



# Full wwPDB X-ray Structure Validation Report ⓘ

May 13, 2020 – 07:16 am BST

PDB ID : 5AQA  
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 : 2.60 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](mailto: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.

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The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity : 4.02b-467  
Mogul : 1.8.5 (274361), CSD as541be (2020)  
Xtriage (Phenix) : 1.13  
EDS : 2.11  
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) : 2.11

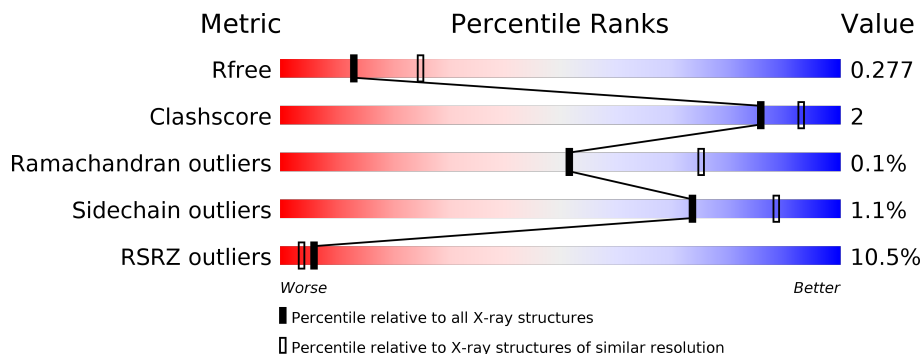
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.60 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))
$R_{free}$	130704	3163 (2.60-2.60)
Clashscore	141614	3518 (2.60-2.60)
Ramachandran outliers	138981	3455 (2.60-2.60)
Sidechain outliers	138945	3455 (2.60-2.60)
RSRZ outliers	127900	3104 (2.60-2.60)

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  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria respectively. 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	418	
1	B	418	

## 2 Entry composition [i](#)

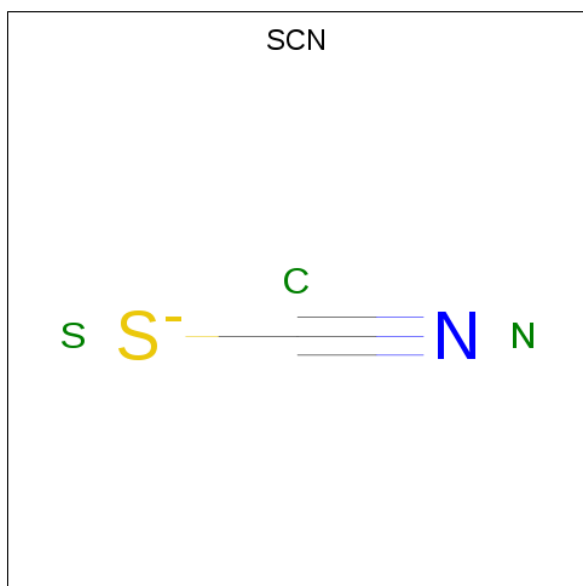
There are 3 unique types of molecules in this entry. The entry contains 12550 atoms, of which 6247 are hydrogens and 0 are deuteriums.

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\_DB04V3.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace	
			Total	C	H	N	O				S
1	A	412	6274	1968	3139	556	597	14	0	0	0
1	B	407	6199	1942	3108	543	592	14	0	0	0

- Molecule 2 is THIOCYANATE ION (three-letter code: SCN) (formula: CNS).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	C	N	S		
2	A	1	3	1	1	1	0	0
2	A	1	3	1	1	1	0	0
2	A	1	3	1	1	1	0	0
2	A	1	3	1	1	1	0	0

- Molecule 3 is water.

<b>Mol</b>	<b>Chain</b>	<b>Residues</b>	<b>Atoms</b>		<b>ZeroOcc</b>	<b>AltConf</b>
3	A	48	Total 48	O 48	0	0
3	B	17	Total 17	O 17	0	0



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 62	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	163.12Å 163.12Å 66.76Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	47.09 – 2.60 47.09 – 2.60	Depositor EDS
% Data completeness (in resolution range)	99.8 (47.09-2.60) 99.8 (47.09-2.60)	Depositor EDS
$R_{merge}$	0.24	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.36 (at 2.61Å)	Xtrriage
Refinement program	PHENIX (PHENIX.REFINE)	Depositor
R, $R_{free}$	0.227 , 0.275 0.228 , 0.277	Depositor DCC
$R_{free}$ test set	1568 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	61.9	Xtrriage
Anisotropy	0.336	Xtrriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.40 , 61.4	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.32$	Xtrriage
Estimated twinning fraction	0.031 for h,-h-k,-l	Xtrriage
$F_o, F_c$ correlation	0.94	EDS
Total number of atoms	12550	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	93.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.47% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical 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](#)

Bond lengths and bond angles in the following residue types are not validated in this section: SCN

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	0.26	0/3192	0.45	0/4329
1	B	0.25	0/3144	0.45	0/4264
All	All	0.26	0/6336	0.45	0/8593

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	3135	3139	3139	12	0
1	B	3091	3108	3108	15	0
2	A	12	0	0	1	0
3	A	48	0	0	2	0
3	B	17	0	0	1	0
All	All	6303	6247	6247	27	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 2.

All (27) 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:235:TYR:OH	1:B:259:MET:O	1.89	0.91
1:B:28:ASP:OD1	1:B:31:ARG:NH2	2.09	0.85
1:B:329:LEU:O	1:B:334:ARG:NH2	2.09	0.84
1:B:33:LEU:O	1:B:36:ASN:ND2	2.20	0.74
1:A:112:ASP:O	1:A:144:LYS:N	2.25	0.70
1:A:45:ASN:ND2	3:A:2004:HOH:O	2.29	0.63
1:B:334:ARG:NH1	3:B:2013:HOH:O	2.37	0.58
1:B:98:VAL:O	1:B:102:ASN:ND2	2.36	0.53
1:B:115:THR:HG22	1:B:118:HIS:ND1	2.23	0.52
1:B:326:GLY:O	1:B:334:ARG:NH2	2.45	0.49
1:A:143:ASP:OD1	1:A:147:LYS:N	2.45	0.49
1:A:229:GLN:N	1:A:243:LEU:HD11	2.27	0.49
1:B:336:GLN:HA	1:B:336:GLN:OE1	2.15	0.47
1:A:126:LYS:HD3	1:A:160:GLU:OE1	2.16	0.45
1:A:406:ALA:HA	2:A:1419:SCN:S	2.57	0.45
1:B:215:ASP:OD1	1:B:333:SER:OG	2.36	0.44
1:A:30:VAL:O	1:A:34:MET:HG2	2.18	0.44
1:A:157:GLY:HA2	1:A:413:ALA:O	2.17	0.44
1:A:162:ALA:O	1:A:166:VAL:HG13	2.18	0.43
1:A:39:ASP:OD1	1:A:41:ASN:N	2.38	0.43
1:A:348:GLY:N	1:A:349:PRO:CD	2.81	0.43
1:A:94:GLU:OE1	3:A:2016:HOH:O	2.22	0.42
1:B:26:GLN:HB3	1:B:29:GLU:HB3	2.01	0.41
1:B:27:ASP:O	1:B:30:VAL:HG12	2.20	0.41
1:B:124:GLY:HA2	1:B:161:ILE:HD12	2.03	0.41
1:B:348:GLY:N	1:B:349:PRO:CD	2.84	0.41
1:B:116:PRO:HA	1:B:119:LEU:HD23	2.03	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	410/418 (98%)	399 (97%)	11 (3%)	0	100	100
1	B	405/418 (97%)	391 (96%)	13 (3%)	1 (0%)	47	71
All	All	815/836 (98%)	790 (97%)	24 (3%)	1 (0%)	51	75

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	235	TYR

### 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	324/329 (98%)	323 (100%)	1 (0%)	92	98
1	B	320/329 (97%)	314 (98%)	6 (2%)	57	79
All	All	644/658 (98%)	637 (99%)	7 (1%)	73	88

All (7) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	94	GLU
1	B	139	VAL
1	B	166	VAL
1	B	232	LEU
1	B	233	VAL
1	B	328	LEU
1	B	405	GLU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (1) such sidechains are listed below:

Mol	Chain	Res	Type
1	B	59	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](#)

4 ligands are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. 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  $|Z| > 2$  is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z  > 2$	Counts	RMSZ	$\# Z  > 2$
2	SCN	A	1420	-	1,2,2	0.89	0	0,1,1	0.00	-
2	SCN	A	1422	-	1,2,2	0.83	0	0,1,1	0.00	-
2	SCN	A	1421	-	1,2,2	0.88	0	0,1,1	0.00	-
2	SCN	A	1419	-	1,2,2	0.80	0	0,1,1	0.00	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	1419	SCN	1	0

## 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, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	A	412/418 (98%)	0.16	0 <b>100</b> <b>100</b>	42, 63, 93, 126	0
1	B	407/418 (97%)	1.05	86 (21%) <b>1</b> <b>0</b>	53, 96, 165, 208	0
All	All	819/836 (97%)	0.60	86 (10%) <b>6</b> <b>4</b>	42, 75, 153, 208	0

All (86) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	32	ILE	9.8
1	B	69	HIS	8.9
1	B	38	ALA	8.4
1	B	18	LEU	8.0
1	B	73	VAL	8.0
1	B	71	ALA	7.4
1	B	12	SER	7.0
1	B	232	LEU	7.0
1	B	65	VAL	6.8
1	B	37	GLY	6.7
1	B	225	ILE	6.3
1	B	50	PRO	6.1
1	B	39	ASP	5.9
1	B	63	VAL	5.9
1	B	15	GLY	5.6
1	B	17	LYS	5.5
1	B	40	VAL	5.5
1	B	67	LEU	5.5
1	B	66	LEU	5.4
1	B	22	ALA	5.3
1	B	244	THR	5.0
1	B	70	GLY	4.9
1	B	51	LEU	4.9
1	B	75	ALA	4.8

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>	<b>RSRZ</b>
1	B	226	HIS	4.8
1	B	220	GLN	4.6
1	B	239	THR	4.4
1	B	25	GLY	4.4
1	B	251	GLU	4.4
1	B	246	GLY	4.4
1	B	243	LEU	4.4
1	B	265	ALA	4.4
1	B	247	MET	4.1
1	B	36	ASN	4.1
1	B	34	MET	3.8
1	B	98	VAL	3.7
1	B	29	GLU	3.6
1	B	229	GLN	3.6
1	B	72	ASP	3.6
1	B	28	ASP	3.5
1	B	252	LEU	3.5
1	B	14	LEU	3.4
1	B	21	ALA	3.4
1	B	13	ASP	3.4
1	B	249	VAL	3.4
1	B	268	LEU	3.3
1	B	54	ALA	3.3
1	B	43	ALA	3.3
1	B	222	GLY	3.3
1	B	272	ILE	3.3
1	B	16	ARG	3.3
1	B	230	ASN	3.3
1	B	227	TYR	3.2
1	B	241	LYS	3.2
1	B	267	LEU	3.2
1	B	55	ALA	3.1
1	B	235	TYR	3.0
1	B	68	LYS	3.0
1	B	19	LEU	2.9
1	B	42	ALA	2.9
1	B	240	GLU	2.9
1	B	100	LEU	2.9
1	B	238	VAL	2.8
1	B	53	LEU	2.7
1	B	269	LEU	2.7
1	B	62	ILE	2.5

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Mol	Chain	Res	Type	RSRZ
1	B	31	ARG	2.5
1	B	104	ALA	2.5
1	B	228	SER	2.5
1	B	60	LEU	2.5
1	B	41	ASN	2.5
1	B	26	GLN	2.4
1	B	48	THR	2.4
1	B	214	ILE	2.4
1	B	414	MET	2.4
1	B	237	PRO	2.4
1	B	35	ALA	2.4
1	B	96	VAL	2.4
1	B	102	ASN	2.4
1	B	221	LEU	2.4
1	B	27	ASP	2.3
1	B	103	GLY	2.3
1	B	33	LEU	2.3
1	B	357	ALA	2.3
1	B	128	ILE	2.2
1	B	331	PRO	2.2

## 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](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
2	SCN	A	1420	3/3	0.58	0.35	112,112,113,113	0
2	SCN	A	1421	3/3	0.71	0.31	100,100,100,101	0
2	SCN	A	1419	3/3	0.75	0.34	77,77,78,80	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
2	SCN	A	1422	3/3	0.92	0.22	87,87,87,87	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.