Full wwPDB X-ray Structure Validation Report ⓘ

Nov 22, 2023 – 07:39 PM JST

PDB ID	:	7Y8V
Title	:	Crystal structure of AlbEF homolog mutant (AlbF-H54A/H58A) from Quasibacillus thermotolerans
Authors	:	Ishida, K.; Nakamura, A.; Kojima, S.
Deposited on	:	2022-06-24
Resolution	:	2.30 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:

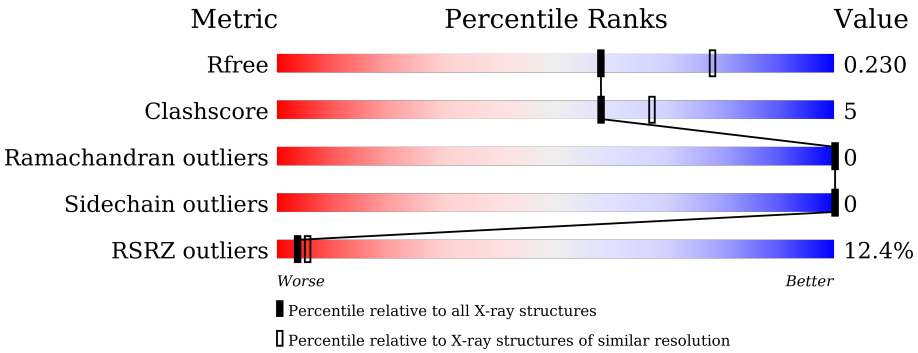
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, 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 2.30 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	5042 (2.30-2.30)
Clashscore	141614	5643 (2.30-2.30)
Ramachandran outliers	138981	5575 (2.30-2.30)
Sidechain outliers	138945	5575 (2.30-2.30)
RSRZ outliers	127900	4938 (2.30-2.30)

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	E	395	16% 79% 16% 5%
2	F	366	7% 87% 7% 6%

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
3	PO4	E	402	-	-	X	-

2 Entry composition (i)

There are 5 unique types of molecules in this entry. The entry contains 6007 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 AlbE homolog.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	E	374	3048	1954	510	572	12	0	0	0

There are 14 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
E	-13	MET	-	initiating methionine	UNP A0A837GIQ1
E	-12	GLY	-	expression tag	UNP A0A837GIQ1
E	-11	SER	-	expression tag	UNP A0A837GIQ1
E	-10	SER	-	expression tag	UNP A0A837GIQ1
E	-9	HIS	-	expression tag	UNP A0A837GIQ1
E	-8	HIS	-	expression tag	UNP A0A837GIQ1
E	-7	HIS	-	expression tag	UNP A0A837GIQ1
E	-6	HIS	-	expression tag	UNP A0A837GIQ1
E	-5	HIS	-	expression tag	UNP A0A837GIQ1
E	-4	HIS	-	expression tag	UNP A0A837GIQ1
E	-3	SER	-	expression tag	UNP A0A837GIQ1
E	-2	GLN	-	expression tag	UNP A0A837GIQ1
E	-1	ASP	-	expression tag	UNP A0A837GIQ1
E	0	PRO	-	expression tag	UNP A0A837GIQ1

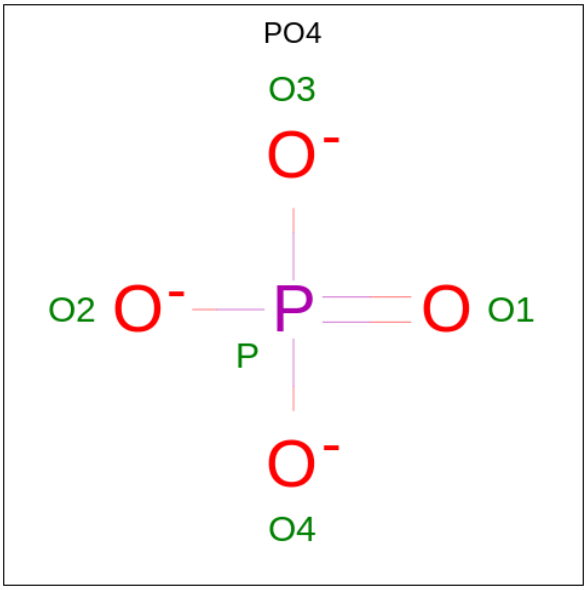
- Molecule 2 is a protein called AlbF homolog H54A/H58A mutant.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
2	F	343	2838	1819	471	537	11	0	4	0

There are 2 discrepancies between the modelled and reference sequences:

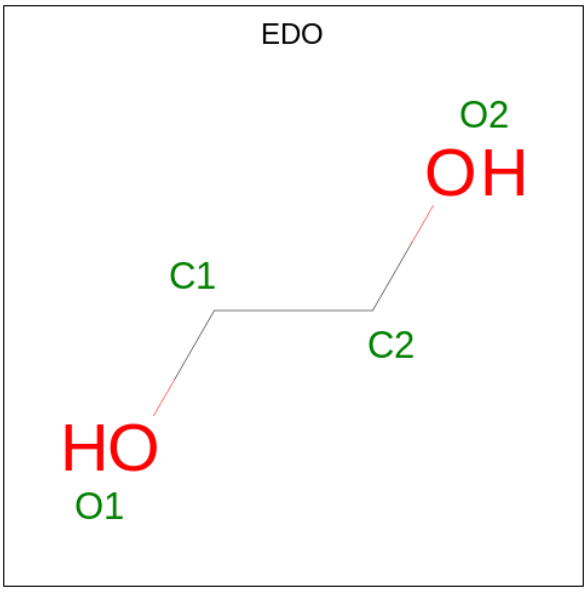
Chain	Residue	Modelled	Actual	Comment	Reference
F	54	ALA	HIS	engineered mutation	UNP A0A837GEN5
F	58	ALA	HIS	engineered mutation	UNP A0A837GEN5

- Molecule 3 is PHOSPHATE ION (three-letter code: PO4) (formula: O_4P).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	E	1	Total O P 5 4 1	0	0
3	E	1	Total O P 5 4 1	0	0
3	E	1	Total O P 5 4 1	0	0
3	E	1	Total O P 5 4 1	0	0
3	F	1	Total O P 5 4 1	0	0
3	F	1	Total O P 5 4 1	0	0
3	F	1	Total O P 5 4 1	0	0

- Molecule 4 is 1,2-ETHANEDIOL (three-letter code: EDO) (formula: $C_2H_6O_2$).



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

- Molecule 5 is water.

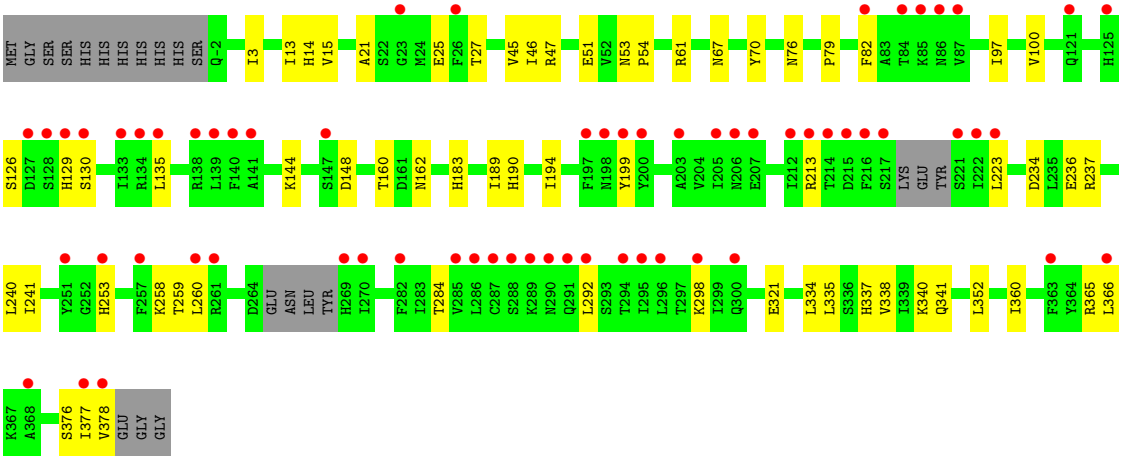
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	E	3	Total O 3 3	0	0
5	F	55	Total O 55 55	0	0

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.

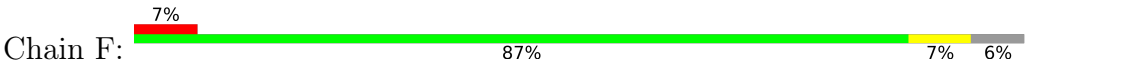
• Molecule 1: AlbE homolog

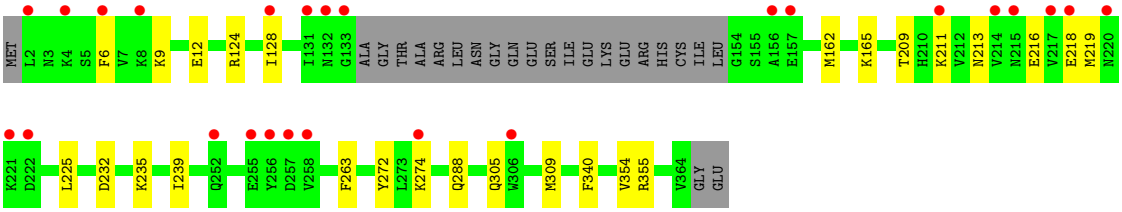
Chain E:



• Molecule 2: AlbF homolog H54A/H58A mutant

Chain F:





4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 31 2 1	Depositor
Cell constants a, b, c, α, β, γ	136.42Å 136.42Å 119.00Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	41.92 – 2.30 44.65 – 2.30	Depositor EDS
% Data completeness (in resolution range)	99.8 (41.92-2.30) 99.8 (44.65-2.30)	Depositor EDS
R_{merge}	0.05	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	4.36 (at 2.29Å)	Xtriage
Refinement program	PHENIX 1.20.1_4487	Depositor
R, R_{free}	0.200 , 0.233 0.198 , 0.230	Depositor DCC
R_{free} test set	2684 reflections (4.71%)	wwPDB-VP
Wilson B-factor (Å^2)	50.4	Xtriage
Anisotropy	0.452	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.34 , 50.6	EDS
L-test for twinning[2]	$< \|L\| > = 0.50$, $< L^2 > = 0.34$	Xtriage
Estimated twinning fraction	0.018 for -h,-k,l	Xtriage
F_o,F_c correlation	0.95	EDS
Total number of atoms	6007	wwPDB-VP
Average B, all atoms (Å^2)	75.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.94% of the height of the origin peak. No significant pseudotranslation is detected.*

[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, PO4

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	E	0.25	0/3110	0.45	0/4191
2	F	0.26	0/2906	0.46	0/3926
All	All	0.26	0/6016	0.45	0/8117

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

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	E	3048	0	3034	37	0
2	F	2838	0	2806	21	0
3	E	20	0	0	2	0
3	F	15	0	0	0	0
4	E	4	0	6	1	0
4	F	24	0	36	1	0
5	E	3	0	0	0	0
5	F	55	0	0	0	0
All	All	6007	0	5882	57	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 5.

All (57) 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)
2:F:225:LEU:HD11	2:F:274:LYS:HZ3	1.43	0.81
1:E:189:ILE:HD13	1:E:338:VAL:HG21	1.78	0.65
2:F:232:ASP:HB3	2:F:235:LYS:HB2	1.79	0.64
1:E:259:THR:HG23	1:E:298:LYS:HE3	1.78	0.64
1:E:236:GLU:OE2	1:E:365:ARG:NH1	2.32	0.62
1:E:234:ASP:OD1	1:E:237:ARG:NH2	2.29	0.62
2:F:218:GLU:HG3	2:F:274:LYS:HZ2	1.66	0.60
1:E:236:GLU:HA	1:E:240:LEU:HB2	1.83	0.60
2:F:263:PHE:HB3	2:F:272:TYR:HB2	1.85	0.59
2:F:225:LEU:CD1	2:F:274:LYS:HZ3	2.14	0.59
1:E:337:HIS:CE1	1:E:341:GLN:HG3	2.38	0.58
2:F:209:THR:HG21	2:F:211:LYS:HE3	1.86	0.58
2:F:218:GLU:HG3	2:F:274:LYS:NZ	2.18	0.58
2:F:263:PHE:HB2	2:F:274:LYS:HE2	1.86	0.57
1:E:241:ILE:HG12	1:E:366:LEU:HD21	1.88	0.55
1:E:253:HIS:HB3	1:E:258:LYS:HD2	1.88	0.55
1:E:321:GLU:HG3	1:E:352:LEU:HD22	1.89	0.55
1:E:213:ARG:HD2	1:E:378:VAL:HG22	1.88	0.54
2:F:165:LYS:HD2	4:F:404:EDO:H22	1.88	0.54
2:F:309:MET:HG2	2:F:340:PHE:CE1	2.43	0.54
2:F:239:ILE:HG21	2:F:354:VAL:HG21	1.88	0.53
1:E:21:ALA:HA	1:E:70:TYR:CD2	2.44	0.53
1:E:223:LEU:HD13	1:E:377:ILE:HG12	1.92	0.52
1:E:13:ILE:HD12	1:E:76:ASN:HB3	1.92	0.51
1:E:46:ILE:HD13	1:E:97:ILE:HG12	1.91	0.51
1:E:47:ARG:NH2	3:E:402:PO4:O1	2.39	0.50
1:E:25:GLU:HG2	1:E:67:ASN:O	2.11	0.50
2:F:219:MET:SD	2:F:225:LEU:HD13	2.51	0.50
2:F:225:LEU:HD11	2:F:274:LYS:NZ	2.21	0.49
1:E:126:SER:HB2	1:E:129:HIS:HB3	1.96	0.48
1:E:14:HIS:CE1	1:E:79:PRO:HB3	2.49	0.47
1:E:199:TYR:OH	1:E:340:LYS:O	2.31	0.47
1:E:259:THR:HG22	1:E:260:LEU:HD12	1.95	0.47
1:E:25:GLU:OE1	1:E:27:THR:OG1	2.26	0.47
2:F:124:ARG:O	2:F:128:ILE:HG12	2.13	0.47
1:E:3:ILE:HD11	1:E:194:ILE:HG13	1.95	0.47
1:E:160:THR:OG1	1:E:162:ASN:OD1	2.29	0.46
2:F:288:GLN:HA	2:F:355:ARG:HH21	1.80	0.46
1:E:82:PHE:HB3	2:F:6:PHE:HB2	1.98	0.46
1:E:126:SER:O	1:E:130:SER:N	2.49	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:9:LYS:O	2:F:12:GLU:HG2	2.16	0.46
2:F:213:ASN:HD21	2:F:216:GLU:HB2	1.80	0.45
2:F:305:GLN:O	2:F:309:MET:HG3	2.17	0.45
1:E:135:LEU:HD11	1:E:376:SER:HB2	1.99	0.45
1:E:53:ASN:OD1	1:E:54:PRO:HA	2.18	0.44
1:E:189:ILE:HD11	1:E:334:LEU:HD21	2.00	0.43
1:E:45:VAL:HG11	1:E:100:VAL:HG13	2.01	0.43
2:F:213:ASN:ND2	2:F:216:GLU:HB2	2.34	0.43
1:E:223:LEU:O	1:E:284:THR:HA	2.19	0.43
1:E:292:LEU:HD11	1:E:377:ILE:HD13	2.01	0.43
2:F:162:MET:HB2	2:F:162:MET:HE3	1.90	0.43
1:E:47:ARG:HG3	1:E:51:GLU:CD	2.39	0.42
1:E:183:HIS:HB3	1:E:190:HIS:HB2	2.00	0.42
1:E:61:ARG:NE	3:E:402:PO4:O2	2.53	0.41
1:E:15:VAL:HG11	1:E:335:LEU:HD22	2.02	0.41
1:E:144:LYS:HA	1:E:148:ASP:HB2	2.03	0.41
1:E:360:ILE:H	4:E:405:EDO:H21	1.86	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	E	368/395 (93%)	357 (97%)	11 (3%)	0	100	100
2	F	343/366 (94%)	334 (97%)	9 (3%)	0	100	100
All	All	711/761 (93%)	691 (97%)	20 (3%)	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	E	344/362 (95%)	344 (100%)	0	100	100
2	F	316/330 (96%)	316 (100%)	0	100	100
All	All	660/692 (95%)	660 (100%)	0	100	100

There are no protein residues with a non-rotameric sidechain to report.

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

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

14 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	$\#\|Z\|>2$
4	EDO	F	405	-	3,3,3	0.46	0	2,2,2	0.33	0
4	EDO	F	406	-	3,3,3	0.47	0	2,2,2	0.31	0
3	PO4	F	402	-	4,4,4	0.91	0	6,6,6	0.44	0
3	PO4	F	401	-	4,4,4	0.86	0	6,6,6	0.50	0
4	EDO	E	405	-	3,3,3	0.47	0	2,2,2	0.23	0
3	PO4	E	404	-	4,4,4	0.99	0	6,6,6	0.52	0
3	PO4	E	401	-	4,4,4	0.93	0	6,6,6	0.44	0
4	EDO	F	404	-	3,3,3	0.47	0	2,2,2	0.16	0
4	EDO	F	409	-	3,3,3	0.49	0	2,2,2	0.28	0
3	PO4	F	403	-	4,4,4	0.90	0	6,6,6	0.44	0
4	EDO	F	408	-	3,3,3	0.47	0	2,2,2	0.28	0
3	PO4	E	403	-	4,4,4	0.90	0	6,6,6	0.44	0
4	EDO	F	407	-	3,3,3	0.50	0	2,2,2	0.22	0
3	PO4	E	402	-	4,4,4	0.92	0	6,6,6	0.46	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
4	EDO	F	405	-	-	0/1/1/1	-
4	EDO	F	406	-	-	0/1/1/1	-
4	EDO	E	405	-	-	0/1/1/1	-
4	EDO	F	404	-	-	0/1/1/1	-
4	EDO	F	409	-	-	0/1/1/1	-
4	EDO	F	408	-	-	0/1/1/1	-
4	EDO	F	407	-	-	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
4	F	407	EDO	O1-C1-C2-O2

There are no ring outliers.

3 monomers are involved in 4 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	E	405	EDO	1	0
4	F	404	EDO	1	0
3	E	402	PO4	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, 95^{th} 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	E	374/395 (94%)	1.03	64 (17%) 1 2	44, 78, 145, 180	0
2	F	343/366 (93%)	0.45	25 (7%) 15 20	35, 57, 119, 160	1 (0%)
All	All	717/761 (94%)	0.75	89 (12%) 4 5	35, 67, 139, 180	1 (0%)

All (89) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	E	286	LEU	12.7
2	F	133	GLY	12.5
1	E	216	PHE	10.8
1	E	205	ILE	9.0
1	E	378	VAL	8.6
1	E	287	CYS	8.5
1	E	292	LEU	8.5
1	E	222	ILE	8.2
1	E	223	LEU	7.7
2	F	257	ASP	7.2
1	E	290	ASN	7.1
1	E	127	ASP	6.9
1	E	197	PHE	6.6
1	E	212	ILE	6.4
1	E	288	SER	6.0
1	E	217	SER	5.9
1	E	138	ARG	5.7
2	F	217	VAL	5.5
1	E	253	HIS	5.5
1	E	377	ILE	5.3
1	E	221	SER	5.3
1	E	213	ARG	5.1
1	E	129	HIS	5.0
1	E	23	GLY	5.0

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Mol	Chain	Res	Type	RSRZ
1	E	141	ALA	5.0
2	F	4	LYS	5.0
2	F	258	VAL	4.9
2	F	256	TYR	4.8
2	F	2	LEU	4.6
2	F	221	LYS	4.4
1	E	206	ASN	4.3
1	E	82	PHE	4.2
1	E	294	THR	4.2
1	E	215	ASP	4.2
1	E	257	PHE	4.1
1	E	125	HIS	4.1
1	E	134	ARG	4.0
2	F	157	GLU	4.0
1	E	260	LEU	3.8
1	E	295	ILE	3.8
1	E	85	LYS	3.8
1	E	86	ASN	3.7
1	E	135	LEU	3.6
1	E	203	ALA	3.6
2	F	132	ASN	3.6
1	E	300	GLN	3.5
1	E	128	SER	3.5
1	E	298	LYS	3.4
2	F	156	ALA	3.4
2	F	220	ASN	3.3
1	E	84	THR	3.3
1	E	139	LEU	3.3
1	E	368	ALA	3.3
1	E	296	LEU	3.3
2	F	215	ASN	3.2
1	E	251	TYR	3.0
1	E	289	LYS	3.0
2	F	211	LYS	3.0
1	E	87	VAL	2.9
2	F	306	TRP	2.9
1	E	199	TYR	2.9
1	E	291	GLN	2.9
1	E	121	GLN	2.8
1	E	140	PHE	2.8
2	F	255	GLU	2.8
2	F	222	ASP	2.7

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Mol	Chain	Res	Type	RSRZ
2	F	252	GLN	2.7
1	E	214	THR	2.6
1	E	200	TYR	2.6
1	E	133	ILE	2.6
2	F	218	GLU	2.6
2	F	128	ILE	2.6
1	E	270	ILE	2.5
2	F	6	PHE	2.5
1	E	261	ARG	2.5
2	F	274	LYS	2.5
1	E	285	VAL	2.4
2	F	214	VAL	2.4
1	E	198	ASN	2.3
2	F	8	LYS	2.2
1	E	26	PHE	2.2
2	F	131	ILE	2.2
1	E	147	SER	2.2
1	E	363	PHE	2.1
1	E	207	GLU	2.0
1	E	269	HIS	2.0
1	E	366	LEU	2.0
1	E	282	PHE	2.0
1	E	130	SER	2.0

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, 95^{th} 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.

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
4	EDO	E	405	4/4	0.41	0.28	75,76,81,90	0
4	EDO	F	407	4/4	0.48	0.33	72,73,76,84	0
4	EDO	F	405	4/4	0.78	0.21	58,60,66,72	0
4	EDO	F	408	4/4	0.80	0.34	72,76,79,81	0
4	EDO	F	409	4/4	0.80	0.21	67,72,76,81	0
4	EDO	F	406	4/4	0.82	0.36	72,73,76,82	0
3	PO4	E	404	5/5	0.82	0.30	114,129,139,219	0
4	EDO	F	404	4/4	0.90	0.14	58,73,73,74	0
3	PO4	F	403	5/5	0.91	0.16	87,89,114,133	0
3	PO4	F	402	5/5	0.92	0.10	77,102,110,121	0
3	PO4	E	403	5/5	0.93	0.19	84,85,95,103	0
3	PO4	E	402	5/5	0.96	0.10	61,73,86,92	0
3	PO4	F	401	5/5	0.98	0.10	59,70,81,84	0
3	PO4	E	401	5/5	0.98	0.22	64,67,81,87	0

6.5 Other polymers (i)

There are no such residues in this entry.