



# Full wwPDB X-ray Structure Validation Report ⓘ

May 22, 2020 – 02:57 pm BST

PDB ID : 2V9I  
Title : L-RHAMNULOSE-1-PHOSPHATE ALDOLASE FROM ESCHERICHIA COLI (MUTANT E192A- K248W-L274stop)  
Authors : Grueninger, D.; Schulz, G.E.  
Deposited on : 2007-08-23  
Resolution : 1.80 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](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.

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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 : 2.11  
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) : 2.11

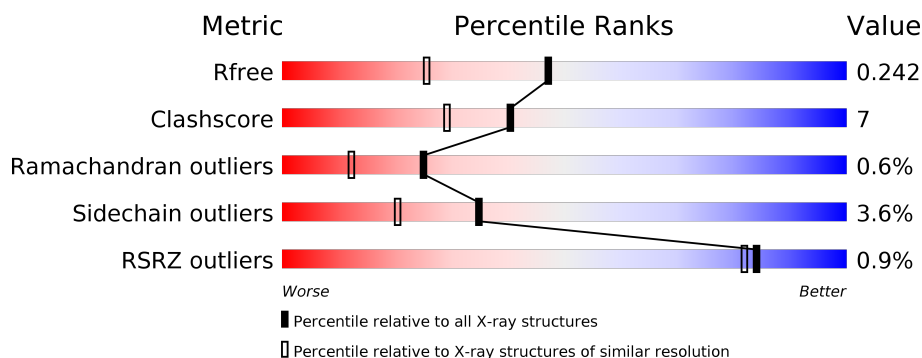
# 1 Overall quality at a glance ⓘ

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 1.80 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	5950 (1.80-1.80)
Clashscore	141614	6793 (1.80-1.80)
Ramachandran outliers	138981	6697 (1.80-1.80)
Sidechain outliers	138945	6696 (1.80-1.80)
RSRZ outliers	127900	5850 (1.80-1.80)

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  $\geq 3$ , 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	273	<div> <div style="width: 100%; height: 10px; background: linear-gradient(to right, red 1%, orange 1%, yellow 1%, green 86%, grey 11%);"></div> <div style="display: flex; justify-content: space-between; width: 100%;"> <span>%</span> <span>86%</span> <span>11%</span> </div> </div>
1	B	273	<div> <div style="width: 100%; height: 10px; background: linear-gradient(to right, red 1%, orange 1%, yellow 1%, green 89%, grey 8%);"></div> <div style="display: flex; justify-content: space-between; width: 100%;"> <span>%</span> <span>89%</span> <span>8%</span> </div> </div>

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	1274	-	X	-	-

## 2 Entry composition [i](#)

There are 4 unique types of molecules in this entry. The entry contains 4661 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 RHAMNULOSE-1-PHOSPHATE ALDOLASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	272	Total	C	N	O	S	0	2	0
			2121	1358	360	393	10			
1	B	272	Total	C	N	O	S	0	1	0
			2115	1354	360	391	10			

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	192	ALA	GLU	engineered mutation	UNP P32169
A	248	TRP	LYS	engineered mutation	UNP P32169
B	192	ALA	GLU	engineered mutation	UNP P32169
B	248	TRP	LYS	engineered mutation	UNP P32169

- Molecule 2 is 1,2-ETHANEDIOL (three-letter code: EDO) (formula: C<sub>2</sub>H<sub>6</sub>O<sub>2</sub>).



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

- Molecule 3 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	B	1	Total Zn 1 1	0	0
3	A	3	Total Zn 3 3	0	0

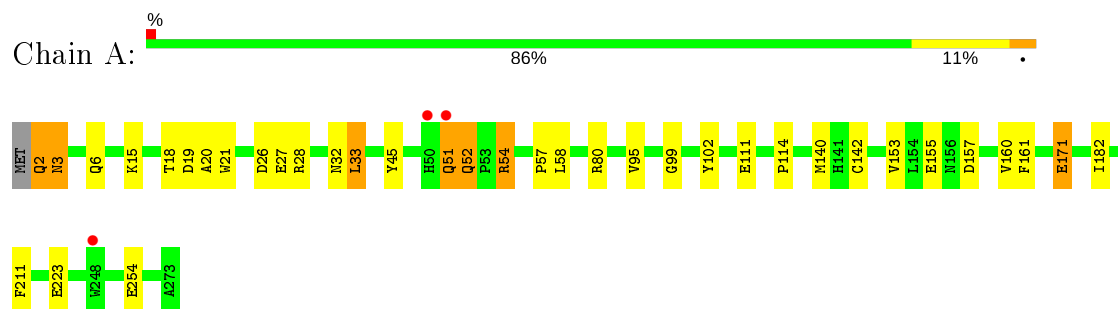
- Molecule 4 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	206	Total O 206 206	0	0
4	B	207	Total O 207 207	0	0

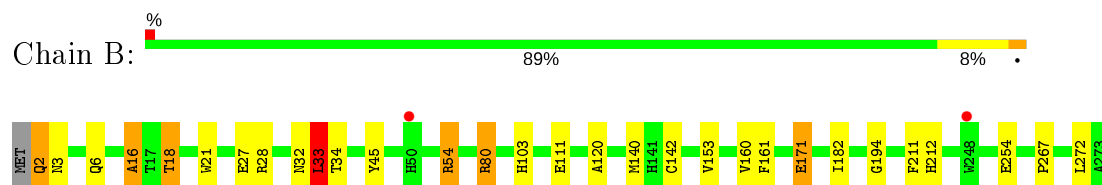
### 3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of 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: RHAMNULOSE-1-PHOSPHATE ALDOLASE



#### • Molecule 1: RHAMNULOSE-1-PHOSPHATE ALDOLASE



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 4	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	85.21Å 85.21Å 90.53Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	14.94 – 1.80 14.94 – 1.80	Depositor EDS
% Data completeness (in resolution range)	93.6 (14.94-1.80) 93.6 (14.94-1.80)	Depositor EDS
$R_{merge}$	0.06	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.68 (at 1.79Å)	Xtriage
Refinement program	REFMAC 5.2.0019	Depositor
R, $R_{free}$	0.208 , 0.238 0.210 , 0.242	Depositor DCC
$R_{free}$ test set	3358 reflections (6.00%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	25.4	Xtriage
Anisotropy	0.649	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.43 , 68.1	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.46$ , $\langle L^2 \rangle = 0.29$	Xtriage
Estimated twinning fraction	0.068 for h,-k,-l	Xtriage
$F_o, F_c$ correlation	0.98	EDS
Total number of atoms	4661	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	28.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 99.51 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 4.1323e-13. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

<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

### 5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: ZN, 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	1.00	6/2183 (0.3%)	0.98	9/2976 (0.3%)
1	B	1.00	7/2174 (0.3%)	0.97	7/2964 (0.2%)
All	All	1.00	13/4357 (0.3%)	0.97	16/5940 (0.3%)

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
1	B	0	1
All	All	0	2

All (13) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	27	GLU	CD-OE1	11.51	1.38	1.25
1	B	16	ALA	CA-CB	10.92	1.75	1.52
1	B	27	GLU	CD-OE1	10.72	1.37	1.25
1	A	18	THR	N-CA	9.79	1.66	1.46
1	B	27	GLU	CB-CG	8.21	1.67	1.52
1	A	27	GLU	CB-CG	7.84	1.67	1.52
1	A	33	LEU	CG-CD2	7.82	1.80	1.51
1	B	33	LEU	CG-CD1	-7.36	1.24	1.51
1	B	18	THR	CB-CG2	7.25	1.76	1.52
1	A	21	TRP	CE3-CZ3	5.71	1.48	1.38
1	B	16	ALA	N-CA	-5.66	1.35	1.46
1	A	18	THR	C-O	5.14	1.33	1.23
1	B	21	TRP	CE3-CZ3	5.05	1.47	1.38



All (16) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	33	LEU	CB-CG-CD2	-13.71	87.69	111.00
1	A	54	ARG	NE-CZ-NH2	-11.56	114.52	120.30
1	B	33	LEU	CA-CB-CG	11.23	141.14	115.30
1	B	54	ARG	NE-CZ-NH2	-10.87	114.87	120.30
1	B	33	LEU	CB-CG-CD1	-9.88	94.20	111.00
1	A	33	LEU	CB-CG-CD1	-9.84	94.26	111.00
1	B	54	ARG	NE-CZ-NH1	9.69	125.14	120.30
1	A	54	ARG	NE-CZ-NH1	9.21	124.90	120.30
1	B	28	ARG	NE-CZ-NH2	-8.30	116.15	120.30
1	A	28	ARG	NE-CZ-NH2	-7.73	116.44	120.30
1	A	51	GLN	N-CA-C	7.25	130.58	111.00
1	B	28	ARG	NE-CZ-NH1	6.35	123.47	120.30
1	B	80	ARG	NE-CZ-NH2	-6.31	117.14	120.30
1	A	33	LEU	CA-CB-CG	-6.28	100.85	115.30
1	A	28	ARG	NE-CZ-NH1	6.24	123.42	120.30
1	A	18	THR	OG1-CB-CG2	-5.57	97.19	110.00

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	2	GLN	Peptide
1	B	2	GLN	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	2121	0	2084	37	0
1	B	2115	0	2078	24	0
2	A	4	0	5	0	0
2	B	4	0	5	0	0
3	A	3	0	0	0	0
3	B	1	0	0	0	0
4	A	206	0	0	16	1
4	B	207	0	0	10	1

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
All	All	4661	0	4172	61	2

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 (61) 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:16:ALA:CA	1:B:16:ALA:CB	1.75	1.59
1:B:18:THR:CB	1:B:18:THR:CG2	1.76	1.57
1:A:33:LEU:CD2	1:A:33:LEU:CG	1.80	1.56
1:A:52:GLN:N	4:A:2062:HOH:O	1.76	1.18
1:A:142:CYS:HB3	4:A:2116:HOH:O	1.41	1.17
1:B:142:CYS:HB3	4:B:2120:HOH:O	1.39	1.17
1:A:171[B]:GLU:HG2	4:A:2132:HOH:O	1.47	1.15
1:B:142:CYS:SG	4:B:2120:HOH:O	2.06	1.12
1:A:33:LEU:CD2	1:A:33:LEU:CB	2.29	1.10
1:A:142:CYS:SG	4:A:2116:HOH:O	2.07	1.09
1:A:142:CYS:CB	4:A:2116:HOH:O	1.96	1.05
1:A:33:LEU:CD2	1:A:33:LEU:CD1	2.44	0.95
1:B:142:CYS:CB	4:B:2120:HOH:O	1.94	0.87
1:A:171[B]:GLU:H	1:A:171[B]:GLU:CD	1.86	0.78
1:B:16:ALA:N	1:B:16:ALA:CB	2.50	0.74
1:B:18:THR:CA	1:B:18:THR:CG2	2.68	0.69
1:A:171[B]:GLU:CG	4:A:2132:HOH:O	2.22	0.67
1:A:33:LEU:CD2	1:A:33:LEU:HD13	2.26	0.65
1:A:223:GLU:HG3	4:A:2157:HOH:O	1.98	0.64
1:B:6:GLN:HG3	4:B:2002:HOH:O	1.99	0.63
1:A:6:GLN:HG3	4:A:2002:HOH:O	1.98	0.63
1:B:140:MET:CE	4:B:2120:HOH:O	2.48	0.61
1:A:51:GLN:CA	4:A:2062:HOH:O	2.49	0.60
1:A:33:LEU:HB2	1:A:33:LEU:CD2	2.31	0.59
1:B:140:MET:HE3	4:B:2120:HOH:O	2.02	0.59
1:A:140:MET:HE3	4:A:2116:HOH:O	2.03	0.58
1:A:140:MET:CE	4:A:2116:HOH:O	2.51	0.57
1:A:33:LEU:HD13	1:A:33:LEU:HD22	1.90	0.53
1:A:20:ALA:HB1	1:A:26:ASP:OD1	2.09	0.53
1:B:33:LEU:C	1:B:34:THR:HG23	2.32	0.50
1:A:254:GLU:H	1:A:254:GLU:CD	2.15	0.49
1:A:51:GLN:N	4:A:2062:HOH:O	2.47	0.48
1:A:2:GLN:HB2	1:A:45:TYR:HE2	1.79	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:33:LEU:HD12	1:A:33:LEU:HA	1.57	0.47
1:A:155:GLU:HG2	1:A:157:ASP:HB2	1.98	0.46
1:B:2:GLN:HB2	1:B:45:TYR:HE2	1.81	0.46
1:A:161:PHE:CB	1:A:182:ILE:HD11	2.45	0.46
1:A:54:ARG:CD	4:A:2061:HOH:O	2.63	0.46
1:B:254:GLU:H	1:B:254:GLU:CD	2.19	0.46
1:A:54:ARG:HD3	4:A:2061:HOH:O	2.16	0.45
1:B:267:PRO:HG2	1:B:272:LEU:HD11	1.98	0.45
1:B:18:THR:CG2	1:B:18:THR:OG1	2.55	0.45
1:B:171:GLU:CD	4:B:2137:HOH:O	2.55	0.44
1:B:212:HIS:CD2	4:B:2154:HOH:O	2.71	0.44
1:B:161:PHE:CB	1:B:182:ILE:HD11	2.48	0.43
1:A:95:VAL:CG1	1:A:99:GLY:HA2	2.47	0.43
1:A:95:VAL:HG12	1:A:99:GLY:HA2	2.00	0.43
1:A:157:ASP:HB3	1:A:160:VAL:HG13	1.99	0.43
1:B:140:MET:HE2	4:B:2120:HOH:O	2.13	0.43
1:B:2:GLN:NE2	1:B:45:TYR:OH	2.53	0.42
1:B:54:ARG:CD	4:B:2061:HOH:O	2.66	0.42
1:A:157:ASP:CG	1:A:160:VAL:HG13	2.40	0.42
1:A:254:GLU:HB3	4:A:2189:HOH:O	2.19	0.41
1:B:120:ALA:HA	1:B:194:GLY:HA2	2.03	0.41
1:B:54:ARG:O	1:B:103:HIS:HA	2.20	0.41
1:A:15:LYS:O	1:A:19:ASP:N	2.48	0.41
1:A:2:GLN:HB3	1:A:3:ASN:O	2.21	0.41
1:B:33:LEU:C	1:B:34:THR:CG2	2.89	0.41
1:A:102:TYR:CE2	1:A:114:PRO:HG2	2.56	0.40
1:A:51:GLN:C	4:A:2062:HOH:O	2.33	0.40

All (2) 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)
4:B:2137:HOH:O	4:B:2154:HOH:O[3_545]	1.88	0.32
4:A:2009:HOH:O	4:A:2009:HOH:O[3_555]	2.18	0.02

## 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	272/273 (100%)	263 (97%)	7 (3%)	2 (1%)	22	10
1	B	271/273 (99%)	264 (97%)	6 (2%)	1 (0%)	34	21
All	All	543/546 (100%)	527 (97%)	13 (2%)	3 (1%)	25	12

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	3	ASN
1	B	3	ASN
1	A	52	GLN

### 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	227/226 (100%)	218 (96%)	9 (4%)	31	16
1	B	226/226 (100%)	218 (96%)	8 (4%)	36	21
All	All	453/452 (100%)	436 (96%)	17 (4%)	35	18

All (17) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	32	ASN
1	A	57	PRO
1	A	58	LEU

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Mol	Chain	Res	Type
1	A	80	ARG
1	A	111	GLU
1	A	153	VAL
1	A	171[A]	GLU
1	A	171[B]	GLU
1	A	211	PHE
1	B	32	ASN
1	B	33	LEU
1	B	80	ARG
1	B	111	GLU
1	B	153	VAL
1	B	160	VAL
1	B	171	GLU
1	B	211	PHE

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (8) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	2	GLN
1	A	156	ASN
1	B	2	GLN
1	B	51	GLN
1	B	52	GLN
1	B	60	GLN
1	B	156	ASN
1	B	195	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 carbohydrates in this entry.

## 5.6 Ligand geometry

Of 6 ligands modelled in this entry, 4 are monoatomic - leaving 2 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	EDO	B	1274	-	3,3,3	2.21	1 (33%)	2,2,2	1.08	0
2	EDO	A	1274	-	3,3,3	1.74	1 (33%)	2,2,2	1.43	1 (50%)

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	B	1274	-	-	1/1/1/1	-
2	EDO	A	1274	-	-	1/1/1/1	-

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	1274	EDO	O2-C2	-3.61	1.23	1.42
2	A	1274	EDO	O2-C2	-2.93	1.26	1.42

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	1274	EDO	O2-C2-C1	2.02	126.41	111.91

There are no chirality outliers.

All (2) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	1274	EDO	O1-C1-C2-O2
2	B	1274	EDO	O1-C1-C2-O2

There are no ring outliers.

No monomer is involved in short contacts.

## 5.7 Other polymers

There are no such residues in this entry.

## 5.8 Polymer linkage issues

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	272/273 (99%)	-0.34	3 (1%) 80 78	14, 26, 36, 45	0
1	B	272/273 (99%)	-0.37	2 (0%) 87 86	14, 25, 36, 45	0
All	All	544/546 (99%)	-0.35	5 (0%) 84 82	14, 26, 36, 45	0

All (5) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	248	TRP	3.6
1	A	248	TRP	3.3
1	A	50	HIS	2.4
1	B	50	HIS	2.3
1	A	51	GLN	2.2

### 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 carbohydrates 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
2	EDO	A	1274	4/4	0.89	0.12	33,37,37,38	0
2	EDO	B	1274	4/4	0.94	0.08	34,37,39,40	0
3	ZN	A	1277	1/1	0.99	0.04	30,30,30,30	0
3	ZN	A	1276	1/1	0.99	0.03	31,31,31,31	0
3	ZN	A	1275	1/1	1.00	0.02	25,25,25,25	0
3	ZN	B	1275	1/1	1.00	0.02	25,25,25,25	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.