



wwPDB X-ray Structure Validation Summary Report

Feb 13, 2017 – 05:00 pm GMT

PDB ID : 3VZ8
Title : Crystal Structure Analysis of the Mini-chaperonin variant with Leu 185, Val 186, Pro 187, Arg 188 and Ser 190 replaced with all Gly
Authors : Saijo, S.; Sato, T.
Deposited on : 2012-10-09
Resolution : 1.90 Å(reported)

This is a wwPDB X-ray Structure Validation Summary 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
Xtrriage (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

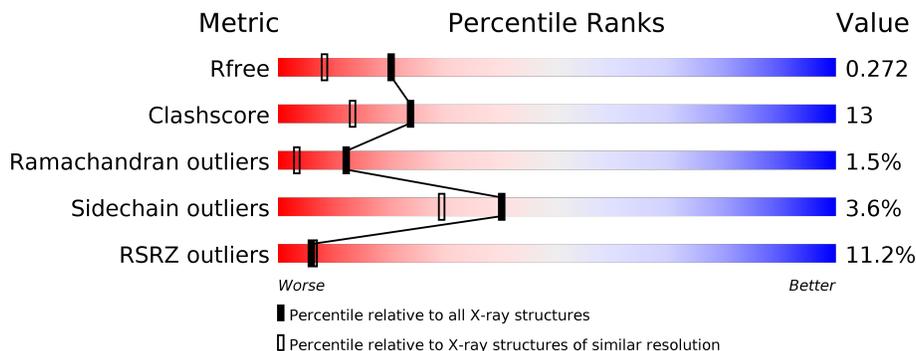
1 Overall quality at a glance

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	199	 10% 70% 21% • 7%
1	B	199	 13% 65% 24% • • 7%
1	C	199	 8% 76% 15% • 7%

2 Entry composition i

There are 2 unique types of molecules in this entry. The entry contains 4396 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 60 kDa chaperonin.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	185	1401	881	240	275	5	0	0	0
1	B	185	1401	881	240	275	5	0	0	0
1	C	185	1401	881	240	275	5	0	0	0

There are 39 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	178	HIS	-	EXPRESSION TAG	UNP P0A6F5
A	179	HIS	-	EXPRESSION TAG	UNP P0A6F5
A	180	HIS	-	EXPRESSION TAG	UNP P0A6F5
A	181	HIS	-	EXPRESSION TAG	UNP P0A6F5
A	182	HIS	-	EXPRESSION TAG	UNP P0A6F5
A	183	HIS	-	EXPRESSION TAG	UNP P0A6F5
A	184	GLY	-	SEE REMARK 999	UNP P0A6F5
A	185	GLY	-	SEE REMARK 999	UNP P0A6F5
A	186	GLY	-	SEE REMARK 999	UNP P0A6F5
A	187	GLY	-	SEE REMARK 999	UNP P0A6F5
A	188	GLY	-	SEE REMARK 999	UNP P0A6F5
A	189	GLY	-	SEE REMARK 999	UNP P0A6F5
A	190	GLY	-	SEE REMARK 999	UNP P0A6F5
B	178	HIS	-	EXPRESSION TAG	UNP P0A6F5
B	179	HIS	-	EXPRESSION TAG	UNP P0A6F5
B	180	HIS	-	EXPRESSION TAG	UNP P0A6F5
B	181	HIS	-	EXPRESSION TAG	UNP P0A6F5
B	182	HIS	-	EXPRESSION TAG	UNP P0A6F5
B	183	HIS	-	EXPRESSION TAG	UNP P0A6F5
B	184	GLY	-	SEE REMARK 999	UNP P0A6F5
B	185	GLY	-	SEE REMARK 999	UNP P0A6F5
B	186	GLY	-	SEE REMARK 999	UNP P0A6F5
B	187	GLY	-	SEE REMARK 999	UNP P0A6F5

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Chain	Residue	Modelled	Actual	Comment	Reference
B	188	GLY	-	SEE REMARK 999	UNP P0A6F5
B	189	GLY	-	SEE REMARK 999	UNP P0A6F5
B	190	GLY	-	SEE REMARK 999	UNP P0A6F5
C	178	HIS	-	EXPRESSION TAG	UNP P0A6F5
C	179	HIS	-	EXPRESSION TAG	UNP P0A6F5
C	180	HIS	-	EXPRESSION TAG	UNP P0A6F5
C	181	HIS	-	EXPRESSION TAG	UNP P0A6F5
C	182	HIS	-	EXPRESSION TAG	UNP P0A6F5
C	183	HIS	-	EXPRESSION TAG	UNP P0A6F5
C	184	GLY	-	SEE REMARK 999	UNP P0A6F5
C	185	GLY	-	SEE REMARK 999	UNP P0A6F5
C	186	GLY	-	SEE REMARK 999	UNP P0A6F5
C	187	GLY	-	SEE REMARK 999	UNP P0A6F5
C	188	GLY	-	SEE REMARK 999	UNP P0A6F5
C	189	GLY	-	SEE REMARK 999	UNP P0A6F5
C	190	GLY	-	SEE REMARK 999	UNP P0A6F5

- Molecule 2 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	62	Total O 62 62	0	0
2	B	64	Total O 64 64	0	0
2	C	67	Total O 67 67	0	0

4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	95.06Å 38.01Å 102.20Å 90.00° 116.23° 90.00°	Depositor
Resolution (Å)	47.51 – 1.90 47.51 – 1.90	Depositor EDS
% Data completeness (in resolution range)	99.4 (47.51-1.90) 99.5 (47.51-1.90)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.24 (at 1.90Å)	Xtrriage
Refinement program	CNS 1.3	Depositor
R, R_{free}	0.263 , 0.272 0.263 , 0.272	Depositor DCC
R_{free} test set	2605 reflections (4.99%)	DCC
Wilson B-factor (Å ²)	22.8	Xtrriage
Anisotropy	0.222	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.38 , 53.1	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.33$	Xtrriage
Estimated twinning fraction	0.015 for h,-k,-h-l	Xtrriage
F_o, F_c correlation	0.91	EDS
Total number of atoms	4396	wwPDB-VP
Average B, all atoms (Å ²)	25.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.54% 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	0.34	0/1413	0.64	0/1903
1	B	0.33	0/1413	0.64	0/1903
1	C	0.32	0/1413	0.63	0/1903
All	All	0.33	0/4239	0.64	0/5709

There are no bond length outliers.

There are no bond angle outliers.

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	1401	0	1455	37	0
1	B	1401	0	1455	42	0
1	C	1401	0	1455	29	0
2	A	62	0	0	3	0
2	B	64	0	0	1	0
2	C	67	0	0	1	0
All	All	4396	0	4365	108	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 13.

The worst 5 of 108 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:C:364:LYS:HA	1:C:364:LYS:NZ	1.94	0.82
1:B:200:LEU:HD21	1:B:277:LYS:HG3	1.63	0.80
1:B:198:GLY:O	1:B:276:VAL:HG23	1.82	0.79
1:C:224:ASP:OD1	1:C:286:LYS:HD3	1.84	0.78
1:A:364:LYS:NZ	1:A:364:LYS:HA	2.01	0.76

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	183/199 (92%)	178 (97%)	4 (2%)	1 (0%)	32	20
1	B	183/199 (92%)	170 (93%)	8 (4%)	5 (3%)	6	1
1	C	183/199 (92%)	174 (95%)	7 (4%)	2 (1%)	17	6
All	All	549/597 (92%)	522 (95%)	19 (4%)	8 (2%)	12	3

5 of 8 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	302	SER
1	C	305	ILE
1	B	305	ILE
1	B	209	GLU
1	C	306	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	147/154 (96%)	140 (95%)	7 (5%)	30	18
1	B	147/154 (96%)	141 (96%)	6 (4%)	35	24
1	C	147/154 (96%)	144 (98%)	3 (2%)	60	55
All	All	441/462 (96%)	425 (96%)	16 (4%)	40	29

5 of 16 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	199	TYR
1	B	209	GLU
1	B	364	LYS
1	A	366	GLN
1	C	345	ARG

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 10 such sidechains are listed below:

Mol	Chain	Res	Type
1	B	265	ASN
1	B	319	GLN
1	B	366	GLN
1	A	343	GLN
1	B	343	GLN

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	185/199 (92%)	0.78	20 (10%) 6 7	12, 22, 47, 54	4 (2%)
1	B	185/199 (92%)	0.86	26 (14%) 3 3	13, 24, 52, 61	4 (2%)
1	C	185/199 (92%)	0.71	16 (8%) 11 12	11, 22, 40, 62	4 (2%)
All	All	555/597 (92%)	0.78	62 (11%) 6 6	11, 23, 47, 62	12 (2%)

The worst 5 of 62 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	376	VAL	7.4
1	C	305	ILE	7.1
1	C	375	GLY	6.7
1	C	374	GLY	6.6
1	A	376	VAL	6.6

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.