



wwPDB X-ray Structure Validation Summary Report ⓘ

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PDB ID : 3KOF / pdb_00003kof
Title : Crystal structure of the double mutant F178Y/R181E of E.coli transaldolase B
Authors : Schneider, S.; Gutierrez, M.; Sandalova, T.; Schneider, G.; Clapes, P.; Sprenger, G.A.; Samland, A.K.
Deposited on : 2009-11-13
Resolution : 1.90 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 Phenix2.0rc1
Mogul : 2022.3.0, CSD as543be (2022)
Xtriage (Phenix) : 2.0rc1
EDS : 3.0
Percentile statistics : 20231227.v01 (using entries in the PDB archive December 27th 2023)
CCP4 : 9.0.006 (Gargrove)
Density-Fitness : 1.0.12
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.43.1

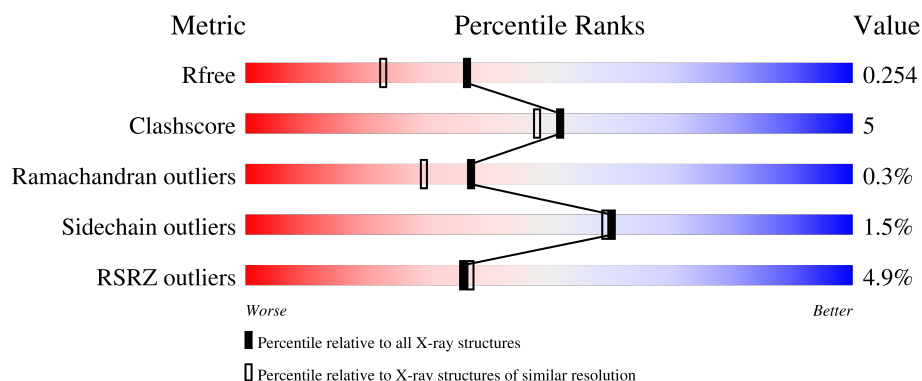
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.90 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	7293 (1.90-1.90)
Clashscore	180529	8090 (1.90-1.90)
Ramachandran outliers	177936	8022 (1.90-1.90)
Sidechain outliers	177891	8022 (1.90-1.90)
RSRZ outliers	164620	7292 (1.90-1.90)

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	337	<div> <div>5%</div> <div> <div></div> <div>83%</div> <div>10%</div> <div>6%</div> </div> </div>
1	B	337	<div> <div>4%</div> <div> <div></div> <div>83%</div> <div>10%</div> <div>6%</div> </div> </div>

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 5523 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 Transaldolase B.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	316	Total	C	N	O	S	0	0	0
			2471	1563	417	484	7			
1	B	316	Total	C	N	O	S	0	0	0
			2471	1563	417	484	7			

There are 46 discrepancies between the modelled and reference sequences:

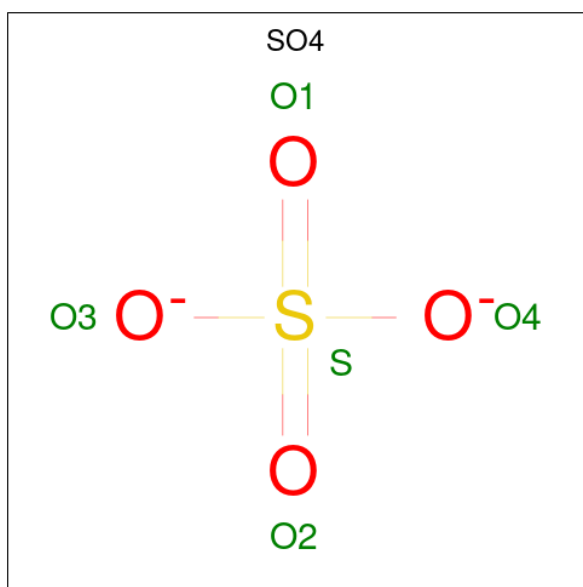
Chain	Residue	Modelled	Actual	Comment	Reference
A	-19	MET	-	expression tag	UNP P0A870
A	-18	GLY	-	expression tag	UNP P0A870
A	-17	SER	-	expression tag	UNP P0A870
A	-16	SER	-	expression tag	UNP P0A870
A	-15	HIS	-	expression tag	UNP P0A870
A	-14	HIS	-	expression tag	UNP P0A870
A	-13	HIS	-	expression tag	UNP P0A870
A	-12	HIS	-	expression tag	UNP P0A870
A	-11	HIS	-	expression tag	UNP P0A870
A	-10	HIS	-	expression tag	UNP P0A870
A	-9	SER	-	expression tag	UNP P0A870
A	-8	SER	-	expression tag	UNP P0A870
A	-7	GLY	-	expression tag	UNP P0A870
A	-6	LEU	-	expression tag	UNP P0A870
A	-5	VAL	-	expression tag	UNP P0A870
A	-4	PRO	-	expression tag	UNP P0A870
A	-3	ARG	-	expression tag	UNP P0A870
A	-2	GLY	-	expression tag	UNP P0A870
A	-1	SER	-	expression tag	UNP P0A870
A	0	HIS	-	expression tag	UNP P0A870
A	178	TYR	PHE	engineered mutation	UNP P0A870
A	181	GLU	ARG	engineered mutation	UNP P0A870
A	247	THR	ALA	engineered mutation	UNP P0A870
B	-19	MET	-	expression tag	UNP P0A870
B	-18	GLY	-	expression tag	UNP P0A870

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Chain	Residue	Modelled	Actual	Comment	Reference
B	-17	SER	-	expression tag	UNP P0A870
B	-16	SER	-	expression tag	UNP P0A870
B	-15	HIS	-	expression tag	UNP P0A870
B	-14	HIS	-	expression tag	UNP P0A870
B	-13	HIS	-	expression tag	UNP P0A870
B	-12	HIS	-	expression tag	UNP P0A870
B	-11	HIS	-	expression tag	UNP P0A870
B	-10	HIS	-	expression tag	UNP P0A870
B	-9	SER	-	expression tag	UNP P0A870
B	-8	SER	-	expression tag	UNP P0A870
B	-7	GLY	-	expression tag	UNP P0A870
B	-6	LEU	-	expression tag	UNP P0A870
B	-5	VAL	-	expression tag	UNP P0A870
B	-4	PRO	-	expression tag	UNP P0A870
B	-3	ARG	-	expression tag	UNP P0A870
B	-2	GLY	-	expression tag	UNP P0A870
B	-1	SER	-	expression tag	UNP P0A870
B	0	HIS	-	expression tag	UNP P0A870
B	178	TYR	PHE	engineered mutation	UNP P0A870
B	181	GLU	ARG	engineered mutation	UNP P0A870
B	247	THR	ALA	engineered mutation	UNP P0A870

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



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

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

- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	287	Total	O	0	0
			287	287		
3	B	274	Total	O	0	0
			274	274		

- Molecule 1: Transaldolase B



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	66.40Å 86.40Å 130.75Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	48.85 – 1.90 48.85 – 1.90	Depositor EDS
% Data completeness (in resolution range)	98.6 (48.85-1.90) 98.6 (48.85-1.90)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.10	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.62 (at 1.90Å)	Xtriage
Refinement program	REFMAC 5.5.0044	Depositor
R, R_{free}	0.203 , 0.248 0.210 , 0.254	Depositor DCC
R_{free} test set	3012 reflections (5.09%)	wwPDB-VP
Wilson B-factor (Å ²)	18.9	Xtriage
Anisotropy	0.344	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.36 , 49.2	EDS
L-test for twinning ²	$\langle L \rangle = 0.53$, $\langle L^2 \rangle = 0.37$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	5523	wwPDB-VP
Average B, all atoms (Å ²)	26.0	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 50.08 % 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 6.8107e-05. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

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: 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	0.73	0/2509	0.83	0/3397
1	B	0.74	0/2509	0.83	0/3397
All	All	0.74	0/5018	0.83	0/6794

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	2471	0	2492	26	0
1	B	2471	0	2492	25	0
2	A	10	0	0	0	0
2	B	10	0	0	1	0
3	A	287	0	0	8	1
3	B	274	0	0	6	1
All	All	5523	0	4984	50	1

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.

The worst 5 of 50 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:101:LEU:HD12	3:B:519:HOH:O	1.56	1.03
1:A:2:THR:HG23	3:A:514:HOH:O	1.67	0.94
1:A:70:ILE:O	1:A:74:THR:HG23	1.69	0.91
1:A:21:ILE:HG23	1:A:48:TYR:OH	1.77	0.84
1:A:92:ARG:HH12	1:A:152:ASN:HD22	1.37	0.72

All (1) 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)
3:A:466:HOH:O	3:B:328:HOH:O[3_645]	2.18	0.02

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	314/337 (93%)	309 (98%)	4 (1%)	1 (0%)	37	29
1	B	314/337 (93%)	309 (98%)	4 (1%)	1 (0%)	37	29
All	All	628/674 (93%)	618 (98%)	8 (1%)	2 (0%)	37	29

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	226	SER
1	B	226	SER

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	261/279 (94%)	257 (98%)	4 (2%)	60	59
1	B	261/279 (94%)	257 (98%)	4 (2%)	60	59
All	All	522/558 (94%)	514 (98%)	8 (2%)	60	59

5 of 8 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	309	LEU
1	B	193	LYS
1	B	44	GLN
1	A	309	LEU
1	B	50	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 9 such sidechains are listed below:

Mol	Chain	Res	Type
1	B	211	GLN
1	B	287	GLN
1	A	163	GLN
1	B	68	GLN
1	B	152	ASN

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 oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

4 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	321	-	4,4,4	0.26	0	6,6,6	0.16	0
2	SO4	A	320	-	4,4,4	0.31	0	6,6,6	0.13	0
2	SO4	B	321	-	4,4,4	0.23	0	6,6,6	0.37	0
2	SO4	B	320	-	4,4,4	0.28	0	6,6,6	0.24	0

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.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	320	SO4	1	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	316/337 (93%)	0.03	18 (5%) 30 32	14, 22, 46, 53	0
1	B	316/337 (93%)	0.03	13 (4%) 42 43	15, 22, 43, 49	0
All	All	632/674 (93%)	0.03	31 (4%) 36 37	14, 22, 44, 53	0

The worst 5 of 31 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	193	LYS	3.7
1	A	269	VAL	3.6
1	B	267	GLY	3.6
1	A	267	GLY	3.5
1	A	268	GLU	3.4

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
2	SO4	B	320	5/5	0.87	0.11	52,53,53,53	0
2	SO4	A	320	5/5	0.91	0.17	40,42,44,44	0
2	SO4	A	321	5/5	0.99	0.03	16,21,22,23	0
2	SO4	B	321	5/5	0.99	0.04	21,21,23,23	0

6.5 Other polymers [i](#)

There are no such residues in this entry.