



Full wwPDB X-ray Structure Validation Report ⓘ

Jun 13, 2024 – 03:57 PM EDT

PDB ID : 8V31
Title : Structure of Alistipes sp. 3-Keto-2-hydroxy-glucal-hydratase AL2
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Deposited on : 2023-11-25
Resolution : 2.65 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 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 : 4.02b-467
Xtriage (Phenix) : 1.13
EDS : 2.36.2
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) : 2.36.2

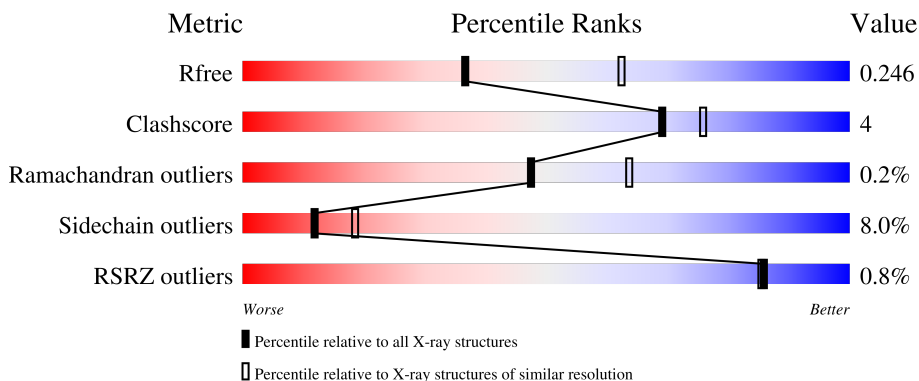
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.65 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	1332 (2.68-2.64)
Clashscore	141614	1374 (2.68-2.64)
Ramachandran outliers	138981	1349 (2.68-2.64)
Sidechain outliers	138945	1349 (2.68-2.64)
RSRZ outliers	127900	1318 (2.68-2.64)

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	277	 % 67% 18% .. 12%
1	C	277	 % 74% 15% .. 9%

2 Entry composition i

There are 3 unique types of molecules in this entry. The entry contains 3980 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 Glycosyl hydrolase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	243	Total	C	N	O	S	0	0	0
			1943	1245	327	365	6			
1	C	251	Total	C	N	O	S	0	0	0
			1995	1273	336	380	6			

There are 14 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	20	MET	-	initiating methionine	UNP A0A4Y1WGD9
A	291	HIS	-	expression tag	UNP A0A4Y1WGD9
A	292	HIS	-	expression tag	UNP A0A4Y1WGD9
A	293	HIS	-	expression tag	UNP A0A4Y1WGD9
A	294	HIS	-	expression tag	UNP A0A4Y1WGD9
A	295	HIS	-	expression tag	UNP A0A4Y1WGD9
A	296	HIS	-	expression tag	UNP A0A4Y1WGD9
C	20	MET	-	initiating methionine	UNP A0A4Y1WGD9
C	291	HIS	-	expression tag	UNP A0A4Y1WGD9
C	292	HIS	-	expression tag	UNP A0A4Y1WGD9
C	293	HIS	-	expression tag	UNP A0A4Y1WGD9
C	294	HIS	-	expression tag	UNP A0A4Y1WGD9
C	295	HIS	-	expression tag	UNP A0A4Y1WGD9
C	296	HIS	-	expression tag	UNP A0A4Y1WGD9

- Molecule 2 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

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

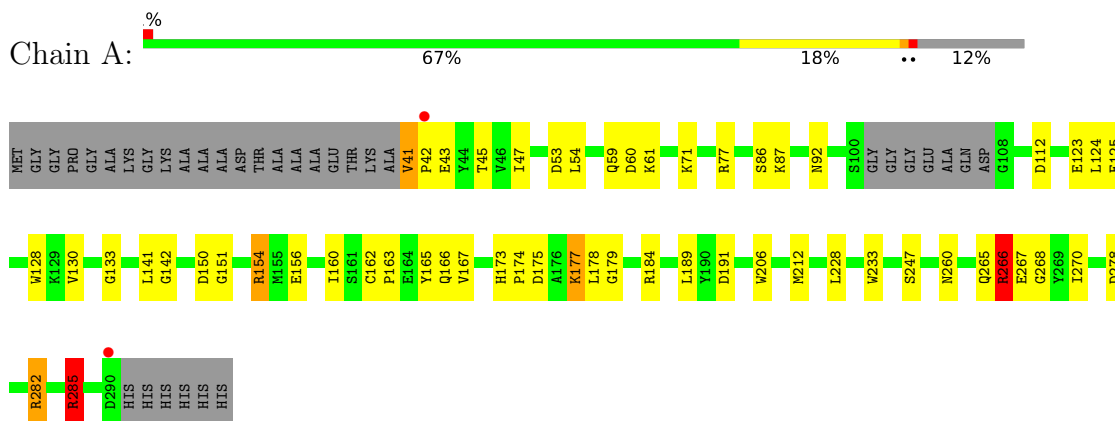
- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	17	Total 17	O 17	0	0
3	C	23	Total 23	O 23	0	0

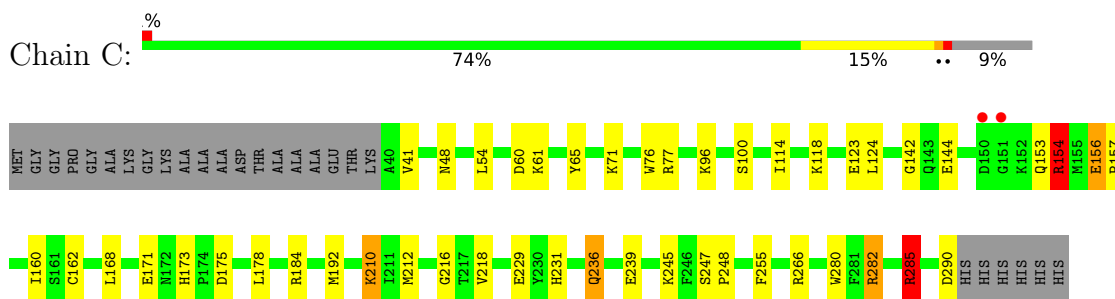
3 Residue-property plots [i](#)

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: Glycosyl hydrolase



- Molecule 1: Glycosyl hydrolase



4 Data and refinement statistics

Property	Value	Source
Space group	P 31 2 1	Depositor
Cell constants a, b, c, α , β , γ	95.09Å 95.09Å 159.54Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	47.54 – 2.65 47.54 – 2.65	Depositor EDS
% Data completeness (in resolution range)	99.1 (47.54-2.65) 98.3 (47.54-2.65)	Depositor EDS
R_{merge}	0.14	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.55 (at 2.65Å)	Xtrriage
Refinement program	REFMAC 5.8.0425	Depositor
R, R_{free}	0.197 , 0.244 0.206 , 0.246	Depositor DCC
R_{free} test set	1222 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å ²)	57.2	Xtrriage
Anisotropy	0.159	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.31 , 33.6	EDS
L-test for twinning ²	$\langle L \rangle = 0.51$, $\langle L^2 \rangle = 0.34$	Xtrriage
Estimated twinning fraction	0.033 for -h,-k,l	Xtrriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	3980	wwPDB-VP
Average B, all atoms (Å ²)	61.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.36% 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: MG

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	0.81	2/1999 (0.1%)	1.40	21/2711 (0.8%)
1	C	0.81	3/2052 (0.1%)	1.40	15/2783 (0.5%)
All	All	0.81	5/4051 (0.1%)	1.40	36/5494 (0.7%)

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	4
1	C	0	3
All	All	0	7

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	156	GLU	CD-OE2	-6.35	1.18	1.25
1	C	144	GLU	CD-OE2	5.72	1.31	1.25
1	C	229	GLU	CD-OE2	5.30	1.31	1.25
1	A	86	SER	CA-CB	-5.20	1.45	1.52
1	C	229	GLU	CD-OE1	5.06	1.31	1.25

All (36) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	184	ARG	NE-CZ-NH1	10.32	125.46	120.30
1	A	282	ARG	NE-CZ-NH1	-8.04	116.28	120.30
1	A	156	GLU	CG-CD-OE1	7.52	133.35	118.30
1	A	285	ARG	NE-CZ-NH2	-7.06	116.77	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	285	ARG	CG-CD-NE	-6.99	97.12	111.80
1	A	178	LEU	C-N-CA	-6.95	107.71	122.30
1	C	178	LEU	C-N-CA	-6.75	108.11	122.30
1	A	260	ASN	CB-CA-C	6.62	123.64	110.40
1	C	154	ARG	NE-CZ-NH2	-6.51	117.05	120.30
1	A	43	GLU	CB-CA-C	-6.39	97.61	110.40
1	C	236	GLN	CB-CA-C	6.27	122.94	110.40
1	A	60	ASP	CB-CG-OD2	-6.22	112.70	118.30
1	A	53	ASP	CB-CA-C	-6.21	97.98	110.40
1	A	45	THR	CA-CB-OG1	-6.19	96.00	109.00
1	C	156	GLU	OE1-CD-OE2	-6.08	116.00	123.30
1	A	278	ASP	CB-CG-OD1	5.93	123.64	118.30
1	C	282	ARG	NE-CZ-NH1	5.86	123.23	120.30
1	A	266	ARG	NE-CZ-NH2	-5.70	117.45	120.30
1	A	59	GLN	N-CA-CB	-5.55	100.61	110.60
1	C	184	ARG	NE-CZ-NH2	-5.51	117.55	120.30
1	A	87	LYS	CD-CE-NZ	-5.49	99.08	111.70
1	A	112	ASP	CB-CA-C	5.47	121.33	110.40
1	A	282	ARG	NE-CZ-NH2	5.38	122.99	120.30
1	C	239	GLU	CG-CD-OE1	-5.29	107.72	118.30
1	A	228	LEU	CB-CG-CD2	-5.28	102.03	111.00
1	C	236	GLN	N-CA-CB	-5.28	101.10	110.60
1	A	156	GLU	OE1-CD-OE2	-5.24	117.02	123.30
1	A	212	MET	CG-SD-CE	-5.23	91.83	100.20
1	C	144	GLU	OE1-CD-OE2	5.20	129.54	123.30
1	A	191	ASP	CB-CG-OD1	-5.19	113.63	118.30
1	A	285	ARG	CG-CD-NE	-5.12	101.06	111.80
1	C	239	GLU	CG-CD-OE2	5.09	128.49	118.30
1	C	154	ARG	NE-CZ-NH1	5.09	122.84	120.30
1	C	77	ARG	N-CA-CB	-5.06	101.50	110.60
1	A	123	GLU	CG-CD-OE1	-5.01	108.27	118.30
1	C	123	GLU	CG-CD-OE1	-5.01	108.28	118.30

There are no chirality outliers.

All (7) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	154	ARG	Sidechain
1	A	177	LYS	Peptide
1	A	285	ARG	Sidechain
1	A	77	ARG	Sidechain
1	C	154	ARG	Sidechain

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Mol	Chain	Res	Type	Group
1	C	282	ARG	Sidechain
1	C	285	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	1943	0	1835	15	0
1	C	1995	0	1877	13	0
2	A	1	0	0	0	0
2	C	1	0	0	0	0
3	A	17	0	0	1	0
3	C	23	0	0	0	0
All	All	3980	0	3712	28	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 (28) 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:173:HIS:CG	1:A:174:PRO:HD2	2.39	0.57
1:C:157:PRO:O	1:C:160:ILE:HG12	2.05	0.57
1:C:142:GLY:HA2	1:C:162:CYS:HB3	1.90	0.53
1:A:166:GLN:HG3	1:A:167:VAL:N	2.23	0.52
1:C:96:LYS:HE3	1:C:280:TRP:CZ2	2.44	0.52
1:A:233:TRP:CE2	1:A:266:ARG:HD2	2.46	0.51
1:A:206:TRP:CZ3	1:A:282:ARG:HG2	2.46	0.50
1:C:156:GLU:HB3	1:C:160:ILE:HD11	1.93	0.50
1:A:141:LEU:HA	1:A:268:GLY:HA3	1.93	0.50
1:C:168:LEU:HD11	1:C:173:HIS:CG	2.48	0.49
1:A:124:LEU:HD22	1:A:270:ILE:HD12	1.96	0.48
1:A:184:ARG:HB2	3:A:402:HOH:O	2.14	0.48
1:A:265:GLN:HB2	1:A:267:GLU:HG2	1.95	0.47
1:A:142:GLY:HA2	1:A:162:CYS:HB3	1.97	0.46
1:A:163:PRO:HB3	1:A:189:LEU:HD11	1.95	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:41:VAL:N	1:A:42:PRO:HD3	2.30	0.46
1:C:60:ASP:OD2	1:C:285:ARG:NH1	2.47	0.46
1:A:133:GLY:O	1:A:173:HIS:HD2	1.99	0.46
1:A:128:TRP:CE3	1:A:167:VAL:HG13	2.51	0.45
1:C:248:PRO:HD3	1:C:255:PHE:CD2	2.53	0.43
1:C:48:ASN:OD1	1:C:118:LYS:NZ	2.48	0.43
1:C:65:TYR:O	1:C:285:ARG:HA	2.19	0.42
1:C:76:TRP:HA	1:C:114:ILE:O	2.20	0.42
1:A:206:TRP:CH2	1:A:282:ARG:HG2	2.55	0.41
1:C:124:LEU:O	1:C:210:LYS:HA	2.20	0.41
1:A:179:GLY:HA3	1:A:184:ARG:HG3	2.03	0.41
1:C:216:GLY:O	1:C:231:HIS:HA	2.20	0.41
1:C:212:MET:O	1:C:218:VAL:HA	2.21	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	239/277 (86%)	229 (96%)	9 (4%)	1 (0%)	34	48
1	C	249/277 (90%)	235 (94%)	14 (6%)	0	100	100
All	All	488/554 (88%)	464 (95%)	23 (5%)	1 (0%)	47	64

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	151	GLY

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	203/224 (91%)	186 (92%)	17 (8%)	11	16
1	C	207/224 (92%)	191 (92%)	16 (8%)	13	20
All	All	410/448 (92%)	377 (92%)	33 (8%)	12	18

All (33) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	41	VAL
1	A	47	ILE
1	A	54	LEU
1	A	61	LYS
1	A	71	LYS
1	A	92	ASN
1	A	125	GLU
1	A	130	VAL
1	A	150	ASP
1	A	154	ARG
1	A	160	ILE
1	A	165	TYR
1	A	175	ASP
1	A	177	LYS
1	A	247	SER
1	A	266	ARG
1	A	285	ARG
1	C	41	VAL
1	C	54	LEU
1	C	61	LYS
1	C	71	LYS
1	C	100	SER
1	C	153	GLN
1	C	154	ARG
1	C	171	GLU
1	C	175	ASP
1	C	192	MET

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Mol	Chain	Res	Type
1	C	210	LYS
1	C	236	GLN
1	C	245	LYS
1	C	247	SER
1	C	266	ARG
1	C	290	ASP

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

Mol	Chain	Res	Type
1	C	236	GLN
1	C	260	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](#)

There are no monosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 2 ligands modelled in this entry, 2 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, 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	243/277 (87%)	-0.48	2 (0%) 86 85	43, 60, 93, 134	0
1	C	251/277 (90%)	-0.57	2 (0%) 86 85	42, 58, 90, 125	0
All	All	494/554 (89%)	-0.52	4 (0%) 86 85	42, 59, 91, 134	0

All (4) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	151	GLY	2.5
1	C	150	ASP	2.5
1	A	42	PRO	2.1
1	A	290	ASP	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](#)

There are no monosaccharides 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, 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	MG	A	301	1/1	0.94	0.10	50,50,50,50	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
2	MG	C	301	1/1	0.98	0.12	34,34,34,34	0

6.5 Other polymers [i](#)

There are no such residues in this entry.