



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 14, 2017 – 11:31 AM EST

PDB ID : 5GQU
Title : Crystal structure of branching enzyme from *Cyanothece* sp. ATCC 51142
Authors : Suzuki, R.; Suzuki, E.
Deposited on : 2016-08-08
Resolution : 1.85 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

<http://wwpdb.org/validation/2016/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 : 1.7.1 (RC1), CSD as537be (2016)
Xtriage (Phenix) : 1.9-1692
EDS : rb-20028442
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)
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) : rb-20028442

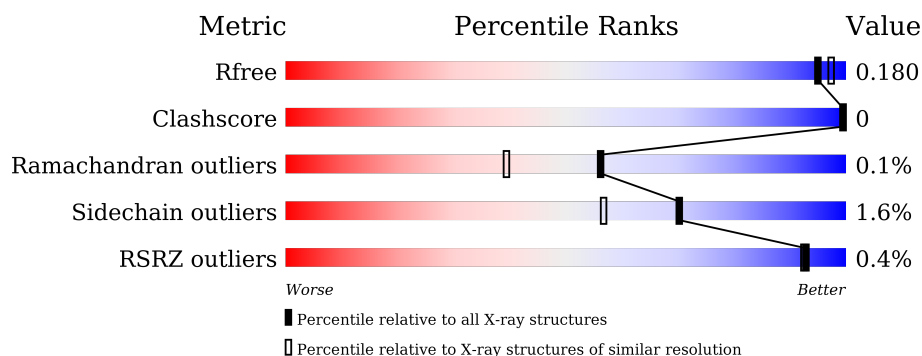
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.85 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}	91344	1745 (1.86-1.86)
Clashscore	102246	1898 (1.86-1.86)
Ramachandran outliers	100387	1875 (1.86-1.86)
Sidechain outliers	100360	1875 (1.86-1.86)
RSRZ outliers	91569	1747 (1.86-1.86)

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. 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	793	

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	GOL	A	801	-	-	-	X
2	GOL	A	802	-	-	-	X

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	GOL	A	803	-	-	-	X
2	GOL	A	804	-	-	-	X
2	GOL	A	806	-	-	-	X

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 7177 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 1,4-alpha-glucan branching enzyme GlgB.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	755	Total	C	N	O	S	0	1	0
			6279	4061	1043	1151	24			

There are 20 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-19	MET	-	initiating methionine	UNP B1WPM8
A	-18	GLY	-	expression tag	UNP B1WPM8
A	-17	SER	-	expression tag	UNP B1WPM8
A	-16	SER	-	expression tag	UNP B1WPM8
A	-15	HIS	-	expression tag	UNP B1WPM8
A	-14	HIS	-	expression tag	UNP B1WPM8
A	-13	HIS	-	expression tag	UNP B1WPM8
A	-12	HIS	-	expression tag	UNP B1WPM8
A	-11	HIS	-	expression tag	UNP B1WPM8
A	-10	HIS	-	expression tag	UNP B1WPM8
A	-9	SER	-	expression tag	UNP B1WPM8
A	-8	SER	-	expression tag	UNP B1WPM8
A	-7	GLY	-	expression tag	UNP B1WPM8
A	-6	LEU	-	expression tag	UNP B1WPM8
A	-5	VAL	-	expression tag	UNP B1WPM8
A	-4	PRO	-	expression tag	UNP B1WPM8
A	-3	ARG	-	expression tag	UNP B1WPM8
A	-2	GLY	-	expression tag	UNP B1WPM8
A	-1	SER	-	expression tag	UNP B1WPM8
A	0	HIS	-	expression tag	UNP B1WPM8

- Molecule 2 is GLYCEROL (three-letter code: GOL) (formula: C₃H₈O₃).



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

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

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	4	Total	Mg	0	0
			4	4		


- Molecule 4 is water.

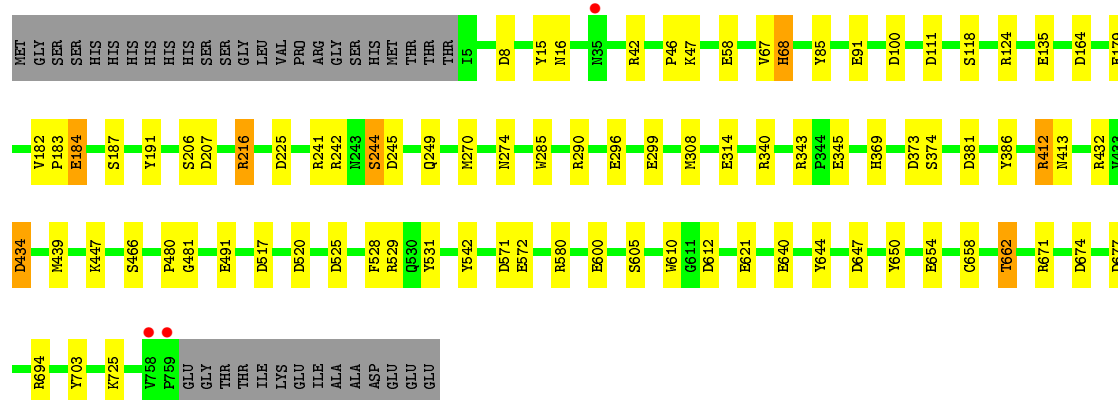
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	852	Total	O	0	0
			852	852		

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 errors 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: 1,4-alpha-glucan branching enzyme GlgB

Chain A:  84% 10% 5%



4 Data and refinement statistics

Property	Value	Source
Space group	P 41 21 2	Depositor
Cell constants a, b, c, α , β , γ	133.75Å 133.75Å 185.90Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	47.29 – 1.85 38.50 – 1.85	Depositor EDS
% Data completeness (in resolution range)	99.9 (47.29-1.85) 100.0 (38.50-1.85)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	9.72 (at 1.85Å)	Xtriage
Refinement program	REFMAC 5.8.0049	Depositor
R, R_{free}	0.147 , 0.170 0.160 , 0.180	Depositor DCC
R_{free} test set	7187 reflections (5.28%)	DCC
Wilson B-factor (Å ²)	21.5	Xtriage
Anisotropy	0.020	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.38 , 48.1	EDS
L-test for twinning ²	$\langle L \rangle = 0.51$, $\langle L^2 \rangle = 0.34$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.97	EDS
Total number of atoms	7177	wwPDB-VP
Average B, all atoms (Å ²)	25.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.63% 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: GOL, 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	1.44	43/6502 (0.7%)	1.29	47/8848 (0.5%)

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

All (43) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	242	ARG	CZ-NH1	9.75	1.45	1.33
1	A	58	GLU	CD-OE2	9.40	1.35	1.25
1	A	285	TRP	CB-CG	-8.90	1.34	1.50
1	A	299	GLU	CD-OE2	8.57	1.35	1.25
1	A	658	CYS	CB-SG	-8.21	1.68	1.82
1	A	654	GLU	CD-OE2	-8.03	1.16	1.25
1	A	343	ARG	CZ-NH2	-7.83	1.22	1.33
1	A	412	ARG	CZ-NH2	7.67	1.43	1.33
1	A	412	ARG	CD-NE	-7.56	1.33	1.46
1	A	187	SER	CB-OG	-7.50	1.32	1.42
1	A	91	GLU	CD-OE1	-7.12	1.17	1.25
1	A	135	GLU	CD-OE2	7.05	1.33	1.25
1	A	703	TYR	CG-CD1	6.90	1.48	1.39
1	A	662	THR	CB-CG2	-6.77	1.30	1.52
1	A	481	GLY	CA-C	6.58	1.62	1.51
1	A	58	GLU	CG-CD	6.51	1.61	1.51
1	A	654	GLU	CD-OE1	-6.50	1.18	1.25
1	A	621	GLU	CD-OE1	-6.50	1.18	1.25

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	85	TYR	CB-CG	-6.43	1.42	1.51
1	A	481	GLY	N-CA	6.27	1.55	1.46
1	A	314	GLU	CD-OE1	-6.12	1.19	1.25
1	A	605	SER	CB-OG	-6.05	1.34	1.42
1	A	610	TRP	CZ3-CH2	-6.04	1.30	1.40
1	A	206	SER	CB-OG	5.93	1.50	1.42
1	A	542	TYR	CG-CD2	5.87	1.46	1.39
1	A	434	ASP	N-CA	5.84	1.58	1.46
1	A	466	SER	CB-OG	-5.81	1.34	1.42
1	A	600	GLU	CG-CD	5.74	1.60	1.51
1	A	542	TYR	CB-CG	5.61	1.60	1.51
1	A	274	ASN	N-CA	5.56	1.57	1.46
1	A	135	GLU	CG-CD	5.45	1.60	1.51
1	A	531	TYR	CE1-CZ	-5.40	1.31	1.38
1	A	244	SER	CB-OG	-5.32	1.35	1.42
1	A	572	GLU	CD-OE2	-5.32	1.19	1.25
1	A	179	GLU	CG-CD	5.31	1.59	1.51
1	A	285	TRP	CG-CD1	5.27	1.44	1.36
1	A	296	GLU	CD-OE2	5.23	1.31	1.25
1	A	15	TYR	CG-CD1	5.20	1.46	1.39
1	A	374	SER	CB-OG	-5.18	1.35	1.42
1	A	179	GLU	CD-OE2	-5.13	1.20	1.25
1	A	644	TYR	CE1-CZ	-5.10	1.31	1.38
1	A	191	TYR	CB-CG	5.05	1.59	1.51
1	A	650	TYR	CB-CG	-5.05	1.44	1.51

All (47) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	412	ARG	NE-CZ-NH2	-24.49	108.05	120.30
1	A	412	ARG	NE-CZ-NH1	17.23	128.92	120.30
1	A	242	ARG	NE-CZ-NH2	-16.65	111.98	120.30
1	A	412	ARG	CD-NE-CZ	12.67	141.33	123.60
1	A	612	ASP	CB-CG-OD1	-9.27	109.96	118.30
1	A	580	ARG	NE-CZ-NH1	8.23	124.41	120.30
1	A	658	CYS	CB-CA-C	7.86	126.12	110.40
1	A	480	PRO	C-N-CA	-7.51	106.53	122.30
1	A	671	ARG	NE-CZ-NH1	7.16	123.88	120.30
1	A	340	ARG	NE-CZ-NH2	7.01	123.80	120.30
1	A	674	ASP	CB-CG-OD2	-6.81	112.17	118.30
1	A	207	ASP	CB-CG-OD2	-6.80	112.18	118.30
1	A	8	ASP	CB-CG-OD1	6.77	124.40	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	571	ASP	CB-CG-OD1	6.49	124.14	118.30
1	A	381	ASP	CB-CG-OD1	6.46	124.11	118.30
1	A	225	ASP	CB-CG-OD2	-6.33	112.61	118.30
1	A	674	ASP	CB-CG-OD1	6.32	123.99	118.30
1	A	662	THR	N-CA-CB	-6.28	98.37	110.30
1	A	647	ASP	CB-CG-OD1	6.27	123.94	118.30
1	A	520	ASP	CB-CG-OD2	-6.16	112.76	118.30
1	A	434	ASP	CB-CG-OD2	5.79	123.51	118.30
1	A	58	GLU	CA-CB-CG	5.70	125.93	113.40
1	A	100	ASP	CB-CG-OD2	-5.67	113.19	118.30
1	A	517	ASP	CB-CG-OD2	-5.63	113.23	118.30
1	A	216	ARG	NE-CZ-NH1	5.62	123.11	120.30
1	A	290	ARG	NE-CZ-NH2	5.61	123.11	120.30
1	A	677	ASP	CB-CG-OD2	-5.56	113.30	118.30
1	A	345	GLU	OE1-CD-OE2	-5.53	116.66	123.30
1	A	529	ARG	NE-CZ-NH1	5.51	123.06	120.30
1	A	68	HIS	N-CA-C	5.50	125.85	111.00
1	A	118	SER	CA-CB-OG	-5.46	96.45	111.20
1	A	111	ASP	CB-CG-OD1	5.46	123.21	118.30
1	A	640	GLU	OE1-CD-OE2	5.44	129.83	123.30
1	A	386	TYR	CB-CG-CD2	5.42	124.25	121.00
1	A	241	ARG	NE-CZ-NH2	-5.40	117.60	120.30
1	A	432	ARG	NE-CZ-NH1	5.37	122.98	120.30
1	A	164	ASP	CB-CG-OD1	5.35	123.12	118.30
1	A	242	ARG	NH1-CZ-NH2	5.31	125.24	119.40
1	A	439	MET	CG-SD-CE	-5.29	91.73	100.20
1	A	525	ASP	CB-CG-OD1	5.28	123.05	118.30
1	A	124	ARG	NE-CZ-NH2	5.22	122.91	120.30
1	A	245	ASP	CB-CG-OD2	-5.17	113.65	118.30
1	A	270	MET	CG-SD-CE	5.15	108.44	100.20
1	A	67	VAL	CG1-CB-CG2	-5.13	102.69	110.90
1	A	694	ARG	NE-CZ-NH2	5.12	122.86	120.30
1	A	308	MET	CA-CB-CG	5.12	122.00	113.30
1	A	42	ARG	NE-CZ-NH2	-5.02	117.79	120.30

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	184	GLU	Mainchain
1	A	412	ARG	Sidechain

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	6279	0	5865	4	0
2	A	42	0	56	2	0
3	A	4	0	0	0	0
4	A	852	0	0	1	0
All	All	7177	0	5921	5	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 0.

All (5) 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:46:PRO:O	1:A:47:LYS:HB2	2.05	0.56
2:A:801:GOL:H2	4:A:967:HOH:O	2.16	0.45
1:A:182:VAL:HA	1:A:183:PRO:HD2	1.94	0.42
1:A:244:SER:HB3	1:A:249:GLN:NE2	2.36	0.40
1:A:528:PHE:CD2	2:A:802:GOL:H2	2.57	0.40

There are no symmetry-related clashes.

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

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	754/793 (95%)	734 (97%)	19 (2%)	1 (0%)	56 39

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	68	HIS

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	669/700 (96%)	658 (98%)	11 (2%)	70 57

All (11) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	16	ASN
1	A	184	GLU
1	A	216	ARG
1	A	369	HIS
1	A	373	ASP
1	A	413	ASN
1	A	434	ASP
1	A	447	LYS
1	A	491	GLU
1	A	662	THR
1	A	725	LYS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (3) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	9	GLN
1	A	16	ASN
1	A	634	ASN

5.3.3 RNA [i](#)

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 ⓘ

There are no carbohydrates in this entry.

5.6 Ligand geometry ⓘ

Of 11 ligands modelled in this entry, 4 are monoatomic - leaving 7 for Mogul analysis.

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	GOL	A	801	-	5,5,5	1.72	2 (40%)	5,5,5	2.59	2 (40%)
2	GOL	A	802	-	5,5,5	2.64	3 (60%)	5,5,5	2.05	1 (20%)
2	GOL	A	803	-	5,5,5	0.91	0	5,5,5	0.41	0
2	GOL	A	804	-	5,5,5	1.05	0	5,5,5	1.26	1 (20%)
2	GOL	A	805	-	5,5,5	0.36	0	5,5,5	1.20	1 (20%)
2	GOL	A	806	-	5,5,5	0.80	0	5,5,5	1.75	1 (20%)
2	GOL	A	807	-	5,5,5	2.01	2 (40%)	5,5,5	2.06	2 (40%)

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	GOL	A	801	-	-	0/4/4/4	0/0/0/0
2	GOL	A	802	-	-	0/4/4/4	0/0/0/0
2	GOL	A	803	-	-	0/4/4/4	0/0/0/0
2	GOL	A	804	-	-	0/4/4/4	0/0/0/0
2	GOL	A	805	-	-	0/4/4/4	0/0/0/0
2	GOL	A	806	-	-	0/4/4/4	0/0/0/0
2	GOL	A	807	-	-	0/4/4/4	0/0/0/0

All (7) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	807	GOL	O2-C2	-2.26	1.36	1.43
2	A	801	GOL	C3-C2	2.11	1.60	1.52
2	A	802	GOL	O2-C2	2.65	1.51	1.43
2	A	801	GOL	O2-C2	2.76	1.51	1.43
2	A	802	GOL	C3-C2	2.77	1.63	1.52
2	A	807	GOL	O3-C3	3.70	1.58	1.42
2	A	802	GOL	O3-C3	4.09	1.60	1.42

All (8) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	805	GOL	O1-C1-C2	2.02	120.23	109.97
2	A	804	GOL	O3-C3-C2	2.44	122.34	109.97
2	A	807	GOL	O3-C3-C2	2.65	123.42	109.97
2	A	807	GOL	O1-C1-C2	3.02	125.31	109.97
2	A	801	GOL	O1-C1-C2	3.15	125.93	109.97
2	A	806	GOL	C3-C2-C1	3.24	124.71	111.06
2	A	802	GOL	O3-C3-C2	3.68	128.63	109.97
2	A	801	GOL	O2-C2-C3	4.26	128.91	108.47

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

2 monomers are involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	801	GOL	1	0
2	A	802	GOL	1	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 ⓘ

6.1 Protein, DNA and RNA chains ⓘ

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	755/793 (95%)	-0.44	3 (0%) 93 92	14, 21, 42, 77	0

All (3) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	758	VAL	3.7
1	A	35	ASN	3.5
1	A	759	PRO	2.5

6.2 Non-standard residues in protein, DNA, RNA chains ⓘ

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

6.3 Carbohydrates ⓘ

There are no carbohydrates in this entry.

6.4 Ligands ⓘ

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, 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	LLDF	B-factors(Å ²)	Q<0.9
2	GOL	A	801	6/6	0.75	0.28	12.06	33,41,43,51	0
2	GOL	A	804	6/6	0.83	0.32	8.23	37,54,58,58	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
2	GOL	A	806	6/6	0.91	0.21	4.77	33,53,59,60	0
2	GOL	A	803	6/6	0.94	0.12	2.30	33,34,35,35	0
2	GOL	A	802	6/6	0.85	0.16	2.04	27,43,55,55	0
2	GOL	A	805	6/6	0.87	0.30	1.90	45,53,58,58	0
2	GOL	A	807	6/6	0.92	0.14	1.73	27,41,44,45	0
3	MG	A	808	1/1	0.98	0.13	-	40,40,40,40	0
3	MG	A	809	1/1	0.98	0.04	-	22,22,22,22	0
3	MG	A	810	1/1	0.98	0.07	-	23,23,23,23	0
3	MG	A	811	1/1	0.89	0.26	-	44,44,44,44	0

6.5 Other polymers [i](#)

There are no such residues in this entry.