



Full wwPDB X-ray Structure Validation Report ⓘ

Oct 29, 2024 – 02:04 pm GMT

PDB ID : 8OTU
Title : The crystal structure of PET44, a PETase enzyme from *Alkalilimnicola ehrlichii*
Authors : Costanzi, E.; Applegate, V.; Smits, S.H.J.
Deposited on : 2023-04-21
Resolution : 1.40 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 : 4.02b-467
Mogul : 1.8.4, CSD as541be (2020)
Xtriage (Phenix) : 1.13
EDS : 3.0
Percentile statistics : 20231227.v01 (using entries in the PDB archive December 27th 2023)
CCP4 : 9.0.003 (Gargrove)
Density-Fitness : 1.0.11
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.39

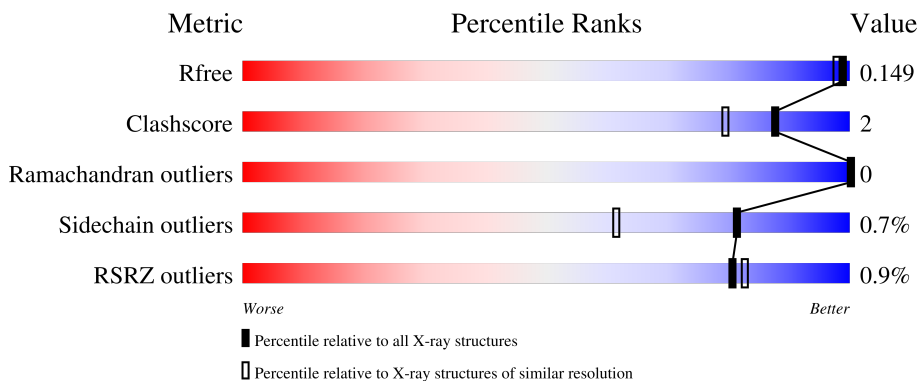
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION


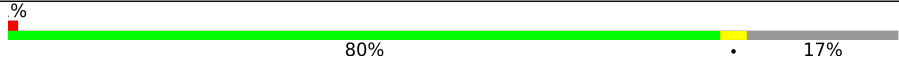
The reported resolution of this entry is 1.40 Å.

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}	164625	2247 (1.40-1.40)
Clashscore	180529	2446 (1.40-1.40)
Ramachandran outliers	177936	2398 (1.40-1.40)
Sidechain outliers	177891	2397 (1.40-1.40)
RSRZ outliers	164620	2246 (1.40-1.40)

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	320	
1	B	320	

2 Entry composition i

There are 5 unique types of molecules in this entry. The entry contains 8762 atoms, of which 4060 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 Dienelactone hydrolase domain-containing protein.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
			Total	C	H	N	O	S			
1	A	264	4019	1290	1954	362	403	10	0	7	0
1	B	266	4010	1287	1956	359	398	10	0	3	0

There are 30 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	306	VAL	-	expression tag	UNP A0A3E0WVY1
A	307	ASP	-	expression tag	UNP A0A3E0WVY1
A	308	LYS	-	expression tag	UNP A0A3E0WVY1
A	309	LEU	-	expression tag	UNP A0A3E0WVY1
A	310	ALA	-	expression tag	UNP A0A3E0WVY1
A	311	ALA	-	expression tag	UNP A0A3E0WVY1
A	312	ALA	-	expression tag	UNP A0A3E0WVY1
A	313	LEU	-	expression tag	UNP A0A3E0WVY1
A	314	GLU	-	expression tag	UNP A0A3E0WVY1
A	315	HIS	-	expression tag	UNP A0A3E0WVY1
A	316	HIS	-	expression tag	UNP A0A3E0WVY1
A	317	HIS	-	expression tag	UNP A0A3E0WVY1
A	318	HIS	-	expression tag	UNP A0A3E0WVY1
A	319	HIS	-	expression tag	UNP A0A3E0WVY1
A	320	HIS	-	expression tag	UNP A0A3E0WVY1
B	306	VAL	-	expression tag	UNP A0A3E0WVY1
B	307	ASP	-	expression tag	UNP A0A3E0WVY1
B	308	LYS	-	expression tag	UNP A0A3E0WVY1
B	309	LEU	-	expression tag	UNP A0A3E0WVY1
B	310	ALA	-	expression tag	UNP A0A3E0WVY1
B	311	ALA	-	expression tag	UNP A0A3E0WVY1
B	312	ALA	-	expression tag	UNP A0A3E0WVY1
B	313	LEU	-	expression tag	UNP A0A3E0WVY1
B	314	GLU	-	expression tag	UNP A0A3E0WVY1
B	315	HIS	-	expression tag	UNP A0A3E0WVY1

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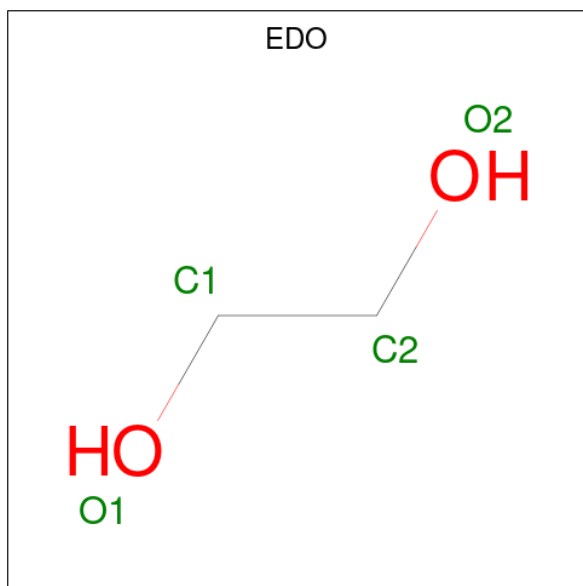
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Chain	Residue	Modelled	Actual	Comment	Reference
B	316	HIS	-	expression tag	UNP A0A3E0WVY1
B	317	HIS	-	expression tag	UNP A0A3E0WVY1
B	318	HIS	-	expression tag	UNP A0A3E0WVY1
B	319	HIS	-	expression tag	UNP A0A3E0WVY1
B	320	HIS	-	expression tag	UNP A0A3E0WVY1

- Molecule 2 is SODIUM ION (three-letter code: NA) (formula: Na).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	1	Total Na 1 1	0	0
2	B	2	Total Na 2 2	0	0

- Molecule 3 is 1,2-ETHANEDIOL (three-letter code: EDO) (formula: C₂H₆O₂).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	1	Total C H O 10 2 6 2	0	0
3	A	1	Total C H O 10 2 6 2	0	0
3	A	1	Total C H O 10 2 6 2	0	0
3	A	1	Total C H O 10 2 6 2	0	0

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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	A	1	Total	C	H	O	0	0
			10	2	6	2		
3	A	1	Total	C	H	O	0	0
			10	2	6	2		
3	A	1	Total	C	H	O	0	0
			10	2	6	2		
3	A	1	Total	C	H	O	0	0
			10	2	6	2		
3	A	1	Total	C	H	O	0	0
			10	2	6	2		
3	A	1	Total	C	H	O	0	0
			10	2	6	2		
3	A	1	Total	C	H	O	0	0
			10	2	6	2		
3	A	1	Total	C	H	O	0	0
			10	2	6	2		
3	A	1	Total	C	H	O	0	0
			10	2	6	2		
3	A	1	Total	C	H	O	0	0
			10	2	6	2		
3	B	1	Total	C	H	O	0	0
			10	2	6	2		
3	B	1	Total	C	H	O	0	0
			10	2	6	2		
3	B	1	Total	C	H	O	0	0
			10	2	6	2		
3	B	1	Total	C	H	O	0	0
			10	2	6	2		
3	B	1	Total	C	H	O	0	0
			10	2	6	2		
3	B	1	Total	C	H	O	0	0
			10	2	6	2		
3	B	1	Total	C	H	O	0	0
			10	2	6	2		

- Molecule 4 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

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

- Molecule 5 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	248	Total O 248 248	0	0
5	B	229	Total O 229 229	0	0

4 Data and refinement statistics i

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	141.13Å 45.66Å 84.19Å 90.00° 97.83° 90.00°	Depositor
Resolution (Å)	50.31 – 1.40 50.31 – 1.40	Depositor EDS
% Data completeness (in resolution range)	95.7 (50.31-1.40) 95.7 (50.31-1.40)	Depositor EDS
R_{merge}	0.04	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.54 (at 1.40Å)	Xtrriage
Refinement program	PHENIX 1.19.2_4158, PHENIX 1.19.2_4158	Depositor
R, R_{free}	0.132 , 0.150 0.131 , 0.149	Depositor DCC
R_{free} test set	5272 reflections (5.02%)	wwPDB-VP
Wilson B-factor (Å ²)	18.1	Xtrriage
Anisotropy	0.530	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.43 , 50.3	EDS
L-test for twinning ²	$\langle L \rangle = 0.51$, $\langle L^2 \rangle = 0.34$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
F_o, F_c correlation	0.98	EDS
Total number of atoms	8762	wwPDB-VP
Average B, all atoms (Å ²)	27.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 6.35% 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: CL, NA, 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	0.57	0/2119	0.78	0/2884
1	B	0.55	0/2111	0.73	0/2874
All	All	0.56	0/4230	0.75	0/5758

There are no bond length outliers.

There are no bond angle outliers.

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	2065	1954	1948	8	0
1	B	2054	1956	1953	8	0
2	A	1	0	0	0	0
2	B	2	0	0	0	0
3	A	64	96	95	4	0
3	B	36	54	54	6	0
4	A	2	0	0	0	0
4	B	1	0	0	0	0
5	A	248	0	0	2	0
5	B	229	0	0	1	0
All	All	4702	4060	4050	16	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 2.

All (16) 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:48:ASP:H	3:A:405:EDO:H21	1.50	0.75
1:A:42:GLY:N	5:A:502:HOH:O	2.26	0.67
1:A:48:ASP:H	3:A:405:EDO:C2	2.15	0.57
1:B:291:GLU:HG3	3:B:408:EDO:H11	1.87	0.57
1:A:262:LEU:HD11	1:A:296:ILE:HD11	1.85	0.57
1:A:48:ASP:N	3:A:405:EDO:H21	2.19	0.56
1:B:188:GLN:HG2	3:B:407:EDO:H11	1.90	0.54
1:A:244:GLU:OE1	3:A:404:EDO:H22	2.09	0.52
1:B:87:GLU:OE2	3:B:410:EDO:O2	2.27	0.51
1:B:186:GLY:O	3:B:405:EDO:H21	2.11	0.50
1:B:205:SER:OG	5:B:501:HOH:O	2.20	0.50
1:A:67[A]:ASN:OD1	5:A:501:HOH:O	2.21	0.45
1:B:188:GLN:CG	3:B:407:EDO:H11	2.47	0.44
1:A:262:LEU:HD11	1:A:296:ILE:CD1	2.50	0.41
1:B:65:THR:HA	1:B:80:ILE:O	2.20	0.41
1:B:186:GLY:O	3:B:405:EDO:C2	2.68	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	269/320 (84%)	264 (98%)	5 (2%)	0	100	100
1	B	268/320 (84%)	264 (98%)	4 (2%)	0	100	100
All	All	537/640 (84%)	528 (98%)	9 (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	220/260 (85%)	219 (100%)	1 (0%)	86	71
1	B	219/260 (84%)	217 (99%)	2 (1%)	75	53
All	All	439/520 (84%)	436 (99%)	3 (1%)	81	61

All (3) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	136	ARG
1	B	136	ARG
1	B	252	CYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

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](#)

Of 31 ligands modelled in this entry, 6 are monoatomic - leaving 25 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
3	EDO	B	406	-	3,3,3	0.67	0	2,2,2	0.53	0
3	EDO	B	405	-	3,3,3	0.46	0	2,2,2	0.66	0
3	EDO	A	407	-	3,3,3	0.41	0	2,2,2	0.60	0
3	EDO	A	405	-	3,3,3	0.42	0	2,2,2	0.53	0
3	EDO	B	403	-	3,3,3	0.49	0	2,2,2	0.56	0
3	EDO	A	406	-	3,3,3	0.40	0	2,2,2	0.24	0
3	EDO	B	410	-	3,3,3	0.48	0	2,2,2	0.13	0
3	EDO	A	410	-	3,3,3	0.50	0	2,2,2	0.20	0
3	EDO	A	403	-	3,3,3	0.40	0	2,2,2	0.84	0
3	EDO	A	404	-	3,3,3	0.46	0	2,2,2	0.35	0
3	EDO	A	414	-	3,3,3	0.45	0	2,2,2	0.51	0
3	EDO	A	415	2	3,3,3	0.47	0	2,2,2	0.04	0
3	EDO	A	413	-	3,3,3	0.47	0	2,2,2	0.34	0
3	EDO	B	409	-	3,3,3	0.52	0	2,2,2	0.53	0
3	EDO	A	409	-	3,3,3	0.50	0	2,2,2	0.63	0
3	EDO	B	408	-	3,3,3	0.41	0	2,2,2	0.33	0
3	EDO	A	408	-	3,3,3	0.54	0	2,2,2	0.36	0
3	EDO	A	412	-	3,3,3	0.43	0	2,2,2	0.71	0
3	EDO	B	411	-	3,3,3	0.58	0	2,2,2	0.24	0
3	EDO	A	411	-	3,3,3	0.45	0	2,2,2	0.36	0
3	EDO	A	417	-	3,3,3	0.42	0	2,2,2	0.30	0
3	EDO	B	407	-	3,3,3	0.42	0	2,2,2	0.52	0
3	EDO	A	416	-	3,3,3	0.42	0	2,2,2	0.48	0
3	EDO	A	402	-	3,3,3	0.47	0	2,2,2	0.72	0
3	EDO	B	404	-	3,3,3	0.44	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
3	EDO	B	406	-	-	0/1/1/1	-
3	EDO	B	405	-	-	1/1/1/1	-
3	EDO	A	407	-	-	0/1/1/1	-
3	EDO	A	405	-	-	0/1/1/1	-
3	EDO	B	403	-	-	0/1/1/1	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	EDO	A	406	-	-	0/1/1/1	-
3	EDO	B	410	-	-	1/1/1/1	-
3	EDO	A	410	-	-	1/1/1/1	-
3	EDO	A	403	-	-	0/1/1/1	-
3	EDO	A	404	-	-	0/1/1/1	-
3	EDO	A	414	-	-	0/1/1/1	-
3	EDO	A	415	2	-	0/1/1/1	-
3	EDO	A	413	-	-	0/1/1/1	-
3	EDO	B	409	-	-	1/1/1/1	-
3	EDO	A	409	-	-	0/1/1/1	-
3	EDO	B	408	-	-	0/1/1/1	-
3	EDO	A	408	-	-	0/1/1/1	-
3	EDO	A	412	-	-	1/1/1/1	-
3	EDO	B	411	-	-	1/1/1/1	-
3	EDO	A	411	-	-	0/1/1/1	-
3	EDO	A	417	-	-	0/1/1/1	-
3	EDO	B	407	-	-	0/1/1/1	-
3	EDO	A	416	-	-	1/1/1/1	-
3	EDO	A	402	-	-	0/1/1/1	-
3	EDO	B	404	-	-	0/1/1/1	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (7) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	410	EDO	O1-C1-C2-O2
3	A	416	EDO	O1-C1-C2-O2
3	B	410	EDO	O1-C1-C2-O2
3	B	405	EDO	O1-C1-C2-O2
3	B	411	EDO	O1-C1-C2-O2
3	B	409	EDO	O1-C1-C2-O2
3	A	412	EDO	O1-C1-C2-O2

There are no ring outliers.

6 monomers are involved in 10 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	B	405	EDO	2	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	405	EDO	3	0
3	B	410	EDO	1	0
3	A	404	EDO	1	0
3	B	408	EDO	1	0
3	B	407	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 [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	264/320 (82%)	-0.55	3 (1%) 77 79	9, 22, 38, 69	7 (2%)
1	B	266/320 (83%)	-0.48	2 (0%) 82 84	6, 24, 40, 79	3 (1%)
All	All	530/640 (82%)	-0.52	5 (0%) 81 83	6, 23, 40, 79	10 (1%)

All (5) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	306	VAL	3.5
1	A	42	GLY	3.1
1	A	305	PHE	2.7
1	A	85	ASN	2.5
1	B	307	ASP	2.3

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
3	EDO	B	406	4/4	0.70	0.24	48,58,60,62	0
3	EDO	A	410	4/4	0.77	0.19	55,66,67,67	0
3	EDO	A	414	4/4	0.79	0.19	63,75,76,76	0
3	EDO	A	403	4/4	0.80	0.22	50,60,60,60	0
3	EDO	B	411	4/4	0.80	0.20	34,41,42,45	10
3	EDO	B	409	4/4	0.83	0.15	58,69,71,72	0
3	EDO	B	403	4/4	0.83	0.14	42,51,52,54	0
3	EDO	B	407	4/4	0.84	0.24	56,67,72,73	0
3	EDO	B	404	4/4	0.84	0.18	43,52,62,63	0
3	EDO	B	410	4/4	0.84	0.14	46,56,58,58	0
3	EDO	A	404	4/4	0.84	0.13	54,65,66,66	0
3	EDO	A	412	4/4	0.85	0.20	69,82,83,84	0
3	EDO	A	415	4/4	0.87	0.12	36,44,52,52	0
3	EDO	A	405	4/4	0.87	0.14	51,62,63,64	0
3	EDO	A	416	4/4	0.88	0.17	47,57,64,65	0
3	EDO	A	411	4/4	0.88	0.16	47,56,64,66	0
3	EDO	A	409	4/4	0.89	0.19	58,70,76,78	0
3	EDO	A	407	4/4	0.89	0.13	46,55,57,57	0
3	EDO	B	405	4/4	0.89	0.16	49,59,64,64	0
3	EDO	A	413	4/4	0.89	0.10	41,49,49,51	0
3	EDO	A	406	4/4	0.91	0.13	31,40,44,48	0
3	EDO	A	417	4/4	0.92	0.10	27,36,41,44	0
3	EDO	A	402	4/4	0.92	0.12	29,35,41,47	0
3	EDO	B	408	4/4	0.92	0.10	34,41,47,47	0
3	EDO	A	408	4/4	0.93	0.10	37,45,50,55	0
2	NA	B	401	1/1	0.94	0.09	27,27,27,27	0
2	NA	B	402	1/1	0.96	0.08	24,24,24,24	0
2	NA	A	401	1/1	0.97	0.07	23,23,23,23	0
4	CL	B	412	1/1	0.98	0.09	40,40,40,40	0
4	CL	A	419	1/1	0.99	0.06	26,26,26,26	1
4	CL	A	418	1/1	1.00	0.01	24,24,24,24	0

6.5 Other polymers [i](#)

There are no such residues in this entry.