



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 06:28 PM UTC

PDB ID : 7O77 / pdb_00007o77
Title : Structure of the PL6 family alginate lyase Pat13640 from *Pseudoalteromonas atlantica* T6c
Authors : Ballut, L.; Violot, S.; Carrique, L.; Aghajari, N.
Deposited on : 2021-04-13
Resolution : 2.32 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 : 4-5-2 with Phenix2.0
Mogul : 2022.3.0, CSD as543be (2022)
Xtriage (Phenix) : 2.0
EDS : 3.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4 : 9.0.010 (Gargrove)
Density-Fitness : 1.0.12
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

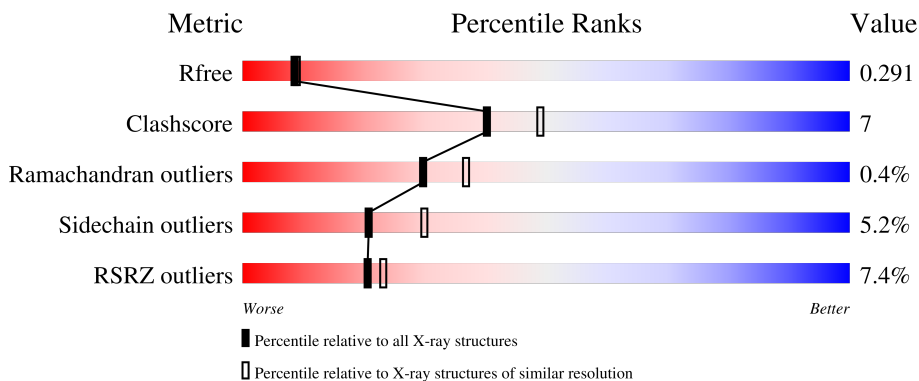
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.32 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}	180053	7754 (2.34-2.30)
Clashscore	190562	8383 (2.34-2.30)
Ramachandran outliers	187476	8303 (2.34-2.30)
Sidechain outliers	187428	8303 (2.34-2.30)
RSRZ outliers	180081	7760 (2.34-2.30)

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	720	

2 Entry composition [i](#)

There are 3 unique types of molecules in this entry. The entry contains 5477 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.

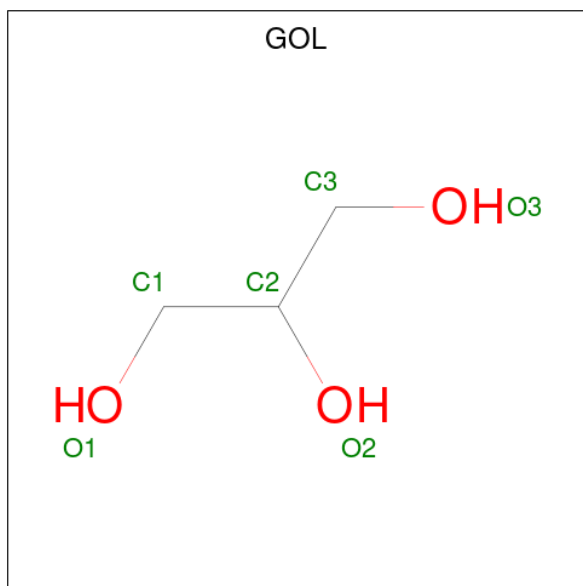
- Molecule 1 is a protein called Poly(Beta-D-mannuronate) lyase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	720	5418	3384	928	1093	13	0	0	0

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	37	MET	-	initiating methionine	UNP Q15PP6

- Molecule 2 is GLYCEROL (CCD ID: GOL) (formula: C₃H₈O₃).



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

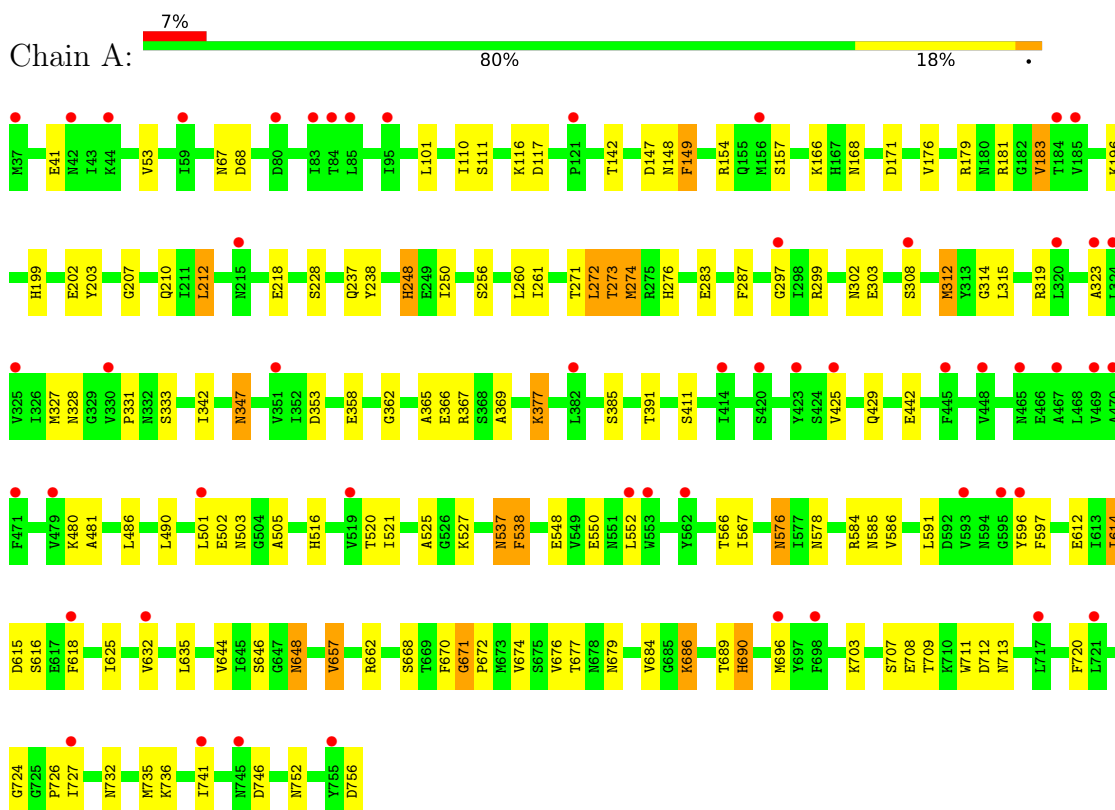
- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	53	Total 53	O 53	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: Poly(Beta-D-mannuronate) lyase



4 Data and refinement statistics

Property	Value	Source
Space group	P 31 2 1	Depositor
Cell constants a, b, c, α , β , γ	79.53Å 79.53Å 269.47Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	48.16 – 2.32 48.16 – 2.32	Depositor EDS
% Data completeness (in resolution range)	96.0 (48.16-2.32) 96.0 (48.16-2.32)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.06 (at 2.32Å)	Xtrriage
Refinement program	BUSTER 2.10.3 (29-NOV-2019)	Depositor
R, R_{free}	0.250 , 0.282 0.260 , 0.291	Depositor DCC
R_{free} test set	2190 reflections (4.99%)	wwPDB-VP
Wilson B-factor (Å ²)	64.7	Xtrriage
Anisotropy	0.570	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.28 , 40.1	EDS
L-test for twinning ²	$\langle L \rangle = 0.51$, $\langle L^2 \rangle = 0.34$	Xtrriage
Estimated twinning fraction	0.029 for -h,-k,l	Xtrriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	5477	wwPDB-VP
Average B, all atoms (Å ²)	79.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.85% 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

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	0.78	2/5521 (0.0%)	1.14	24/7520 (0.3%)

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	525	ALA	CA-C	11.06	1.62	1.53
1	A	319	ARG	CA-C	5.28	1.57	1.52

All (24) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	576	ASN	CA-CB-CG	7.74	120.34	112.60
1	A	250	ILE	N-CA-C	-6.99	104.04	110.82
1	A	333	SER	N-CA-C	6.61	118.03	109.64
1	A	538	PHE	CA-CB-CG	6.21	120.01	113.80
1	A	591	LEU	N-CA-C	-6.17	102.88	110.65
1	A	657	VAL	N-CA-C	-6.12	104.78	110.53
1	A	41	GLU	CB-CG-CD	5.69	122.27	112.60
1	A	272	LEU	N-CA-C	-5.61	99.39	108.41
1	A	377	LYS	N-CA-C	5.55	118.50	109.24
1	A	365	ALA	CA-C-N	5.50	128.12	120.63
1	A	365	ALA	C-N-CA	5.50	128.12	120.63
1	A	166	LYS	CA-C-N	5.45	129.86	122.07
1	A	166	LYS	C-N-CA	5.45	129.86	122.07
1	A	303	GLU	N-CA-C	5.44	118.86	110.42
1	A	274	MET	N-CA-C	-5.31	101.65	109.62
1	A	720	PHE	CA-CB-CG	-5.31	108.49	113.80
1	A	597	PHE	CA-CB-CG	5.22	119.02	113.80
1	A	149	PHE	CA-CB-CG	-5.09	108.70	113.80
1	A	648	ASN	N-CA-C	5.05	117.83	109.85

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	614	ILE	N-CA-C	5.03	115.96	108.46
1	A	712	ASP	CA-CB-CG	5.02	117.62	112.60
1	A	347	ASN	CA-CB-CG	5.02	117.62	112.60
1	A	327	MET	N-CA-C	5.02	117.15	110.53
1	A	674	VAL	N-CA-C	5.01	115.80	108.53

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	5418	0	5100	69	0
2	A	6	0	8	0	0
3	A	53	0	0	1	0
All	All	5477	0	5108	69	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 7.

All (69) 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:736:LYS:HA	1:A:756:ASP:HA	1.56	0.88
1:A:148:ASN:ND2	1:A:179:ARG:NH1	2.37	0.71
1:A:248:HIS:CE1	1:A:668:SER:HA	2.30	0.67
1:A:657:VAL:HG23	1:A:684:VAL:HG11	1.77	0.67
1:A:347:ASN:HD22	1:A:377:LYS:H	1.41	0.65
1:A:176:VAL:HG12	1:A:207:GLY:HA3	1.80	0.62
1:A:690:HIS:CD2	1:A:690:HIS:H	2.16	0.62
1:A:711:TRP:HB2	1:A:735:MET:HG2	1.82	0.61
1:A:287:PHE:HB2	1:A:312:MET:HG3	1.84	0.59
1:A:670:PHE:O	1:A:671:GLY:O	2.21	0.57
1:A:181:ARG:HG2	1:A:212:LEU:CD1	2.34	0.57
1:A:312:MET:HG2	1:A:315:LEU:HD11	1.87	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:690:HIS:H	1:A:690:HIS:HD2	1.54	0.56
1:A:314:GLY:HA2	1:A:353:ASP:O	2.04	0.56
1:A:538:PHE:HB2	1:A:567:ILE:O	2.07	0.54
1:A:67:ASN:OD1	1:A:68:ASP:OD1	2.26	0.53
1:A:724:GLY:O	1:A:726:PRO:HD3	2.08	0.53
1:A:347:ASN:ND2	1:A:377:LYS:H	2.06	0.52
1:A:183:VAL:HG13	1:A:218:GLU:HG2	1.91	0.52
1:A:616:SER:HB2	1:A:648:ASN:ND2	2.24	0.52
1:A:260:LEU:HD12	1:A:272:LEU:HD21	1.92	0.52
1:A:168:ASN:HD22	1:A:199:HIS:CE1	2.28	0.52
1:A:618:PHE:HE1	1:A:648:ASN:HD22	1.58	0.51
1:A:312:MET:HG2	1:A:315:LEU:CD1	2.41	0.51
1:A:148:ASN:HD21	1:A:179:ARG:NH1	2.06	0.50
1:A:585:ASN:HA	1:A:615:ASP:O	2.11	0.50
1:A:101:LEU:HD21	1:A:110:ILE:HG12	1.93	0.50
1:A:550:GLU:HG3	1:A:584:ARG:HB3	1.93	0.50
1:A:676:VAL:HG11	1:A:696:MET:HE1	1.94	0.49
1:A:210:GLN:HE22	1:A:578:ASN:H	1.60	0.49
1:A:283:GLU:CB	1:A:308:SER:O	2.61	0.49
1:A:616:SER:HB2	1:A:648:ASN:HD21	1.77	0.49
1:A:358:GLU:OE1	1:A:391:THR:HB	2.11	0.49
1:A:331:PRO:HG3	1:A:369:ALA:HB2	1.96	0.48
1:A:686:LYS:HD2	1:A:713:ASN:O	2.13	0.48
1:A:228:SER:HB2	1:A:276:HIS:HB3	1.96	0.47
1:A:273:THR:HG21	1:A:299:ARG:HH21	1.77	0.47
1:A:362:GLY:O	1:A:367:ARG:HD2	2.16	0.46
1:A:481:ALA:HB2	1:A:505:ALA:HB1	1.97	0.46
1:A:171:ASP:HA	1:A:202:GLU:O	2.16	0.46
1:A:111:SER:HA	1:A:142:THR:O	2.15	0.45
1:A:503:ASN:HB3	1:A:527:LYS:CB	2.47	0.45
1:A:157:SER:HB3	1:A:181:ARG:HB2	1.99	0.45
1:A:148:ASN:HD21	1:A:179:ARG:HH11	1.63	0.44
1:A:486:LEU:HD13	1:A:501:LEU:HD11	1.99	0.44
1:A:679:ASN:H	1:A:709:THR:HG22	1.81	0.44
1:A:203:TYR:HA	1:A:238:TYR:O	2.17	0.44
1:A:596:TYR:CE1	1:A:689:THR:HB	2.53	0.44
1:A:480:LYS:HA	1:A:502:GLU:OE2	2.19	0.43
1:A:237:GLN:HA	1:A:261:ILE:O	2.18	0.43
1:A:724:GLY:C	1:A:726:PRO:HD3	2.43	0.43
1:A:521:ILE:HG22	1:A:552:LEU:HD11	2.01	0.43
1:A:181:ARG:HG2	1:A:212:LEU:HD11	2.01	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:614:ILE:HA	1:A:646:SER:O	2.19	0.42
1:A:202:GLU:HA	1:A:237:GLN:O	2.19	0.42
1:A:271:THR:OG1	1:A:273:THR:HG22	2.20	0.42
1:A:537:ASN:HA	1:A:566:THR:O	2.19	0.42
1:A:625:ILE:HB	1:A:657:VAL:O	2.18	0.42
1:A:520:THR:HG23	1:A:548:GLU:HG3	2.02	0.42
1:A:707:SER:O	1:A:709:THR:HG23	2.19	0.42
1:A:612:GLU:HG2	1:A:644:VAL:HB	2.01	0.41
1:A:116:LYS:HA	1:A:147:ASP:O	2.20	0.41
1:A:516:HIS:HD2	3:A:923:HOH:O	2.03	0.41
1:A:677:THR:HA	1:A:707:SER:O	2.21	0.41
1:A:297:GLY:HA3	1:A:323:ALA:O	2.20	0.41
1:A:732:ASN:H	1:A:752:ASN:HB2	1.84	0.41
1:A:312:MET:HE2	1:A:312:MET:HB2	1.96	0.41
1:A:662:ARG:HD3	1:A:672:PRO:HD3	2.03	0.41
1:A:154:ARG:HB3	1:A:576:ASN:HA	2.02	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	718/720 (100%)	676 (94%)	39 (5%)	3 (0%)	30 37

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	671	GLY
1	A	117	ASP
1	A	741	ILE

5.3.2 Protein sidechains

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	575/613 (94%)	545 (95%)	30 (5%)	21 30

All (30) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	53	VAL
1	A	149	PHE
1	A	183	VAL
1	A	196	LYS
1	A	212	LEU
1	A	248	HIS
1	A	256	SER
1	A	273	THR
1	A	274	MET
1	A	302	ASN
1	A	312	MET
1	A	328	ASN
1	A	342	ILE
1	A	366	GLU
1	A	385	SER
1	A	411	SER
1	A	425	VAL
1	A	429	GLN
1	A	442	GLU
1	A	490	LEU
1	A	537	ASN
1	A	586	VAL
1	A	632	VAL
1	A	635	LEU
1	A	686	LYS
1	A	690	HIS
1	A	703	LYS
1	A	708	GLU
1	A	727	ILE
1	A	746	ASP

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (18) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	67	ASN
1	A	148	ASN
1	A	168	ASN
1	A	210	GLN
1	A	248	HIS
1	A	347	ASN
1	A	478	HIS
1	A	494	GLN
1	A	516	HIS
1	A	517	HIS
1	A	537	ASN
1	A	540	ASN
1	A	580	ASN
1	A	603	ASN
1	A	620	ASN
1	A	648	ASN
1	A	690	HIS
1	A	702	GLN

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 oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

1 ligand is 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	GOL	A	801	-	5,5,5	0.10	0	5,5,5	0.30	0

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	-	-	2/4/4/4	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (2) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	801	GOL	O1-C1-C2-C3
2	A	801	GOL	O1-C1-C2-O2

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

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	720/720 (100%)	0.80	53 (7%) 20 23	58, 77, 102, 114	0

All (53) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	717	LEU	3.8
1	A	324	LEU	3.7
1	A	297	GLY	3.3
1	A	121	PRO	3.2
1	A	469	VAL	3.1
1	A	552	LEU	3.1
1	A	80	ASP	3.0
1	A	320	LEU	3.0
1	A	414	ILE	3.0
1	A	562	TYR	3.0
1	A	470	ALA	2.9
1	A	698	PHE	2.8
1	A	465	ASN	2.8
1	A	85	LEU	2.7
1	A	84	THR	2.7
1	A	721	LEU	2.7
1	A	215	ASN	2.6
1	A	553	TRP	2.6
1	A	755	TYR	2.6
1	A	632	VAL	2.6
1	A	59	ILE	2.6
1	A	42	ASN	2.5
1	A	696	MET	2.5
1	A	479	VAL	2.5
1	A	382	LEU	2.5
1	A	618	PHE	2.4
1	A	83	ILE	2.4

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Mol	Chain	Res	Type	RSRZ
1	A	425	VAL	2.4
1	A	593	VAL	2.4
1	A	741	ILE	2.4
1	A	37	MET	2.4
1	A	330	VAL	2.4
1	A	501	LEU	2.4
1	A	95	ILE	2.3
1	A	423	TYR	2.3
1	A	595	GLY	2.3
1	A	596	TYR	2.3
1	A	325	VAL	2.3
1	A	445	PHE	2.2
1	A	351	VAL	2.2
1	A	471	PHE	2.2
1	A	156	MET	2.1
1	A	727	ILE	2.1
1	A	185	VAL	2.1
1	A	519	VAL	2.1
1	A	308	SER	2.1
1	A	420	SER	2.1
1	A	44	LYS	2.1
1	A	323	ALA	2.1
1	A	467	ALA	2.0
1	A	448	VAL	2.0
1	A	184	THR	2.0
1	A	745	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 [\(i\)](#)

There are no oligosaccharides 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(\AA^2)	Q<0.9
2	GOL	A	801	6/6	0.79	0.16	79,79,80,80	0

6.5 Other polymers [i](#)

There are no such residues in this entry.