



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 10, 2026 – 03:33 AM UTC

PDB ID : 4YWI / pdb_00004ywi
Title : F96S/L167V Double mutant of Plasmodium Falciparum Triosephosphate Isomerase
Authors : Pareek, V.; Balaram, P.; Murthy, M.R.N.
Deposited on : 2015-03-20
Resolution : 1.85 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 : 4-5-2 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

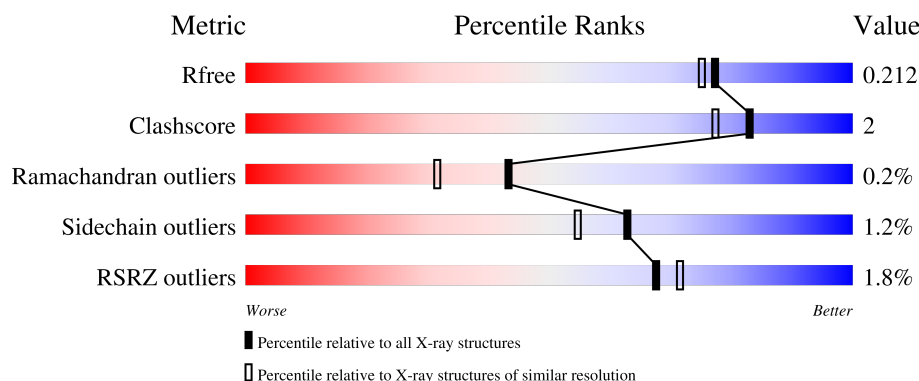
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.85 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	3428 (1.86-1.86)
Clashscore	190562	3579 (1.86-1.86)
Ramachandran outliers	187476	3553 (1.86-1.86)
Sidechain outliers	187428	3553 (1.86-1.86)
RSRZ outliers	180081	3429 (1.86-1.86)

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	248	2% 56% 40% ..
1	B	248	2% 56% 42% .

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 4306 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 Triosephosphate isomerase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	246	Total	C	N	O	S	0	1	2
			1921	1216	323	377	5			
1	B	247	Total	C	N	O	S	0	1	1
			1926	1222	325	374	5			

There are 6 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	96	SER	PHE	engineered mutation	UNP Q07412
A	163	VAL	ALA	engineered mutation	UNP Q07412
A	167	VAL	LEU	engineered mutation	UNP Q07412
B	96	SER	PHE	engineered mutation	UNP Q07412
B	163	VAL	ALA	engineered mutation	UNP Q07412
B	167	VAL	LEU	engineered mutation	UNP Q07412

- Molecule 2 is SULFATE ION (CCD ID: SO4) (formula: O₄S).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	1	Total O S 5 4 1	0	0
2	B	1	Total O S 5 4 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 4 2 2	0	0
3	A	1	Total C O 4 2 2	0	0
3	A	1	Total C O 4 2 2	0	0
3	B	1	Total C O 4 2 2	0	0
3	B	1	Total C O 4 2 2	0	0
3	B	1	Total C O 4 2 2	0	0
3	B	1	Total C O 4 2 2	0	0

- Molecule 4 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	234	Total O 234 234	0	0

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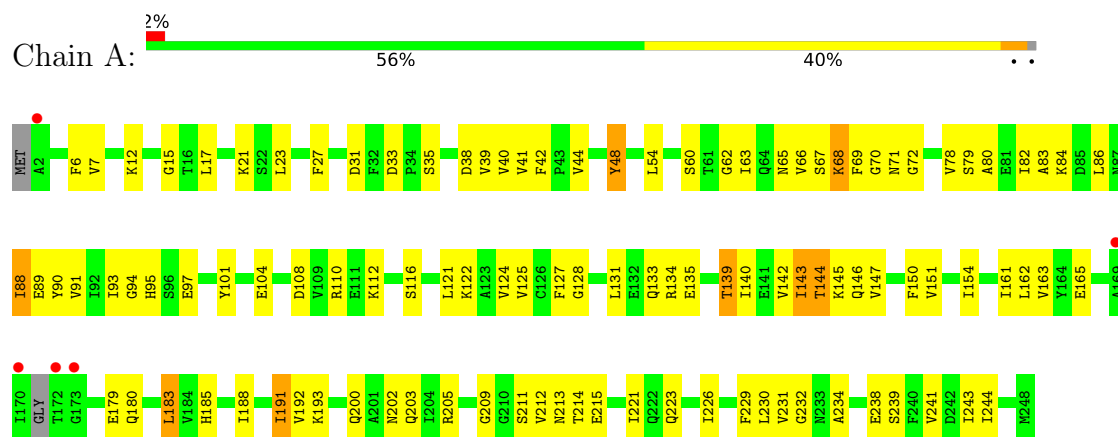
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	B	187	Total	O	0	0
			187	187		

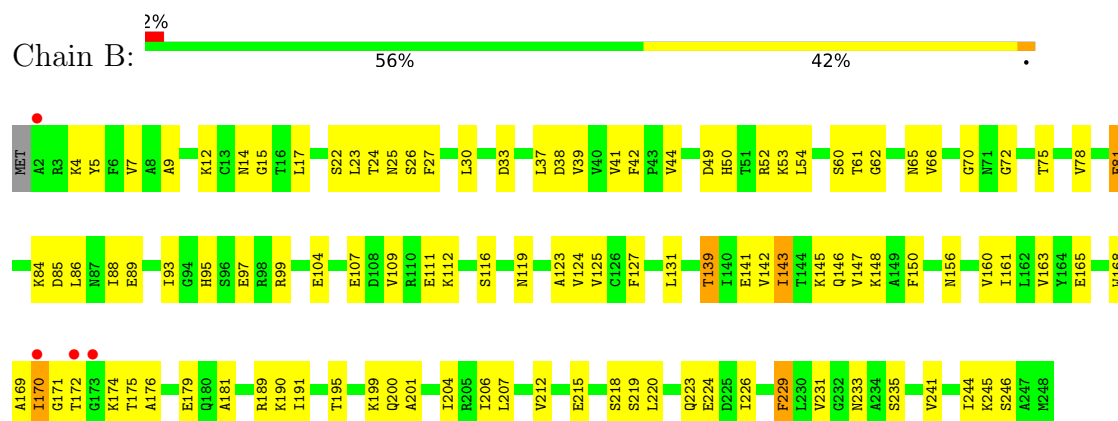
3 Residue-property plots [i](#)

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: Triosephosphate isomerase



• Molecule 1: Triosephosphate isomerase



4 Data and refinement statistics

Property	Value	Source
Space group	P 2 ₁ 2 ₁ 2 ₁	Depositor
Cell constants a, b, c, α , β , γ	50.93Å 53.81Å 174.50Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	33.89 – 1.85 33.89 – 1.85	Depositor EDS
% Data completeness (in resolution range)	83.6 (33.89-1.85) 82.6 (33.89-1.85)	Depositor EDS
R_{merge}	0.08	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	9.81 (at 1.85Å)	Xtriage
Refinement program	REFMAC 5.8.0049	Depositor
R, R_{free}	0.162 , 0.203 0.175 , 0.212	Depositor DCC
R_{free} test set	1759 reflections (3.59%)	wwPDB-VP
Wilson B-factor (Å ²)	21.1	Xtriage
Anisotropy	0.042	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.35 , 43.4	EDS
L-test for twinning ²	$\langle L \rangle = 0.46$, $\langle L^2 \rangle = 0.29$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	4306	wwPDB-VP
Average B, all atoms (Å ²)	20.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.74% 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: EDO, SO4

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	2.08	94/1950 (4.8%)	1.02	4/2632 (0.2%)
1	B	2.07	90/1958 (4.6%)	1.08	9/2636 (0.3%)
All	All	2.08	184/3908 (4.7%)	1.05	13/5268 (0.2%)

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	B	0	1

All (184) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	62	GLY	C-O	-9.33	1.14	1.23
1	B	93	ILE	C-O	-8.84	1.14	1.24
1	A	161	ILE	C-O	-8.36	1.15	1.24
1	A	209	GLY	C-O	-8.36	1.18	1.24
1	B	207	LEU	C-O	-7.96	1.14	1.23
1	A	80	ALA	C-O	-7.95	1.14	1.24
1	A	70	GLY	C-O	-7.71	1.16	1.23
1	A	142	VAL	C-O	-7.61	1.15	1.24
1	B	7	VAL	C-O	-7.53	1.16	1.24
1	A	150	PHE	C-O	-7.48	1.15	1.24
1	A	230	LEU	C-O	-7.45	1.15	1.24
1	B	12	LYS	C-O	-7.34	1.16	1.24
1	B	165	GLU	C-O	-7.24	1.15	1.24
1	B	244	ILE	C-O	-7.23	1.15	1.24
1	B	107	GLU	C-O	-7.04	1.15	1.24
1	B	116	SER	C-O	-7.03	1.15	1.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	154	ILE	C-O	-7.00	1.17	1.24
1	A	223	GLN	C-O	-6.98	1.15	1.23
1	B	160	VAL	C-O	-6.90	1.16	1.24
1	B	95	HIS	C-O	-6.87	1.15	1.23
1	A	139	THR	C-O	-6.87	1.16	1.24
1	A	27	PHE	C-O	-6.85	1.16	1.24
1	B	246	SER	C-O	-6.82	1.15	1.24
1	A	226	ILE	C-O	-6.76	1.16	1.24
1	B	88	ILE	C-O	-6.74	1.17	1.23
1	B	44	VAL	C-O	-6.74	1.16	1.24
1	B	39	VAL	C-O	-6.72	1.16	1.24
1	B	33	ASP	C-O	-6.72	1.15	1.24
1	B	42	PHE	C-O	-6.71	1.16	1.24
1	B	37	LEU	C-O	-6.69	1.15	1.23
1	A	193	LYS	C-O	-6.68	1.16	1.24
1	A	7	VAL	C-O	-6.68	1.16	1.24
1	A	244	ILE	C-O	-6.67	1.16	1.24
1	A	145	LYS	C-O	-6.62	1.16	1.24
1	A	212	VAL	C-O	-6.62	1.17	1.24
1	A	23	LEU	C-O	-6.60	1.16	1.24
1	A	125	VAL	C-O	-6.57	1.16	1.24
1	A	67	SER	C-O	-6.56	1.15	1.23
1	A	42	PHE	C-O	-6.56	1.16	1.24
1	B	78	VAL	C-O	-6.49	1.17	1.24
1	B	191	ILE	C-O	-6.49	1.16	1.24
1	A	84	LYS	C-O	-6.41	1.16	1.24
1	A	243	ILE	C-O	-6.39	1.16	1.24
1	A	205	ARG	C-O	-6.39	1.16	1.23
1	A	93	ILE	C-O	-6.39	1.17	1.24
1	B	49	ASP	C-O	-6.39	1.16	1.24
1	B	139	THR	C-O	-6.38	1.16	1.24
1	A	48	TYR	C-O	-6.38	1.16	1.24
1	A	116	SER	C-O	-6.38	1.16	1.24
1	A	146	GLN	C-O	-6.37	1.16	1.24
1	A	39	VAL	C-O	-6.30	1.17	1.24
1	A	82	ILE	C-O	-6.29	1.16	1.24
1	A	238	GLU	C-O	-6.29	1.16	1.24
1	B	163	VAL	C-O	-6.27	1.17	1.24
1	B	190	LYS	C-O	-6.26	1.16	1.24
1	B	226	ILE	C-O	-6.26	1.17	1.24
1	B	61	THR	C-O	-6.25	1.16	1.23
1	A	40	VAL	C-O	-6.23	1.17	1.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	33	ASP	C-O	-6.22	1.17	1.24
1	A	124	VAL	C-O	-6.19	1.17	1.24
1	B	199	LYS	C-O	-6.18	1.16	1.24
1	B	23	LEU	C-O	-6.16	1.17	1.24
1	A	188	ILE	C-O	-6.16	1.17	1.24
1	A	127	PHE	C-O	-6.14	1.16	1.23
1	A	163	VAL	C-O	-6.12	1.17	1.24
1	A	165	GLU	C-O	-6.11	1.17	1.24
1	A	231	VAL	C-O	-6.11	1.16	1.24
1	A	221	ILE	C-O	-6.09	1.16	1.24
1	A	65	ASN	C-O	-6.09	1.16	1.23
1	B	241	VAL	C-O	-6.07	1.16	1.24
1	A	213	ASN	C-O	-6.03	1.16	1.24
1	B	104	GLU	C-O	-6.03	1.16	1.23
1	A	234	ALA	C-O	-5.98	1.16	1.24
1	B	70	GLY	C-O	-5.96	1.18	1.23
1	B	206	ILE	C-O	-5.95	1.17	1.24
1	B	17	LEU	C-O	-5.93	1.17	1.24
1	B	212	VAL	C-O	-5.92	1.18	1.24
1	A	12	LYS	C-O	-5.89	1.18	1.24
1	B	15	GLY	C-O	-5.87	1.18	1.23
1	B	124	VAL	C-O	-5.87	1.17	1.24
1	B	170	ILE	C-O	-5.85	1.18	1.24
1	A	110	ARG	C-O	-5.83	1.17	1.24
1	A	62	GLY	C-O	-5.82	1.18	1.23
1	A	134	ARG	C-O	-5.82	1.17	1.24
1	B	161	ILE	C-O	-5.80	1.18	1.24
1	A	44	VAL	C-O	-5.79	1.17	1.24
1	B	53	LYS	C-O	-5.79	1.17	1.24
1	B	38	ASP	C-O	-5.78	1.17	1.24
1	A	203	GLN	C-O	-5.78	1.17	1.24
1	B	150	PHE	C-O	-5.77	1.17	1.24
1	A	191	ILE	C-O	-5.77	1.17	1.24
1	B	204	ILE	C-O	-5.76	1.17	1.24
1	A	78	VAL	C-O	-5.75	1.17	1.24
1	A	6	PHE	C-O	-5.74	1.17	1.23
1	A	41	VAL	C-O	-5.74	1.17	1.24
1	B	231	VAL	C-O	-5.74	1.16	1.24
1	B	145	LYS	C-O	-5.73	1.17	1.24
1	B	189	ARG	C-O	-5.72	1.17	1.24
1	A	104	GLU	C-O	-5.70	1.17	1.23
1	B	9	ALA	C-O	-5.70	1.17	1.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	128	GLY	C-O	-5.69	1.15	1.23
1	A	200	GLN	C-O	-5.68	1.17	1.24
1	A	162	LEU	C-O	-5.68	1.17	1.23
1	B	119	ASN	C-O	-5.67	1.16	1.24
1	B	147	VAL	C-O	-5.65	1.17	1.24
1	B	127	PHE	C-O	-5.64	1.17	1.23
1	A	68	LYS	C-O	-5.64	1.16	1.24
1	B	109	VAL	C-O	-5.63	1.17	1.24
1	A	112	LYS	C-O	-5.63	1.17	1.24
1	A	192	VAL	C-O	-5.62	1.17	1.24
1	A	131	LEU	C-O	-5.61	1.17	1.24
1	B	25	ASN	C-O	-5.61	1.17	1.24
1	B	97	GLU	C-O	-5.61	1.17	1.24
1	B	66	VAL	C-O	-5.60	1.18	1.23
1	B	24	THR	C-O	-5.59	1.17	1.24
1	A	211	SER	C-O	-5.59	1.17	1.24
1	B	52	ARG	C-O	-5.59	1.17	1.24
1	B	111	GLU	C-O	-5.58	1.17	1.24
1	A	144	THR	C-O	-5.54	1.17	1.24
1	A	183	LEU	C-O	-5.54	1.17	1.24
1	A	21	LYS	C-O	-5.53	1.17	1.24
1	A	179	GLU	C-O	-5.52	1.17	1.24
1	B	233	ASN	C-O	-5.52	1.17	1.24
1	B	219	SER	C-O	-5.50	1.17	1.24
1	A	15	GLY	C-O	-5.49	1.17	1.23
1	B	50	HIS	C-O	-5.48	1.17	1.24
1	A	214	THR	C-O	-5.47	1.17	1.24
1	A	83	ALA	C-O	-5.47	1.17	1.24
1	A	60	SER	C-O	-5.46	1.16	1.23
1	A	63	ILE	C-O	-5.45	1.17	1.23
1	B	81	GLU	C-O	-5.45	1.17	1.24
1	B	99	ARG	C-O	-5.44	1.17	1.24
1	B	41	VAL	C-O	-5.43	1.18	1.24
1	A	133	GLN	C-O	-5.41	1.17	1.24
1	A	108	ASP	C-O	-5.40	1.17	1.24
1	A	232	GLY	C-O	-5.38	1.16	1.23
1	B	75	THR	C-O	-5.38	1.17	1.23
1	B	142	VAL	C-O	-5.37	1.18	1.24
1	A	95	HIS	C-O	-5.37	1.17	1.23
1	B	84	LYS	C-O	-5.37	1.17	1.24
1	A	31	ASP	C-O	-5.36	1.17	1.24
1	B	146	GLN	C-O	-5.35	1.17	1.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	60	SER	C-O	-5.34	1.16	1.23
1	A	215	GLU	C-O	-5.34	1.18	1.24
1	A	66	VAL	C-O	-5.33	1.17	1.23
1	A	143	ILE	C-O	-5.33	1.18	1.24
1	B	123	ALA	C-O	-5.28	1.17	1.24
1	A	241	VAL	C-O	-5.28	1.17	1.24
1	B	125	VAL	C-O	-5.28	1.18	1.24
1	B	5	TYR	C-O	-5.26	1.16	1.23
1	A	91	VAL	C-O	-5.25	1.18	1.24
1	B	179	GLU	C-O	-5.24	1.17	1.24
1	B	4	LYS	C-O	-5.24	1.17	1.24
1	A	72	GLY	C-O	-5.24	1.16	1.23
1	A	180	GLN	C-O	-5.24	1.18	1.24
1	A	97	GLU	C-O	-5.22	1.18	1.24
1	B	156	ASN	C-O	-5.21	1.18	1.24
1	A	147	VAL	C-O	-5.20	1.18	1.24
1	B	229	PHE	C-O	-5.20	1.17	1.23
1	A	86	LEU	C-O	-5.20	1.17	1.24
1	B	65	ASN	C-O	-5.18	1.17	1.23
1	A	121	LEU	C-O	-5.18	1.17	1.23
1	B	245	LYS	C-O	-5.17	1.17	1.24
1	A	38	ASP	C-O	-5.17	1.17	1.24
1	A	151	VAL	C-O	-5.17	1.17	1.24
1	B	218	SER	C-O	-5.16	1.18	1.24
1	A	185	HIS	C-O	-5.16	1.18	1.24
1	B	201	ALA	C-O	-5.15	1.17	1.24
1	B	200	GLN	C-O	-5.12	1.18	1.24
1	B	72	GLY	C-O	-5.12	1.17	1.23
1	B	141	GLU	C-O	-5.12	1.18	1.24
1	A	35	SER	C-O	-5.11	1.17	1.24
1	B	27	PHE	C-O	-5.09	1.18	1.24
1	B	30	LEU	C-O	-5.08	1.17	1.24
1	B	22	SER	C-O	-5.08	1.18	1.24
1	B	112	LYS	C-O	-5.06	1.18	1.24
1	B	85	ASP	C-O	-5.06	1.18	1.24
1	B	181	ALA	C-O	-5.04	1.18	1.24
1	A	94	GLY	C-O	-5.03	1.17	1.23
1	B	235	SER	C-O	-5.03	1.17	1.24
1	B	14	ASN	C-O	-5.02	1.17	1.23
1	A	88	ILE	C-O	-5.02	1.18	1.23
1	B	223	GLN	C-O	-5.00	1.18	1.23
1	A	239	SER	C-O	-5.00	1.16	1.24

All (13) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	26[A]	SER	N-CA-C	8.01	120.01	111.28
1	B	26[B]	SER	N-CA-C	8.01	120.01	111.28
1	B	26[A]	SER	CA-C-O	7.99	129.02	120.55
1	B	26[B]	SER	CA-C-O	7.99	129.02	120.55
1	A	101	TYR	N-CA-C	7.90	119.97	111.36
1	B	89	GLU	N-CA-C	7.67	119.72	111.36
1	A	89	GLU	N-CA-C	7.64	119.69	111.36
1	B	169	ALA	N-CA-C	6.61	118.56	111.36
1	B	54	LEU	N-CA-C	6.06	117.97	111.36
1	B	220	LEU	N-CA-C	5.47	117.05	111.14
1	B	215	GLU	N-CA-C	5.38	117.22	111.36
1	A	54	LEU	N-CA-C	5.24	117.07	111.36
1	A	215	GLU	N-CA-C	5.11	116.66	111.14

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	B	170	ILE	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	1921	0	1857	12	0
1	B	1926	0	1887	6	0
2	A	5	0	0	0	0
2	B	5	0	0	0	0
3	A	12	0	18	2	0
3	B	16	0	24	1	0
4	A	234	0	0	3	0
4	B	187	0	0	1	0
All	All	4306	0	3786	18	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 (18) 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:135:GLU:OE2	4:A:402:HOH:O	1.92	0.86
1:A:140:ILE:HD11	3:A:302:EDO:H11	1.62	0.79
1:A:140:ILE:HD11	3:A:302:EDO:C1	2.33	0.58
3:B:304:EDO:H11	4:B:515:HOH:O	2.07	0.54
1:B:171:GLY:HA2	1:B:172:THR:CA	2.36	0.54
1:A:17:LEU:HD21	1:B:86:LEU:HD21	1.93	0.49
1:A:68:LYS:HE3	1:A:69:PHE:CZ	2.49	0.46
1:A:202:ASN:ND2	4:A:408:HOH:O	2.49	0.46
1:A:139:THR:O	1:A:143:ILE:HG12	2.17	0.45
1:A:144:THR:HA	1:A:191:ILE:HD13	2.00	0.44
1:A:71:ASN:ND2	1:A:79:SER:OG	2.51	0.44
1:B:175:THR:HG23	1:B:176:ALA:O	2.18	0.44
1:A:90:TYR:HA	1:A:122:LYS:O	2.19	0.43
1:A:183:LEU:HB3	4:A:401:HOH:O	2.18	0.42
1:B:139:THR:O	1:B:143:ILE:HD13	2.20	0.42
1:A:48:TYR:CZ	1:A:88:ILE:HG12	2.56	0.41
1:B:148:LYS:HD3	1:B:195:THR:HG21	2.02	0.41
1:B:131:LEU:HA	1:B:168:TRP:CB	2.51	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	241/248 (97%)	238 (99%)	3 (1%)	0	100	100
1	B	243/248 (98%)	239 (98%)	3 (1%)	1 (0%)	30	17
All	All	484/496 (98%)	477 (99%)	6 (1%)	1 (0%)	43	31

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	174	LYS

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	206/220 (94%)	205 (100%)	1 (0%)	81	77
1	B	208/220 (94%)	204 (98%)	4 (2%)	50	38
All	All	414/440 (94%)	409 (99%)	5 (1%)	63	55

All (5) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	229	PHE
1	B	81	GLU
1	B	143	ILE
1	B	224	GLU
1	B	229	PHE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (9) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	71	ASN
1	A	120	ASN
1	A	136	GLN
1	A	159	ASN
1	A	202	ASN
1	A	203	GLN
1	B	71	ASN
1	B	159	ASN
1	B	202	ASN

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](#)

9 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	$\# Z > 2$
2	SO4	A	301	-	4,4,4	0.34	0	6,6,6	0.20	0
2	SO4	B	301	-	4,4,4	0.34	0	6,6,6	0.23	0
3	EDO	B	305	-	3,3,3	0.33	0	2,2,2	0.34	0
3	EDO	A	304	-	3,3,3	0.40	0	2,2,2	0.23	0
3	EDO	B	304	-	3,3,3	0.35	0	2,2,2	0.44	0
3	EDO	A	302	-	3,3,3	0.35	0	2,2,2	0.49	0
3	EDO	B	302	-	3,3,3	0.28	0	2,2,2	0.25	0
3	EDO	B	303	-	3,3,3	0.43	0	2,2,2	0.28	0
3	EDO	A	303	-	3,3,3	0.31	0	2,2,2	0.52	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	305	-	-	1/1/1/1	-
3	EDO	A	304	-	-	0/1/1/1	-
3	EDO	B	304	-	-	1/1/1/1	-
3	EDO	A	302	-	-	0/1/1/1	-
3	EDO	B	302	-	-	0/1/1/1	-
3	EDO	B	303	-	-	1/1/1/1	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	EDO	A	303	-	-	1/1/1/1	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (4) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	303	EDO	O1-C1-C2-O2
3	B	303	EDO	O1-C1-C2-O2
3	B	305	EDO	O1-C1-C2-O2
3	B	304	EDO	O1-C1-C2-O2

There are no ring outliers.

2 monomers are involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	B	304	EDO	1	0
3	A	302	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	246/248 (99%)	-0.40	5 (2%) 65 68	8, 18, 29, 54	1 (0%)
1	B	247/248 (99%)	-0.32	4 (1%) 70 74	12, 19, 32, 52	1 (0%)
All	All	493/496 (99%)	-0.36	9 (1%) 67 71	8, 18, 30, 54	2 (0%)

All (9) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	170	ILE	4.7
1	A	172	THR	4.0
1	B	172	THR	3.9
1	A	173	GLY	3.1
1	A	169	ALA	2.6
1	B	2	ALA	2.3
1	B	173	GLY	2.2
1	A	2	ALA	2.1
1	B	170	ILE	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 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	A	303	4/4	0.87	0.13	36,36,37,38	0
3	EDO	B	304	4/4	0.87	0.14	41,42,42,44	0
3	EDO	A	302	4/4	0.90	0.13	28,32,32,34	0
3	EDO	B	303	4/4	0.93	0.11	23,27,27,30	0
3	EDO	B	305	4/4	0.93	0.14	24,25,25,26	0
3	EDO	B	302	4/4	0.95	0.07	28,28,29,30	0
3	EDO	A	304	4/4	0.95	0.08	27,27,27,28	0
2	SO4	A	301	5/5	0.97	0.06	33,33,35,37	0
2	SO4	B	301	5/5	0.98	0.05	26,27,27,27	0

6.5 Other polymers [i](#)

There are no such residues in this entry.