



# wwPDB X-ray Structure Validation Summary Report ⓘ

Mar 9, 2026 – 09:37 PM UTC

PDB ID : 6AA1 / pdb\_00006aa1  
Title : Crystal structure of putative amino acid binding periplasmic ABC transporter protein from Candidatus Liberibacter asiaticus bound with citrate  
Authors : Kumar, P.; Kesari, P.; Ghosh, D.K.; Kumar, P.; Sharma, A.K.  
Deposited on : 2018-07-16  
Resolution : 1.86 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

<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>.

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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

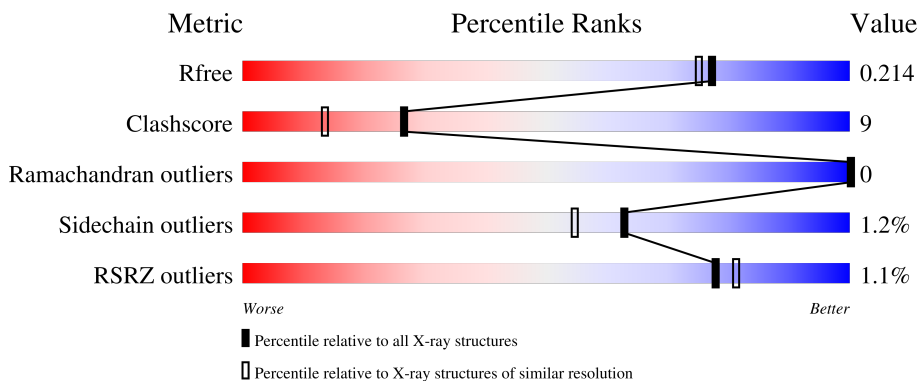
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 1.86 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	3428 (1.86-1.86)
Clashscore	190562	3579 (1.86-1.86)
Ramachandran outliers	187476	3553 (1.86-1.86)
Sidechain outliers	187428	3553 (1.86-1.86)
RSRZ outliers	180081	3429 (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 of 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	241	 80% 17% •
1	B	241	 2% 87% 9% ••

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	322	-	-	X	-
3	EDO	B	307	-	-	X	-
4	CIT	A	321	-	X	-	-

## 2 Entry composition [i](#)

There are 6 unique types of molecules in this entry. The entry contains 4476 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.

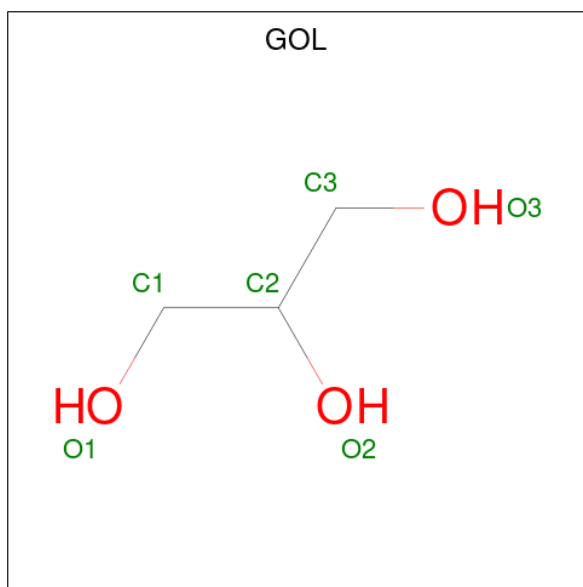
- Molecule 1 is a protein called Putative amino acid-binding periplasmic ABC transporter protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	234	Total 2002	C 1265	N 359	O 370	S 8	0	15	0
1	B	234	Total 1994	C 1262	N 353	O 370	S 9	0	15	0

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	1	MET	-	initiating methionine	UNP C6XGT2
B	1	MET	-	initiating methionine	UNP C6XGT2

- Molecule 2 is GLYCEROL (CCD ID: GOL) (formula: C<sub>3</sub>H<sub>8</sub>O<sub>3</sub>).



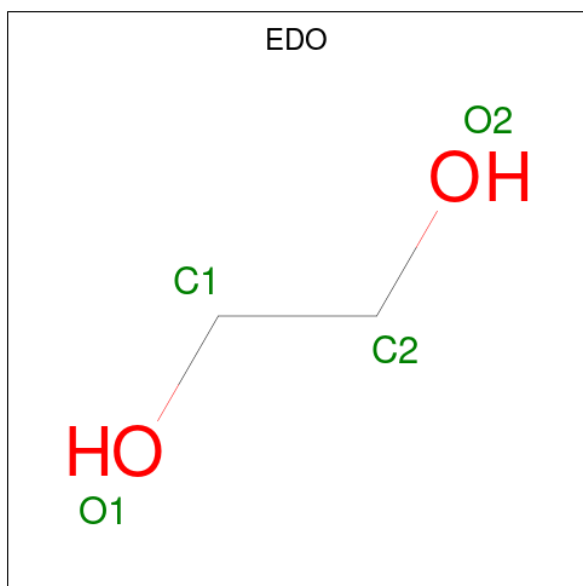
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	C	O		
2	A	1	Total 6	C 3	O 3	0	0

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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	B	1	Total	C	O	0	0
			6	3	3		
2	B	1	Total	C	O	0	0
			6	3	3		
2	B	1	Total	C	O	0	0
			6	3	3		

- Molecule 3 is 1,2-ETHANEDIOL (CCD ID: EDO) (formula: C<sub>2</sub>H<sub>6</sub>O<sub>2</sub>).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	C	O	0	0
			4	2	2		
3	A	1	Total	C	O	0	0
			4	2	2		
3	A	1	Total	C	O	0	0
			4	2	2		
3	A	1	Total	C	O	0	0
			4	2	2		
3	A	1	Total	C	O	0	0
			4	2	2		

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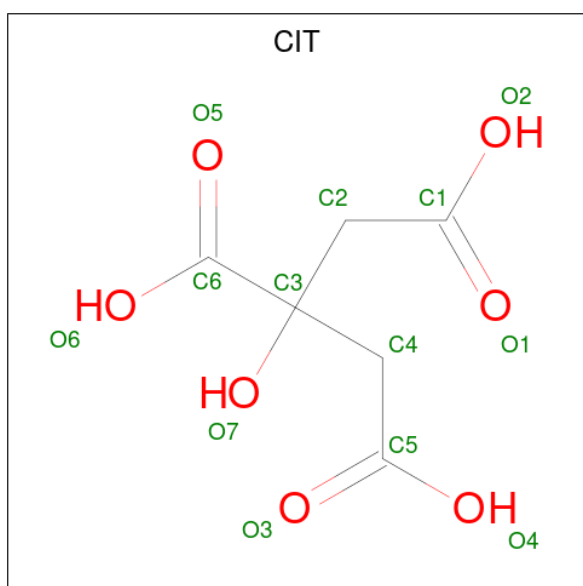
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	1	Total C O 4 2 2	0	0
3	A	1	Total C O 4 2 2	0	0
3	A	1	Total C O 4 2 2	0	0
3	A	1	Total C O 4 2 2	0	0
3	A	1	Total C O 4 2 2	0	0
3	A	1	Total C O 4 2 2	0	0
3	A	1	Total C O 4 2 2	0	0
3	A	1	Total C O 4 2 2	0	0
3	A	1	Total C O 4 2 2	0	0
3	A	1	Total C O 4 2 2	0	0
3	A	1	Total C O 4 2 2	0	0
3	A	1	Total C O 4 2 2	0	0
3	A	1	Total C O 4 2 2	0	0
3	A	1	Total C O 4 2 2	0	0
3	A	1	Total C O 4 2 2	0	0
3	A	1	Total C O 4 2 2	0	0
3	B	1	Total C O 4 2 2	0	0
3	B	1	Total C O 4 2 2	0	0
3	B	1	Total C O 4 2 2	0	0
3	B	1	Total C O 4 2 2	0	0
3	B	1	Total C O 4 2 2	0	0
3	B	1	Total C O 4 2 2	0	0

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	B	1	Total	C	O	0	0
			4	2	2		
3	B	1	Total	C	O	0	0
			4	2	2		
3	B	1	Total	C	O	0	0
			4	2	2		
3	B	1	Total	C	O	0	0
			4	2	2		
3	B	1	Total	C	O	0	0
			4	2	2		
3	B	1	Total	C	O	0	0
			4	2	2		
3	B	1	Total	C	O	0	0
			4	2	2		
3	B	1	Total	C	O	0	0
			4	2	2		

- Molecule 4 is CITRIC ACID (CCD ID: CIT) (formula:  $C_6H_8O_7$ ).



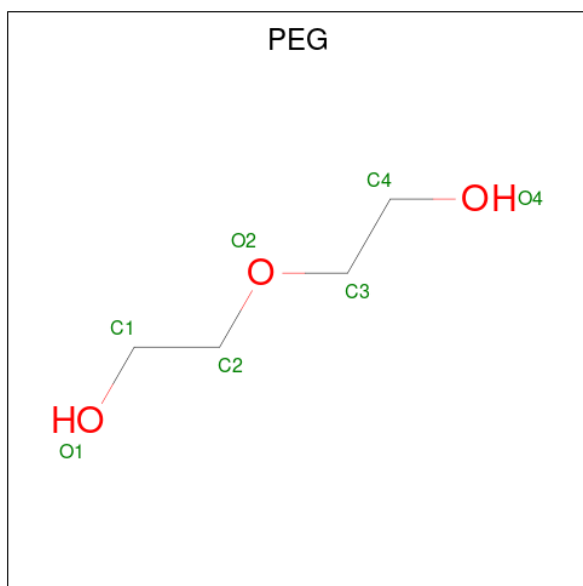
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total	C	O	0	0
			13	6	7		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	B	1	Total	C	O	0	0
			13	6	7		

- Molecule 5 is DI(HYDROXYETHYL)ETHER (CCD ID: PEG) (formula:  $C_4H_{10}O_3$ ).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	B	1	Total	C	O	0	0
			7	4	3		

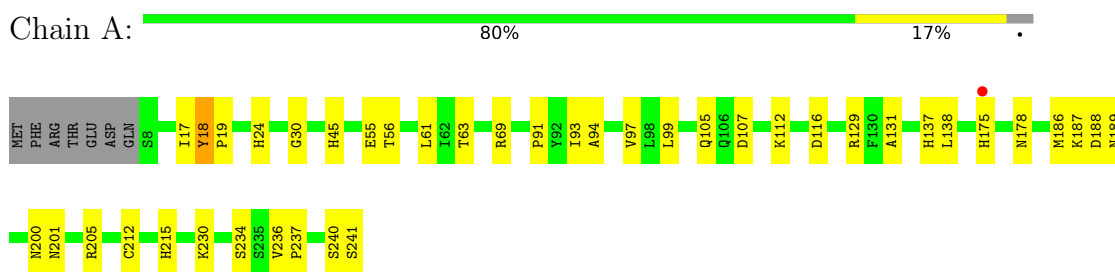
- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	126	Total	O	0	0
			126	126		
6	B	135	Total	O	0	0
			135	135		

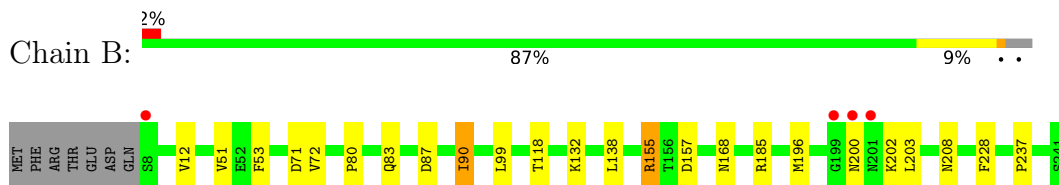
### 3 Residue-property plots [i](#)

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: Putative amino acid-binding periplasmic ABC transporter protein



- Molecule 1: Putative amino acid-binding periplasmic ABC transporter protein



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	46.07Å 86.96Å 121.80Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	70.77 – 1.86 70.77 – 1.86	Depositor EDS
% Data completeness (in resolution range)	99.9 (70.77-1.86) 99.9 (70.77-1.86)	Depositor EDS
$R_{merge}$	0.14	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.88 (at 1.86Å)	Xtrriage
Refinement program	REFMAC 5.8.0218	Depositor
R, $R_{free}$	0.186 , 0.225 (Not available) , 0.214	Depositor DCC
$R_{free}$ test set	2016 reflections (4.78%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	25.3	Xtrriage
Anisotropy	0.355	Xtrriage
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>	$\langle  L  \rangle = 0.50$ , $\langle L^2 \rangle = 0.33$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
$F_o, F_c$ correlation	0.96	EDS
Total number of atoms	4476	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	25.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.78% 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: EDO, CIT, PEG, 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	1.02	2/2040 (0.1%)	1.00	3/2751 (0.1%)
1	B	1.02	0/2031	0.99	0/2739
All	All	1.02	2/4071 (0.0%)	0.99	3/5490 (0.1%)

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	19	PRO	C-O	-9.19	1.17	1.25
1	A	18	TYR	N-CA	-5.17	1.41	1.46

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	240	SER	CA-C-N	5.44	131.49	121.70
1	A	240	SER	C-N-CA	5.44	131.49	121.70
1	A	241	SER	CA-CB-OG	-5.08	100.94	111.10

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	2002	0	1992	46	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	B	1994	0	1990	36	0
2	A	24	0	32	8	0
2	B	18	0	24	5	0
3	A	80	0	120	5	0
3	B	64	0	96	8	0
4	A	13	0	5	1	0
4	B	13	0	5	0	0
5	B	7	0	10	0	0
6	A	126	0	0	9	0
6	B	135	0	0	2	0
All	All	4476	0	4274	79	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 9.

The worst 5 of 79 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:155[B]:ARG:HH11	1:B:155[B]:ARG:CB	1.13	1.61
1:B:155[B]:ARG:HB2	1:B:155[B]:ARG:NH1	1.09	1.38
1:A:69[B]:ARG:CG	1:A:69[B]:ARG:HH21	1.79	0.95
1:B:83:GLN:HG2	3:B:307:EDO:H22	1.51	0.90
1:B:155[B]:ARG:HH11	1:B:155[B]:ARG:CG	1.85	0.89

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	247/241 (102%)	243 (98%)	4 (2%)	0	100	100
1	B	247/241 (102%)	243 (98%)	4 (2%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
All	All	494/482 (102%)	486 (98%)	8 (2%)	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	224/216 (104%)	222 (99%)	2 (1%)	70	64
1	B	217/216 (100%)	212 (98%)	5 (2%)	44	30
All	All	441/432 (102%)	434 (98%)	7 (2%)	63	44

5 of 7 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	90[B]	ILE
1	B	99	LEU
1	B	155[B]	ARG
1	B	155[A]	ARG
1	B	90[A]	ILE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 6 such sidechains are listed below:

Mol	Chain	Res	Type
1	A	201	ASN
1	B	175	HIS
1	B	178	ASN
1	A	142	HIS
1	A	137	HIS

### 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](#)

46 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	GOL	B	320	-	5,5,5	0.44	0	5,5,5	0.39	0
3	EDO	A	304	-	3,3,3	0.50	0	2,2,2	0.22	0
3	EDO	A	313	-	3,3,3	0.43	0	2,2,2	0.63	0
3	EDO	A	317	-	3,3,3	0.57	0	2,2,2	0.42	0
3	EDO	B	303	-	3,3,3	0.44	0	2,2,2	0.43	0
3	EDO	B	310	-	3,3,3	0.87	0	2,2,2	0.32	0
3	EDO	B	315	-	3,3,3	0.27	0	2,2,2	0.95	0
2	GOL	B	319	-	5,5,5	0.38	0	5,5,5	0.80	0
3	EDO	A	302	-	3,3,3	0.32	0	2,2,2	0.82	0
3	EDO	B	316	-	3,3,3	0.47	0	2,2,2	0.23	0
3	EDO	A	311	-	3,3,3	0.23	0	2,2,2	0.66	0
3	EDO	A	312	-	3,3,3	0.48	0	2,2,2	0.37	0
3	EDO	B	306	-	3,3,3	0.65	0	2,2,2	0.05	0
3	EDO	A	315	-	3,3,3	0.34	0	2,2,2	0.33	0
3	EDO	A	309	-	3,3,3	0.35	0	2,2,2	0.60	0
2	GOL	A	301	-	5,5,5	0.64	0	5,5,5	0.75	0
2	GOL	A	322	-	5,5,5	0.65	0	5,5,5	1.36	1 (20%)
3	EDO	A	325	-	3,3,3	0.54	0	2,2,2	0.24	0
3	EDO	A	310	-	3,3,3	0.47	0	2,2,2	0.27	0
3	EDO	B	307	-	3,3,3	0.86	0	2,2,2	0.73	0
3	EDO	B	312	-	3,3,3	0.48	0	2,2,2	0.33	0
3	EDO	B	302	-	3,3,3	0.49	0	2,2,2	0.35	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
3	EDO	A	303	-	3,3,3	0.62	0	2,2,2	0.27	0
3	EDO	A	319	-	3,3,3	0.43	0	2,2,2	0.45	0
3	EDO	A	316	-	3,3,3	0.44	0	2,2,2	0.57	0
3	EDO	A	305	-	3,3,3	0.40	0	2,2,2	0.45	0
3	EDO	B	309	-	3,3,3	0.35	0	2,2,2	0.54	0
5	PEG	B	321	-	6,6,6	0.42	0	5,5,5	0.71	0
2	GOL	B	318	-	5,5,5	0.45	0	5,5,5	0.41	0
3	EDO	B	314	-	3,3,3	0.31	0	2,2,2	0.60	0
3	EDO	A	306	-	3,3,3	0.53	0	2,2,2	0.15	0
3	EDO	A	308	-	3,3,3	0.28	0	2,2,2	0.61	0
4	CIT	A	321	-	12,12,12	2.04	5 (41%)	17,17,17	2.74	10 (58%)
3	EDO	A	320	-	3,3,3	0.49	0	2,2,2	0.08	0
3	EDO	B	313	-	3,3,3	0.53	0	2,2,2	0.48	0
3	EDO	B	308	-	3,3,3	0.38	0	2,2,2	0.52	0
3	EDO	B	305	-	3,3,3	0.42	0	2,2,2	0.21	0
3	EDO	A	307	-	3,3,3	0.42	0	2,2,2	0.53	0
3	EDO	A	314	-	3,3,3	0.57	0	2,2,2	0.18	0
3	EDO	B	311	-	3,3,3	0.73	0	2,2,2	0.17	0
3	EDO	B	304	-	3,3,3	0.36	0	2,2,2	0.40	0
4	CIT	B	317	-	12,12,12	1.66	3 (25%)	17,17,17	1.71	3 (17%)
2	GOL	A	324	-	5,5,5	0.57	0	5,5,5	1.50	2 (40%)
3	EDO	B	301	-	3,3,3	0.49	0	2,2,2	0.33	0
3	EDO	A	318	-	3,3,3	0.37	0	2,2,2	0.64	0
2	GOL	A	323	-	5,5,5	0.32	0	5,5,5	0.34	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	B	320	-	-	2/4/4/4	-
3	EDO	A	304	-	-	1/1/1/1	-
3	EDO	A	313	-	-	0/1/1/1	-
3	EDO	A	317	-	-	1/1/1/1	-
3	EDO	B	303	-	-	0/1/1/1	-
3	EDO	B	310	-	-	0/1/1/1	-
3	EDO	B	315	-	-	1/1/1/1	-
2	GOL	B	319	-	-	4/4/4/4	-
3	EDO	A	302	-	-	1/1/1/1	-
3	EDO	B	316	-	-	1/1/1/1	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	EDO	A	311	-	-	1/1/1/1	-
3	EDO	A	312	-	-	1/1/1/1	-
3	EDO	B	306	-	-	0/1/1/1	-
3	EDO	A	315	-	-	0/1/1/1	-
3	EDO	A	309	-	-	1/1/1/1	-
2	GOL	A	301	-	-	3/4/4/4	-
2	GOL	A	322	-	-	3/4/4/4	-
3	EDO	A	325	-	-	1/1/1/1	-
3	EDO	A	310	-	-	1/1/1/1	-
3	EDO	B	307	-	-	1/1/1/1	-
3	EDO	B	312	-	-	1/1/1/1	-
3	EDO	B	302	-	-	1/1/1/1	-
3	EDO	A	303	-	-	0/1/1/1	-
3	EDO	A	319	-	-	0/1/1/1	-
3	EDO	A	316	-	-	1/1/1/1	-
3	EDO	A	305	-	-	1/1/1/1	-
3	EDO	B	309	-	-	0/1/1/1	-
5	PEG	B	321	-	-	2/4/4/4	-
2	GOL	B	318	-	-	0/4/4/4	-
3	EDO	B	314	-	-	0/1/1/1	-
3	EDO	A	306	-	-	0/1/1/1	-
3	EDO	A	308	-	-	1/1/1/1	-
4	CIT	A	321	-	-	7/16/16/16	-
3	EDO	A	320	-	-	0/1/1/1	-
3	EDO	B	313	-	-	0/1/1/1	-
3	EDO	B	308	-	-	0/1/1/1	-
3	EDO	B	305	-	-	0/1/1/1	-
3	EDO	A	307	-	-	0/1/1/1	-
3	EDO	A	314	-	-	1/1/1/1	-
3	EDO	B	311	-	-	0/1/1/1	-
3	EDO	B	304	-	-	1/1/1/1	-
4	CIT	B	317	-	-	7/16/16/16	-
2	GOL	A	324	-	-	2/4/4/4	-
3	EDO	B	301	-	-	1/1/1/1	-
3	EDO	A	318	-	-	1/1/1/1	-
2	GOL	A	323	-	-	4/4/4/4	-

The worst 5 of 8 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	321	CIT	C2-C3	4.08	1.59	1.54

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	B	317	CIT	O1-C1	2.86	1.31	1.22
4	A	321	CIT	O5-C6	2.59	1.30	1.22
4	A	321	CIT	O7-C3	2.45	1.47	1.43
4	B	317	CIT	O4-C5	-2.40	1.22	1.30

The worst 5 of 16 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	321	CIT	O1-C1-C2	-5.76	106.65	122.95
4	A	321	CIT	O7-C3-C2	4.53	119.70	109.38
4	A	321	CIT	O7-C3-C6	-3.79	103.58	108.96
4	A	321	CIT	O2-C1-C2	3.77	126.30	114.35
4	B	317	CIT	O7-C3-C2	3.60	117.59	109.38

There are no chirality outliers.

5 of 54 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	301	GOL	C1-C2-C3-O3
2	A	322	GOL	O1-C1-C2-C3
2	A	323	GOL	O1-C1-C2-C3
2	A	323	GOL	C1-C2-C3-O3
2	A	324	GOL	C1-C2-C3-O3

There are no ring outliers.

13 monomers are involved in 27 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	313	EDO	1	0
2	B	319	GOL	2	0
3	A	315	EDO	1	0
2	A	301	GOL	1	0
2	A	322	GOL	4	0
3	A	310	EDO	2	0
3	B	307	EDO	6	0
3	B	312	EDO	1	0
2	B	318	GOL	3	0
4	A	321	CIT	1	0
2	A	324	GOL	3	0
3	B	301	EDO	2	0
3	A	318	EDO	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 [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	234/241 (97%)	0.00	1 (0%) 88 91	7, 21, 38, 46	15 (6%)
1	B	234/241 (97%)	0.03	4 (1%) 69 73	8, 21, 41, 56	15 (6%)
All	All	468/482 (97%)	0.01	5 (1%) 78 81	7, 21, 39, 56	30 (6%)

All (5) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	200	ASN	3.3
1	B	201	ASN	2.9
1	B	199	GLY	2.8
1	A	175	HIS	2.5
1	B	8	SER	2.4

### 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, 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( $\text{\AA}^2$ )	Q<0.9
3	EDO	B	316	4/4	0.65	0.22	66,71,74,74	0
3	EDO	B	308	4/4	0.74	0.17	50,51,53,58	0
3	EDO	A	302	4/4	0.74	0.18	51,53,53,57	0
3	EDO	A	320	4/4	0.75	0.21	55,56,56,59	0
3	EDO	A	310	4/4	0.76	0.18	55,56,56,56	0
2	GOL	B	318	6/6	0.76	0.17	49,50,53,54	0
3	EDO	A	312	4/4	0.77	0.20	57,61,62,63	0
2	GOL	A	324	6/6	0.77	0.18	50,55,58,61	0
3	EDO	B	303	4/4	0.78	0.18	53,54,54,60	0
5	PEG	B	321	7/7	0.78	0.17	45,53,57,57	0
3	EDO	A	317	4/4	0.80	0.16	49,49,51,54	0
3	EDO	A	314	4/4	0.80	0.18	54,57,58,65	0
3	EDO	B	311	4/4	0.81	0.15	36,40,41,47	0
3	EDO	B	315	4/4	0.81	0.15	42,47,48,53	0
2	GOL	A	323	6/6	0.82	0.15	51,53,55,56	0
3	EDO	A	325	4/4	0.82	0.16	52,53,54,57	0
3	EDO	A	316	4/4	0.82	0.24	35,45,48,56	0
2	GOL	A	322	6/6	0.82	0.16	39,47,54,57	0
3	EDO	A	313	4/4	0.83	0.15	50,52,53,54	0
3	EDO	B	301	4/4	0.83	0.16	38,38,42,50	0
3	EDO	A	319	4/4	0.84	0.17	46,50,51,58	0
3	EDO	A	318	4/4	0.84	0.17	49,49,49,55	0
4	CIT	A	321	13/13	0.84	0.13	23,36,38,43	0
3	EDO	B	302	4/4	0.84	0.14	39,46,49,52	0
3	EDO	B	304	4/4	0.85	0.15	44,45,49,50	0
3	EDO	B	307	4/4	0.85	0.14	35,37,37,41	0
3	EDO	A	308	4/4	0.85	0.16	53,54,57,59	0
2	GOL	B	320	6/6	0.85	0.13	46,49,52,56	0
3	EDO	A	304	4/4	0.86	0.13	43,43,44,45	0
3	EDO	B	314	4/4	0.86	0.11	41,42,45,45	0
2	GOL	A	301	6/6	0.86	0.14	39,45,50,51	0
3	EDO	B	312	4/4	0.88	0.15	38,47,49,54	0
3	EDO	A	303	4/4	0.88	0.12	36,40,40,41	0
2	GOL	B	319	6/6	0.88	0.12	37,41,42,44	0
3	EDO	A	309	4/4	0.89	0.15	34,39,43,43	0
3	EDO	A	311	4/4	0.89	0.12	41,45,45,50	0
3	EDO	A	315	4/4	0.90	0.12	37,38,42,42	0
3	EDO	B	310	4/4	0.90	0.14	27,34,38,40	0
3	EDO	A	306	4/4	0.90	0.11	48,50,51,52	0
4	CIT	B	317	13/13	0.92	0.08	24,30,33,35	0
3	EDO	B	313	4/4	0.92	0.09	32,32,33,35	0
3	EDO	B	309	4/4	0.93	0.09	33,33,34,34	0
3	EDO	A	305	4/4	0.94	0.08	26,29,30,32	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
3	EDO	B	306	4/4	0.95	0.07	18,19,20,20	0
3	EDO	A	307	4/4	0.96	0.06	25,25,26,26	0
3	EDO	B	305	4/4	0.96	0.07	21,27,31,33	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.