



wwPDB X-ray Structure Validation Summary Report ⓘ

May 12, 2016 – 06:05 PM EDT

PDB ID : 5AQ9
Title : DARPIn-based Crystallization Chaperones exploit Molecular Geometry as a Screening Dimension in Protein Crystallography
Authors : Batyuk, A.; Wu, Y.; Honegger, A.; Heberling, M.; Plueckthun, A.
Deposited on : 2015-09-21
Resolution : 1.86 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
Mogul : unknown
Xtriage (Phenix) : 1.9-1692
EDS : rb-20027457
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-20027457

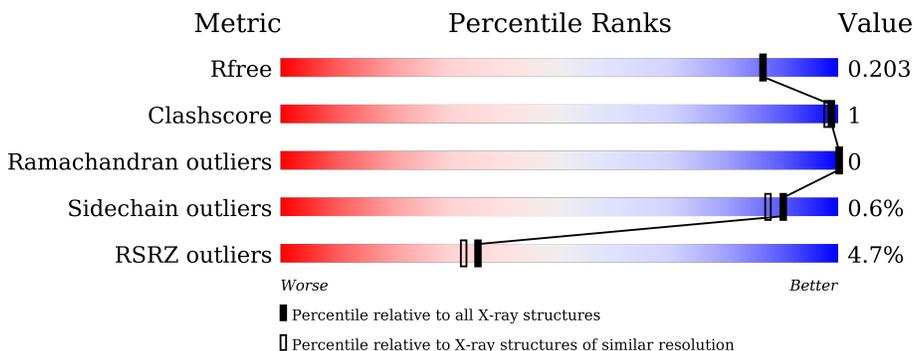
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.86 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	1745 (1.86-1.86)
Clashscore	102246	1898 (1.86-1.86)
Ramachandran outliers	100387	1875 (1.86-1.86)
Sidechain outliers	100360	1875 (1.86-1.86)
RSRZ outliers	91569	1747 (1.86-1.86)

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	422	97%
1	C	422	97%
2	B	395	11% 91%
2	D	395	7% 93%

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 25157 atoms, of which 11966 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 OFF7_DB08V4.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
			Total	C	H	N	O	S			
1	A	419	6379	2006	3172	563	624	14	0	5	0
1	C	419	6374	2005	3169	563	622	15	0	4	0

- Molecule 2 is a protein called MALTOSE-BINDING PERIPLASMIC PROTEIN.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
			Total	C	H	N	O	S			
2	B	371	5672	1837	2812	465	552	6	0	0	0
2	D	371	5673	1837	2813	465	552	6	0	0	0

There are 70 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	1	MET	-	INITIATING METHIONINE	UNP P0AEX9
B	2	ARG	-	EXPRESSION TAG	UNP P0AEX9
B	3	GLY	-	EXPRESSION TAG	UNP P0AEX9
B	4	SER	-	EXPRESSION TAG	UNP P0AEX9
B	5	HIS	-	EXPRESSION TAG	UNP P0AEX9
B	6	HIS	-	EXPRESSION TAG	UNP P0AEX9
B	7	HIS	-	EXPRESSION TAG	UNP P0AEX9
B	8	HIS	-	EXPRESSION TAG	UNP P0AEX9
B	9	HIS	-	EXPRESSION TAG	UNP P0AEX9
B	10	HIS	-	EXPRESSION TAG	UNP P0AEX9
B	11	GLY	-	EXPRESSION TAG	UNP P0AEX9
B	12	SER	-	EXPRESSION TAG	UNP P0AEX9
B	13	GLY	-	EXPRESSION TAG	UNP P0AEX9
B	14	SER	-	EXPRESSION TAG	UNP P0AEX9
B	15	MET	-	EXPRESSION TAG	UNP P0AEX9
B	16	LYS	-	EXPRESSION TAG	UNP P0AEX9

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Chain	Residue	Modelled	Actual	Comment	Reference
B	17	THR	-	EXPRESSION TAG	UNP P0AEX9
B	18	GLU	-	EXPRESSION TAG	UNP P0AEX9
B	19	GLU	-	EXPRESSION TAG	UNP P0AEX9
B	20	GLY	-	EXPRESSION TAG	UNP P0AEX9
B	21	ASN	-	EXPRESSION TAG	UNP P0AEX9
B	382	GLY	-	EXPRESSION TAG	UNP P0AEX9
B	383	SER	-	EXPRESSION TAG	UNP P0AEX9
B	384	GLY	-	EXPRESSION TAG	UNP P0AEX9
B	385	GLY	-	EXPRESSION TAG	UNP P0AEX9
B	386	THR	-	EXPRESSION TAG	UNP P0AEX9
B	387	PRO	-	EXPRESSION TAG	UNP P0AEX9
B	388	GLY	-	EXPRESSION TAG	UNP P0AEX9
B	389	ARG	-	EXPRESSION TAG	UNP P0AEX9
B	390	PRO	-	EXPRESSION TAG	UNP P0AEX9
B	391	ALA	-	EXPRESSION TAG	UNP P0AEX9
B	392	ALA	-	EXPRESSION TAG	UNP P0AEX9
B	393	LYS	-	EXPRESSION TAG	UNP P0AEX9
B	394	LEU	-	EXPRESSION TAG	UNP P0AEX9
B	395	ASN	-	EXPRESSION TAG	UNP P0AEX9
D	1	MET	-	INITIATING METHIONINE	UNP P0AEX9
D	2	ARG	-	EXPRESSION TAG	UNP P0AEX9
D	3	GLY	-	EXPRESSION TAG	UNP P0AEX9
D	4	SER	-	EXPRESSION TAG	UNP P0AEX9
D	5	HIS	-	EXPRESSION TAG	UNP P0AEX9
D	6	HIS	-	EXPRESSION TAG	UNP P0AEX9
D	7	HIS	-	EXPRESSION TAG	UNP P0AEX9
D	8	HIS	-	EXPRESSION TAG	UNP P0AEX9
D	9	HIS	-	EXPRESSION TAG	UNP P0AEX9
D	10	HIS	-	EXPRESSION TAG	UNP P0AEX9
D	11	GLY	-	EXPRESSION TAG	UNP P0AEX9
D	12	SER	-	EXPRESSION TAG	UNP P0AEX9
D	13	GLY	-	EXPRESSION TAG	UNP P0AEX9
D	14	SER	-	EXPRESSION TAG	UNP P0AEX9
D	15	MET	-	EXPRESSION TAG	UNP P0AEX9
D	16	LYS	-	EXPRESSION TAG	UNP P0AEX9
D	17	THR	-	EXPRESSION TAG	UNP P0AEX9
D	18	GLU	-	EXPRESSION TAG	UNP P0AEX9
D	19	GLU	-	EXPRESSION TAG	UNP P0AEX9
D	20	GLY	-	EXPRESSION TAG	UNP P0AEX9
D	21	ASN	-	EXPRESSION TAG	UNP P0AEX9
D	382	GLY	-	EXPRESSION TAG	UNP P0AEX9
D	383	SER	-	EXPRESSION TAG	UNP P0AEX9

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Chain	Residue	Modelled	Actual	Comment	Reference
D	384	GLY	-	EXPRESSION TAG	UNP P0AEX9
D	385	GLY	-	EXPRESSION TAG	UNP P0AEX9
D	386	THR	-	EXPRESSION TAG	UNP P0AEX9
D	387	PRO	-	EXPRESSION TAG	UNP P0AEX9
D	388	GLY	-	EXPRESSION TAG	UNP P0AEX9
D	389	ARG	-	EXPRESSION TAG	UNP P0AEX9
D	390	PRO	-	EXPRESSION TAG	UNP P0AEX9
D	391	ALA	-	EXPRESSION TAG	UNP P0AEX9
D	392	ALA	-	EXPRESSION TAG	UNP P0AEX9
D	393	LYS	-	EXPRESSION TAG	UNP P0AEX9
D	394	LEU	-	EXPRESSION TAG	UNP P0AEX9
D	395	ASN	-	EXPRESSION TAG	UNP P0AEX9

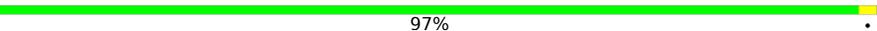
- Molecule 3 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	409	Total O 409 409	0	0
3	B	101	Total O 101 101	0	0
3	C	336	Total O 336 336	0	0
3	D	213	Total O 213 213	0	0

3 Residue-property plots [i](#)

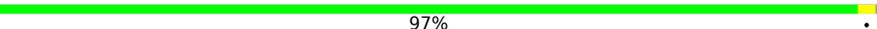
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according 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 ($RSRZ > 2$). 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: OFF7_DB08V4

Chain A:  97%



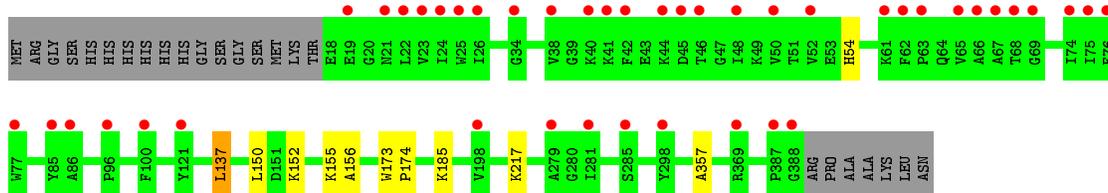
- Molecule 1: OFF7_DB08V4

Chain C:  97%

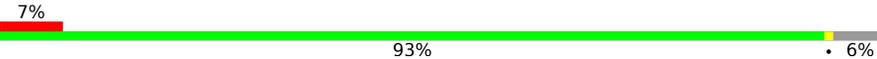


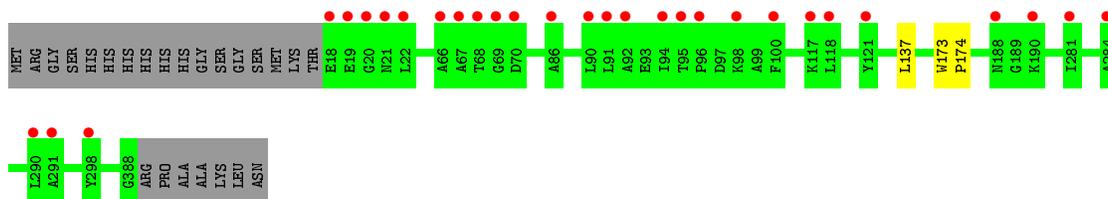
- Molecule 2: MALTOSE-BINDING PERIPLASMIC PROTEIN

Chain B:  11% 91% 6%



- Molecule 2: MALTOSE-BINDING PERIPLASMIC PROTEIN

Chain D:  7% 93% 6%



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	41.48Å 191.12Å 219.51Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	48.05 – 1.86 48.05 – 1.86	Depositor EDS
% Data completeness (in resolution range)	100.0 (48.05-1.86) 100.0 (48.05-1.86)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.04 (at 1.86Å)	Xtrriage
Refinement program	PHENIX (PHENIX.REFINE)	Depositor
R, R_{free}	0.182 , 0.204 0.179 , 0.203	Depositor DCC
R_{free} test set	7408 reflections (5.00%)	DCC
Wilson B-factor (Å ²)	29.7	Xtrriage
Anisotropy	0.281	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.38 , 47.4	EDS
L-test for twinning ²	$\langle L \rangle = 0.47$, $\langle L^2 \rangle = 0.30$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	25157	wwPDB-VP
Average B, all atoms (Å ²)	52.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.31% 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, 0.375 respectively for untwinned datasets, and 0.333, 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	0.27	0/3281	0.48	0/4454
1	C	0.26	0/3276	0.46	0/4446
2	B	0.25	0/2930	0.41	0/3980
2	D	0.26	0/2930	0.41	0/3980
All	All	0.26	0/12417	0.44	0/16860

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	3207	3172	3172	6	0
1	C	3205	3169	3169	6	0
2	B	2860	2812	2812	7	0
2	D	2860	2813	2812	1	0
3	A	409	0	0	2	3
3	B	101	0	0	1	0
3	C	336	0	0	4	0
3	D	213	0	0	0	0
All	All	13191	11966	11965	18	3

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.

The worst 5 of 18 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:125:TYR:OH	2:B:152:LYS:NZ	2.17	0.75
1:A:151:ASP:OD1	3:A:2134:HOH:O	2.07	0.72
1:C:326:LYS:NZ	3:C:2244:HOH:O	2.21	0.72
2:B:357:ALA:O	3:B:2096:HOH:O	2.13	0.66
2:B:54:HIS:ND1	2:B:54:HIS:O	2.32	0.61

All (3) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:2061:HOH:O	3:A:2249:HOH:O[4_455]	2.05	0.15
3:A:2065:HOH:O	3:A:2306:HOH:O[4_555]	2.16	0.04
3:A:2223:HOH:O	3:A:2357:HOH:O[4_455]	2.17	0.03

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	422/422 (100%)	416 (99%)	6 (1%)	0	100	100
1	C	421/422 (100%)	416 (99%)	5 (1%)	0	100	100
2	B	369/395 (93%)	360 (98%)	9 (2%)	0	100	100
2	D	369/395 (93%)	361 (98%)	8 (2%)	0	100	100
All	All	1581/1634 (97%)	1553 (98%)	28 (2%)	0	100	100

There are no Ramachandran outliers to report.

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	338/335 (101%)	336 (99%)	2 (1%)	90	87
1	C	337/335 (101%)	335 (99%)	2 (1%)	90	87
2	B	294/313 (94%)	292 (99%)	2 (1%)	88	84
2	D	294/313 (94%)	293 (100%)	1 (0%)	94	94
All	All	1263/1296 (98%)	1256 (99%)	7 (1%)	90	87

5 of 7 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	B	185	LYS
2	D	137	LEU
1	C	56	TYR
1	A	264	SER
1	C	264	SER

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

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	419/422 (99%)	0.07	1 (0%) 95 94	17, 34, 70, 107	0
1	C	419/422 (99%)	-0.05	1 (0%) 95 94	22, 35, 55, 106	0
2	B	371/395 (93%)	0.61	43 (11%) 6 6	48, 62, 98, 144	0
2	D	371/395 (93%)	0.31	29 (7%) 16 15	34, 49, 84, 120	0
All	All	1580/1634 (96%)	0.22	74 (4%) 35 33	17, 45, 83, 144	0

The worst 5 of 74 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	D	67	ALA	7.5
2	B	68	THR	6.9
2	B	24	ILE	5.8
2	D	66	ALA	4.8
2	B	38	VAL	4.6

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

There are no such residues in this entry.