



wwPDB X-ray Structure Validation Summary Report ⓘ

Sep 14, 2020 – 02:02 AM BST

PDB ID : 5WQ3
Title : Crystal structure of type-II LOG from *Corynebacterium glutamicum*
Authors : Seo, H.; Kim, K.-J.
Deposited on : 2016-11-22
Resolution : 1.95 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

A user guide is available at

<https://www.wwpdb.org/validation/2017/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 : 1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix) : 1.13
EDS : 2.14.4.dev1
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) : 2.14.4.dev1

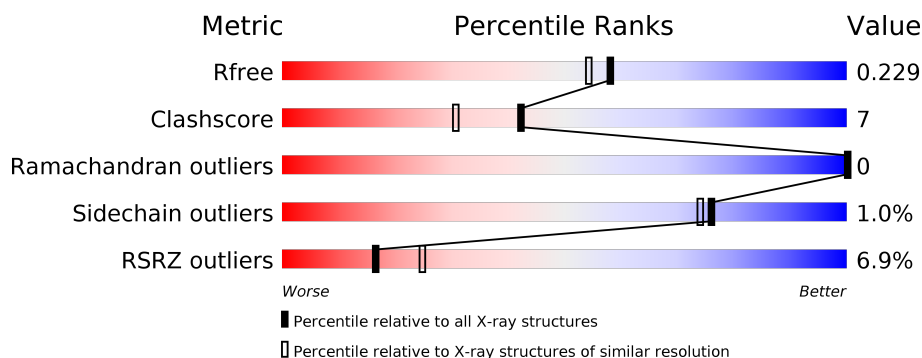
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.95 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	2580 (1.96-1.96)
Clashscore	141614	2705 (1.96-1.96)
Ramachandran outliers	138981	2678 (1.96-1.96)
Sidechain outliers	138945	2678 (1.96-1.96)
RSRZ outliers	127900	2539 (1.96-1.96)

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 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	264	<div> <div>7%</div> <div> <div></div> <div>68%</div> <div>10%</div> <div>22%</div> </div> </div>
1	B	264	<div> <div>4%</div> <div> <div></div> <div>70%</div> <div>8%</div> <div>22%</div> </div> </div>
1	C	264	<div> <div>5%</div> <div> <div></div> <div>67%</div> <div>11%</div> <div>21%</div> </div> </div>

2 Entry composition

There are 8 unique types of molecules in this entry. The entry contains 5281 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 Cytokinin riboside 5'-monophosphate phosphoribohydrolase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	206	Total	C	N	O	S	0	6	0
			1663	1081	276	296	10			
1	B	206	Total	C	N	O	S	0	3	0
			1634	1055	272	298	9			
1	C	208	Total	C	N	O	S	0	8	0
			1695	1094	285	306	10			

There are 24 discrepancies between the modelled and reference sequences:

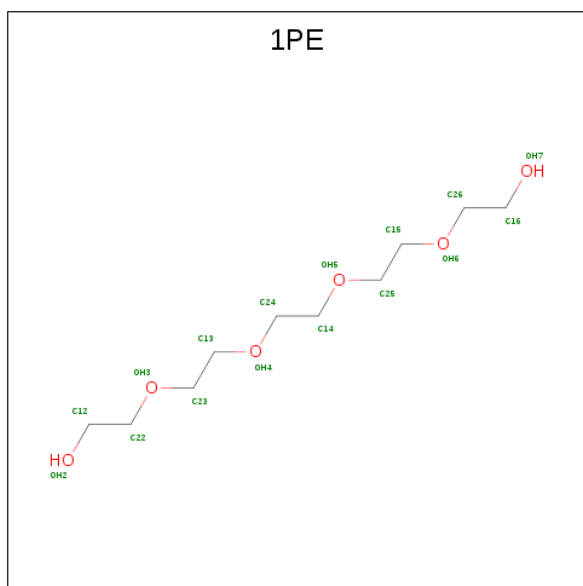
Chain	Residue	Modelled	Actual	Comment	Reference
A	257	LEU	-	expression tag	UNP A0A1B4WK77
A	258	GLU	-	expression tag	UNP A0A1B4WK77
A	259	HIS	-	expression tag	UNP A0A1B4WK77
A	260	HIS	-	expression tag	UNP A0A1B4WK77
A	261	HIS	-	expression tag	UNP A0A1B4WK77
A	262	HIS	-	expression tag	UNP A0A1B4WK77
A	263	HIS	-	expression tag	UNP A0A1B4WK77
A	264	HIS	-	expression tag	UNP A0A1B4WK77
B	257	LEU	-	expression tag	UNP A0A1B4WK77
B	258	GLU	-	expression tag	UNP A0A1B4WK77
B	259	HIS	-	expression tag	UNP A0A1B4WK77
B	260	HIS	-	expression tag	UNP A0A1B4WK77
B	261	HIS	-	expression tag	UNP A0A1B4WK77
B	262	HIS	-	expression tag	UNP A0A1B4WK77
B	263	HIS	-	expression tag	UNP A0A1B4WK77
B	264	HIS	-	expression tag	UNP A0A1B4WK77
C	257	LEU	-	expression tag	UNP A0A1B4WK77
C	258	GLU	-	expression tag	UNP A0A1B4WK77
C	259	HIS	-	expression tag	UNP A0A1B4WK77
C	260	HIS	-	expression tag	UNP A0A1B4WK77
C	261	HIS	-	expression tag	UNP A0A1B4WK77
C	262	HIS	-	expression tag	UNP A0A1B4WK77
C	263	HIS	-	expression tag	UNP A0A1B4WK77

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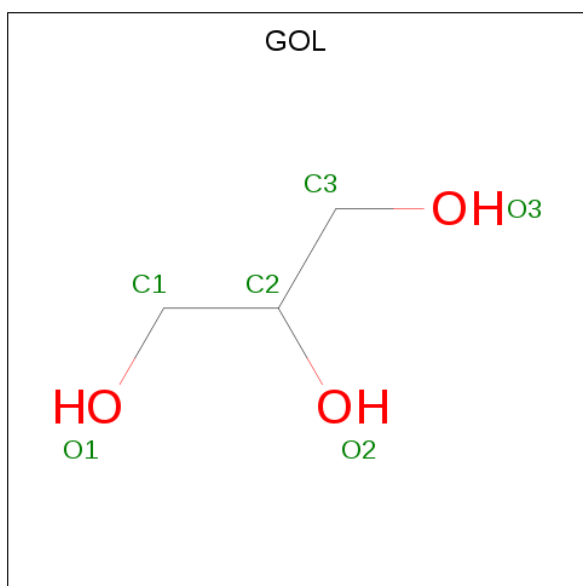
Chain	Residue	Modelled	Actual	Comment	Reference
C	264	HIS	-	expression tag	UNP A0A1B4WK77

- Molecule 2 is PENTAETHYLENE GLYCOL (three-letter code: 1PE) (formula: $C_{10}H_{22}O_6$).



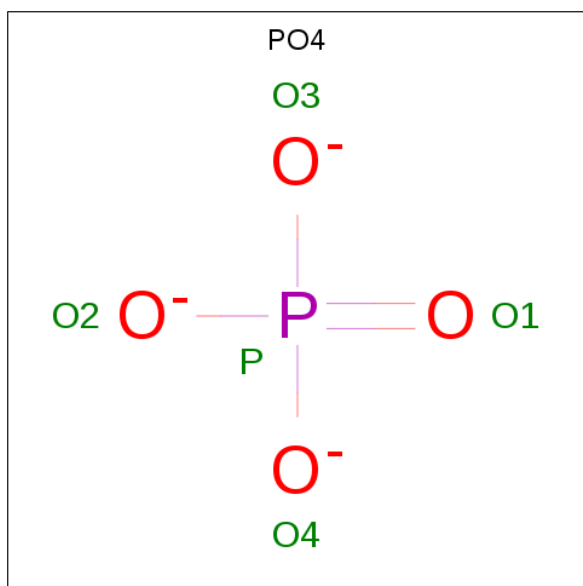
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total	C	O	0	0
			9	6	3		

- Molecule 3 is GLYCEROL (three-letter code: GOL) (formula: $C_3H_8O_3$).



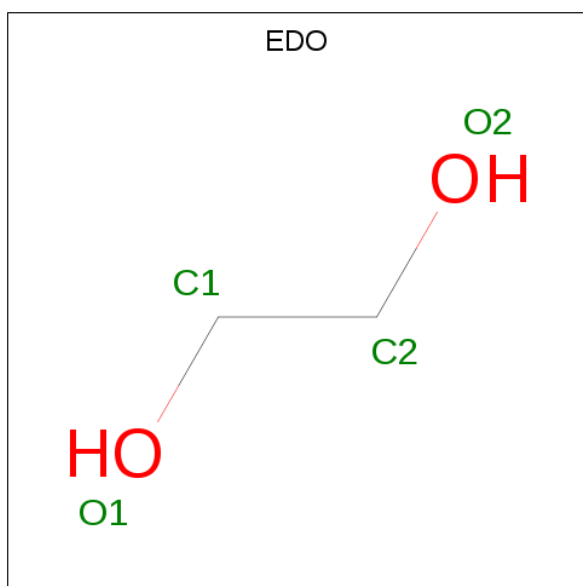
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	C	O	0	0
			6	3	3		

- Molecule 4 is PHOSPHATE ION (three-letter code: PO4) (formula: O_4P).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total	O	P	0	0
			5	4	1		

- Molecule 5 is 1,2-ETHANEDIOL (three-letter code: EDO) (formula: $C_2H_6O_2$).

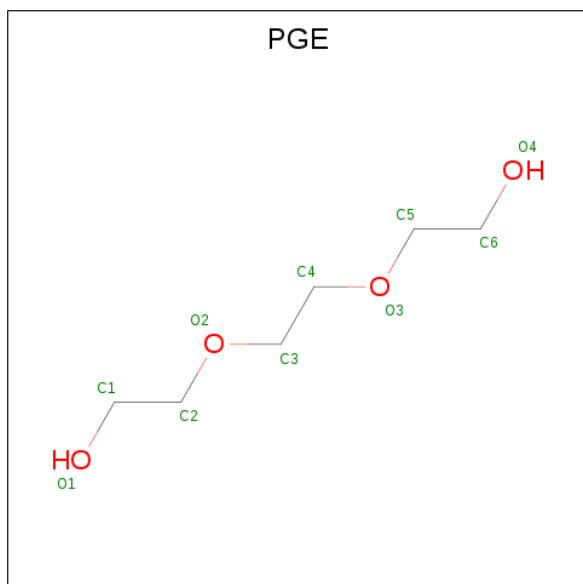


Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	B	1	Total C O 4 2 2	0	0
5	B	1	Total C O 4 2 2	0	0
5	B	1	Total C O 4 2 2	0	0
5	C	1	Total C O 4 2 2	0	0

- Molecule 6 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	B	2	Total Cl 2 2	0	0
6	C	3	Total Cl 3 3	0	0

- Molecule 7 is TRIETHYLENE GLYCOL (three-letter code: PGE) (formula: C₆H₁₄O₄).



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

- Molecule 8 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
8	A	49	Total 49	O 49	0	0
8	B	84	Total 84	O 84	0	0
8	C	111	Total 111	O 111	0	0

4 Data and refinement statistics

Property	Value	Source
Space group	C 2 2 21	Depositor
Cell constants a, b, c, α , β , γ	98.70Å 173.62Å 79.90Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	50.00 – 1.95 23.44 – 1.95	Depositor EDS
% Data completeness (in resolution range)	95.4 (50.00-1.95) 95.5 (23.44-1.95)	Depositor EDS
R_{merge}	0.08	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	4.46 (at 1.95Å)	Xtriage
Refinement program	REFMAC 5.8.0073	Depositor
R, R_{free}	0.178 , 0.227 0.185 , 0.229	Depositor DCC
R_{free} test set	2296 reflections (4.79%)	wwPDB-VP
Wilson B-factor (Å ²)	25.3	Xtriage
Anisotropy	0.318	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.40 , 51.2	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	0.013 for 1/2*h-1/2*k,-3/2*h-1/2*k,-l 0.021 for 1/2*h+1/2*k,3/2*h-1/2*k,-l	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	5281	wwPDB-VP
Average B, all atoms (Å ²)	32.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.00% 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, PGE, CL, PO4, EDO, IPE

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	0.96	0/1707	0.88	2/2313 (0.1%)
1	B	0.97	0/1673	0.90	3/2266 (0.1%)
1	C	0.96	0/1738	0.92	3/2355 (0.1%)
All	All	0.97	0/5118	0.90	8/6934 (0.1%)

There are no bond length outliers.

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

Mol	Chain	Res	Type	Atoms	Z	Observed($^{\circ}$)	Ideal($^{\circ}$)
1	B	49	ARG	NE-CZ-NH2	7.99	124.30	120.30
1	C	133	LEU	C-N-CD	6.04	141.09	128.40
1	C	49[A]	ARG	NE-CZ-NH1	-5.57	117.52	120.30
1	C	49[B]	ARG	NE-CZ-NH1	-5.57	117.52	120.30
1	A	140	ASN	C-N-CD	5.34	139.61	128.40

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	1663	0	1625	33	0
1	B	1634	0	1599	18	0
1	C	1695	0	1647	27	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	A	9	0	11	2	1
3	A	6	0	8	0	0
4	A	5	0	0	0	0
5	B	12	0	18	0	0
5	C	4	0	6	0	0
6	B	2	0	0	0	0
6	C	3	0	0	1	0
7	C	4	0	5	0	0
8	A	49	0	0	3	0
8	B	84	0	0	1	0
8	C	111	0	0	3	0
All	All	5281	0	4919	69	1

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.

The worst 5 of 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:C:74:PHE:HD2	1:C:166[B]:PHE:CE1	1.70	1.10
1:C:74:PHE:CD2	1:C:166[B]:PHE:CE1	2.59	0.90
1:A:213[B]:HIS:ND1	1:A:213[B]:HIS:O	2.06	0.89
1:A:171:GLY:C	1:B:220:MET:HE3	2.00	0.82
1:C:166[B]:PHE:HD2	1:C:182[B]:VAL:HG21	1.44	0.81

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:301:1PE:C14	2:A:301:1PE:C24[3_556]	1.91	0.29

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	208/264 (79%)	204 (98%)	4 (2%)	0	100	100
1	B	205/264 (78%)	199 (97%)	6 (3%)	0	100	100
1	C	212/264 (80%)	210 (99%)	2 (1%)	0	100	100
All	All	625/792 (79%)	613 (98%)	12 (2%)	0	100	100

There are no Ramachandran outliers to report.

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	173/220 (79%)	172 (99%)	1 (1%)	86	85
1	B	170/220 (77%)	166 (98%)	4 (2%)	49	40
1	C	177/220 (80%)	177 (100%)	0	100	100
All	All	520/660 (79%)	515 (99%)	5 (1%)	76	74

All (5) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	43	LYS
1	B	137	GLN
1	B	192	THR
1	B	214	ARG
1	B	229	MET

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (1) such sidechains are listed below:

Mol	Chain	Res	Type
1	B	138	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 monosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 13 ligands modelled in this entry, 5 are monoatomic - leaving 8 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	$\# Z > 2$
5	EDO	C	301	-	3,3,3	0.22	0	2,2,2	0.60	0
5	EDO	B	303	-	3,3,3	0.33	0	2,2,2	0.33	0
5	EDO	B	301	-	3,3,3	0.38	0	2,2,2	0.18	0
3	GOL	A	302	-	5,5,5	0.36	0	5,5,5	0.72	0
4	PO4	A	303	-	4,4,4	0.92	0	6,6,6	0.43	0
2	1PE	A	301	-	8,8,15	0.54	0	7,7,14	0.96	0
7	PGE	C	302	-	3,3,9	0.38	0	2,2,8	0.54	0
5	EDO	B	302	-	3,3,3	0.26	0	2,2,2	0.59	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
5	EDO	C	301	-	-	1/1/1/1	-
5	EDO	B	303	-	-	1/1/1/1	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	GOL	A	302	-	-	0/4/4/4	-
5	EDO	B	301	-	-	0/1/1/1	-
2	1PE	A	301	-	-	4/6/6/13	-
7	PGE	C	302	-	-	0/1/1/7	-
5	EDO	B	302	-	-	1/1/1/1	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

5 of 7 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	301	1PE	OH7-C16-C26-OH6
2	A	301	1PE	OH6-C15-C25-OH5
5	C	301	EDO	O1-C1-C2-O2
5	B	303	EDO	O1-C1-C2-O2
2	A	301	1PE	C24-C14-OH5-C25

There are no ring outliers.

1 monomer is involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	301	1PE	2	1

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	206/264 (78%)	0.61	18 (8%) 10 16	17, 33, 56, 87	0
1	B	206/264 (78%)	0.28	11 (5%) 26 35	17, 28, 53, 76	0
1	C	208/264 (78%)	0.25	14 (6%) 17 26	17, 26, 53, 75	0
All	All	620/792 (78%)	0.38	43 (6%) 16 25	17, 29, 54, 87	0

The worst 5 of 43 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	133	LEU	10.3
1	A	249	LEU	8.9
1	B	133	LEU	7.2
1	A	135	HIS	5.7
1	A	42	TRP	5.4

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 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(\AA^2)	Q<0.9
5	EDO	B	301	4/4	0.77	0.16	56,58,61,62	0
5	EDO	B	303	4/4	0.84	0.30	52,57,60,62	0
5	EDO	C	301	4/4	0.85	0.14	52,54,58,64	0
6	CL	B	305	1/1	0.85	0.09	57,57,57,57	0
7	PGE	C	302	4/10	0.87	0.27	39,50,55,57	0
4	PO4	A	303	5/5	0.90	0.29	20,20,20,20	0
3	GOL	A	302	6/6	0.91	0.17	38,42,44,48	0
2	1PE	A	301	9/16	0.93	0.12	25,37,40,42	1
5	EDO	B	302	4/4	0.94	0.36	56,58,58,59	0
6	CL	C	305	1/1	0.94	0.07	63,63,63,63	0
6	CL	B	304	1/1	0.96	0.05	39,39,39,39	0
6	CL	C	303	1/1	0.98	0.08	33,33,33,33	0
6	CL	C	304	1/1	0.99	0.20	46,46,46,46	1

6.5 Other polymers [i](#)

There are no such residues in this entry.