



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 13, 2017 – 03:35 pm GMT

PDB ID : 4IK0
Title : Crystal structure of diaminopimelate epimerase Y268A mutant from Escherichia coli
Authors : Hor, L.; Dobson, R.C.J.; Hutton, C.A.; Perugini, M.A.
Deposited on : 2012-12-24
Resolution : 2.05 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

<http://wwpdb.org/validation/2016/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.9-1692
EDS	:	trunk28620
Percentile statistics	:	20161228.v01 (using entries in the PDB archive December 28th 2016)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	recalc28949

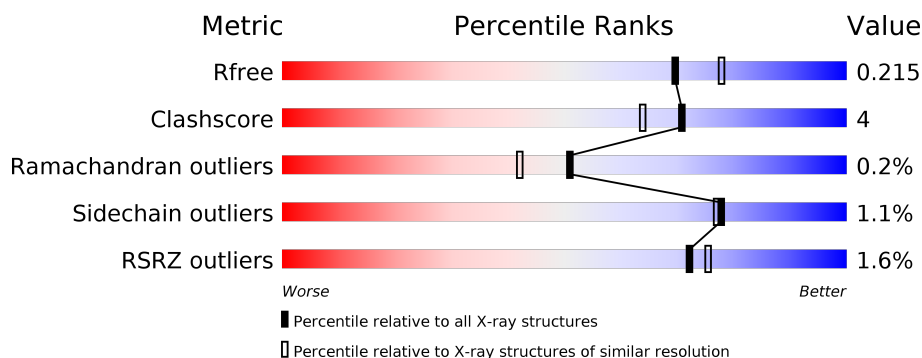
1 Overall quality at a glance

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}	100719	1316 (2.04-2.04)
Clashscore	112137	1394 (2.04-2.04)
Ramachandran outliers	110173	1383 (2.04-2.04)
Sidechain outliers	110143	1383 (2.04-2.04)
RSRZ outliers	101464	1319 (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 on the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria. 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	280	<div> <div style="width: 100%; height: 10px; background: linear-gradient(to right, red 1%, orange 1%, yellow 1%, green 93%, grey 5%);"></div> <div style="display: flex; justify-content: space-between; width: 100%;"> % 93% 5% • </div> </div>
1	B	280	<div> <div style="width: 100%; height: 10px; background: linear-gradient(to right, red 2%, orange 2%, yellow 1%, green 88%, grey 9%);"></div> <div style="display: flex; justify-content: space-between; width: 100%;"> 2% 88% 9% • • </div> </div>

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 4648 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 Diaminopimelate epimerase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	274	Total	C	N	O	S	0	1	0
			2117	1330	386	386	15			
1	B	275	Total	C	N	O	S	0	1	0
			2123	1334	390	384	15			

There are 14 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	268	ALA	TYR	ENGINEERED MUTATION	UNP P0A6K1
A	275	HIS	-	EXPRESSION TAG	UNP P0A6K1
A	276	HIS	-	EXPRESSION TAG	UNP P0A6K1
A	277	HIS	-	EXPRESSION TAG	UNP P0A6K1
A	278	HIS	-	EXPRESSION TAG	UNP P0A6K1
A	279	HIS	-	EXPRESSION TAG	UNP P0A6K1
A	280	HIS	-	EXPRESSION TAG	UNP P0A6K1
B	268	ALA	TYR	ENGINEERED MUTATION	UNP P0A6K1
B	275	HIS	-	EXPRESSION TAG	UNP P0A6K1
B	276	HIS	-	EXPRESSION TAG	UNP P0A6K1
B	277	HIS	-	EXPRESSION TAG	UNP P0A6K1
B	278	HIS	-	EXPRESSION TAG	UNP P0A6K1
B	279	HIS	-	EXPRESSION TAG	UNP P0A6K1
B	280	HIS	-	EXPRESSION TAG	UNP P0A6K1

- Molecule 2 is IODIDE ION (three-letter code: IOD) (formula: I).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	B	7	Total	I	0	0
			7	7		
2	A	6	Total	I	0	0
			6	6		

- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	178	Total 178	O 178	0	0
3	B	217	Total 217	O 217	0	0

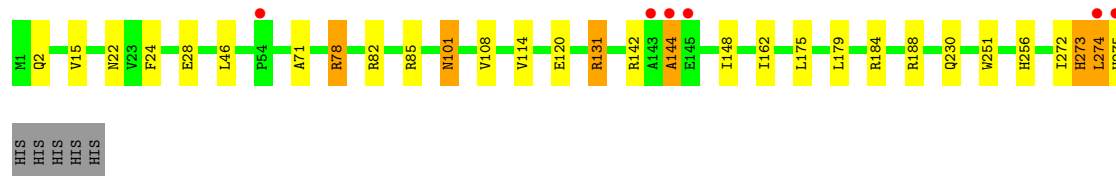
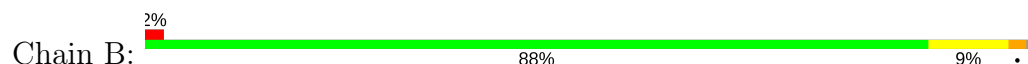
3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA and DNA 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: Diaminopimelate epimerase



- Molecule 1: Diaminopimelate epimerase



4 Data and refinement statistics

Property	Value	Source
Space group	P 41 21 2	Depositor
Cell constants a, b, c, α , β , γ	89.18Å 89.18Å 179.45Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	49.68 – 2.05 49.68 – 2.05	Depositor EDS
% Data completeness (in resolution range)	100.0 (49.68-2.05) 100.0 (49.68-2.05)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.13	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.69 (at 2.05Å)	Xtriage
Refinement program	REFMAC 5.6.0117	Depositor
R, R_{free}	0.176 , 0.217 0.175 , 0.215	Depositor DCC
R_{free} test set	1863 reflections (4.20%)	DCC
Wilson B-factor (Å ²)	24.7	Xtriage
Anisotropy	0.022	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.37 , 56.3	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.34$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	4648	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 24.68 % 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 3.6630e-03. 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 [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: IOD

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	0.74	1/2163 (0.0%)	0.79	0/2929
1	B	0.77	1/2170 (0.0%)	1.01	8/2939 (0.3%)
All	All	0.75	2/4333 (0.0%)	0.91	8/5868 (0.1%)

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	251	TRP	CD2-CE2	5.91	1.48	1.41
1	B	251	TRP	CD2-CE2	5.61	1.48	1.41

All (8) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	78	ARG	NE-CZ-NH1	-17.85	111.38	120.30
1	B	78	ARG	NE-CZ-NH2	13.41	127.01	120.30
1	B	82	ARG	NE-CZ-NH2	-12.29	114.15	120.30
1	B	82	ARG	NE-CZ-NH1	7.55	124.07	120.30
1	B	78	ARG	CD-NE-CZ	6.70	132.97	123.60
1	B	131	ARG	NE-CZ-NH2	-5.48	117.56	120.30
1	B	131	ARG	NE-CZ-NH1	5.41	123.00	120.30
1	B	78	ARG	CG-CD-NE	-5.03	101.24	111.80

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	2117	0	2095	10	0
1	B	2123	0	2100	25	0
2	A	6	0	0	1	0
2	B	7	0	0	2	0
3	A	178	0	0	1	0
3	B	217	0	0	9	0
All	All	4648	0	4195	35	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.

All (35) 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:208:GLU:OE2	1:A:214:THR:HG21	1.28	1.26
1:A:208:GLU:OE2	1:A:214:THR:CG2	2.03	1.06
1:B:188:ARG:HD3	3:B:596:HOH:O	1.72	0.89
1:A:80:PHE:CE2	1:A:97:VAL:HG11	2.22	0.74
1:B:273:HIS:CD2	1:B:273:HIS:H	2.08	0.71
1:B:131:ARG:HD3	1:B:184:ARG:HA	1.75	0.68
1:B:272:ILE:HG12	1:B:274:LEU:HD13	1.78	0.65
1:B:28:GLU:OE1	3:B:613:HOH:O	2.13	0.64
1:B:230:GLN:HG3	3:B:610:HOH:O	1.97	0.64
1:B:131:ARG:NH1	3:B:567:HOH:O	2.27	0.63
1:B:22:ASN:HB3	1:B:24:PHE:CZ	2.38	0.57
1:A:274:LEU:HB2	3:A:505:HOH:O	2.05	0.56
1:A:1:MET:SD	1:A:23:VAL:HG13	2.46	0.56
1:A:208:GLU:OE2	1:A:214:THR:CB	2.55	0.55
1:B:144:ALA:HB3	3:B:602:HOH:O	2.07	0.54
1:B:142[A]:ARG:NE	1:B:144:ALA:O	2.27	0.52
1:A:142:ARG:O	1:A:142:ARG:HG2	2.11	0.51
1:B:78:ARG:NH1	2:B:303:IOD:I	2.94	0.50
1:B:148:ILE:HD11	1:B:175:LEU:HD21	1.96	0.47
1:B:162:ILE:HD11	1:B:179:LEU:HD13	1.98	0.46
1:B:2:GLN:HG3	3:B:573:HOH:O	2.16	0.45
1:B:120:GLU:HG3	1:B:256:HIS:O	2.17	0.45
1:B:85:ARG:HD3	1:B:108:VAL:HG21	1.98	0.45
1:B:78:ARG:HG2	1:B:114:VAL:HB	1.99	0.45
1:A:175:LEU:HD12	2:A:304:IOD:I	2.87	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:101:ASN:OD1	1:B:101:ASN:N	2.50	0.44
1:A:273:HIS:H	1:A:273:HIS:CD2	2.35	0.44
1:B:78:ARG:HB2	2:B:301:IOD:I	2.87	0.43
1:B:230:GLN:CG	3:B:610:HOH:O	2.62	0.43
1:B:15:VAL:HG13	1:B:46:LEU:HG	2.01	0.43
1:B:22:ASN:HB3	1:B:24:PHE:CE1	2.54	0.42
1:B:71:ALA:C	1:B:101:ASN:HD21	2.23	0.42
1:B:22:ASN:ND2	3:B:541:HOH:O	2.32	0.41
1:B:275:HIS:CE1	3:B:598:HOH:O	2.74	0.41
1:A:187:GLU:O	1:A:188[B]:ARG:HB2	2.22	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	273/280 (98%)	266 (97%)	7 (3%)	0	100	100
1	B	274/280 (98%)	270 (98%)	3 (1%)	1 (0%)	38	27
All	All	547/560 (98%)	536 (98%)	10 (2%)	1 (0%)	51	42

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	144	ALA

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	223/229 (97%)	221 (99%)	2 (1%)	82	82
1	B	223/229 (97%)	220 (99%)	3 (1%)	73	72
All	All	446/458 (97%)	441 (99%)	5 (1%)	78	77

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

Mol	Chain	Res	Type
1	A	93	ARG
1	A	274	LEU
1	B	101	ASN
1	B	273	HIS
1	B	274	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (1) such sidechains are listed below:

Mol	Chain	Res	Type
1	B	273	HIS

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 carbohydrates in this entry.

5.6 Ligand geometry ⓘ

Of 13 ligands modelled in this entry, 13 are monoatomic - leaving 0 for Mogul analysis.

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

There are no such residues in this entry.

5.8 Polymer linkage issues

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	274/280 (97%)	-0.01	3 (1%) 80 83	12, 23, 40, 54	0
1	B	275/280 (98%)	-0.07	6 (2%) 62 67	13, 21, 43, 73	0
All	All	549/560 (98%)	-0.04	9 (1%) 72 75	12, 22, 41, 73	0

All (9) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	274	LEU	4.1
1	B	275	HIS	3.8
1	B	144	ALA	3.3
1	A	255	GLY	3.0
1	A	254	PRO	2.6
1	B	145	GLU	2.5
1	B	143	ALA	2.3
1	B	274	LEU	2.3
1	B	54	PRO	2.1

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 carbohydrates 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. LLDF column lists the quality of electron

density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. 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	LLDF	B-factors(Å ²)	Q<0.9
2	IOD	B	304	1/1	0.98	0.08	-1.25	67,67,67,67	0
2	IOD	A	302	1/1	0.99	0.07	-1.67	28,28,28,28	0
2	IOD	A	304	1/1	0.99	0.06	-1.89	59,59,59,59	0
2	IOD	B	301	1/1	1.00	0.08	-1.96	19,19,19,19	0
2	IOD	B	302	1/1	0.99	0.07	-2.46	28,28,28,28	0
2	IOD	A	301	1/1	1.00	0.07	-2.65	21,21,21,21	0
2	IOD	B	303	1/1	1.00	0.05	-3.61	28,28,28,28	0
2	IOD	A	303	1/1	1.00	0.04	-4.87	28,28,28,28	0
2	IOD	A	305	1/1	0.99	0.17	-	75,75,75,75	0
2	IOD	B	305	1/1	0.97	0.12	-	84,84,84,84	0
2	IOD	B	306	1/1	0.98	0.17	-	67,67,67,67	0
2	IOD	A	306	1/1	0.98	0.18	-	83,83,83,83	0
2	IOD	B	307	1/1	0.97	0.10	-	91,91,91,91	0

6.5 Other polymers

There are no such residues in this entry.