



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 14, 2017 – 02:49 am GMT

PDB ID : 1X13
Title : Crystal structure of E. coli transhydrogenase domain I
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Deposited on : 2005-03-31
Resolution : 1.90 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

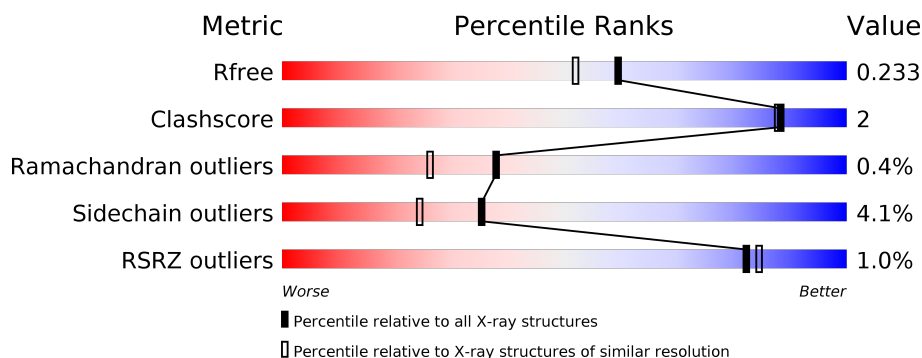
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION



The reported resolution of this entry is 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}	100719	5047 (1.90-1.90)
Clashscore	112137	5731 (1.90-1.90)
Ramachandran outliers	110173	5669 (1.90-1.90)
Sidechain outliers	110143	5670 (1.90-1.90)
RSRZ outliers	101464	5100 (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 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	401	
1	B	401	

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 5946 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 NAD(P) transhydrogenase subunit alpha.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	368	Total	C	N	O	S	0	0	0
			2745	1741	465	527	12			
1	B	364	Total	C	N	O	S	0	0	0
			2721	1724	464	522	11			

There are 16 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	994	MET	-	EXPRESSION TAG	UNP P07001
A	995	HIS	-	EXPRESSION TAG	UNP P07001
A	996	HIS	-	EXPRESSION TAG	UNP P07001
A	997	HIS	-	EXPRESSION TAG	UNP P07001
A	998	HIS	-	EXPRESSION TAG	UNP P07001
A	999	HIS	-	EXPRESSION TAG	UNP P07001
A	1000	HIS	-	EXPRESSION TAG	UNP P07001
A	1001	GLY	-	EXPRESSION TAG	UNP P07001
B	994	MET	-	EXPRESSION TAG	UNP P07001
B	995	HIS	-	EXPRESSION TAG	UNP P07001
B	996	HIS	-	EXPRESSION TAG	UNP P07001
B	997	HIS	-	EXPRESSION TAG	UNP P07001
B	998	HIS	-	EXPRESSION TAG	UNP P07001
B	999	HIS	-	EXPRESSION TAG	UNP P07001
B	1000	HIS	-	EXPRESSION TAG	UNP P07001
B	1001	GLY	-	EXPRESSION TAG	UNP P07001

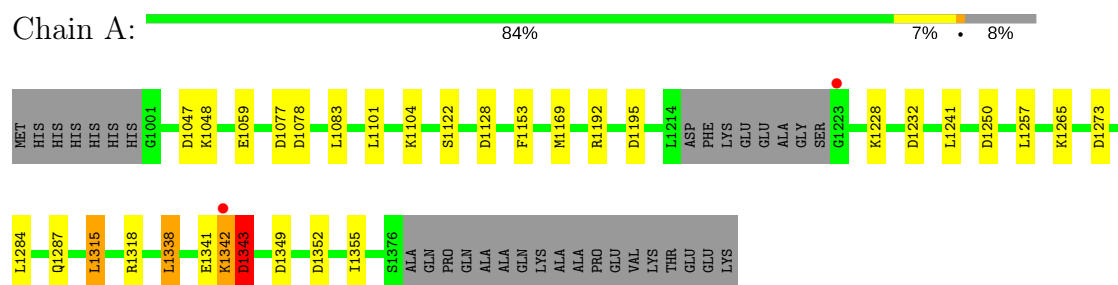
- Molecule 2 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	227	Total	O	0	0
			227	227		
2	B	253	Total	O	0	0
			253	253		

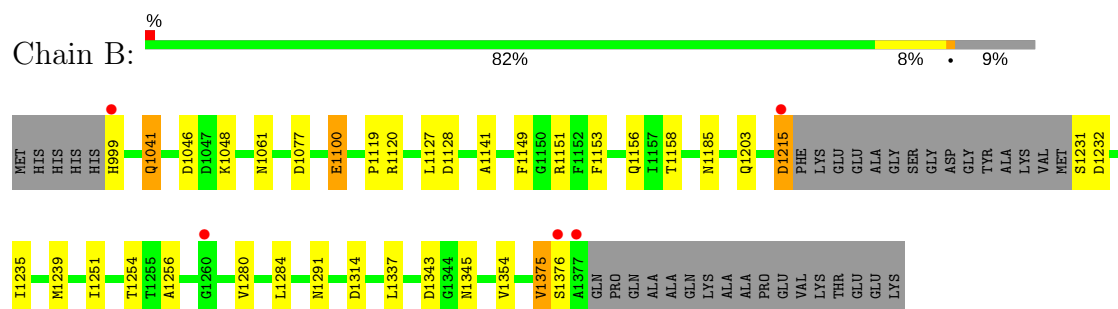
3 Residue-property plots [i](#)

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: NAD(P) transhydrogenase subunit alpha



- Molecule 1: NAD(P) transhydrogenase subunit alpha



4 Data and refinement statistics

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α , β , γ	38.76Å 66.90Å 76.30Å 67.11° 80.66° 81.23°	Depositor
Resolution (Å)	30.00 – 1.90 69.84 – 1.70	Depositor EDS
% Data completeness (in resolution range)	(Not available) (30.00-1.90) 77.6 (69.84-1.70)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.44 (at 1.70Å)	Xtriage
Refinement program	REFMAC 5.1.24	Depositor
R, R_{free}	0.179 , 0.224 0.188 , 0.233	Depositor DCC
R_{free} test set	2591 reflections (5.29%)	DCC
Wilson B-factor (Å ²)	22.4	Xtriage
Anisotropy	0.366	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.37 , 43.4	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	0.96	EDS
Total number of atoms	5946	wwPDB-VP
Average B, all atoms (Å ²)	31.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 6.37% 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

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	0.56	0/2787	0.79	12/3785 (0.3%)
1	B	0.64	0/2764	0.80	8/3756 (0.2%)
All	All	0.60	0/5551	0.79	20/7541 (0.3%)

There are no bond length outliers.

All (20) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	1128	ASP	CB-CG-OD2	7.00	124.60	118.30
1	B	1343	ASP	CB-CG-OD2	6.87	124.48	118.30
1	B	1077	ASP	CB-CG-OD2	6.38	124.04	118.30
1	A	1273	ASP	CB-CG-OD2	6.12	123.81	118.30
1	A	1250	ASP	CB-CG-OD2	6.07	123.77	118.30
1	B	1128	ASP	CB-CG-OD2	5.91	123.62	118.30
1	A	1047	ASP	CB-CG-OD2	5.89	123.60	118.30
1	A	1077	ASP	CB-CG-OD2	5.85	123.57	118.30
1	A	1318	ARG	NE-CZ-NH2	-5.71	117.44	120.30
1	A	1078	ASP	CB-CG-OD2	5.66	123.40	118.30
1	A	1195	ASP	CB-CG-OD2	5.53	123.28	118.30
1	B	1215	ASP	CB-CG-OD2	5.37	123.13	118.30
1	A	1352	ASP	CB-CG-OD2	5.31	123.08	118.30
1	B	1232	ASP	CB-CG-OD2	5.31	123.08	118.30
1	A	1232	ASP	CB-CG-OD2	5.21	122.99	118.30
1	B	1127	LEU	CA-CB-CG	5.20	127.26	115.30
1	A	1318	ARG	NE-CZ-NH1	5.09	122.84	120.30
1	B	1314	ASP	CB-CG-OD1	5.06	122.85	118.30
1	B	1046	ASP	CB-CG-OD2	5.03	122.82	118.30
1	A	1349	ASP	CB-CG-OD2	5.02	122.81	118.30

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	2745	0	2804	5	0
1	B	2721	0	2772	20	1
2	A	227	0	0	0	0
2	B	253	0	0	5	1
All	All	5946	0	5576	25	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 2.

All (25) 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:1100:GLU:N	1:B:1100:GLU:OE1	2.31	0.64
1:B:1048:LYS:HG2	2:B:73:HOH:O	1.97	0.64
1:B:1375:VAL:HG12	1:B:1376:SER:N	2.17	0.58
1:B:1041:GLN:NE2	2:B:410:HOH:O	2.43	0.52
1:B:1100:GLU:CD	1:B:1100:GLU:H	2.13	0.51
1:A:1341:GLU:O	1:A:1342:LYS:C	2.52	0.48
1:B:1141:ALA:HB2	1:B:1284:LEU:HD11	1.95	0.48
1:A:1342:LYS:N	1:A:1343:ASP:HB3	2.29	0.48
1:B:1375:VAL:HG12	1:B:1376:SER:H	1.81	0.46
1:B:1156:GLN:HE21	1:B:1158:THR:HG22	1.82	0.45
1:B:1185:ASN:ND2	2:B:86:HOH:O	2.50	0.45
1:B:1256:ALA:H	1:B:1291:ASN:HD21	1.64	0.45
1:B:1254:THR:HG21	1:B:1291:ASN:HB2	2.00	0.44
1:B:1120:ARG:HB2	1:B:1375:VAL:CG1	2.48	0.44
1:A:1169:MET:HA	1:A:1192:ARG:O	2.17	0.44
1:B:1120:ARG:O	1:B:1375:VAL:HG13	2.17	0.44
1:A:1338:LEU:CD1	1:A:1355:ILE:HD12	2.49	0.43
1:B:1156:GLN:NE2	2:B:319:HOH:O	2.52	0.43
1:B:1251:ILE:HA	1:B:1280:VAL:O	2.20	0.41
1:A:1284:LEU:HD22	1:A:1315:LEU:CD2	2.50	0.41
1:B:1119:PRO:HG2	1:B:1354:VAL:HA	2.02	0.41
1:B:1048:LYS:HG3	2:B:254:HOH:O	2.21	0.41
1:B:1235:ILE:O	1:B:1239:MET:HG2	2.22	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1185:ASN:HA	1:B:1185:ASN:HD22	1.72	0.40
1:B:1149:PHE:CE2	1:B:1151:ARG:HB2	2.57	0.40

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)
1:B:999:HIS:NE2	2:B:261:HOH:O[1_565]	2.12	0.08

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	364/401 (91%)	357 (98%)	5 (1%)	2 (0%)	32	20
1	B	360/401 (90%)	352 (98%)	7 (2%)	1 (0%)	44	34
All	All	724/802 (90%)	709 (98%)	12 (2%)	3 (0%)	38	26

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	1342	LYS
1	A	1343	ASP
1	B	1375	VAL

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	291/317 (92%)	276 (95%)	15 (5%)	27	16
1	B	289/317 (91%)	280 (97%)	9 (3%)	45	36
All	All	580/634 (92%)	556 (96%)	24 (4%)	35	24

All (24) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	1048	LYS
1	A	1059	GLU
1	A	1083	LEU
1	A	1101	LEU
1	A	1104	LYS
1	A	1122	SER
1	A	1153	PHE
1	A	1228	LYS
1	A	1241	LEU
1	A	1257	LEU
1	A	1265	LYS
1	A	1287	GLN
1	A	1315	LEU
1	A	1338	LEU
1	A	1343	ASP
1	B	1041	GLN
1	B	1061	ASN
1	B	1100	GLU
1	B	1153	PHE
1	B	1203	GLN
1	B	1215	ASP
1	B	1231	SER
1	B	1337	LEU
1	B	1345	ASN

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (13) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	1052	GLN
1	A	1135	ASN
1	A	1205	GLN
1	A	1288	ASN

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Mol	Chain	Res	Type
1	A	1325	GLN
1	A	1330	ASN
1	A	1374	GLN
1	B	1135	ASN
1	B	1156	GLN
1	B	1185	ASN
1	B	1203	GLN
1	B	1288	ASN
1	B	1291	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 carbohydrates in this entry.

5.6 Ligand geometry [i](#)

There are no ligands in this entry.

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	368/401 (91%)	-0.37	2 (0%) 90 92	17, 31, 47, 55	0
1	B	364/401 (90%)	-0.43	5 (1%) 75 78	15, 27, 45, 61	0
All	All	732/802 (91%)	-0.40	7 (0%) 82 84	15, 29, 47, 61	0

All (7) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	999	HIS	4.8
1	B	1377	ALA	4.3
1	B	1376	SER	3.7
1	B	1215	ASP	3.7
1	A	1342	LYS	3.5
1	B	1260	GLY	2.3
1	A	1223	GLY	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](#)

There are no ligands in this entry.

6.5 Other polymers [i](#)

There are no such residues in this entry.