



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 13, 2017 – 12:52 am GMT

PDB ID : 1LZL
Title : Bacterial Heroin Esterase
Authors : Zhu, X.; Larsen, N.A.; Basran, A.; Bruce, N.C.; Wilson, I.A.
Deposited on : 2002-06-10
Resolution : 1.30 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

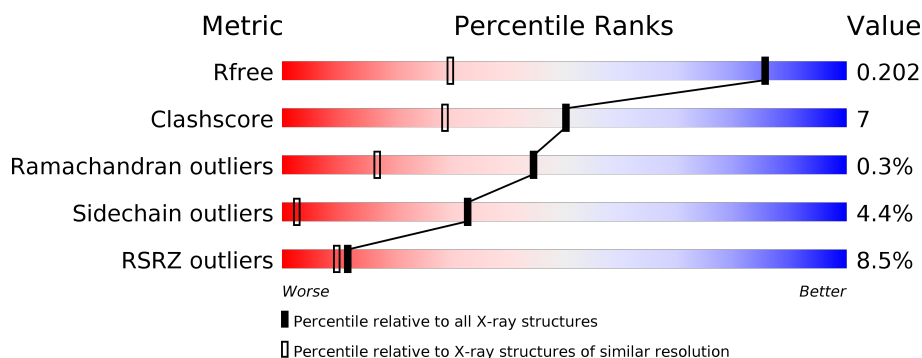
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.30 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	1131 (1.32-1.28)
Clashscore	112137	1185 (1.32-1.28)
Ramachandran outliers	110173	1138 (1.32-1.28)
Sidechain outliers	110143	1138 (1.32-1.28)
RSRZ outliers	101464	1133 (1.32-1.28)

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	323	<div> <div>8%</div> <div>84%</div> <div>12%</div> <div>••</div> </div>

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 2699 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 HEROIN ESTERASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	317	Total	C	N	O	S	0	4	0
			2386	1522	393	465	6			

There are 19 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	159	GLN	GLU	SEE REMARK 999	UNP O06441
A	299	ALA	GLY	SEE REMARK 999	UNP O06441
A	301	SER	ARG	SEE REMARK 999	UNP O06441
A	307	GLU	LYS	SEE REMARK 999	UNP O06441
A	308	ALA	PRO	SEE REMARK 999	UNP O06441
A	309	LEU	HIS	SEE REMARK 999	UNP O06441
A	310	THR	CYS	SEE REMARK 999	UNP O06441
A	311	ALA	ASP	SEE REMARK 999	UNP O06441
A	312	ILE	PRO	SEE REMARK 999	UNP O06441
A	313	ARG	GLU	SEE REMARK 999	UNP O06441
A	315	GLY	VAL	SEE REMARK 999	UNP O06441
A	316	LEU	ALA	SEE REMARK 999	UNP O06441
A	317	ARG	PHE	SEE REMARK 999	UNP O06441
A	318	SER	ALA	SEE REMARK 999	UNP O06441
A	319	LEU	VAL	SEE REMARK 999	UNP O06441
A	320	SER	ALA	SEE REMARK 999	UNP O06441
A	321	PRO	VAL	SEE REMARK 999	UNP O06441
A	322	VAL	SER	SEE REMARK 999	UNP O06441
A	323	SER	-	SEE REMARK 999	UNP O06441

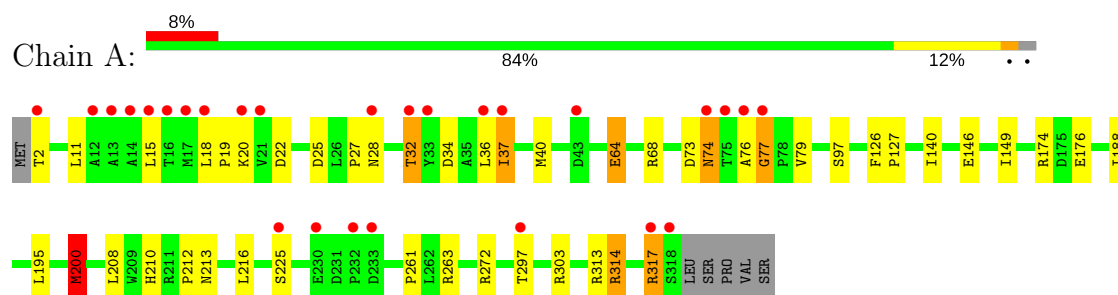
- Molecule 2 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	313	Total	O	0	0
			313	313		

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: HEROIN ESTERASE



4 Data and refinement statistics

Property	Value	Source
Space group	P 32 2 1	Depositor
Cell constants a, b, c, α , β , γ	71.43Å 71.43Å 105.67Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	26.70 – 1.30 26.69 – 1.30	Depositor EDS
% Data completeness (in resolution range)	99.7 (26.70-1.30) 93.9 (26.69-1.30)	Depositor EDS
R_{merge}	0.04	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.48 (at 1.30Å)	Xtriage
Refinement program	SHELXL-97	Depositor
R, R_{free}	0.153 , 0.213 0.151 , 0.202	Depositor DCC
R_{free} test set	3700 reflections (5.38%)	DCC
Wilson B-factor (Å ²)	12.8	Xtriage
Anisotropy	0.192	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.35 , 63.3	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	0.028 for -h,-k,l	Xtriage
F_o, F_c correlation	0.98	EDS
Total number of atoms	2699	wwPDB-VP
Average B, all atoms (Å ²)	19.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 7.92% 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	0.66	0/2461	1.35	16/3369 (0.5%)

There are no bond length outliers.

All (16) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	272	ARG	CD-NE-CZ	19.91	151.47	123.60
1	A	314	ARG	CD-NE-CZ	19.86	151.41	123.60
1	A	314	ARG	NE-CZ-NH2	-13.31	113.64	120.30
1	A	272	ARG	NE-CZ-NH2	-10.29	115.16	120.30
1	A	314	ARG	NE-CZ-NH1	8.21	124.40	120.30
1	A	303	ARG	NE-CZ-NH1	7.06	123.83	120.30
1	A	200	MET	CA-CB-CG	6.62	124.56	113.30
1	A	68	ARG	NE-CZ-NH2	-6.47	117.06	120.30
1	A	34	ASP	CB-CG-OD1	5.94	123.65	118.30
1	A	317	ARG	NE-CZ-NH1	-5.74	117.43	120.30
1	A	176	GLU	OE1-CD-OE2	-5.46	116.75	123.30
1	A	74	ASN	C-N-CA	-5.40	108.21	121.70
1	A	297	THR	CA-CB-CG2	-5.30	104.98	112.40
1	A	174	ARG	NE-CZ-NH2	-5.25	117.67	120.30
1	A	263	ARG	NE-CZ-NH2	-5.02	117.79	120.30
1	A	303	ARG	NH1-CZ-NH2	-5.02	113.88	119.40

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	2386	0	2333	31	0
2	A	313	0	0	5	0
All	All	2699	0	2333	31	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 7.

All (31) 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:317:ARG:HD3	2:A:617:HOH:O	1.85	0.76
1:A:18:LEU:HD22	1:A:208:LEU:HD21	1.72	0.71
1:A:15:LEU:HA	1:A:18:LEU:HD12	1.76	0.67
1:A:25:ASP:OD1	1:A:27:PRO:HD2	2.01	0.60
1:A:210:HIS:CD2	1:A:213:ASN:H	2.24	0.55
1:A:210:HIS:HD2	1:A:213:ASN:H	1.56	0.54
1:A:195:LEU:HA	1:A:200:MET:HG3	1.89	0.53
1:A:64:GLU:HG3	2:A:621:HOH:O	2.09	0.52
1:A:15:LEU:HD12	1:A:18:LEU:CD1	2.41	0.50
1:A:73:ASP:O	1:A:74:ASN:HB2	2.12	0.50
1:A:314:ARG:HG3	1:A:317:ARG:HH11	1.77	0.48
1:A:18:LEU:CD2	1:A:208:LEU:HD21	2.41	0.47
1:A:210:HIS:HA	1:A:261:PRO:HG3	1.97	0.46
1:A:28:ASN:O	1:A:32:THR:HG23	2.15	0.46
1:A:76:ALA:O	1:A:77:GLY:O	2.33	0.46
1:A:210:HIS:CD2	1:A:212:PRO:HD2	2.51	0.45
1:A:140[B]:ILE:HG23	1:A:149:ILE:HD13	1.99	0.45
1:A:313:ARG:NH2	2:A:582:HOH:O	2.50	0.45
1:A:126:PHE:CD1	1:A:127:PRO:HA	2.52	0.45
1:A:140[B]:ILE:HG23	1:A:149:ILE:CD1	2.47	0.43
1:A:126:PHE:CG	1:A:127:PRO:HA	2.53	0.43
1:A:37:ILE:CG1	1:A:97:SER:HB2	2.49	0.43
1:A:313:ARG:NH1	2:A:586:HOH:O	2.52	0.42
1:A:225:SER:HB3	2:A:477:HOH:O	2.18	0.42
1:A:77:GLY:HA2	1:A:79:VAL:HG13	2.00	0.42
1:A:15:LEU:HD12	1:A:18:LEU:HD12	2.01	0.41
1:A:18:LEU:HA	1:A:19:PRO:HD2	1.43	0.41
1:A:313:ARG:HH11	1:A:313:ARG:HD3	1.68	0.41
1:A:37:ILE:HG21	1:A:97:SER:CB	2.50	0.41
1:A:11:LEU:HD23	1:A:11:LEU:HA	1.91	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	319/323 (99%)	308 (97%)	10 (3%)	1 (0%)	44 17

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	77	GLY

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	252/254 (99%)	241 (96%)	11 (4%)	33 2

All (11) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	2	THR
1	A	20	LYS
1	A	22	ASP
1	A	32	THR
1	A	36	LEU
1	A	37	ILE
1	A	40	MET
1	A	64	GLU
1	A	146	GLU
1	A	200	MET

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Mol	Chain	Res	Type
1	A	216	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	A	210	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	317/323 (98%)	0.19	27 (8%) 11 10	8, 14, 42, 65	0

All (27) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	37	ILE	7.9
1	A	18	LEU	6.8
1	A	76	ALA	6.1
1	A	17	MET	5.8
1	A	36	LEU	5.8
1	A	75	THR	4.9
1	A	318	SER	4.7
1	A	32	THR	4.5
1	A	74	ASN	4.4
1	A	232	PRO	4.1
1	A	21	VAL	3.7
1	A	33	TYR	3.7
1	A	233	ASP	3.6
1	A	16	THR	3.3
1	A	13	ALA	3.1
1	A	15	LEU	3.0
1	A	77	GLY	2.9
1	A	230	GLU	2.9
1	A	2	THR	2.9
1	A	20	LYS	2.7
1	A	14	ALA	2.5
1	A	297	THR	2.4
1	A	12	ALA	2.3
1	A	43	ASP	2.3
1	A	317	ARG	2.1
1	A	225	SER	2.1
1	A	28	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.