



wwPDB X-ray Structure Validation Summary Report ⓘ

Aug 7, 2017 – 09:21 PM EDT

PDB ID : 4IVJ
Title : Structure of a 16 nm protein cage designed by fusing symmetric oligomeric domains, triple mutant, I222 form
Authors : Lai, Y.-T.; Sawaya, M.R.; Yeates, T.O.
Deposited on : unknown
Resolution : 7.35 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
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20029824
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)	:	rb-20029824

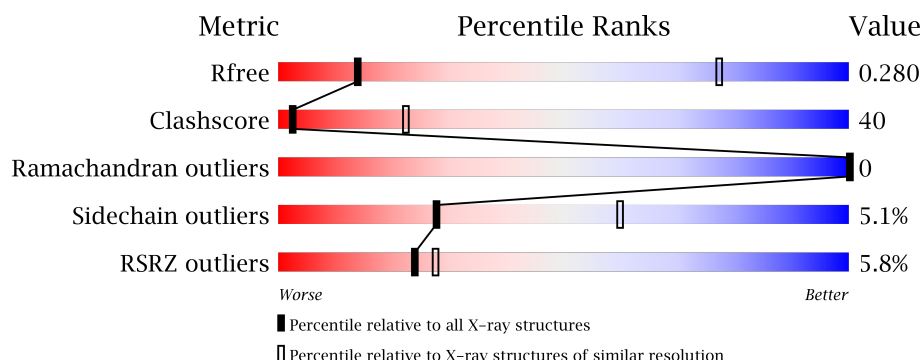
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 7.35 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	1100 (10.00-3.70)
Clashscore	112137	1035 (10.00-3.80)
Ramachandran outliers	110173	1003 (10.00-3.76)
Sidechain outliers	110143	1098 (10.00-3.70)
RSRZ outliers	101464	1003 (10.00-3.72)

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	456	<div> <div>3%</div> <div>58%</div> <div>35%</div> <div>• •</div> </div>
1	B	456	<div> <div>9%</div> <div>55%</div> <div>37%</div> <div>5% •</div> </div>
1	C	456	<div> <div>4%</div> <div>54%</div> <div>39%</div> <div>• •</div> </div>

2 Entry composition

There is only 1 type of molecule in this entry. The entry contains 10194 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 Non-haem bromoperoxidase BPO-A2, Matrix protein 1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	440	Total	C	N	O	S	0	0	0
			3398	2166	572	652	8			
1	B	440	Total	C	N	O	S	0	0	0
			3398	2166	572	652	8			
1	C	440	Total	C	N	O	S	0	0	0
			3398	2166	572	652	8			

There are 54 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	24	THR	GLN	ENGINEERED MUTATION	UNP P29715
A	118	ALA	LYS	ENGINEERED MUTATION	UNP P29715
A	278	ALA	-	LINKER	UNP P03485
A	279	GLN	-	LINKER	UNP P03485
A	280	GLU	-	LINKER	UNP P03485
A	281	ALA	-	LINKER	UNP P03485
A	282	GLN	-	LINKER	UNP P03485
A	283	LYS	-	LINKER	UNP P03485
A	284	GLN	-	LINKER	UNP P03485
A	285	LYS	-	LINKER	UNP P03485
A	448	LEU	-	EXPRESSION TAG	UNP P03485
A	449	GLU	-	EXPRESSION TAG	UNP P03485
A	450	HIS	-	EXPRESSION TAG	UNP P03485
A	451	HIS	-	EXPRESSION TAG	UNP P03485
A	452	HIS	-	EXPRESSION TAG	UNP P03485
A	453	HIS	-	EXPRESSION TAG	UNP P03485
A	454	HIS	-	EXPRESSION TAG	UNP P03485
A	455	HIS	-	EXPRESSION TAG	UNP P03485
B	24	THR	GLN	ENGINEERED MUTATION	UNP P29715
B	118	ALA	LYS	ENGINEERED MUTATION	UNP P29715
B	278	ALA	-	LINKER	UNP P03485
B	279	GLN	-	LINKER	UNP P03485
B	280	GLU	-	LINKER	UNP P03485

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Chain	Residue	Modelled	Actual	Comment	Reference
B	281	ALA	-	LINKER	UNP P03485
B	282	GLN	-	LINKER	UNP P03485
B	283	LYS	-	LINKER	UNP P03485
B	284	GLN	-	LINKER	UNP P03485
B	285	LYS	-	LINKER	UNP P03485
B	448	LEU	-	EXPRESSION TAG	UNP P03485
B	449	GLU	-	EXPRESSION TAG	UNP P03485
B	450	HIS	-	EXPRESSION TAG	UNP P03485
B	451	HIS	-	EXPRESSION TAG	UNP P03485
B	452	HIS	-	EXPRESSION TAG	UNP P03485
B	453	HIS	-	EXPRESSION TAG	UNP P03485
B	454	HIS	-	EXPRESSION TAG	UNP P03485
B	455	HIS	-	EXPRESSION TAG	UNP P03485
C	24	THR	GLN	ENGINEERED MUTATION	UNP P29715
C	118	ALA	LYS	ENGINEERED MUTATION	UNP P29715
C	278	ALA	-	LINKER	UNP P03485
C	279	GLN	-	LINKER	UNP P03485
C	280	GLU	-	LINKER	UNP P03485
C	281	ALA	-	LINKER	UNP P03485
C	282	GLN	-	LINKER	UNP P03485
C	283	LYS	-	LINKER	UNP P03485
C	284	GLN	-	LINKER	UNP P03485
C	285	LYS	-	LINKER	UNP P03485
C	448	LEU	-	EXPRESSION TAG	UNP P03485
C	449	GLU	-	EXPRESSION TAG	UNP P03485
C	450	HIS	-	EXPRESSION TAG	UNP P03485
C	451	HIS	-	EXPRESSION TAG	UNP P03485
C	452	HIS	-	EXPRESSION TAG	UNP P03485
C	453	HIS	-	EXPRESSION TAG	UNP P03485
C	454	HIS	-	EXPRESSION TAG	UNP P03485
C	455	HIS	-	EXPRESSION TAG	UNP P03485

4 Data and refinement statistics

Property	Value	Source
Space group	I 2 2 2	Depositor
Cell constants a, b, c, α , β , γ	129.67Å 160.98Å 167.63Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	28.42 – 7.35 29.28 – 7.35	Depositor EDS
% Data completeness (in resolution range)	97.0 (28.42-7.35) 97.2 (29.28-7.35)	Depositor EDS
R_{merge}	0.08	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.21 (at 7.22Å)	Xtriage
Refinement program	PHENIX 1.8.1 _1168	Depositor
R, R_{free}	0.276 , 0.288 0.270 , 0.280	Depositor DCC
R_{free} test set	121 reflections (4.98%)	DCC
Wilson B-factor (Å ²)	400.2	Xtriage
Anisotropy	0.357	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.24 , 204.7	EDS
L-test for twinning ²	$\langle L \rangle = 0.45$, $\langle L^2 \rangle = 0.28$	Xtriage
Estimated twinning fraction	0.038 for -h,-l,-k	Xtriage
F_o, F_c correlation	0.79	EDS
Total number of atoms	10194	wwPDB-VP
Average B, all atoms (Å ²)	318.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 7.27% 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	0.79	2/3475 (0.1%)	1.23	22/4729 (0.5%)
1	B	0.75	2/3475 (0.1%)	1.17	20/4729 (0.4%)
1	C	0.77	3/3475 (0.1%)	1.16	21/4729 (0.4%)
All	All	0.77	7/10425 (0.1%)	1.19	63/14187 (0.4%)

The worst 5 of 7 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	192	SER	CB-OG	5.35	1.49	1.42
1	C	136	PRO	N-CD	5.28	1.55	1.47
1	A	192	SER	CB-OG	5.16	1.49	1.42
1	C	192	SER	CB-OG	5.15	1.49	1.42
1	B	337	PRO	N-CD	5.07	1.54	1.47

The worst 5 of 63 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	17	TYR	CZ-CE2-CD2	-5.99	114.41	119.80
1	C	53	VAL	CA-CB-CG2	5.98	119.87	110.90
1	C	98	SER	CB-CA-C	5.98	121.46	110.10
1	A	98	SER	CB-CA-C	5.97	121.45	110.10
1	A	53	VAL	CA-CB-CG2	5.96	119.84	110.90

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	3398	0	3326	245	0
1	B	3398	0	3326	352	0
1	C	3398	0	3326	323	0
All	All	10194	0	9978	814	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 40.

The worst 5 of 814 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:303:LEU:CD1	1:B:334:ILE:HB	1.46	1.46
1:B:10:SER:CB	1:C:87:LEU:HD22	1.53	1.39
1:B:303:LEU:HD12	1:B:334:ILE:CB	1.53	1.38
1:C:298:ILE:HD13	1:C:307:ILE:CD1	1.61	1.30
1:B:11:THR:HG22	1:C:17:TYR:CZ	1.65	1.29

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	438/456 (96%)	427 (98%)	11 (2%)	0	100	100
1	B	438/456 (96%)	428 (98%)	10 (2%)	0	100	100
1	C	438/456 (96%)	427 (98%)	11 (2%)	0	100	100
All	All	1314/1368 (96%)	1282 (98%)	32 (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	354/370 (96%)	337 (95%)	17 (5%)	30	61
1	B	354/370 (96%)	334 (94%)	20 (6%)	25	57
1	C	354/370 (96%)	337 (95%)	17 (5%)	30	61
All	All	1062/1110 (96%)	1008 (95%)	54 (5%)	28	60

5 of 54 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	165	ASN
1	B	290	VAL
1	C	338	LEU
1	B	177	ARG
1	B	238	ARG

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 16 such sidechains are listed below:

Mol	Chain	Res	Type
1	B	135	ASN
1	B	173	ASN
1	C	42	GLN
1	B	90	GLN
1	C	135	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

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	440/456 (96%)	0.11	14 (3%) 48 46	184, 286, 365, 403	0
1	B	440/456 (96%)	0.68	43 (9%) 8 15	268, 397, 443, 467	0
1	C	440/456 (96%)	0.16	20 (4%) 34 35	165, 260, 336, 373	0
All	All	1320/1368 (96%)	0.32	77 (5%) 24 27	165, 306, 426, 467	0

The worst 5 of 77 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	100	GLY	9.9
1	B	96	GLY	9.3
1	B	101	THR	8.6
1	B	30	HIS	8.1
1	A	30	HIS	7.8

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.