



wwPDB X-ray Structure Validation Summary Report ⓘ

Mar 7, 2026 – 01:35 AM UTC

PDB ID : 8EGY / pdb_00008egy
Title : Engineered holo tyrosine synthase (TmTyrS1) derived from *T. maritima* TrpB
Authors : Porter, N.J.; Almhjell, P.J.; Arnold, F.H.
Deposited on : 2022-09-13
Resolution : 2.05 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 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	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

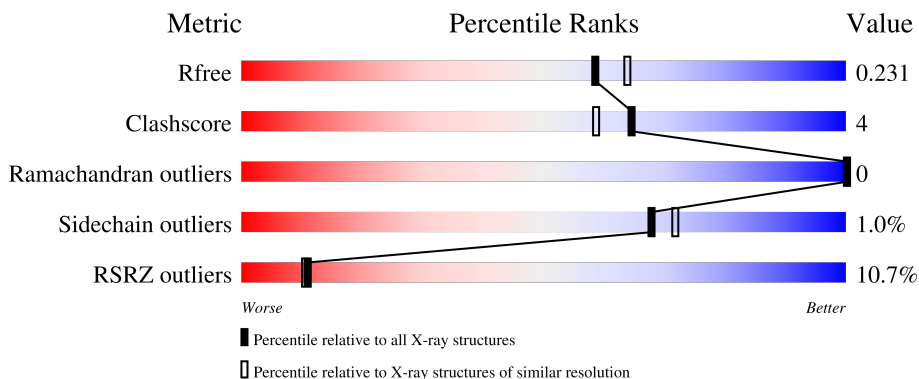
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.05 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}	180053	2260 (2.04-2.04)
Clashscore	190562	2333 (2.04-2.04)
Ramachandran outliers	187476	2318 (2.04-2.04)
Sidechain outliers	187428	2318 (2.04-2.04)
RSRZ outliers	180081	2260 (2.04-2.04)

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	397	5% 90% 6% ••
1	B	397	16% 84% 12% •

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 6201 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 Engineered tyrosine synthase (TmTyrS1).

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	385	Total	C	N	O	P	S	26	1	0
			2990	1903	516	562	1	8			
1	B	382	Total	C	N	O	P	S	71	2	0
			2966	1887	512	558	1	8			

There are 52 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	4	ASN	TYR	engineered mutation	UNP P50909
A	12	ASN	TYR	engineered mutation	UNP P50909
A	19	GLY	PRO	engineered mutation	UNP P50909
A	30	GLY	GLU	engineered mutation	UNP P50909
A	41	TYR	PHE	engineered mutation	UNP P50909
A	69	VAL	ILE	engineered mutation	UNP P50909
A	96	LEU	LYS	engineered mutation	UNP P50909
A	103	THR	ILE	engineered mutation	UNP P50909
A	105	GLY	GLU	engineered mutation	UNP P50909
A	140	LEU	PRO	engineered mutation	UNP P50909
A	167	ASP	ASN	engineered mutation	UNP P50909
A	184	PRO	ILE	engineered mutation	UNP P50909
A	213	PRO	LEU	engineered mutation	UNP P50909
A	228	SER	GLY	engineered mutation	UNP P50909
A	291	ALA	VAL	engineered mutation	UNP P50909
A	292	SER	THR	engineered mutation	UNP P50909
A	302	PRO	SER	engineered mutation	UNP P50909
A	389	HIS	ARG	engineered mutation	UNP P50909
A	390	LEU	-	expression tag	UNP P50909
A	391	GLU	-	expression tag	UNP P50909
A	392	HIS	-	expression tag	UNP P50909
A	393	HIS	-	expression tag	UNP P50909
A	394	HIS	-	expression tag	UNP P50909
A	395	HIS	-	expression tag	UNP P50909
A	396	HIS	-	expression tag	UNP P50909

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Chain	Residue	Modelled	Actual	Comment	Reference
A	397	HIS	-	expression tag	UNP P50909
B	4	ASN	TYR	engineered mutation	UNP P50909
B	12	ASN	TYR	engineered mutation	UNP P50909
B	19	GLY	PRO	engineered mutation	UNP P50909
B	30	GLY	GLU	engineered mutation	UNP P50909
B	41	TYR	PHE	engineered mutation	UNP P50909
B	69	VAL	ILE	engineered mutation	UNP P50909
B	96	LEU	LYS	engineered mutation	UNP P50909
B	103	THR	ILE	engineered mutation	UNP P50909
B	105	GLY	GLU	engineered mutation	UNP P50909
B	140	LEU	PRO	engineered mutation	UNP P50909
B	167	ASP	ASN	engineered mutation	UNP P50909
B	184	PRO	ILE	engineered mutation	UNP P50909
B	213	PRO	LEU	engineered mutation	UNP P50909
B	228	SER	GLY	engineered mutation	UNP P50909
B	291	ALA	VAL	engineered mutation	UNP P50909
B	292	SER	THR	engineered mutation	UNP P50909
B	302	PRO	SER	engineered mutation	UNP P50909
B	389	HIS	ARG	engineered mutation	UNP P50909
B	390	LEU	-	expression tag	UNP P50909
B	391	GLU	-	expression tag	UNP P50909
B	392	HIS	-	expression tag	UNP P50909
B	393	HIS	-	expression tag	UNP P50909
B	394	HIS	-	expression tag	UNP P50909
B	395	HIS	-	expression tag	UNP P50909
B	396	HIS	-	expression tag	UNP P50909
B	397	HIS	-	expression tag	UNP P50909

- Molecule 2 is POTASSIUM ION (CCD ID: K) (formula: K).

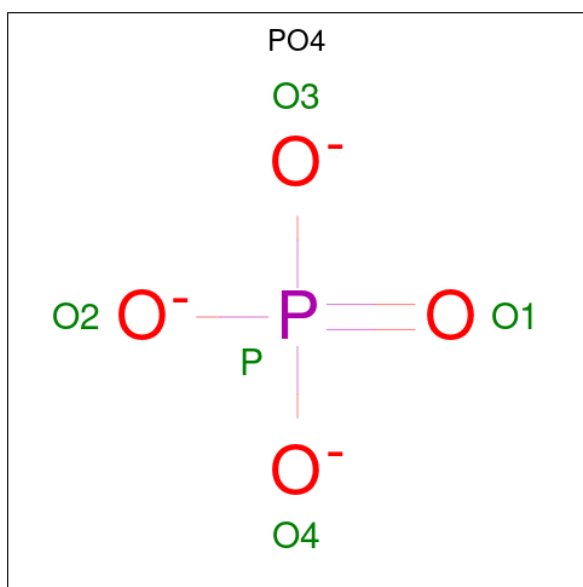
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	1	Total K 1 1	0	0
2	B	1	Total K 1 1	0	0

- Molecule 3 is 1,2-ETHANEDIOL (CCD ID: EDO) (formula: C₂H₆O₂).



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

- Molecule 4 is PHOSPHATE ION (CCD ID: PO4) (formula: O_4P).



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

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

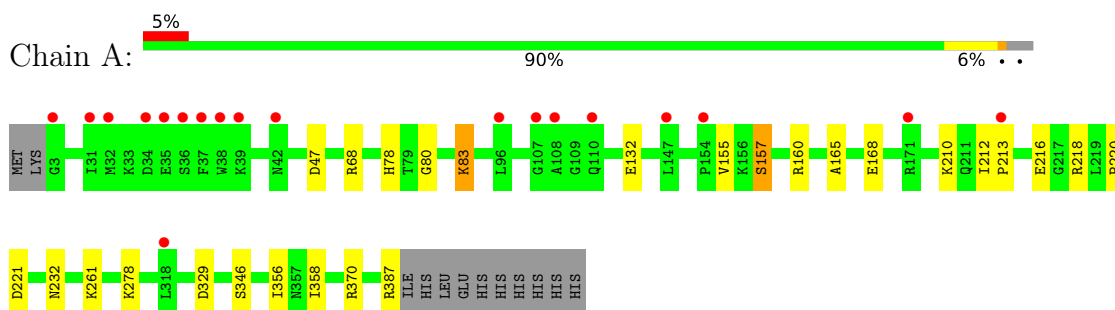
- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	149	Total	O	0	2
			151	151		
5	B	69	Total	O	0	1
			70	70		

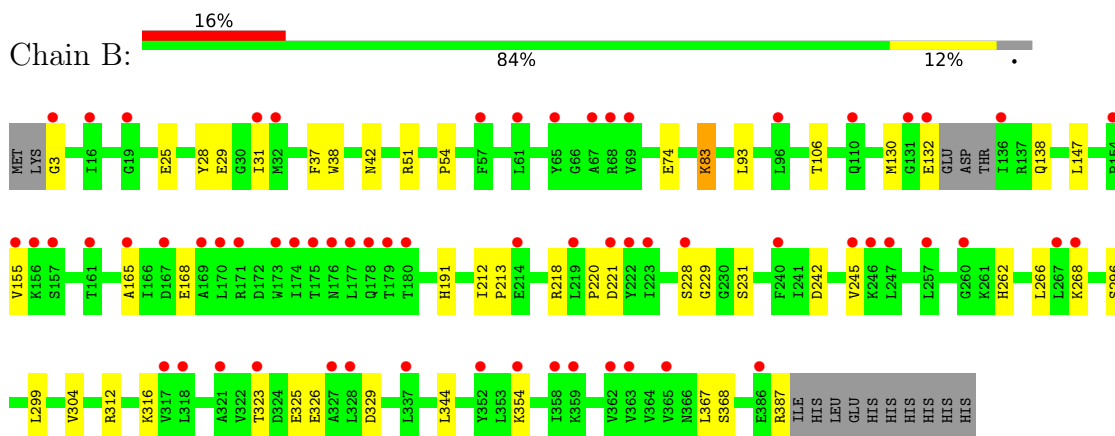
3 Residue-property plots

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: Engineered tyrosine synthase (TmTyrS1)



- Molecule 1: Engineered tyrosine synthase (TmTyrS1)



4 Data and refinement statistics

Property	Value	Source
Space group	I 4	Depositor
Cell constants a, b, c, α , β , γ	164.61Å 164.61Å 83.14Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	38.80 – 2.05 38.80 – 2.05	Depositor EDS
% Data completeness (in resolution range)	99.9 (38.80-2.05) 99.9 (38.80-2.05)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.56 (at 2.05Å)	Xtriage
Refinement program	PHENIX 1.20.1_4487	Depositor
R, R_{free}	0.216 , 0.232 0.216 , 0.231	Depositor DCC
R_{free} test set	3488 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å ²)	45.5	Xtriage
Anisotropy	0.341	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 41.2	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	0.019 for -k,-h,-l	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	6201	wwPDB-VP
Average B, all atoms (Å ²)	52.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.05% 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

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: K, PO4, EDO, LLP

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	0.09	0/3029	0.25	0/4095
1	B	0.09	0/3001	0.24	0/4057
All	All	0.09	0/6030	0.25	0/8152

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	A	2990	0	2995	16	0
1	B	2966	0	2955	30	0
2	A	1	0	0	0	0
2	B	1	0	0	0	0
3	A	8	0	12	0	0
3	B	4	0	6	0	0
4	A	5	0	0	0	0
4	B	5	0	0	0	0
5	A	151	0	0	3	0
5	B	70	0	0	1	0
All	All	6201	0	5968	45	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 4.

The worst 5 of 45 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:132:GLU:HA	1:B:138:GLN:HE22	1.48	0.77
1:B:51:ARG:NH2	1:B:74:GLU:OE1	2.29	0.65
1:A:356:ILE:HG13	1:A:358:ILE:HG23	1.79	0.64
1:B:323:THR:HB	1:B:326:GLU:HG3	1.82	0.62
1:A:261:LYS:NZ	5:A:502:HOH:O	2.32	0.62

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	383/397 (96%)	377 (98%)	6 (2%)	0	100	100
1	B	379/397 (96%)	362 (96%)	17 (4%)	0	100	100
All	All	762/794 (96%)	739 (97%)	23 (3%)	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	307/318 (96%)	304 (99%)	3 (1%)	68	72
1	B	303/318 (95%)	300 (99%)	3 (1%)	68	72
All	All	610/636 (96%)	604 (99%)	6 (1%)	68	72

5 of 6 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	147	LEU
1	B	367	LEU
1	B	368	SER
1	A	346	SER
1	A	157	SER

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (4) such sidechains are listed below:

Mol	Chain	Res	Type
1	B	111	HIS
1	B	138	GLN
1	B	290	GLN
1	B	380	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

2 non-standard protein/DNA/RNA residues 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	$\# Z > 2$
1	LLP	B	83	1	23,24,25	2.48	6 (26%)	25,32,34	1.31	4 (16%)
1	LLP	A	83	1	23,24,25	2.49	6 (26%)	25,32,34	1.28	4 (16%)

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
1	LLP	B	83	1	-	6/16/17/19	0/1/1/1
1	LLP	A	83	1	-	3/16/17/19	0/1/1/1

The worst 5 of 12 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	83	LLP	C4-C4'	7.24	1.62	1.46
1	B	83	LLP	C4-C4'	7.18	1.61	1.46
1	B	83	LLP	C4'-NZ	5.01	1.43	1.27
1	A	83	LLP	C4'-NZ	5.00	1.43	1.27
1	A	83	LLP	C2'-C2	3.78	1.56	1.50

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

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	83	LLP	C4-C4'-NZ	-3.60	107.45	124.04
1	A	83	LLP	C4-C4'-NZ	-3.23	109.11	124.04
1	A	83	LLP	CE-NZ-C4'	-2.60	110.39	118.72
1	B	83	LLP	CE-NZ-C4'	-2.55	110.56	118.72
1	A	83	LLP	C5-C6-N1	-2.35	120.00	123.83

There are no chirality outliers.

5 of 9 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	A	83	LLP	C4-C4'-NZ-CE
1	A	83	LLP	CG-CD-CE-NZ
1	B	83	LLP	C4-C4'-NZ-CE
1	B	83	LLP	CE-CD-CG-CB
1	B	83	LLP	CA-CB-CG-CD

There are no ring outliers.

2 monomers are involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	B	83	LLP	2	0
1	A	83	LLP	1	0

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 7 ligands modelled in this entry, 2 are monoatomic - leaving 5 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	$\# Z > 2$
4	PO4	B	404	-	4,4,4	0.97	0	6,6,6	0.46	0
4	PO4	A	405	-	4,4,4	0.96	0	6,6,6	0.48	0
3	EDO	A	403	-	3,3,3	0.43	0	2,2,2	0.37	0
3	EDO	B	403	-	3,3,3	0.43	0	2,2,2	0.34	0
3	EDO	A	404	-	3,3,3	0.43	0	2,2,2	0.38	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	A	403	-	-	0/1/1/1	-
3	EDO	B	403	-	-	0/1/1/1	-
3	EDO	A	404	-	-	0/1/1/1	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

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	384/397 (96%)	0.46	19 (4%)	35 35	25, 46, 65, 89	8 (2%)
1	B	381/397 (95%)	1.08	63 (16%)	4 4	23, 53, 78, 93	21 (5%)
All	All	765/794 (96%)	0.77	82 (10%)	11 10	23, 49, 73, 93	29 (3%)

The worst 5 of 82 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	174	ILE	6.1
1	B	358	ILE	4.2
1	B	245	VAL	3.8
1	B	175	THR	3.7
1	B	228[A]	SER	3.6

6.2 Non-standard residues in protein, DNA, RNA chains [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(Å ²)	Q<0.9
1	LLP	B	83	24/25	0.95	0.10	34,45,58,61	0
1	LLP	A	83	24/25	0.96	0.09	32,41,48,55	0

6.3 Carbohydrates [i](#)

There are no oligosaccharides 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(Å ²)	Q<0.9
3	EDO	B	403	4/4	0.81	0.24	53,56,63,64	0
3	EDO	A	404	4/4	0.86	0.18	59,69,78,81	0
4	PO4	B	404	5/5	0.91	0.13	50,51,54,63	0
3	EDO	A	403	4/4	0.92	0.14	48,51,70,70	0
4	PO4	A	405	5/5	0.94	0.08	49,58,61,61	0
2	K	B	402	1/1	0.96	0.07	49,49,49,49	0
2	K	A	402	1/1	0.99	0.04	39,39,39,39	0

6.5 Other polymers [i](#)

There are no such residues in this entry.