



Full wwPDB X-ray Structure Validation Report ⓘ

Jan 1, 2017 – 04:29 AM EST

PDB ID : 5TZ5
Title : Crystal Structure of CurK Dehydratase H996F Inactive Mutant
Authors : Dodge, G.J.; Smith, J.L.
Deposited on : 2016-11-21
Resolution : 1.43 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
Mogul	:	unknown
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20028442
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
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)	:	rb-20028442

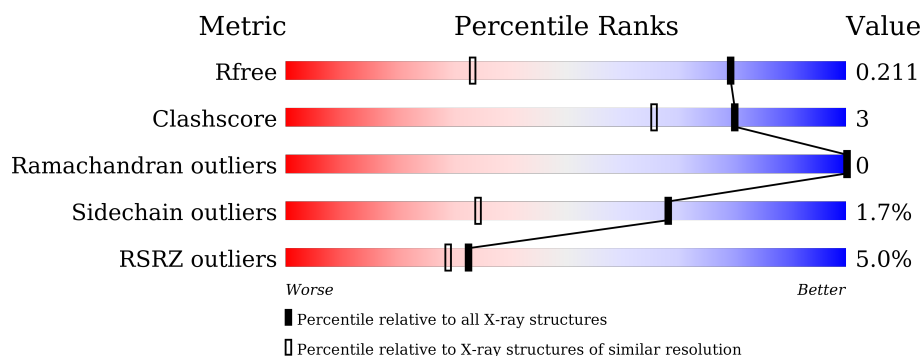
1 Overall quality at a glance ⓘ

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.43 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}	91344	1632 (1.44-1.40)
Clashscore	102246	1743 (1.44-1.40)
Ramachandran outliers	100387	1698 (1.44-1.40)
Sidechain outliers	100360	1697 (1.44-1.40)
RSRZ outliers	91569	1632 (1.44-1.40)

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	296	<div> <div>5%</div> <div> <div></div> <div>89%</div> <div>6%</div> <div>5%</div> </div> </div>
1	B	296	<div> <div>4%</div> <div> <div></div> <div>84%</div> <div>9%</div> <div>6%</div> </div> </div>

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 4612 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 CurK.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	281	Total	C	N	O	S	0	5	0
			2233	1419	375	438	1			
1	B	279	Total	C	N	O	S	4	3	0
			2211	1409	373	428	1			

There are 8 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	955	SER	-	expression tag	UNP F4Y425
A	956	ASN	-	expression tag	UNP F4Y425
A	957	ALA	-	expression tag	UNP F4Y425
A	996	PHE	HIS	engineered mutation	UNP F4Y425
B	955	SER	-	expression tag	UNP F4Y425
B	956	ASN	-	expression tag	UNP F4Y425
B	957	ALA	-	expression tag	UNP F4Y425
B	996	PHE	HIS	engineered mutation	UNP F4Y425

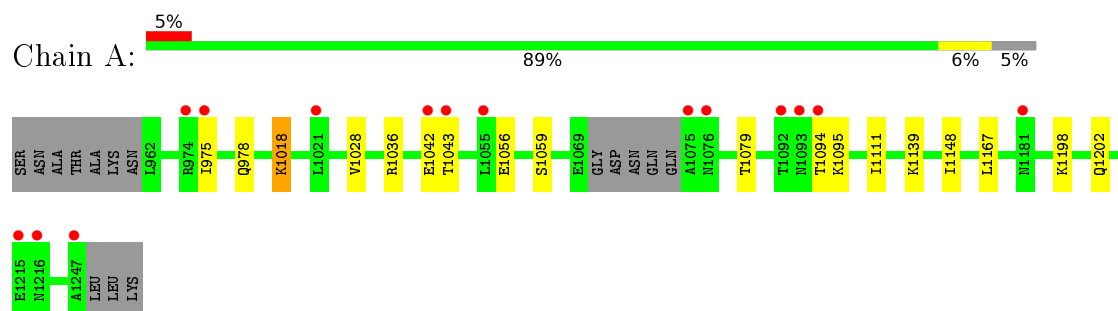
- Molecule 2 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	105	Total	O	0	0
			105	105		
2	B	63	Total	O	0	0
			63	63		

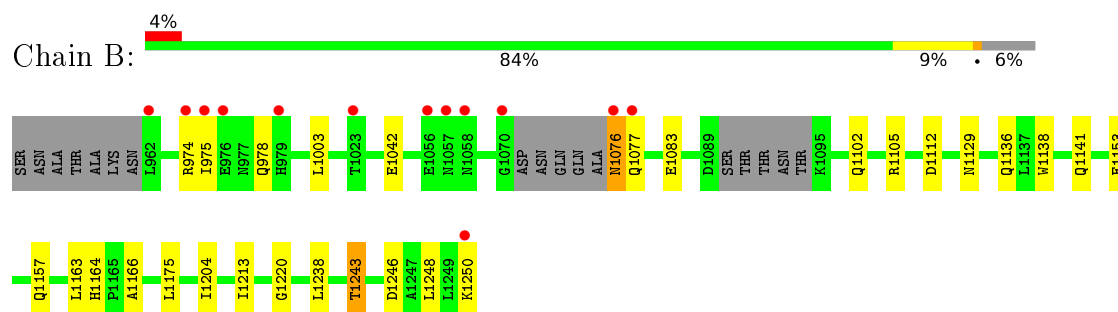
3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors 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 ($\text{RSRZ} > 2$). 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: CurK



• Molecule 1: CurK



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	38.11Å 94.57Å 152.00Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	40.15 – 1.43 47.28 – 1.43	Depositor EDS
% Data completeness (in resolution range)	97.2 (40.15-1.43) 97.2 (47.28-1.43)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.93 (at 1.43Å)	Xtriage
Refinement program	PHENIX	Depositor
R, R_{free}	0.187 , 0.211 0.187 , 0.211	Depositor DCC
R_{free} test set	4984 reflections (4.98%)	DCC
Wilson B-factor (Å ²)	19.4	Xtriage
Anisotropy	0.044	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.36 , 42.7	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.97	EDS
Total number of atoms	4612	wwPDB-VP
Average B, all atoms (Å ²)	28.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.07% 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](#)

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	0.68	0/2270	0.84	0/3082
1	B	0.62	1/2247 (0.0%)	0.76	1/3046 (0.0%)
All	All	0.65	1/4517 (0.0%)	0.80	1/6128 (0.0%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	1243	THR	CB-CG2	-5.09	1.35	1.52

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	1112	ASP	CB-CG-OD1	7.57	125.11	118.30

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	2233	0	2237	11	0
1	B	2211	0	2223	19	0
2	A	105	0	0	0	0
2	B	63	0	0	1	0
All	All	4612	0	4460	30	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 3.

All (30) 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:1164:HIS:HD2	1:B:1166:ALA:H	1.12	0.97
1:A:1042:GLU:HG2	1:A:1043:THR:HG23	1.50	0.93
1:B:1129[B]:ASN:ND2	1:B:1153:GLU:OE2	2.10	0.85
1:B:1102:GLN:OE1	1:B:1105:ARG:NH2	2.14	0.75
1:B:1042:GLU:OE1	2:B:1301:HOH:O	2.05	0.73
1:B:1175:LEU:HD11	1:B:1238:LEU:HD21	1.71	0.71
1:B:1164:HIS:CD2	1:B:1166:ALA:H	2.03	0.67
1:B:1213:ILE:HD13	1:B:1220:GLY:HA3	1.77	0.67
1:A:1018:LYS:HE3	1:A:1202:GLN:NE2	2.12	0.65
1:B:1136:GLN:HE21	1:B:1138:TRP:HE1	1.44	0.64
1:B:1175:LEU:HD21	1:B:1238:LEU:HD23	1.83	0.59
1:A:1056:GLU:HG2	1:A:1059:SER:HB3	1.83	0.59
1:B:1163:LEU:HD21	1:B:1204:ILE:HD12	1.85	0.59
1:A:1036:ARG:HD2	1:A:1079:THR:CG2	2.35	0.57
1:B:1157:GLN:OE1	1:B:1164:HIS:HE1	1.88	0.56
1:B:1003:LEU:HD21	1:B:1248:LEU:HB3	1.91	0.52
1:B:1164:HIS:HD2	1:B:1166:ALA:N	1.95	0.52
1:A:1148:ILE:HG22	1:A:1167[B]:LEU:HD11	1.93	0.50
1:B:975:ILE:HG22	1:B:978:GLN:HB2	1.93	0.50
1:B:1246[B]:ASP:O	1:B:1250:LYS:HG2	2.12	0.49
1:B:1246[A]:ASP:O	1:B:1250:LYS:HG2	2.13	0.47
1:A:1018:LYS:HE3	1:A:1202:GLN:HE22	1.80	0.47
1:A:1028:VAL:HG22	1:A:1198:LYS:HE3	1.96	0.47
1:A:1202:GLN:OE1	1:A:1202:GLN:HA	2.18	0.43
1:A:1111:ILE:HD11	1:A:1139:LYS:HE2	2.01	0.43
1:B:1076:ASN:HB2	1:B:1077:GLN:H	1.56	0.42
1:A:975:ILE:CG2	1:A:978:GLN:HB3	2.50	0.42
1:A:1148:ILE:HG22	1:A:1167[B]:LEU:CD1	2.50	0.41
1:B:1076:ASN:OD1	1:B:1076:ASN:N	2.53	0.41
1:B:975:ILE:CG2	1:B:978:GLN:HB2	2.50	0.41

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	282/296 (95%)	276 (98%)	6 (2%)	0	100	100
1	B	276/296 (93%)	268 (97%)	8 (3%)	0	100	100
All	All	558/592 (94%)	544 (98%)	14 (2%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains

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	243/250 (97%)	240 (99%)	3 (1%)	78	51
1	B	239/250 (96%)	234 (98%)	5 (2%)	61	24
All	All	482/500 (96%)	474 (98%)	8 (2%)	68	34

All (8) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	1018	LYS
1	A	1094	THR
1	A	1095	LYS
1	B	974	ARG
1	B	1076	ASN
1	B	1083	GLU
1	B	1141	GLN
1	B	1243	THR

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (7) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	980	HIS
1	A	1058	ASN
1	A	1104	GLN
1	A	1115	GLN
1	B	1104	GLN
1	B	1136	GLN
1	B	1164	HIS

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 ⓘ

6.1 Protein, DNA and RNA chains ⓘ

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	281/296 (94%)	0.02	15 (5%)	30 26	12, 22, 53, 87	2 (0%)
1	B	279/296 (94%)	0.03	13 (4%)	35 32	16, 26, 49, 81	4 (1%)
All	All	560/592 (94%)	0.03	28 (5%)	32 29	12, 24, 51, 87	6 (1%)

All (28) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	1094	THR	6.6
1	B	975	ILE	4.7
1	A	1076	ASN	4.6
1	B	1076	ASN	4.3
1	A	1043	THR	4.0
1	A	975	ILE	3.9
1	A	1075	ALA	3.7
1	B	1056	GLU	3.6
1	A	1092	THR	3.5
1	A	974	ARG	3.4
1	A	1021	LEU	3.2
1	B	1058	ASN	3.0
1	A	1093	ASN	3.0
1	A	1042	GLU	2.9
1	A	1215	GLU	2.7
1	B	1023	THR	2.6
1	A	1247	ALA	2.5
1	A	1216	ASN	2.5
1	B	979	HIS	2.5
1	A	1055	LEU	2.5
1	B	1250	LYS	2.4
1	B	974	ARG	2.4
1	A	1181	ASN	2.3
1	B	1070	GLY	2.3

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Mol	Chain	Res	Type	RSRZ
1	B	962	LEU	2.2
1	B	1077	GLN	2.2
1	B	976	GLU	2.0
1	B	1057	ASN	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 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.