Full wwPDB X-ray Structure Validation Report ⓘ

Dec 16, 2023 – 09:15 AM EST

PDB ID	:	2OLU
Title	:	Structural Insight Into the Transglycosylation Step Of Bacterial Cell Wall Biosynthesis : Apoenzyme
Authors	:	Lovering, A.L.; De Castro, L.H.; Lim, D.; Strynadka, N.C.
Deposited on	:	2007-01-19
Resolution	:	2.90 Å(reported)

The following versions of software and data (see references ⓘ) were used in the production of this report:

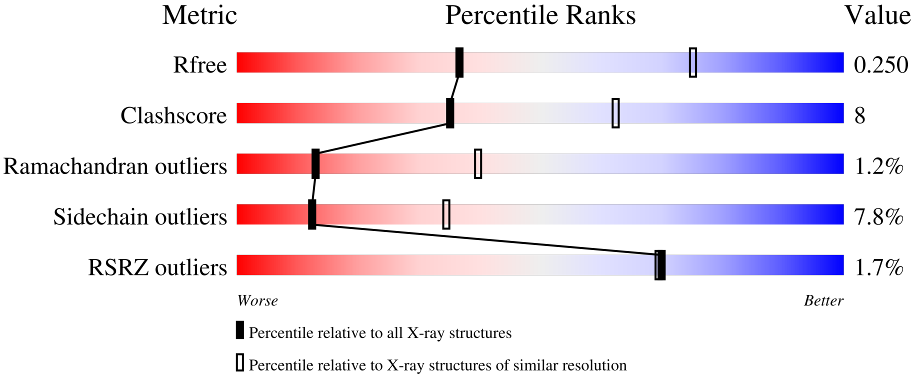
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

1 Overall quality at a glance ⓘ

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

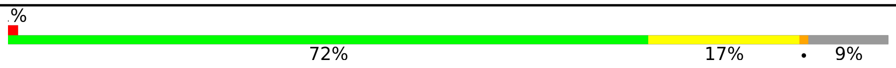
The reported resolution of this entry is 2.90 Å.

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	1957 (2.90-2.90)
Clashscore	141614	2172 (2.90-2.90)
Ramachandran outliers	138981	2115 (2.90-2.90)
Sidechain outliers	138945	2117 (2.90-2.90)
RSRZ outliers	127900	1906 (2.90-2.90)

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 <=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	669	

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	EDO	A	728	-	-	-	X

2 Entry composition ⓘ

There are 3 unique types of molecules in this entry. The entry contains 4803 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.

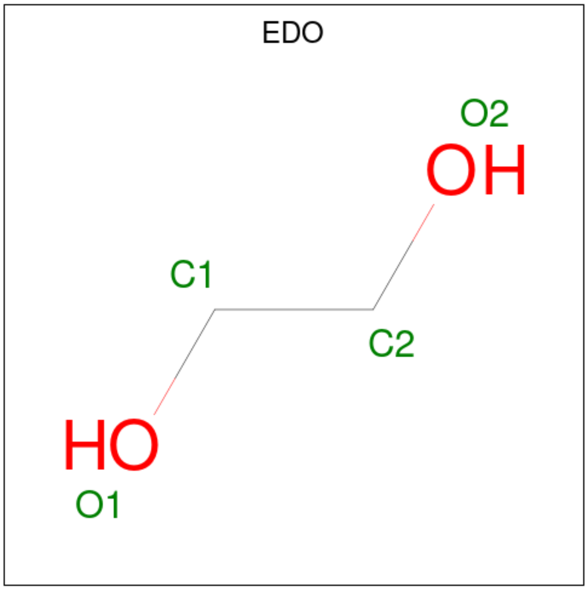
- Molecule 1 is a protein called Penicillin-binding protein 2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	Se			
1	A	608	4777	2990	819	956	12	0	0	0

There are 15 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	59	MSE	-	initiating methionine	UNP Q2YY56
A	106	MSE	MET	modified residue	UNP Q2YY56
A	257	MSE	MET	modified residue	UNP Q2YY56
A	285	PRO	ALA	SEE REMARK 999	UNP Q2YY56
A	311	MSE	MET	modified residue	UNP Q2YY56
A	335	MSE	MET	modified residue	UNP Q2YY56
A	413	MSE	MET	modified residue	UNP Q2YY56
A	439	THR	VAL	SEE REMARK 999	UNP Q2YY56
A	548	MSE	MET	modified residue	UNP Q2YY56
A	555	MSE	MET	modified residue	UNP Q2YY56
A	559	MSE	MET	modified residue	UNP Q2YY56
A	580	MSE	MET	modified residue	UNP Q2YY56
A	618	MSE	MET	modified residue	UNP Q2YY56
A	622	MSE	MET	modified residue	UNP Q2YY56
A	652	MSE	MET	modified residue	UNP Q2YY56

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



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

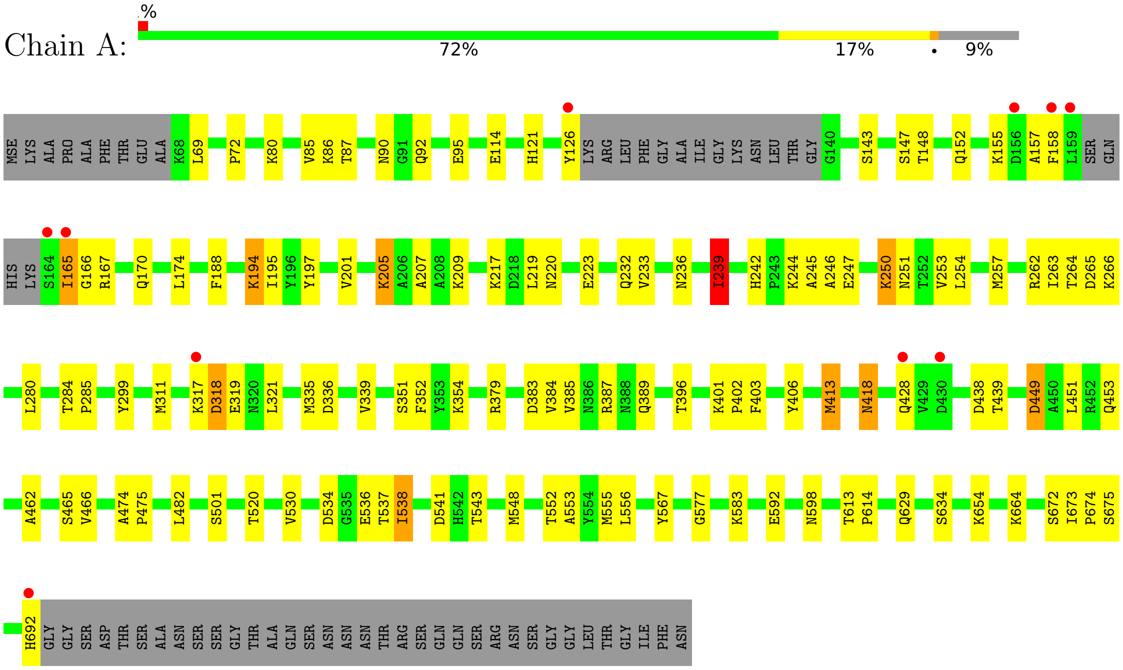
- Molecule 3 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	22	Total O 22 22	0	0

3 Residue-property plots ⓘ

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: Penicillin-binding protein 2



4 Data and refinement statistics ⓘ

Property	**Value**	**Source**
Space group	C 2 2 21	Depositor
Cell constants a, b, c, α, β, γ	70.50Å 249.89Å 103.16Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	24.60 – 2.90 24.61 – 2.90	Depositor EDS
% Data completeness (in resolution range)	99.8 (24.60-2.90) 99.8 (24.61-2.90)	Depositor EDS
R_{merge}	0.13	Depositor
R_{sym}	0.13	Depositor
$< I/\sigma(I) >$ [1]	68.72 (at 2.89Å)	Xtriage
Refinement program	REFMAC	Depositor
R, R_{free}	0.191 , 0.246 0.196 , 0.250	Depositor DCC
R_{free} test set	1043 reflections (5.06%)	wwPDB-VP
Wilson B-factor (Å^2)	43.8	Xtriage
Anisotropy	0.063	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.30 , 36.0	EDS
L-test for twinning[2]	$< \|L\| > = 0.45$, $< L^2 > = 0.28$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.91	EDS
Total number of atoms	4803	wwPDB-VP
Average B, all atoms (Å^2)	22.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.50% of the height of the origin peak. No significant pseudotranslation is detected.*

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[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality ⓘ

5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: EDO

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	0.77	1/4867 (0.0%)	0.74	2/6561 (0.0%)

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	1

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	555	MSE	CG-SE	-5.03	1.78	1.95

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	239	ILE	CB-CA-C	-5.03	101.53	111.60
1	A	449	ASP	CB-CG-OD1	5.03	122.83	118.30

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	577	GLY	Peptide

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	4777	0	4572	77	0
2	A	4	0	6	2	0
3	A	22	0	0	1	0
All	All	4803	0	4578	77	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 8.

All (77) 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:438:ASP:O	1:A:439:THR:HG22	1.56	1.06
1:A:165:ILE:HG22	1:A:166:GLY:H	1.27	0.95
1:A:548:MSE:HE3	1:A:552:THR:HG22	1.55	0.88
1:A:165:ILE:HG22	1:A:166:GLY:N	1.97	0.80
1:A:548:MSE:HE3	1:A:552:THR:CG2	2.13	0.79
1:A:548:MSE:HE2	1:A:553:ALA:HA	1.63	0.79
1:A:548:MSE:HE2	1:A:553:ALA:CA	2.14	0.77
1:A:85:VAL:HG11	1:A:335:MSE:HE1	1.69	0.74
1:A:195:ILE:HD11	1:A:197:TYR:CZ	2.25	0.70
1:A:438:ASP:O	1:A:439:THR:CG2	2.38	0.66
1:A:548:MSE:HE2	1:A:553:ALA:N	2.12	0.65
1:A:95:GLU:HB2	1:A:205:LYS:HG2	1.80	0.64
1:A:148:THR:O	1:A:152:GLN:HG2	1.99	0.62
1:A:239:ILE:CD1	1:A:280:LEU:HD13	2.29	0.62
1:A:254:LEU:HD23	1:A:257:MSE:CE	2.29	0.62
1:A:165:ILE:CG2	1:A:166:GLY:N	2.62	0.62
1:A:165:ILE:CG2	1:A:166:GLY:H	2.10	0.61
1:A:239:ILE:HD12	1:A:280:LEU:HD13	1.83	0.61
1:A:548:MSE:HE1	1:A:556:LEU:HD12	1.84	0.60
1:A:462:ALA:O	1:A:466:VAL:HG23	2.02	0.60
1:A:598:ASN:ND2	1:A:629:GLN:OE1	2.35	0.60
1:A:157:ALA:HB2	1:A:194:LYS:NZ	2.17	0.59
1:A:354:LYS:NZ	1:A:634:SER:O	2.33	0.59
1:A:548:MSE:CE	1:A:552:THR:HG22	2.31	0.58

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Atom-1	**Atom-2**	**Interatomic distance (Å)**	**Clash overlap (Å)**
1:A:254:LEU:HD23	1:A:257:MSE:HE3	1.84	0.58
1:A:530:VAL:HB	1:A:538:ILE:HG23	1.85	0.56
1:A:239:ILE:HD12	1:A:280:LEU:CD1	2.36	0.55
1:A:567:TYR:CD1	1:A:692:HIS:HB2	2.41	0.54
1:A:254:LEU:HA	1:A:257:MSE:HE3	1.91	0.52
1:A:418:ASN:HD22	1:A:675:SER:HA	1.75	0.52
1:A:85:VAL:HG11	1:A:335:MSE:CE	2.39	0.52
1:A:239:ILE:HD12	1:A:280:LEU:HD22	1.92	0.51
1:A:253:VAL:HG12	1:A:257:MSE:HE2	1.93	0.51
1:A:396:THR:HG23	1:A:501:SER:O	2.12	0.50
1:A:219:LEU:HD22	1:A:223:GLU:HB3	1.94	0.49
1:A:90:ASN:HB2	1:A:92:GLN:HG2	1.95	0.49
1:A:548:MSE:HE3	1:A:552:THR:CB	2.42	0.48
1:A:232:GLN:HG2	1:A:233:VAL:HG23	1.96	0.48
1:A:157:ALA:HB2	1:A:194:LYS:HZ1	1.78	0.48
1:A:239:ILE:HD12	1:A:280:LEU:CD2	2.44	0.47
1:A:195:ILE:CD1	1:A:197:TYR:CE1	2.98	0.47
1:A:284:THR:HB	1:A:285:PRO:HD2	1.96	0.47
1:A:201:VAL:HG11	1:A:207:ALA:HA	1.98	0.46
1:A:318:ASP:N	1:A:318:ASP:OD1	2.48	0.46
1:A:401:LYS:N	1:A:402:PRO:CD	2.79	0.46
1:A:233:VAL:HG12	1:A:236:ASN:HB2	1.98	0.46
1:A:311:MSE:HG3	1:A:321:LEU:HD13	1.98	0.46
1:A:242:HIS:HB3	2:A:728:EDO:H11	1.97	0.45
1:A:264:THR:HG22	1:A:265:ASP:N	2.31	0.45
1:A:158:PHE:CZ	1:A:170:GLN:NE2	2.85	0.44
1:A:262:ARG:O	1:A:263:ILE:HG23	2.17	0.44
1:A:613:THR:HB	1:A:614:PRO:HD2	1.98	0.44
1:A:250:LYS:NZ	1:A:251:ASN:OD1	2.48	0.44
1:A:239:ILE:HG23	1:A:246:ALA:CB	2.47	0.44
1:A:247:GLU:OE2	1:A:250:LYS:NZ	2.49	0.44
1:A:406:TYR:CD2	1:A:451:LEU:HD13	2.53	0.43
1:A:474:ALA:N	1:A:475:PRO:CD	2.81	0.43
1:A:534:ASP:OD1	1:A:534:ASP:N	2.51	0.43
1:A:239:ILE:HD11	1:A:280:LEU:HD13	2.00	0.43
1:A:449:ASP:O	1:A:453:GLN:HG2	2.18	0.43
1:A:239:ILE:HD13	1:A:239:ILE:HG21	1.84	0.43
1:A:195:ILE:HD11	1:A:197:TYR:CE1	2.54	0.42
1:A:195:ILE:HD12	1:A:197:TYR:CE1	2.54	0.42
1:A:121:HIS:CB	3:A:11:HOH:O	2.68	0.42
1:A:673:ILE:HG23	1:A:674:PRO:HA	2.02	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:195:ILE:CD1	1:A:197:TYR:CZ	3.01	0.42
1:A:541:ASP:OD2	1:A:541:ASP:N	2.52	0.41
1:A:336:ASP:OD1	1:A:339:VAL:HG23	2.21	0.41
1:A:245:ALA:H	2:A:728:EDO:H21	1.85	0.41
1:A:403:PHE:CD2	1:A:482:LEU:HD13	2.55	0.41
1:A:548:MSE:CE	1:A:553:ALA:HA	2.42	0.41
1:A:220:ASN:OD1	1:A:220:ASN:C	2.59	0.41
1:A:195:ILE:HD11	1:A:197:TYR:OH	2.20	0.40
1:A:413:MSE:HE2	1:A:413:MSE:HB3	1.93	0.40
1:A:548:MSE:HE3	1:A:552:THR:HB	2.02	0.40
1:A:85:VAL:HG13	1:A:299:TYR:CE1	2.55	0.40
1:A:567:TYR:CE1	1:A:692:HIS:HB2	2.56	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	602/669 (90%)	557 (92%)	38 (6%)	7 (1%)	13 40

All (7) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	143	SER
1	A	536	GLU
1	A	80	LYS
1	A	165	ILE
1	A	72	PRO
1	A	317	LYS
1	A	383	ASP

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	513/546 (94%)	473 (92%)	40 (8%)	12 34

All (40) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	69	LEU
1	A	86	LYS
1	A	87	THR
1	A	114	GLU
1	A	126	TYR
1	A	147	SER
1	A	155	LYS
1	A	167	ARG
1	A	174	LEU
1	A	188	PHE
1	A	194	LYS
1	A	205	LYS
1	A	209	LYS
1	A	217	LYS
1	A	239	ILE
1	A	244	LYS
1	A	250	LYS
1	A	266	LYS
1	A	318	ASP
1	A	319	GLU
1	A	351	SER
1	A	352	PHE
1	A	379	ARG
1	A	384	VAL
1	A	385	VAL
1	A	387	ARG
1	A	389	GLN
1	A	413	MSE
1	A	418	ASN
1	A	428	GLN

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Mol	Chain	Res	Type
1	A	465	SER
1	A	520	THR
1	A	537	THR
1	A	538	ILE
1	A	543	THR
1	A	583	LYS
1	A	592	GLU
1	A	654	LYS
1	A	664	LYS
1	A	672	SER

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

Mol	Chain	Res	Type
1	A	152	GLN
1	A	598	ASN
1	A	629	GLN

5.3.3 RNA ⓘ

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 monosaccharides in this entry.

5.6 Ligand geometry ⓘ

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	EDO	A	728	-	3,3,3	0.74	0	2,2,2	0.84	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	EDO	A	728	-	-	1/1/1/1	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (1) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	728	EDO	O1-C1-C2-O2

There are no ring outliers.

1 monomer is involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	728	EDO	2	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	596/669 (89%)	-0.14	10 (1%)	70	69	10, 21, 38, 57	0

All (10) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	159	LEU	4.5
1	A	317	LYS	2.6
1	A	428	GLN	2.5
1	A	164	SER	2.5
1	A	156	ASP	2.3
1	A	165	ILE	2.3
1	A	126	TYR	2.2
1	A	692	HIS	2.2
1	A	158	PHE	2.2
1	A	430	ASP	2.1

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 monosaccharides 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. 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	EDO	A	728	4/4	0.64	0.43	46,47,47,47	0

6.5 Other polymers ⓘ

There are no such residues in this entry.