



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 21, 2020 – 10:35 PM EST

PDB ID : 5B0R  
Title : Beta-1,2-Mannobiose phosphorylase from *Listeria innocua* - beta-1,2-mannobiose complex  
Authors : Tsuda, T.; Arakawa, T.; Fushinobu, S.  
Deposited on : 2015-11-02  
Resolution : 1.80 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](mailto: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.

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The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity : 4.02b-467  
Mogul : 1.8.0 (224370), CSD as540be (2019)  
Xtriage (Phenix) : 1.13  
EDS : 2.8  
Percentile statistics : 20171227.v01 (using entries in the PDB archive December 27th 2017)  
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) : 2.8

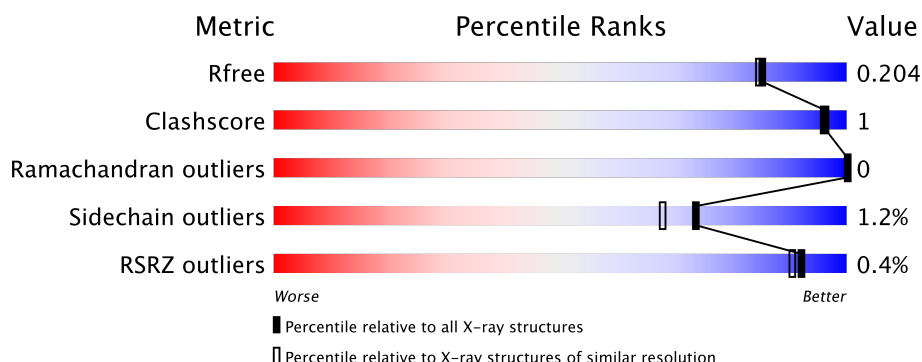
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*



The reported resolution of this entry is 1.80 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))
$R_{free}$	111664	5253 (1.80-1.80)
Clashscore	122126	6077 (1.80-1.80)
Ramachandran outliers	120053	6011 (1.80-1.80)
Sidechain outliers	120020	6010 (1.80-1.80)
RSRZ outliers	108989	5157 (1.80-1.80)

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  $\geq 3$ , 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	363	 84% 13% •
1	B	363	 89% 8% •

## 2 Entry composition

There are 7 unique types of molecules in this entry. The entry contains 6311 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.

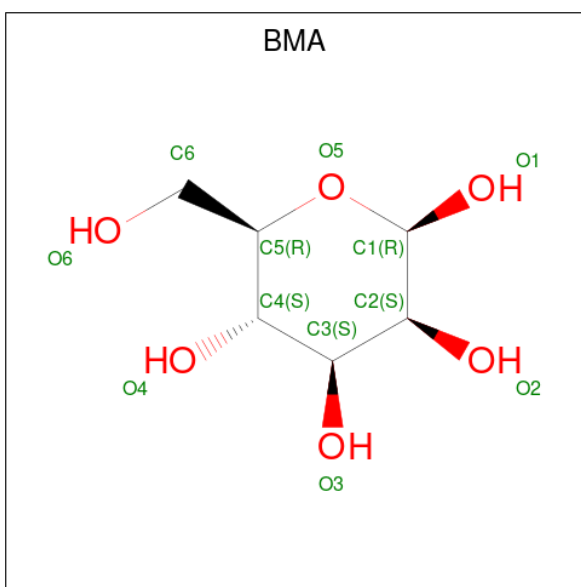
- Molecule 1 is a protein called Lin0857 protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	353	Total	C	N	O	S	0	1	0
			2816	1803	461	543	9			
1	B	353	Total	C	N	O	S	0	1	0
			2816	1803	461	543	9			

There are 16 discrepancies between the modelled and reference sequences:

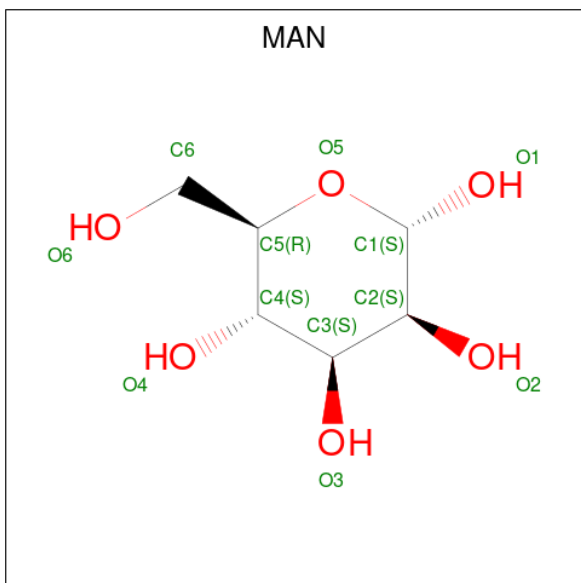
Chain	Residue	Modelled	Actual	Comment	Reference
A	356	LEU	-	expression tag	UNP Q92DF6
A	357	GLU	-	expression tag	UNP Q92DF6
A	358	HIS	-	expression tag	UNP Q92DF6
A	359	HIS	-	expression tag	UNP Q92DF6
A	360	HIS	-	expression tag	UNP Q92DF6
A	361	HIS	-	expression tag	UNP Q92DF6
A	362	HIS	-	expression tag	UNP Q92DF6
A	363	HIS	-	expression tag	UNP Q92DF6
B	356	LEU	-	expression tag	UNP Q92DF6
B	357	GLU	-	expression tag	UNP Q92DF6
B	358	HIS	-	expression tag	UNP Q92DF6
B	359	HIS	-	expression tag	UNP Q92DF6
B	360	HIS	-	expression tag	UNP Q92DF6
B	361	HIS	-	expression tag	UNP Q92DF6
B	362	HIS	-	expression tag	UNP Q92DF6
B	363	HIS	-	expression tag	UNP Q92DF6

- Molecule 2 is BETA-D-MANNOSE (three-letter code: BMA) (formula:  $C_6H_{12}O_6$ ).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total	C	O	0	0
			11	6	5		
2	A	1	Total	C	O	0	1
			12	6	6		
2	B	1	Total	C	O	0	0
			11	6	5		
2	B	1	Total	C	O	0	1
			12	6	6		

- Molecule 3 is ALPHA-D-MANNOSE (three-letter code: MAN) (formula: C<sub>6</sub>H<sub>12</sub>O<sub>6</sub>).



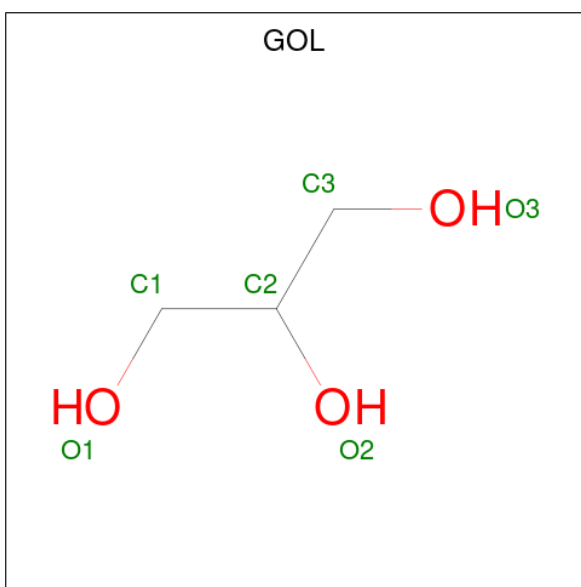
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	C	O	0	1
			12	6	6		
3	B	1	Total	C	O	0	1
			12	6	6		

- Molecule 4 is SULFATE ION (three-letter code: SO4) (formula: O<sub>4</sub>S).



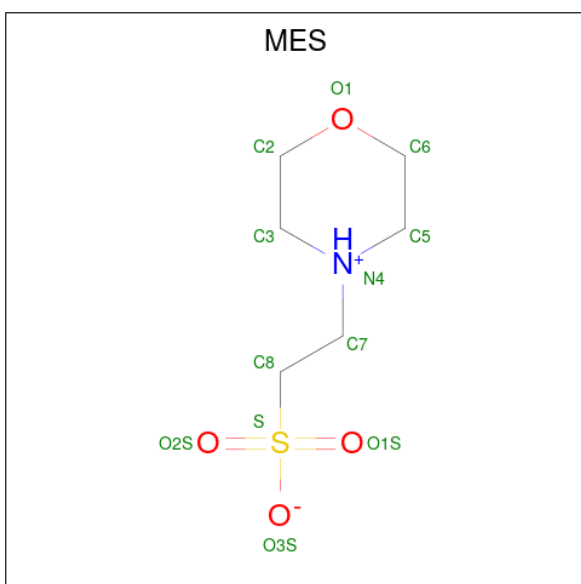
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total	O	S	0	0
			5	4	1		
4	A	1	Total	O	S	0	0
			5	4	1		
4	A	1	Total	O	S	0	0
			5	4	1		
4	B	1	Total	O	S	0	0
			5	4	1		
4	B	1	Total	O	S	0	0
			5	4	1		
4	B	1	Total	O	S	0	0
			5	4	1		
4	B	1	Total	O	S	0	0
			5	4	1		

- Molecule 5 is GLYCEROL (three-letter code: GOL) (formula: C<sub>3</sub>H<sub>8</sub>O<sub>3</sub>).



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	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-(N-MORPHOLINO)-ETHANESULFONIC ACID (three-letter code: MES) (formula:  $C_6H_{13}NO_4S$ ).



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

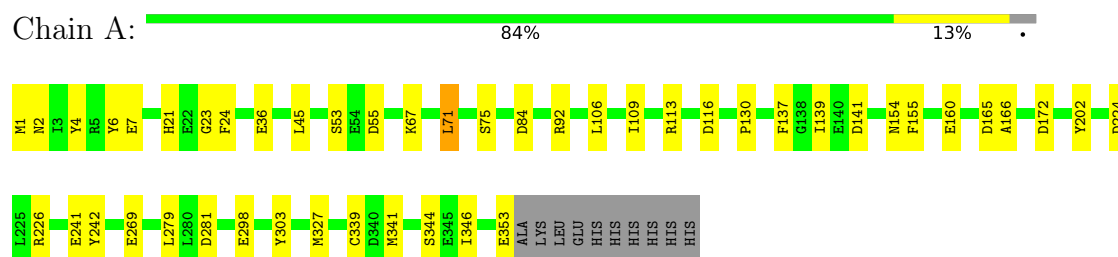
- Molecule 7 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	A	281	Total	O	0	0
			281	281		
7	B	240	Total	O	0	0
			240	240		

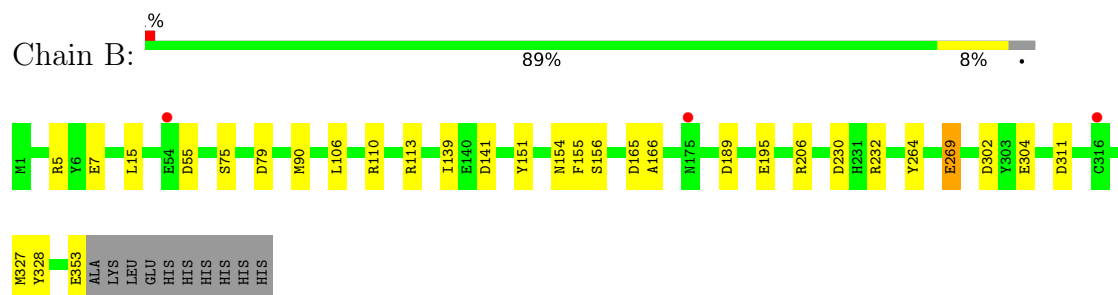
### 3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA and DNA 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: Lin0857 protein



#### • Molecule 1: Lin0857 protein





## 4 Data and refinement statistics

Property	Value	Source
Space group	P 31 2 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	145.77Å 145.77Å 105.77Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	32.93 – 1.80 32.93 – 1.80	Depositor EDS
% Data completeness (in resolution range)	99.8 (32.93-1.80) 99.8 (32.93-1.80)	Depositor EDS
$R_{merge}$	0.05	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	6.09 (at 1.81Å)	Xtriage
Refinement program	REFMAC 5.8.0107	Depositor
R, $R_{free}$	0.165 , 0.193 0.178 , 0.204	Depositor DCC
$R_{free}$ test set	5996 reflections (5.01%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	24.1	Xtriage
Anisotropy	0.012	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.37 , 45.8	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.52$ , $\langle L^2 \rangle = 0.35$	Xtriage
Estimated twinning fraction	0.010 for -h,-k,l	Xtriage
$F_o, F_c$ correlation	0.97	EDS
Total number of atoms	6311	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	29.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.08% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>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, SO4, 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	1.44	13/2887 (0.5%)	1.37	23/3915 (0.6%)
1	B	1.41	9/2887 (0.3%)	1.29	18/3915 (0.5%)
All	All	1.42	22/5774 (0.4%)	1.33	41/7830 (0.5%)

All (22) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	160	GLU	CD-OE2	8.39	1.34	1.25
1	B	269	GLU	CG-CD	7.33	1.62	1.51
1	A	241	GLU	CD-OE2	7.07	1.33	1.25
1	B	264	TYR	CE1-CZ	7.04	1.47	1.38
1	A	2	ASN	CG-OD1	6.71	1.38	1.24
1	A	298	GLU	CD-OE2	-6.67	1.18	1.25
1	B	151	TYR	CE1-CZ	6.30	1.46	1.38
1	A	160	GLU	CG-CD	6.00	1.60	1.51
1	A	23	GLY	C-O	5.98	1.33	1.23
1	B	156	SER	CA-CB	-5.80	1.44	1.52
1	A	344	SER	CA-CB	5.79	1.61	1.52
1	A	242	TYR	CE2-CZ	-5.71	1.31	1.38
1	A	303	TYR	CE1-CZ	5.53	1.45	1.38
1	A	202	TYR	CE2-CZ	-5.51	1.31	1.38
1	B	195	GLU	CG-CD	5.42	1.60	1.51
1	A	67	LYS	N-CA	5.34	1.57	1.46
1	B	264	TYR	CG-CD2	5.29	1.46	1.39
1	A	75	SER	CB-OG	-5.22	1.35	1.42
1	B	195	GLU	CD-OE2	-5.14	1.20	1.25
1	B	75	SER	CA-CB	5.14	1.60	1.52
1	A	7	GLU	CD-OE2	5.02	1.31	1.25
1	B	232	ARG	CG-CD	-5.01	1.39	1.51

All (41) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	327	MET	CG-SD-CE	-10.92	82.72	100.20
1	A	281	ASP	CB-CG-OD1	-9.18	110.04	118.30
1	A	226	ARG	NE-CZ-NH2	8.96	124.78	120.30
1	B	110	ARG	NE-CZ-NH2	8.79	124.70	120.30
1	A	113	ARG	NE-CZ-NH1	8.36	124.48	120.30
1	B	79	ASP	CB-CG-OD1	8.34	125.81	118.30
1	A	172	ASP	CB-CG-OD1	8.00	125.50	118.30
1	A	224	ASP	CB-CG-OD1	7.28	124.85	118.30
1	A	141	ASP	CB-CG-OD1	7.27	124.84	118.30
1	A	116	ASP	CB-CG-OD1	7.11	124.70	118.30
1	A	55	ASP	CB-CG-OD1	6.77	124.40	118.30
1	B	302	ASP	CB-CG-OD1	6.57	124.21	118.30
1	B	141	ASP	CB-CG-OD1	6.39	124.05	118.30
1	B	230	ASP	CB-CG-OD1	6.38	124.04	118.30
1	A	36[A]	GLU	OE1-CD-OE2	-6.22	115.83	123.30
1	A	36[B]	GLU	OE1-CD-OE2	-6.22	115.83	123.30
1	B	353	GLU	CA-C-O	-6.07	107.36	120.10
1	B	328	TYR	CB-CG-CD2	-5.96	117.42	121.00
1	A	353	GLU	CA-C-O	-5.91	107.69	120.10
1	A	165	ASP	CB-CG-OD1	5.90	123.61	118.30
1	A	113	ARG	NE-CZ-NH2	-5.79	117.41	120.30
1	A	137	PHE	CB-CG-CD2	-5.78	116.75	120.80
1	A	226	ARG	NE-CZ-NH1	-5.71	117.44	120.30
1	B	113	ARG	NE-CZ-NH2	5.67	123.14	120.30
1	A	84	ASP	CB-CG-OD2	5.65	123.39	118.30
1	B	206	ARG	NE-CZ-NH2	5.64	123.12	120.30
1	B	110	ARG	NE-CZ-NH1	-5.57	117.52	120.30
1	A	242	TYR	CZ-CE2-CD2	5.47	124.72	119.80
1	B	55	ASP	CB-CG-OD2	-5.45	113.40	118.30
1	A	141	ASP	CB-CG-OD2	-5.43	113.42	118.30
1	B	327	MET	CG-SD-CE	-5.37	91.61	100.20
1	B	189	ASP	CB-CG-OD1	5.34	123.10	118.30
1	A	92	ARG	NE-CZ-NH1	-5.31	117.64	120.30
1	B	165	ASP	CB-CG-OD1	-5.29	113.54	118.30
1	B	5	ARG	NE-CZ-NH1	5.27	122.93	120.30
1	B	90	MET	CG-SD-CE	5.16	108.45	100.20
1	B	304	GLU	OE1-CD-OE2	5.15	129.48	123.30
1	A	1	MET	CB-CA-C	-5.14	100.12	110.40
1	A	279	LEU	CB-CG-CD2	-5.11	102.31	111.00
1	A	6	TYR	CB-CG-CD1	5.11	124.06	121.00
1	B	311	ASP	CB-CG-OD2	-5.06	113.74	118.30

There are no chirality outliers.

There are no planarity outliers.

## 5.2 Too-close contacts

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2816	0	2731	9	0
1	B	2816	0	2731	3	0
2	A	23	0	21	0	0
2	B	23	0	21	0	0
3	A	12	0	11	0	0
3	B	12	0	11	0	0
4	A	15	0	0	0	0
4	B	25	0	0	0	0
5	A	12	0	16	0	0
5	B	12	0	16	0	0
6	A	12	0	13	0	0
6	B	12	0	13	0	0
7	A	281	0	0	2	0
7	B	240	0	0	0	0
All	All	6311	0	5584	12	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 1.

All (12) 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:269:GLU:HG3	7:A:629:HOH:O	1.97	0.63
1:A:341:MET:HE3	1:A:346:ILE:HD11	1.91	0.51
1:A:21:HIS:CD2	1:A:71:LEU:HD22	2.51	0.46
1:B:139:ILE:HG23	1:B:155:PHE:CD1	2.54	0.42
1:A:154:ASN:HA	1:A:166:ALA:O	2.20	0.42
1:A:4:TYR:O	1:A:339:CYS:HA	2.20	0.42
1:B:154:ASN:HA	1:B:166:ALA:O	2.20	0.41
1:A:24:PHE:CZ	1:A:71:LEU:HD23	2.55	0.41
1:A:139:ILE:HG23	1:A:155:PHE:CD1	2.56	0.41
1:A:45:LEU:O	1:A:109:ILE:HA	2.20	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:269:GLU:CG	7:A:629:HOH:O	2.64	0.40
1:B:269:GLU:CD	1:B:269:GLU:H	2.25	0.40

There are no symmetry-related clashes.

## 5.3 Torsion angles [i](#)

### 5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	352/363 (97%)	338 (96%)	14 (4%)	0	100	100
1	B	352/363 (97%)	339 (96%)	13 (4%)	0	100	100
All	All	704/726 (97%)	677 (96%)	27 (4%)	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	303/311 (97%)	299 (99%)	4 (1%)	71	65
1	B	303/311 (97%)	300 (99%)	3 (1%)	78	74
All	All	606/622 (97%)	599 (99%)	7 (1%)	74	68

All (7) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	53	SER
1	A	71	LEU
1	A	106	LEU
1	A	130	PRO
1	B	7	GLU
1	B	15	LEU
1	B	106	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

### 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](#)

There are no carbohydrates in this entry.

## 5.6 Ligand geometry [i](#)

20 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	$\# Z  > 2$
2	BMA	A	501	3,2	11,11,12	1.36	2 (18%)	15,15,17	1.92	4 (26%)
2	BMA	A	502[A]	2	12,12,12	1.03	1 (8%)	17,17,17	2.18	7 (41%)
3	MAN	A	503[B]	2	12,12,12	1.17	2 (16%)	17,17,17	1.38	2 (11%)
4	SO4	A	504	-	4,4,4	0.59	0	6,6,6	0.56	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
4	SO4	A	505	-	4,4,4	1.16	0	6,6,6	0.76	0
4	SO4	A	506	-	4,4,4	1.12	0	6,6,6	1.39	1 (16%)
5	GOL	A	507	-	5,5,5	1.07	0	5,5,5	1.22	0
5	GOL	A	508	-	5,5,5	0.56	0	5,5,5	0.74	0
6	MES	A	509	-	12,12,12	1.62	3 (25%)	14,16,16	3.10	5 (35%)
2	BMA	B	501	3,2	11,11,12	1.60	3 (27%)	15,15,17	1.78	6 (40%)
2	BMA	B	502[A]	2	12,12,12	0.73	0	17,17,17	2.76	6 (35%)
3	MAN	B	503[B]	2	12,12,12	1.00	1 (8%)	17,17,17	1.43	2 (11%)
4	SO4	B	504	-	4,4,4	0.52	0	6,6,6	0.80	0
4	SO4	B	505	-	4,4,4	0.67	0	6,6,6	0.94	0
4	SO4	B	506	-	4,4,4	1.00	0	6,6,6	1.30	0
4	SO4	B	507	-	4,4,4	0.61	0	6,6,6	0.49	0
4	SO4	B	508	-	4,4,4	1.66	1 (25%)	6,6,6	1.23	1 (16%)
5	GOL	B	509	-	5,5,5	0.63	0	5,5,5	1.14	0
5	GOL	B	510	-	5,5,5	0.54	0	5,5,5	1.17	1 (20%)
6	MES	B	511	-	12,12,12	1.73	2 (16%)	14,16,16	1.97	4 (28%)

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	BMA	A	501	3,2	-	0/2/19/22	1/1/1/1
2	BMA	A	502[A]	2	-	0/2/22/22	0/1/1/1
3	MAN	A	503[B]	2	-	0/2/22/22	0/1/1/1
5	GOL	A	507	-	-	4/4/4/4	-
5	GOL	A	508	-	-	2/4/4/4	-
6	MES	A	509	-	-	0/6/14/14	0/1/1/1
2	BMA	B	501	3,2	-	0/2/19/22	1/1/1/1
2	BMA	B	502[A]	2	-	0/2/22/22	0/1/1/1
3	MAN	B	503[B]	2	-	0/2/22/22	0/1/1/1
5	GOL	B	509	-	-	0/4/4/4	-
5	GOL	B	510	-	-	4/4/4/4	-
6	MES	B	511	-	-	0/6/14/14	0/1/1/1

All (15) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	B	511	MES	C8-S	-4.49	1.71	1.77

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	A	509	MES	C8-S	-4.17	1.71	1.77
2	B	501	BMA	O5-C1	-2.93	1.39	1.43
2	A	502[A]	BMA	O4-C4	2.83	1.49	1.43
3	A	503[B]	MAN	O4-C4	2.82	1.49	1.43
4	B	508	SO4	O1-S	2.61	1.59	1.45
2	A	501	BMA	O5-C5	2.49	1.48	1.43
3	B	503[B]	MAN	O1-C1	2.47	1.47	1.39
2	B	501	BMA	O4-C4	2.34	1.48	1.43
3	A	503[B]	MAN	O1-C1	2.32	1.47	1.39
2	A	501	BMA	C2-C3	2.24	1.55	1.52
6	A	509	MES	C3-N4	2.16	1.52	1.47
6	A	509	MES	O2S-S	2.07	1.51	1.45
2	B	501	BMA	O2-C2	-2.07	1.38	1.43
6	B	511	MES	O1S-S	2.03	1.51	1.45

All (39) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	A	509	MES	O2S-S-C8	9.12	117.90	106.92
2	B	502[A]	BMA	O1-C1-O5	-5.98	92.40	110.41
2	A	501	BMA	C1-O5-C5	5.08	119.11	112.20
2	B	502[A]	BMA	C1-O5-C5	-4.88	104.35	113.68
2	B	502[A]	BMA	C1-C2-C3	-4.60	100.69	110.31
6	B	511	MES	O2S-S-C8	4.44	112.27	106.92
2	A	502[A]	BMA	C1-O5-C5	-3.85	106.32	113.68
2	B	502[A]	BMA	O5-C1-C2	3.82	117.16	110.31
2	A	502[A]	BMA	O1-C1-O5	-3.64	99.46	110.41
2	B	502[A]	BMA	O2-C2-C1	3.59	117.52	109.14
6	A	509	MES	O3S-S-O1S	3.56	119.97	111.27
6	B	511	MES	O3S-S-O1S	3.52	119.86	111.27
6	A	509	MES	C2-C3-N4	-3.49	104.75	110.09
2	B	501	BMA	C1-O5-C5	3.27	116.65	112.20
6	A	509	MES	O3S-S-O2S	-3.27	103.28	111.27
2	A	502[A]	BMA	O5-C1-C2	3.17	116.00	110.31
2	A	502[A]	BMA	C3-C4-C5	3.03	115.68	110.23
2	B	502[A]	BMA	C3-C4-C5	3.03	115.67	110.23
6	B	511	MES	O2S-S-O1S	-2.99	103.62	113.95
2	A	501	BMA	C2-C3-C4	2.98	116.06	110.89
2	A	502[A]	BMA	O2-C2-C1	2.87	115.83	109.14
3	B	503[B]	MAN	O1-C1-O5	2.77	118.75	110.41
3	A	503[B]	MAN	C3-C4-C5	2.73	115.13	110.23
3	B	503[B]	MAN	C3-C4-C5	2.68	115.04	110.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	501	BMA	O3-C3-C2	2.67	114.98	110.02
2	A	502[A]	BMA	C1-C2-C3	-2.63	104.80	110.31
3	A	503[B]	MAN	O2-C2-C3	-2.60	104.30	110.34
2	B	501	BMA	O2-C2-C1	2.55	114.35	109.17
2	B	501	BMA	O2-C2-C3	2.49	115.02	110.16
4	B	508	SO4	O3-S-O2	2.44	122.44	109.37
4	A	506	SO4	O3-S-O2	2.41	122.29	109.37
2	A	501	BMA	O2-C2-C3	2.37	114.81	110.16
6	B	511	MES	O3S-S-C8	-2.33	102.00	105.77
2	B	501	BMA	O3-C3-C4	2.31	115.70	110.34
2	A	502[A]	BMA	O2-C2-C3	-2.30	105.01	110.34
2	B	501	BMA	C3-C4-C5	2.14	114.08	110.23
6	A	509	MES	O2S-S-O1S	-2.13	106.57	113.95
2	A	501	BMA	C1-C2-C3	-2.13	107.04	109.66
5	B	510	GOL	O1-C1-C2	-2.09	100.02	110.12

There are no chirality outliers.

All (10) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	A	508	GOL	O1-C1-C2-C3
5	A	507	GOL	O1-C1-C2-C3
5	A	507	GOL	C1-C2-C3-O3
5	A	507	GOL	O1-C1-C2-O2
5	A	507	GOL	O2-C2-C3-O3
5	B	510	GOL	O1-C1-C2-O2
5	B	510	GOL	O1-C1-C2-C3
5	B	510	GOL	C1-C2-C3-O3
5	A	508	GOL	O1-C1-C2-O2
5	B	510	GOL	O2-C2-C3-O3

All (2) ring outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	B	501	BMA	C1-C2-C3-C4-C5-O5
2	A	501	BMA	C1-C2-C3-C4-C5-O5

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, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	A	353/363 (97%)	-0.39	0	100   100	18, 26, 42, 59	0
1	B	353/363 (97%)	-0.23	3 (0%)	86   84	19, 28, 46, 75	0
All	All	706/726 (97%)	-0.31	3 (0%)	92   90	18, 27, 43, 75	0

All (3) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	54	GLU	3.7
1	B	175	ASN	2.2
1	B	316	CYS	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](#)

There are no carbohydrates in this entry.

### 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, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
5	GOL	A	508	6/6	0.90	0.21	47,60,66,72	0
5	GOL	A	507	6/6	0.94	0.18	29,42,43,43	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
4	SO4	A	506	5/5	0.94	0.24	44,57,60,62	0
4	SO4	B	507	5/5	0.94	0.30	77,80,88,90	0
4	SO4	B	506	5/5	0.95	0.25	52,59,66,79	0
4	SO4	B	508	5/5	0.95	0.34	40,47,52,60	0
5	GOL	B	509	6/6	0.95	0.17	29,47,49,49	0
5	GOL	B	510	6/6	0.95	0.14	40,55,58,62	0
6	MES	A	509	12/12	0.96	0.20	40,51,58,59	0
6	MES	B	511	12/12	0.96	0.20	47,48,51,56	0
2	BMA	B	501	11/12	0.98	0.14	19,21,22,23	0
3	MAN	B	503[B]	12/12	0.98	0.09	17,20,21,23	12
4	SO4	A	505	5/5	0.98	0.21	34,40,45,47	0
2	BMA	B	502[A]	12/12	0.98	0.09	19,21,23,24	12
3	MAN	A	503[B]	12/12	0.99	0.11	15,18,19,21	12
4	SO4	B	504	5/5	0.99	0.07	20,21,21,21	0
4	SO4	B	505	5/5	0.99	0.20	41,45,51,52	0
2	BMA	A	502[A]	12/12	0.99	0.10	17,19,19,22	12
2	BMA	A	501	11/12	0.99	0.12	17,18,19,20	0
4	SO4	A	504	5/5	1.00	0.07	18,18,18,19	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.