



Full wwPDB X-ray Structure Validation Report ⓘ

Dec 14, 2020 – 12:15 PM JST

PDB ID : 6LRW
Title : Marsupenaeus japonicus ferritin mutant(T158H) pH 7.0
Authors : Zhao, G.; Tan, X.; Zhang, T.
Deposited on : 2020-01-16
Resolution : 2.40 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

<https://www.wwpdb.org/validation/2017/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:

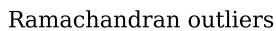
MolProbity : 4.02b-467
Xtriage (Phenix) : 1.13
EDS : 2.15.1
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac : 5.8.0158
CCP4 : 7.0.044 (Gargrove)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.15.1

i

X-RAY DIFFRACTION

A.

Metric	Percentile Rank	Value
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 R_{free}

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.

1

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 2818 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 Ferritin.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	169	Total	C	N	O	S	0	0	0
			1362	854	230	271	7			
1	B	169	Total	C	N	O	S	0	0	0
			1362	854	230	271	7			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	158	HIS	THR	engineered mutation	UNP T2B7E1
B	158	HIS	THR	engineered mutation	UNP T2B7E1


- Molecule 2 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	43	Total	O	0	0
			43	43		
2	B	51	Total	O	0	0
			51	51		

3 Residue-property plots [i](#)


These plots are drawn for all protein, RNA, DNA and oligosaccharide 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.

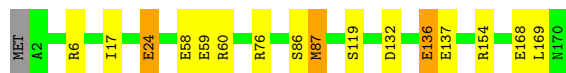
- Molecule 1: Ferritin

Chain A:  91% 6% ..



- Molecule 1: Ferritin

Chain B:  90% 8% ..



4 Data and refinement statistics

Property	Value	Source
Space group	P 2 3	Depositor
Cell constants a, b, c, α , β , γ	117.11Å 117.11Å 117.11Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	50.00 – 2.40 47.81 – 2.40	Depositor EDS
% Data completeness (in resolution range)	100.0 (50.00-2.40) 100.0 (47.81-2.40)	Depositor EDS
R_{merge}	0.14	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	5.56 (at 2.39Å)	Xtriage
Refinement program	REFMAC 5.8.0103	Depositor
R, R_{free}	0.176 , 0.228 0.185 , 0.234	Depositor DCC
R_{free} test set	1118 reflections (5.27%)	wwPDB-VP
Wilson B-factor (Å ²)	20.1	Xtriage
Anisotropy	0.000	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.35 , -1.2	EDS
L-test for twinning ²	$\langle L \rangle = 0.51$, $\langle L^2 \rangle = 0.34$	Xtriage
Estimated twinning fraction	0.489 for l,-k,h	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	2818	wwPDB-VP
Average B, all atoms (Å ²)	23.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 6.06% 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	0.90	2/1387 (0.1%)	0.95	7/1864 (0.4%)
1	B	0.87	1/1387 (0.1%)	0.93	5/1864 (0.3%)
All	All	0.88	3/2774 (0.1%)	0.94	12/3728 (0.3%)

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	24	GLU	CD-OE1	8.06	1.34	1.25
1	A	141	SER	CB-OG	-5.67	1.34	1.42
1	B	24	GLU	CD-OE1	5.15	1.31	1.25

All (12) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	76	ARG	NE-CZ-NH1	7.30	123.95	120.30
1	A	60	ARG	NE-CZ-NH1	6.75	123.67	120.30
1	A	76	ARG	NE-CZ-NH1	6.64	123.62	120.30
1	A	154	ARG	NE-CZ-NH1	6.34	123.47	120.30
1	A	24	GLU	CG-CD-OE1	6.17	130.65	118.30
1	B	87	MET	CG-SD-CE	6.00	109.79	100.20
1	A	87	MET	CG-SD-CE	5.71	109.34	100.20
1	A	24	GLU	CG-CD-OE2	-5.69	106.92	118.30
1	B	6	ARG	NE-CZ-NH2	5.46	123.03	120.30
1	B	24	GLU	CG-CD-OE1	5.39	129.08	118.30
1	A	154	ARG	NE-CZ-NH2	-5.27	117.67	120.30
1	B	154	ARG	NE-CZ-NH1	5.17	122.89	120.30

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	1362	0	1311	3	0
1	B	1362	0	1311	4	0
2	A	43	0	0	0	0
2	B	51	0	0	2	0
All	All	2818	0	2622	6	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 1.

All (6) 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:60:ARG:HD3	2:B:244:HOH:O	1.95	0.65
1:A:24:GLU:OE1	1:A:59:GLU:OE1	2.16	0.63
1:B:24:GLU:OE1	1:B:59:GLU:OE1	2.24	0.56
1:B:136:GLU:HG3	2:B:229:HOH:O	2.13	0.48
1:A:60:ARG:HD2	1:B:60:ARG:NH1	2.35	0.42
1:A:46:PRO:HB2	1:A:170:ASN:HD21	1.84	0.42

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	167/170 (98%)	165 (99%)	2 (1%)	0	100 100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	B	167/170 (98%)	165 (99%)	2 (1%)	0	100	100
All	All	334/340 (98%)	330 (99%)	4 (1%)	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	145/146 (99%)	137 (94%)	8 (6%)	21	35
1	B	145/146 (99%)	135 (93%)	10 (7%)	15	25
All	All	290/292 (99%)	272 (94%)	18 (6%)	18	29

All (18) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	17	ILE
1	A	81	GLN
1	A	86	SER
1	A	87	MET
1	A	102	ASP
1	A	136	GLU
1	A	141	SER
1	A	168	GLU
1	B	17	ILE
1	B	58	GLU
1	B	86	SER
1	B	87	MET
1	B	119	SER
1	B	132	ASP
1	B	136	GLU
1	B	137	GLU
1	B	168	GLU
1	B	169	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (3) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	81	GLN
1	A	170	ASN
1	B	121	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 monosaccharides 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	169/170 (99%)	-0.62	0 100 100	16, 21, 37, 46	0
1	B	169/170 (99%)	-0.62	0 100 100	16, 21, 36, 44	0
All	All	338/340 (99%)	-0.62	0 100 100	16, 21, 36, 46	0

There are no RSRZ outliers to report.

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](#)

There are no ligands in this entry.

6.5 Other polymers [i](#)

There are no such residues in this entry.