Full wwPDB X-ray Structure Validation Report ⓘ

May 23, 2020 – 04:26 am BST

PDB ID	:	5LEE
Title	:	Crystal structure of DARPin-DARPin rigid fusion, variant DDD_D12_12_D12_12_D12
Authors	:	Batyuk, A.; Wu, Y.; Mittl, P.R.; Plueckthun, A.
Deposited on	:	2016-06-29
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:

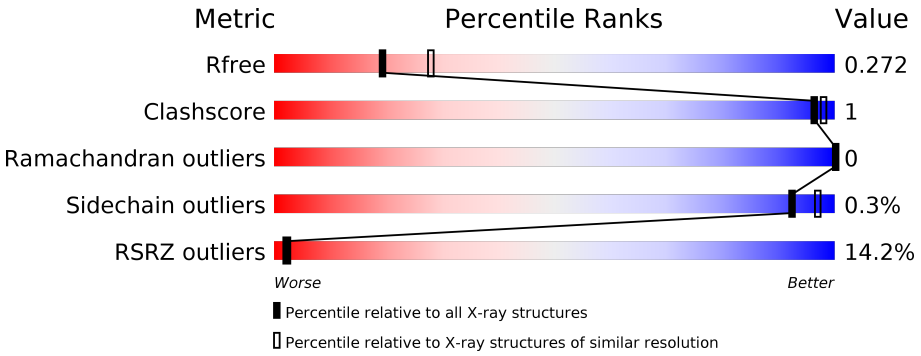
MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.13
EDS	:	2.11
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.11

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 2.40 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	3907 (2.40-2.40)
Clashscore	141614	4398 (2.40-2.40)
Ramachandran outliers	138981	4318 (2.40-2.40)
Sidechain outliers	138945	4319 (2.40-2.40)
RSRZ outliers	127900	3811 (2.40-2.40)

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 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 <=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	485	14% 95%

2 Entry composition (i)

There is only 1 type of molecule in this entry. The entry contains 7150 atoms, of which 3566 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 DDD_D12_12_D12_12_D12.

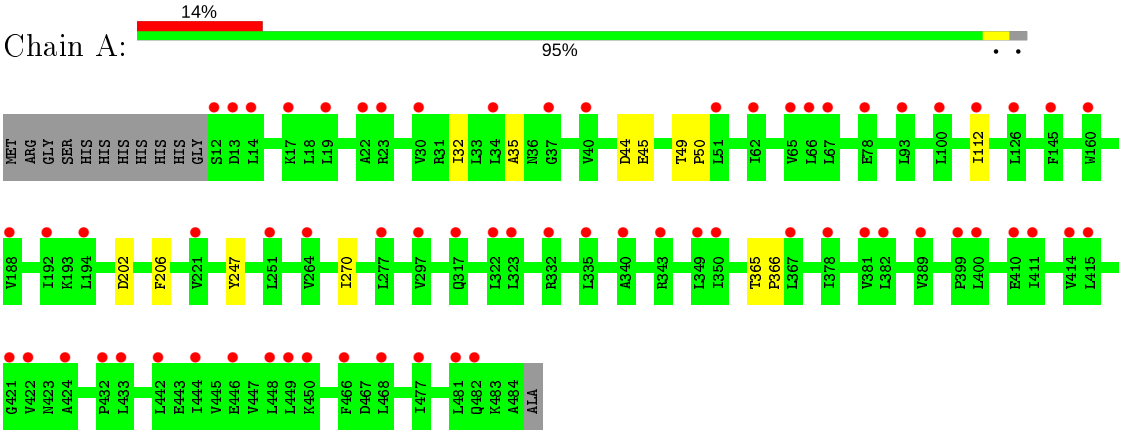
Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
			Total	C	H	N	O	S			
1	A	473	7150	2258	3566	638	685	3	0	0	0

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 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: DDD_D12_12_D12_12_D12

Chain A:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 32 2 1	Depositor
Cell constants a, b, c, α, β, γ	69.26Å 69.26Å 230.49Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	47.28 – 2.40 47.28 – 2.40	Depositor EDS
% Data completeness (in resolution range)	96.7 (47.28-2.40) 97.1 (47.28-2.40)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	0.95 (at 2.39Å)	Xtriage
Refinement program	PHENIX (dev_2400)	Depositor
R, R_{free}	0.249 , 0.274 0.249 , 0.272	Depositor DCC
R_{free} test set	1258 reflections (4.99%)	wwPDB-VP
Wilson B-factor (Å^2)	93.4	Xtriage
Anisotropy	0.326	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.37 , 86.9	EDS
L-test for twinning[2]	$< \|L\| > = 0.50$, $< L^2 > = 0.33$	Xtriage
Estimated twinning fraction	0.025 for -h,-k,l	Xtriage
F_o,F_c correlation	0.96	EDS
Total number of atoms	7150	wwPDB-VP
Average B, all atoms (Å^2)	149.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 16.94% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ 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	0.23	0/3646	0.38	0/4953

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

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	3584	3566	3577	7	1
All	All	3584	3566	3577	7	1

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 (7) 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:44:ASP:OD1	1:A:45:GLU:N	2.31	0.64
1:A:32:ILE:O	1:A:35:ALA:N	2.44	0.51
1:A:202:ASP:OD1	1:A:206:PHE:N	2.51	0.43
1:A:270:ILE:HG22	1:A:270:ILE:O	2.18	0.43
1:A:365:THR:HB	1:A:366:PRO:HD2	2.00	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:49:THR:HB	1:A:50:PRO:HD2	2.02	0.42
1:A:112:ILE:O	1:A:112:ILE:HG22	2.21	0.41

All (1) 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)
1:A:32:ILE:CD1	1:A:32:ILE:CD1[5_554]	1.93	0.27

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	471/485 (97%)	452 (96%)	19 (4%)	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	361/370 (98%)	360 (100%)	1 (0%)	92 97

All (1) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	247	TYR

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

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

There are no carbohydrates in this entry.

5.6 Ligand geometry

There are no ligands in this entry.

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

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^{th} 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	473/485 (97%)	0.96	67 (14%) 2 2	85, 128, 198, 232	0

All (67) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	433	LEU	5.7
1	A	481	LEU	5.4
1	A	13	ASP	5.3
1	A	19	LEU	4.6
1	A	389	VAL	4.4
1	A	12	SER	4.3
1	A	367	LEU	4.2
1	A	400	LEU	4.1
1	A	468	LEU	4.1
1	A	448	LEU	4.0
1	A	382	LEU	3.9
1	A	446	GLU	3.7
1	A	381	VAL	3.4
1	A	340	ALA	3.4
1	A	399	PRO	3.3
1	A	415	LEU	3.1
1	A	432	PRO	3.1
1	A	335	LEU	3.1
1	A	62	ILE	3.0
1	A	449	LEU	3.0
1	A	65	VAL	3.0
1	A	421	GLY	3.0
1	A	411	ILE	2.9
1	A	22	ALA	2.9
1	A	93	LEU	2.9
1	A	477	ILE	2.8
1	A	442	LEU	2.8

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Mol	Chain	Res	Type	RSRZ
1	A	188	VAL	2.8
1	A	34	LEU	2.7
1	A	482	GLN	2.7
1	A	23	ARG	2.7
1	A	317	GLN	2.7
1	A	349	LEU	2.7
1	A	194	LEU	2.6
1	A	160	TRP	2.5
1	A	466	PHE	2.5
1	A	323	LEU	2.5
1	A	332	ARG	2.5
1	A	67	LEU	2.5
1	A	192	ILE	2.5
1	A	40	VAL	2.4
1	A	14	LEU	2.4
1	A	17	LYS	2.4
1	A	37	GLY	2.4
1	A	424	ALA	2.4
1	A	78	GLU	2.4
1	A	264	VAL	2.3
1	A	343	ARG	2.3
1	A	450	LYS	2.3
1	A	378	ILE	2.3
1	A	422	VAL	2.3
1	A	251	LEU	2.3
1	A	297	VAL	2.3
1	A	444	ILE	2.3
1	A	112	ILE	2.2
1	A	221	VAL	2.2
1	A	410	GLU	2.2
1	A	66	LEU	2.2
1	A	30	VAL	2.1
1	A	100	LEU	2.1
1	A	51	LEU	2.1
1	A	350	ILE	2.1
1	A	322	LEU	2.1
1	A	414	VAL	2.1
1	A	145	PHE	2.1
1	A	277	LEU	2.1
1	A	126	LEU	2.0

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.