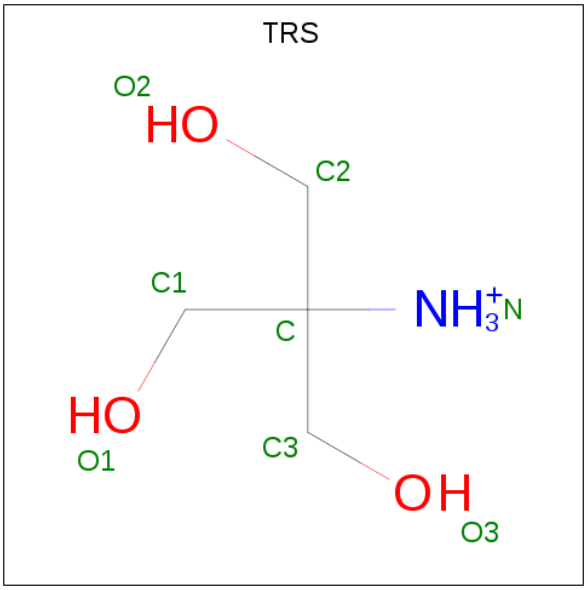
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	414	3386	2162	568	635	21	0	9	0

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



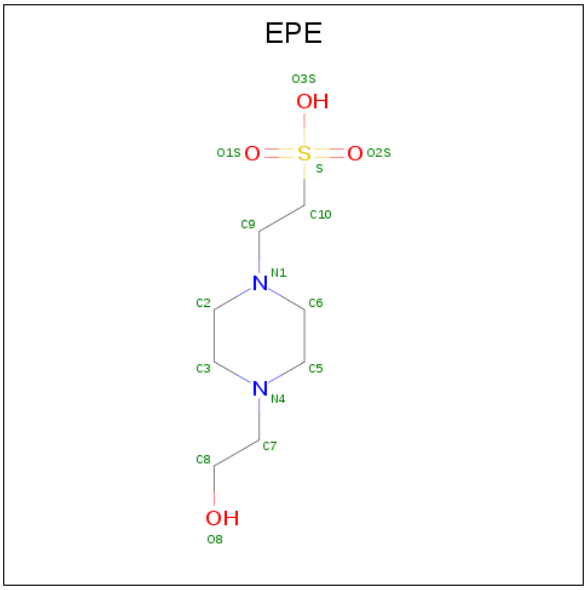
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf	Trace
			Total	C	O			
2	B	3	32	17	15	0	0	0

- Molecule 3 is 2-AMINO-2-HYDROXYMETHYL-PROPANE-1,3-DIOL (three-letter code: TRS) (formula: $C_4H_{12}NO_3$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	C	N	O		
3	A	1	8	4	1	3	0	0
			Total	C	N	O		
3	A	1	8	4	1	3	0	0

- Molecule 4 is 4-(2-HYDROXYETHYL)-1-PIPERAZINE ETHANESULFONIC ACID (three-letter code: EPE) (formula: $C_8H_{18}N_2O_4S$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
			Total	C	N	O	S		
4	A	1	15	8	2	4	1	0	0

- Molecule 5 is water.

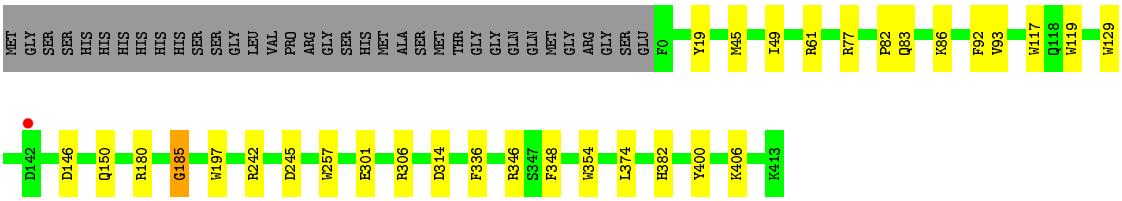
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
5	A	400	400	400	0	0

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: Exo-beta-1,4-mannosidase

Chain A: 85% 7% 8%



• Molecule 2: beta-D-mannopyranose-(1-4)-beta-D-mannopyranose-(1-4)-alpha-D-mannopyranose

Chain B: 67% 33%

4 Data and refinement statistics (i)

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α, β, γ	131.17Å 76.55Å 54.84Å 90.00° 113.36° 90.00°	Depositor
Resolution (Å)	50.00 – 2.00 30.47 – 2.00	Depositor EDS
% Data completeness (in resolution range)	94.4 (50.00-2.00) 94.5 (30.47-2.00)	Depositor EDS
R_{merge}	0.04	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	18.67 (at 2.00Å)	Xtriage
Refinement program	REFMAC 5.6.0117	Depositor
R, R_{free}	0.125 , 0.163 0.125 , 0.163	Depositor DCC
R_{free} test set	1592 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å^2)	8.6	Xtriage
Anisotropy	0.297	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.43 , 59.3	EDS
L-test for twinning[2]	$< \|L\| > = 0.50$, $< L^2 > = 0.33$	Xtriage
Estimated twinning fraction	0.020 for -h-2*l,-k,l	Xtriage
F_o,F_c correlation	0.96	EDS
Total number of atoms	3849	wwPDB-VP
Average B, all atoms (Å^2)	9.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.53% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ 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: TRS, EPE, BMA, 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	1.34	8/3521 (0.2%)	1.04	6/4783 (0.1%)

All (8) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	257	TRP	CD2-CE2	6.27	1.48	1.41
1	A	117	TRP	CD2-CE2	6.11	1.48	1.41
1	A	129	TRP	CD2-CE2	5.98	1.48	1.41
1	A	354	TRP	CD2-CE2	5.89	1.48	1.41
1	A	197	TRP	CD2-CE2	5.62	1.48	1.41
1	A	19	TYR	CE1-CZ	5.54	1.45	1.38
1	A	185	GLY	N-CA	5.39	1.54	1.46
1	A	119	TRP	CD2-CE2	5.11	1.47	1.41

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	61	ARG	NE-CZ-NH2	-6.30	117.15	120.30
1	A	306	ARG	NE-CZ-NH1	-6.27	117.17	120.30
1	A	306	ARG	NE-CZ-NH2	5.91	123.26	120.30
1	A	77	ARG	NE-CZ-NH2	-5.84	117.38	120.30
1	A	301	GLU	CB-CA-C	-5.01	100.37	110.40
1	A	314	ASP	CB-CG-OD1	5.00	122.80	118.30

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	3386	0	3195	18	0
2	B	32	0	26	1	0
3	A	16	0	24	2	0
4	A	15	0	17	0	0
5	A	400	0	0	8	1
All	All	3849	0	3262	19	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 3.

All (19) 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:346[A]:ARG:HH21	1:A:346[A]:ARG:HG2	1.21	1.01
1:A:346[A]:ARG:NH2	1:A:346[A]:ARG:HG2	1.93	0.82
1:A:382:HIS:HD2	5:A:619:HOH:O	1.73	0.71
1:A:93[B]:VAL:CG1	5:A:809:HOH:O	2.48	0.61
1:A:180[B]:ARG:HD2	1:A:185:GLY:O	2.01	0.59
1:A:245:ASP:HB3	3:A:505:TRS:H31	1.85	0.58
1:A:180[B]:ARG:CD	1:A:185:GLY:O	2.52	0.57
5:A:933:HOH:O	2:B:2:BMA:H5	2.03	0.57
1:A:93[B]:VAL:HG13	5:A:809:HOH:O	2.10	0.52
1:A:146:ASP:O	1:A:150:GLN:HG3	2.08	0.52
1:A:86:LYS:HD2	5:A:937:HOH:O	2.11	0.49
1:A:242:ARG:HA	3:A:505:TRS:H12	1.97	0.47
1:A:45[A]:MET:SD	1:A:49:ILE:HD12	2.54	0.47
1:A:83:GLN:HG3	5:A:869:HOH:O	2.17	0.44
1:A:82:PRO:HD2	1:A:86:LYS:O	2.19	0.42
1:A:93[B]:VAL:HG11	5:A:861:HOH:O	2.18	0.42
1:A:346[A]:ARG:HH21	1:A:346[A]:ARG:CG	2.03	0.41
1:A:83:GLN:CD	5:A:937:HOH:O	2.58	0.41
1:A:336:PHE:HB3	1:A:400:TYR:CD1	2.57	0.40

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)
5:A:957:HOH:O	5:A:964:HOH:O[2_858]	1.90	0.30

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	421/449 (94%)	413 (98%)	8 (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	359/380 (94%)	355 (99%)	4 (1%)	73 78

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

Mol	Chain	Res	Type
1	A	92	PHE
1	A	348	PHE
1	A	374	LEU
1	A	406	LYS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (1) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	382	HIS

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)

3 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	MAN	B	1	2	10,10,12	0.94	0	14,14,17	2.26	5 (35%)
2	BMA	B	2	2	11,11,12	1.49	3 (27%)	15,15,17	1.22	1 (6%)
2	BMA	B	3	2	11,11,12	1.51	2 (18%)	15,15,17	3.00	8 (53%)

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	MAN	B	1	2	-	-	0/1/1/1
2	BMA	B	2	2	-	0/2/19/22	0/1/1/1
2	BMA	B	3	2	-	0/2/19/22	1/1/1/1

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	3	BMA	O3-C3	3.20	1.50	1.43
2	B	2	BMA	C1-C2	2.97	1.59	1.52
2	B	2	BMA	C4-C3	2.49	1.58	1.52
2	B	3	BMA	C4-C3	2.19	1.57	1.52
2	B	2	BMA	O2-C2	-2.01	1.39	1.43

All (14) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	B	3	BMA	O5-C5-C6	-6.35	97.25	107.20
2	B	3	BMA	O3-C3-C4	5.63	123.36	110.35
2	B	1	MAN	C5-C4-C3	5.31	116.19	109.67
2	B	3	BMA	O4-C4-C3	4.62	121.04	110.35
2	B	1	MAN	O5-C1-C2	3.81	115.10	109.43
2	B	3	BMA	C1-O5-C5	3.17	116.49	112.19
2	B	2	BMA	O3-C3-C2	3.00	115.75	109.99
2	B	3	BMA	C2-C3-C4	-2.94	105.80	110.89
2	B	1	MAN	C4-C3-C2	2.83	115.78	110.89
2	B	3	BMA	O5-C1-C2	-2.57	106.80	110.77
2	B	3	BMA	C1-C2-C3	-2.55	106.53	109.67
2	B	3	BMA	O3-C3-C2	-2.53	105.15	109.99
2	B	1	MAN	C5-O5-C1	2.50	116.92	112.71
2	B	1	MAN	O1-C1-C2	-2.29	102.58	109.03

There are no chirality outliers.

There are no torsion outliers.

All (1) ring outliers are listed below:

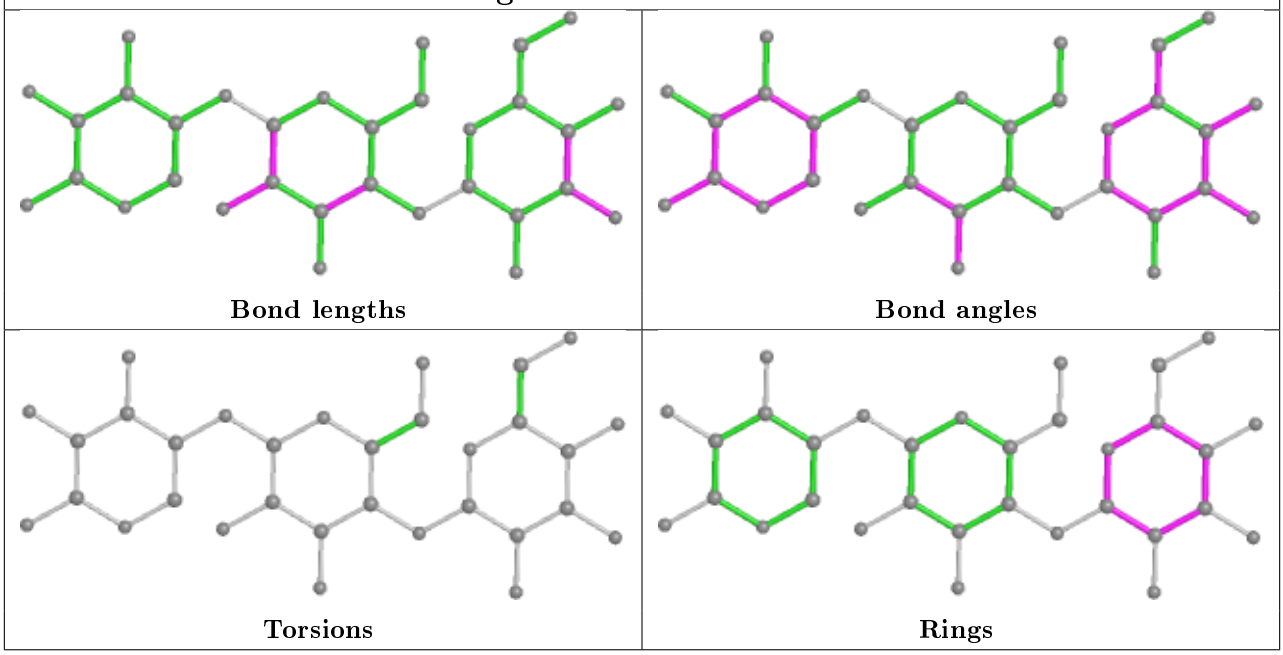
Mol	Chain	Res	Type	Atoms
2	B	3	BMA	C1-C2-C3-C4-C5-O5

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	2	BMA	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.

Oligosaccharide Chain B



5.6 Ligand geometry (i)

3 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	EPE	A	506	-	15,15,15	2.48	3 (20%)	18,20,20	7.05	8 (44%)
3	TRS	A	504	-	7,7,7	0.54	0	9,9,9	1.93	4 (44%)
3	TRS	A	505	-	7,7,7	0.92	0	9,9,9	1.60	2 (22%)

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	EPE	A	506	-	-	7/9/19/19	0/1/1/1
3	TRS	A	504	-	-	8/9/9/9	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	TRS	A	505	-	-	6/9/9/9	-

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	506	EPE	O2S-S	7.00	1.65	1.45
4	A	506	EPE	C10-S	-5.53	1.69	1.77
4	A	506	EPE	C5-N4	2.24	1.53	1.46

All (14) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	A	506	EPE	O2S-S-C10	-20.99	81.63	106.92
4	A	506	EPE	O1S-S-C10	16.43	126.70	106.92
4	A	506	EPE	O3S-S-C10	8.47	119.47	105.77
4	A	506	EPE	O2S-S-O1S	-7.63	87.53	113.95
4	A	506	EPE	O3S-S-O2S	-5.27	98.39	111.27
3	A	504	TRS	O1-C1-C	-4.16	97.80	111.00
3	A	505	TRS	O1-C1-C	3.14	120.96	111.00
4	A	506	EPE	C9-N1-C6	2.66	118.04	111.23
3	A	504	TRS	O2-C2-C	2.45	118.75	111.00
4	A	506	EPE	C6-C5-N4	2.30	115.35	110.64
3	A	504	TRS	C2-C-C1	-2.21	103.97	110.81
3	A	505	TRS	C1-C-N	2.17	114.45	107.98
4	A	506	EPE	C2-C3-N4	-2.06	106.42	110.64
3	A	504	TRS	C2-C-N	2.05	114.11	107.98

There are no chirality outliers.

All (21) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	A	506	EPE	C10-C9-N1-C6
4	A	506	EPE	C9-C10-S-O2S
3	A	504	TRS	C3-C-C2-O2
3	A	504	TRS	C1-C-C2-O2
4	A	506	EPE	C8-C7-N4-C3
4	A	506	EPE	N4-C7-C8-O8
4	A	506	EPE	C8-C7-N4-C5
3	A	504	TRS	C3-C-C1-O1
3	A	504	TRS	N-C-C1-O1
3	A	504	TRS	N-C-C2-O2

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Mol	Chain	Res	Type	Atoms
3	A	504	TRS	N-C-C3-O3
3	A	505	TRS	C3-C-C1-O1
3	A	505	TRS	N-C-C1-O1
3	A	505	TRS	C2-C-C3-O3
3	A	505	TRS	N-C-C3-O3
4	A	506	EPE	C9-C10-S-O1S
4	A	506	EPE	C10-C9-N1-C2
3	A	504	TRS	C2-C-C1-O1
3	A	504	TRS	C1-C-C3-O3
3	A	505	TRS	C2-C-C1-O1
3	A	505	TRS	C1-C-C3-O3

There are no ring outliers.

1 monomer is involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	505	TRS	2	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 (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	414/449 (92%)	-0.87	1 (0%) 95 94	3, 6, 19, 43	0

All (1) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	142	ASP	2.2

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)

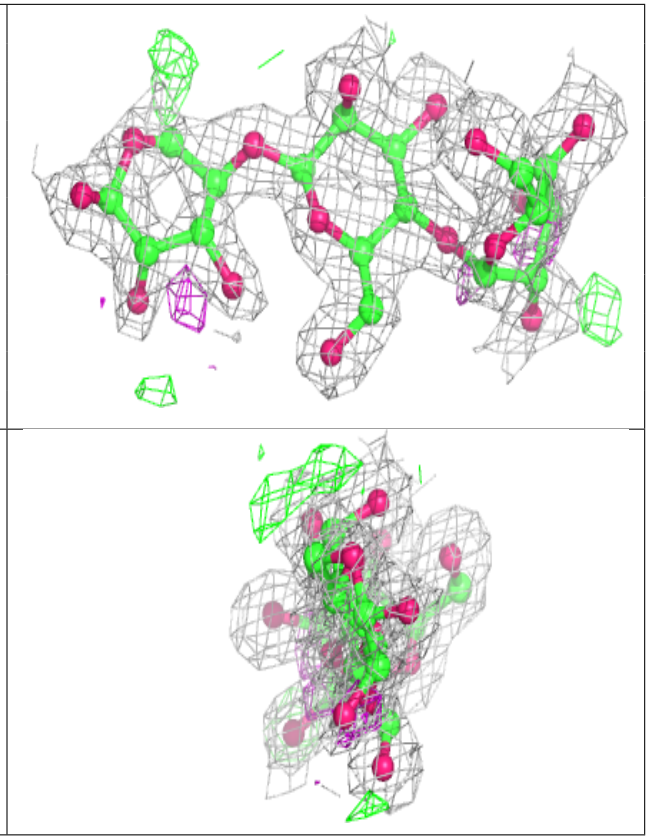
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
2	MAN	B	1	10/12	0.91	0.25	27,30,36,37	0
2	BMA	B	2	11/12	0.94	0.10	19,21,23,24	0
2	BMA	B	3	11/12	0.94	0.12	12,15,22,22	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.

Electron density around Chain B:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



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
3	TRS	A	505	8/8	0.90	0.24	28,34,41,42	0
3	TRS	A	504	8/8	0.92	0.23	19,32,40,44	0
4	EPE	A	506	15/15	0.93	0.18	23,33,51,54	0

6.5 Other polymers (i)

There are no such residues in this entry.