



# wwPDB X-ray Structure Validation Summary Report ⓘ

Feb 14, 2017 – 09:35 pm GMT

PDB ID : 1MPN  
Title : MALTOPORIN MALTOTRIOSE COMPLEX  
Authors : Dutzler, R.; Schirmer, T.  
Deposited on : 1996-01-11  
Resolution : 3.20 Å(reported)

This is a wwPDB X-ray Structure Validation Summary Report for a publicly released PDB entry.

We welcome your comments at [validation@mail.wwpdb.org](mailto:validation@mail.wwpdb.org)

A user guide is available at

<http://wwpdb.org/validation/2016/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 : 1.7.2 (RC1), CSD as538be (2017)  
Xtriage (Phenix) : 1.9-1692  
EDS : trunk28620  
Percentile statistics : 20161228.v01 (using entries in the PDB archive December 28th 2016)  
Refmac : 5.8.0135  
CCP4 : 6.5.0  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : recalc28949

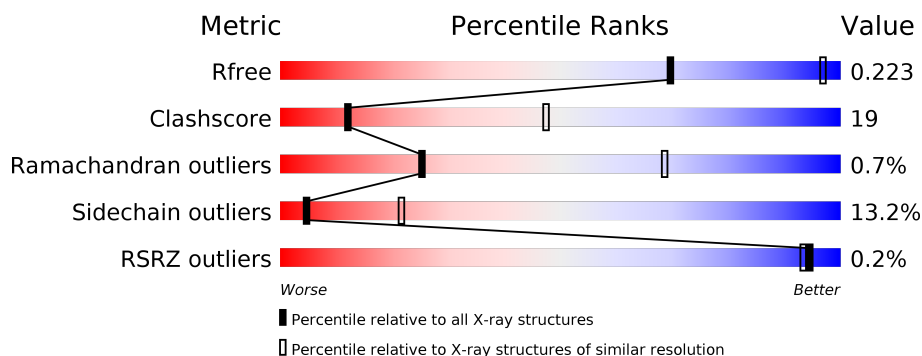
# 1 Overall quality at a glance ⓘ

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 3.20 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))
$R_{free}$	100719	1015 (3.22-3.18)
Clashscore	112137	1009 (3.20-3.20)
Ramachandran outliers	110173	1118 (3.22-3.18)
Sidechain outliers	110143	1117 (3.22-3.18)
RSRZ outliers	101464	1020 (3.22-3.18)

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. 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	421	 67% 27% 6%
1	B	421	 67% 27% 6%
1	C	421	 67% 27% 6%

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	GLC	A	431	-	-	-	X
2	GLC	A	433	-	-	-	X
2	GLC	B	431	-	-	-	X
2	GLC	B	433	-	-	-	X
2	GLC	C	431	-	-	-	X
2	GLC	C	433	-	-	-	X

## 2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 10155 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 MALTOPORIN.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	421	Total	C	N	O	S	127	0	0
			3350	2110	571	655	14			
1	B	421	Total	C	N	O	S	127	0	0
			3350	2110	571	655	14			
1	C	421	Total	C	N	O	S	127	0	0
			3350	2110	571	655	14			

- Molecule 2 is a polymer of unknown type called SUGAR (3-MER).

Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	3	Total	C	O	0	0
			34	18	16		
2	B	3	Total	C	O	0	0
			34	18	16		
2	C	3	Total	C	O	0	0
			34	18	16		

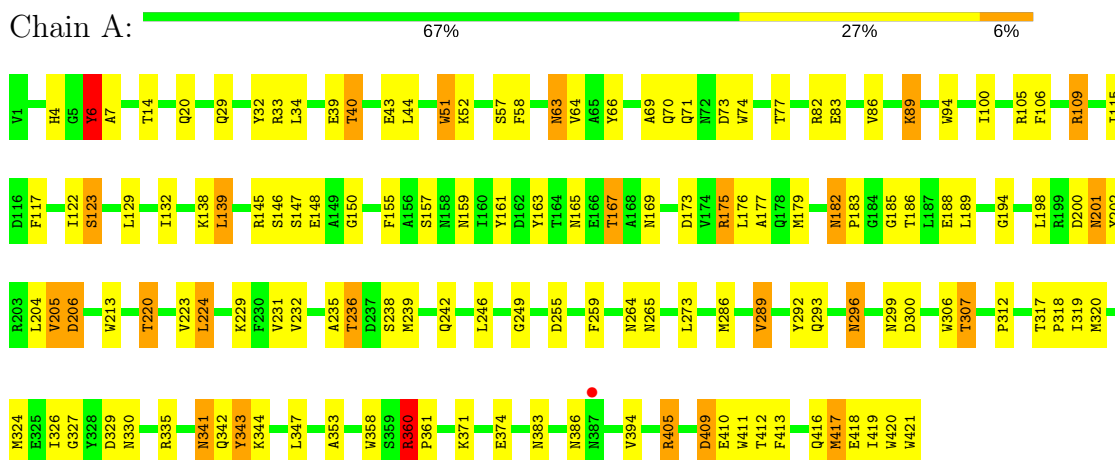
- Molecule 3 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	B	1	Total	Mg	0	0
			1	1		
3	A	1	Total	Mg	0	0
			1	1		
3	C	1	Total	Mg	0	0
			1	1		

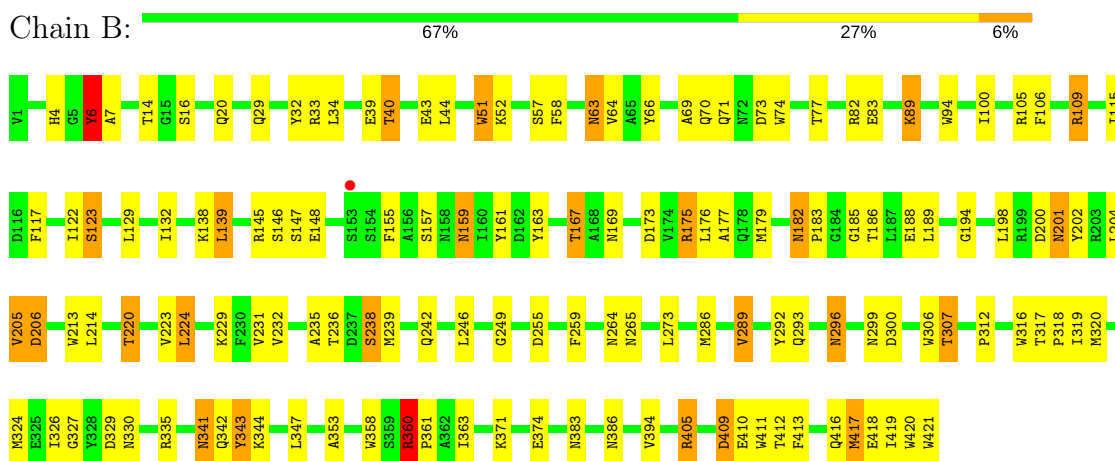
### 3 Residue-property plots

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.

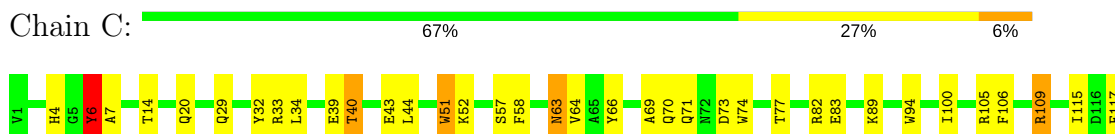
#### • Molecule 1: MALTOPORIN



#### • Molecule 1: MALTOPORIN



#### • Molecule 1: MALTOPORIN



	M324	E325	I326	G327	Y328	D329	N330		R335		N341	Q342	Y343	K344		L347		A353		W358	S359	R360	P361		K371		E374		N383		N386		Y394		R405		D409	E410	W411	T412	F413		Q416	P417	E418	I419	W420	W421													
	Y202	R203	L204	V205	D206		W213		T220		V223	L224		K229	F230	V231	V232		A235	T236	D237	S238	M239		Q242		L246		G249		D255		F259		N264	N265		L273		M286		V289		Y292	Q293		N296		N299	D300		W306	T307		P312		T317	P318	I319	M320	
	D121	I122	S123		L129		I132		F136	G137	K138	L139		R145	S146	S147	E148		A149	G150		F155	A156	S157	N158	N159	I160	Y161		D162	Y163	T164	N165	E166	T167	A168	N169		D173	W174	R175	L176	A177	Q178	M179		N182	P183	G184	G185	T186	L187	E188	L189		G194		L198	R199	D200	N201

## 4 Data and refinement statistics

Property	Value	Source
Space group	C 2 2 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	131.90Å 214.80Å 220.20Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	8.00 – 3.20 38.95 – 3.20	Depositor EDS
% Data completeness (in resolution range)	96.1 (8.00-3.20) 98.8 (38.95-3.20)	Depositor EDS
$R_{merge}$	0.10	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	5.98 (at 3.18Å)	Xtriage
Refinement program	X-PLOR 3.1	Depositor
R, $R_{free}$	0.218 , 0.231 0.211 , 0.223	Depositor DCC
$R_{free}$ test set	4760 reflections (9.93%)	DCC
Wilson B-factor (Å <sup>2</sup> )	57.3	Xtriage
Anisotropy	0.282	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.30 , 102.0	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.47$ , $\langle L^2 \rangle = 0.30$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.90	EDS
Total number of atoms	10155	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	28.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.65% 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

### 5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: MG, GLC

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	0.77	1/3443 (0.0%)	0.95	2/4668 (0.0%)
1	B	0.77	2/3443 (0.1%)	0.95	2/4668 (0.0%)
1	C	0.77	1/3443 (0.0%)	0.95	2/4668 (0.0%)
All	All	0.77	4/10329 (0.0%)	0.95	6/14004 (0.0%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	2
1	B	0	2
1	C	0	2
All	All	0	6

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	358	TRP	CB-CG	-5.97	1.39	1.50
1	A	358	TRP	CB-CG	-5.96	1.39	1.50
1	C	358	TRP	CB-CG	-5.92	1.39	1.50
1	B	316	TRP	CB-CG	-5.00	1.41	1.50

The worst 5 of 6 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	289	VAL	CB-CA-C	-8.61	95.04	111.40
1	C	289	VAL	CB-CA-C	-8.61	95.05	111.40
1	B	289	VAL	CB-CA-C	-8.59	95.08	111.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	73	ASP	CB-CG-OD1	5.76	123.48	118.30
1	B	73	ASP	CB-CG-OD1	5.75	123.47	118.30

There are no chirality outliers.

5 of 6 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	360	ARG	Peptide
1	A	6	TYR	Sidechain
1	B	360	ARG	Peptide
1	B	6	TYR	Sidechain
1	C	6	TYR	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	3350	0	3070	124	0
1	B	3350	0	3070	127	0
1	C	3350	0	3070	128	0
2	A	34	0	30	3	0
2	B	34	0	30	3	0
2	C	34	0	30	3	0
3	A	1	0	0	0	0
3	B	1	0	0	1	0
3	C	1	0	0	1	0
All	All	10155	0	9300	355	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 19.

The worst 5 of 355 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:B:145:ARG:CD	1:C:71:GLN:HE22	1.70	1.04

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:353:ALA:HB2	1:C:58:PHE:CD2	1.98	0.99
1:A:71:GLN:HE22	1:C:145:ARG:CD	1.74	0.98
1:B:58:PHE:CD2	1:C:353:ALA:HB2	2.03	0.93
1:B:145:ARG:HD3	1:C:71:GLN:NE2	1.84	0.91

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	419/421 (100%)	380 (91%)	36 (9%)	3 (1%)	25	68
1	B	419/421 (100%)	380 (91%)	36 (9%)	3 (1%)	25	68
1	C	419/421 (100%)	380 (91%)	36 (9%)	3 (1%)	25	68
All	All	1257/1263 (100%)	1140 (91%)	108 (9%)	9 (1%)	25	68

5 of 9 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	224	LEU
1	A	264	ASN
1	B	224	LEU
1	B	264	ASN
1	C	224	LEU

### 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	340/340 (100%)	295 (87%)	45 (13%)	5	21
1	B	340/340 (100%)	295 (87%)	45 (13%)	5	21
1	C	340/340 (100%)	295 (87%)	45 (13%)	5	21
All	All	1020/1020 (100%)	885 (87%)	135 (13%)	5	21

5 of 135 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	159	ASN
1	B	289	VAL
1	C	307	THR
1	B	167	THR
1	B	206	ASP

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 50 such sidechains are listed below:

Mol	Chain	Res	Type
1	B	159	ASN
1	B	265	ASN
1	C	296	ASN
1	B	169	ASN
1	B	221	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 carbohydrates 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	GLC	A	431	2	11,11,12	0.51	0	13,15,17	1.10	1 (7%)
2	GLC	A	432	2	11,11,12	0.48	0	13,15,17	0.90	1 (7%)
2	GLC	A	433	2	12,12,12	0.85	0	17,17,17	0.97	2 (11%)
2	GLC	B	431	2	11,11,12	0.52	0	13,15,17	1.11	1 (7%)
2	GLC	B	432	2	11,11,12	0.49	0	13,15,17	0.90	1 (7%)
2	GLC	B	433	2	12,12,12	0.85	0	17,17,17	0.97	2 (11%)
2	GLC	C	431	2	11,11,12	0.50	0	13,15,17	1.11	1 (7%)
2	GLC	C	432	2	11,11,12	0.48	0	13,15,17	0.91	1 (7%)
2	GLC	C	433	2	12,12,12	0.84	0	17,17,17	0.97	2 (11%)

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	GLC	A	431	2	-	0/2/19/22	0/1/1/1
2	GLC	A	432	2	-	0/2/19/22	0/1/1/1
2	GLC	A	433	2	-	0/2/22/22	0/1/1/1
2	GLC	B	431	2	-	0/2/19/22	0/1/1/1
2	GLC	B	432	2	-	0/2/19/22	0/1/1/1
2	GLC	B	433	2	-	0/2/22/22	0/1/1/1
2	GLC	C	431	2	-	0/2/19/22	0/1/1/1
2	GLC	C	432	2	-	0/2/19/22	0/1/1/1
2	GLC	C	433	2	-	0/2/22/22	0/1/1/1

There are no bond length outliers.

The worst 5 of 12 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	433	GLC	C1-C2-C3	2.12	114.48	110.65
2	A	433	GLC	C1-C2-C3	2.13	114.51	110.65
2	C	433	GLC	C1-C2-C3	2.14	114.52	110.65
2	B	432	GLC	C1-O5-C5	2.26	115.28	112.17
2	C	433	GLC	C4-C3-C2	2.26	114.82	110.84

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

6 monomers are involved in 9 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	432	GLC	2	0
2	A	433	GLC	2	0
2	B	432	GLC	2	0
2	B	433	GLC	2	0
2	C	432	GLC	2	0
2	C	433	GLC	2	0

## 5.6 Ligand geometry [i](#)

Of 3 ligands modelled in this entry, 3 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

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, 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	421/421 (100%)	-0.45	1 (0%) 94 93	9, 26, 47, 58	45 (10%)
1	B	421/421 (100%)	-0.41	1 (0%) 94 93	9, 26, 47, 58	45 (10%)
1	C	421/421 (100%)	-0.46	0 100 100	9, 26, 47, 58	45 (10%)
All	All	1263/1263 (100%)	-0.44	2 (0%) 94 93	9, 27, 47, 58	135 (10%)

All (2) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	153	SER	2.4
1	A	387	ASN	2.0

### 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. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. 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	LLDF	B-factors(Å <sup>2</sup> )	Q<0.9
2	GLC	A	433	12/12	0.81	0.36	21.47	81,81,81,81	0
2	GLC	B	431	11/12	0.88	0.28	7.01	54,54,54,54	0
2	GLC	C	431	11/12	0.85	0.25	5.36	54,54,54,54	0
2	GLC	B	433	12/12	0.86	0.28	5.08	81,81,81,81	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
2	GLC	C	433	12/12	0.88	0.28	5.04	81,81,81,81	0
2	GLC	A	431	11/12	0.88	0.25	2.84	54,54,54,54	0
2	GLC	A	432	11/12	0.94	0.18	1.18	46,46,46,46	0
2	GLC	B	432	11/12	0.93	0.18	0.85	46,46,46,46	0
2	GLC	C	432	11/12	0.95	0.16	0.67	46,46,46,46	0

## 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. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. 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	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
3	MG	B	422	1/1	0.95	0.12	-	11,11,11,11	1
3	MG	A	422	1/1	0.96	0.13	-	11,11,11,11	1
3	MG	C	422	1/1	0.96	0.13	-	11,11,11,11	1

## 6.5 Other polymers [i](#)

There are no such residues in this entry.