Full wwPDB X-ray Structure Validation Report (i)

Nov 15, 2021 – 01:02 pm GMT

PDB ID	:	7B4V
Title	:	Broadly neutralizing DARPin bnD.2 in complex with the HIV-1 envelope variable loop 3 crown mimetic peptide V3-IF (BG505)
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Deposited on	:	2020-12-02
Resolution	:	1.40 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 (i) symbol.

The following versions of software and data (see references (1)) were used in the production of this report:

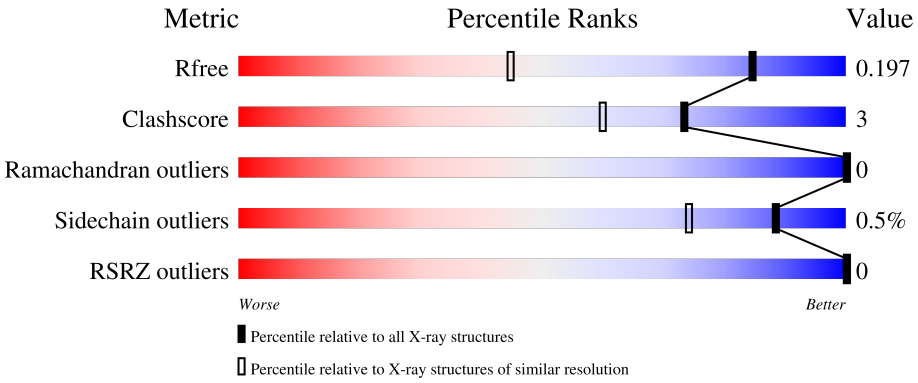
MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.13
EDS	:	2.23.2
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0267
CCP4	:	7.1.010 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.23.2

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 1.40 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	1714 (1.40-1.40)
Clashscore	141614	1812 (1.40-1.40)
Ramachandran outliers	138981	1763 (1.40-1.40)
Sidechain outliers	138945	1762 (1.40-1.40)
RSRZ outliers	127900	1674 (1.40-1.40)

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 of 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	132	91% 5% • •
1	C	132	91% 5% 5%
2	B	15	93% 7%
2	D	15	100%

2 Entry composition (i)

There are 5 unique types of molecules in this entry. The entry contains 4873 atoms, of which 2258 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 Broadly neutralizing DARPin bnD.2.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	C	126	Total	C	H	N	O	S	0	12	0
			1953	613	981	168	190	1			
1	A	128	Total	C	H	N	O	S	0	16	0
			2048	640	1033	176	198	1			

- Molecule 2 is a protein called HIV-1 envelope variable loop 3 crown mimetic peptide V3-IF (BG505).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	15	Total	C	H	N	O	0	2	0
			249	81	128	21	19			
2	D	15	Total	C	H	N	O	0	0	0
			229	75	116	20	18			

- Molecule 3 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	C	2	Total	Cl	0	0
			2	2		
3	A	3	Total	Cl	0	0
			3	3		

- Molecule 4 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	C	2	Total	Mg	0	0
			2	2		
4	A	1	Total	Mg	0	0
			1	1		
4	B	1	Total	Mg	0	0
			1	1		

- Molecule 5 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	C	175	Total O 175 175	0	0
5	A	163	Total O 163 163	0	0
5	B	22	Total O 22 22	0	0
5	D	25	Total O 25 25	0	0

3 Residue-property plots (i)

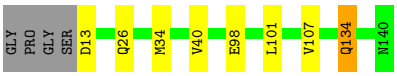
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. 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: Broadly neutralizing DARPin bnD.2

Chain C:

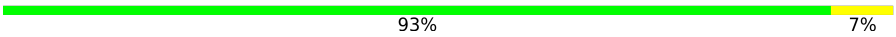
• Molecule 1: Broadly neutralizing DARPin bnD.2

Chain A:



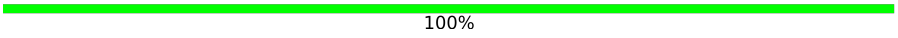
• Molecule 2: HIV-1 envelope variable loop 3 crown mimetic peptide V3-IF (BG505)

Chain B:



• Molecule 2: HIV-1 envelope variable loop 3 crown mimetic peptide V3-IF (BG505)

Chain D:



There are no outlier residues recorded for this chain.

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	50.63Å 69.34Å 69.92Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	49.23 – 1.40 49.23 – 1.40	Depositor EDS
% Data completeness (in resolution range)	100.0 (49.23-1.40) 100.0 (49.23-1.40)	Depositor EDS
R_{merge}	0.16	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.64 (at 1.40Å)	Xtriage
Refinement program	PHENIX 1.10_2155	Depositor
R, R_{free}	0.165 , 0.196 0.165 , 0.197	Depositor DCC
R_{free} test set	2471 reflections (5.02%)	wwPDB-VP
Wilson B-factor (Å^2)	14.2	Xtriage
Anisotropy	0.421	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	(Not available) , (Not available)	EDS
L-test for twinning[2]	$< \|L\| > = 0.46$, $< L^2 > = 0.29$	Xtriage
Estimated twinning fraction	0.028 for -h,l,k	Xtriage
F_o,F_c correlation	0.97	EDS
Total number of atoms	4873	wwPDB-VP
Average B, all atoms (Å^2)	22.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 10.07% 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

Bond lengths and bond angles in the following residue types are not validated in this section: MG, CL, DPR

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	0/1105	0.46	0/1500
1	C	0.26	0/1030	0.48	0/1402
2	B	0.32	0/120	0.57	0/159
2	D	0.33	0/108	0.46	0/142
All	All	0.27	0/2363	0.48	0/3203

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	1015	1033	952	8	0
1	C	972	981	925	5	0
2	B	121	128	124	1	0
2	D	113	116	116	0	0
3	A	3	0	0	1	0
3	C	2	0	0	0	0
4	A	1	0	0	0	0
4	B	1	0	0	0	0
4	C	2	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
5	A	163	0	0	6	4
5	B	22	0	0	1	2
5	C	175	0	0	4	5
5	D	25	0	0	1	0
All	All	2615	2258	2117	15	7

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 3.

All (15) 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:26[B]:GLN:OE1	5:A:301:HOH:O	1.89	0.91
1:A:26[A]:GLN:NE2	5:A:303:HOH:O	2.03	0.90
1:A:134[B]:GLN:OE1	5:A:302:HOH:O	1.93	0.86
1:A:134[B]:GLN:NE2	5:A:305:HOH:O	2.09	0.85
1:C:27:ASP:OD1	5:C:301:HOH:O	2.00	0.80
2:B:4:ARG:NH2	5:B:201:HOH:O	2.19	0.76
3:A:201:CL:CL	5:D:101:HOH:O	2.42	0.73
1:A:98:GLU:OE2	5:A:304:HOH:O	2.06	0.73
1:C:16[A]:LYS:NZ	5:C:304:HOH:O	2.25	0.69
1:C:123:ASP:OD1	5:C:302:HOH:O	2.11	0.68
1:C:13:ASP:N	5:C:306:HOH:O	2.31	0.64
1:A:34:MET:SD	1:A:40[B]:VAL:HG12	2.53	0.48
1:C:96:ILE:HA	1:C:99[B]:VAL:HG12	1.96	0.47
1:A:101[A]:LEU:CD2	1:A:107:VAL:HG22	2.49	0.42
1:A:13:ASP:OD1	5:A:306:HOH:O	2.22	0.41

All (7) 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)
5:C:346:HOH:O	5:A:431:HOH:O[2_455]	1.88	0.32
5:A:448:HOH:O	5:B:221:HOH:O[3_554]	1.99	0.21
5:C:334:HOH:O	5:B:218:HOH:O[2_455]	2.03	0.17
5:A:457:HOH:O	5:A:459:HOH:O[3_544]	2.04	0.16
5:C:468:HOH:O	5:A:319:HOH:O[2_555]	2.07	0.13
5:C:458:HOH:O	5:C:475:HOH:O[4_545]	2.12	0.08
5:C:340:HOH:O	5:C:458:HOH:O[4_445]	2.14	0.06

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	142/132 (108%)	139 (98%)	3 (2%)	0	100	100
1	C	136/132 (103%)	136 (100%)	0	0	100	100
2	B	14/15 (93%)	12 (86%)	2 (14%)	0	100	100
2	D	12/15 (80%)	12 (100%)	0	0	100	100
All	All	304/294 (103%)	299 (98%)	5 (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	111/97 (114%)	109 (98%)	2 (2%)	59	28
1	C	103/97 (106%)	103 (100%)	0	100	100
2	B	11/10 (110%)	11 (100%)	0	100	100
2	D	10/10 (100%)	10 (100%)	0	100	100
All	All	235/214 (110%)	233 (99%)	2 (1%)	88	58

All (2) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	134[A]	GLN
1	A	134[B]	GLN

Sometimes 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

2 non-standard protein/DNA/RNA residues are modelled in this entry.

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.

No monomer is involved in short contacts.

5.5 Carbohydrates

There are no monosaccharides in this entry.

5.6 Ligand geometry

Of 9 ligands modelled in this entry, 9 are monoatomic - leaving 0 for Mogul analysis.

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.

No monomer is involved in short contacts.

5.7 Other polymers

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^{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	128/132 (96%)	-0.40	0	100	100	12, 18, 39, 53	0
1	C	126/132 (95%)	-0.42	0	100	100	11, 16, 38, 53	0
2	B	14/15 (93%)	-0.33	0	100	100	13, 17, 23, 34	0
2	D	14/15 (93%)	-0.52	0	100	100	12, 14, 17, 21	0
All	All	282/294 (95%)	-0.41	0	100	100	11, 17, 38, 53	0

There are no RSRZ outliers to report.

6.2 Non-standard residues in protein, DNA, RNA chains

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^{th} 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(Å^2)	Q<0.9
2	DPR	B	14	7/8	0.95	0.07	12,14,16,16	0
2	DPR	D	14	7/8	0.95	0.07	12,16,20,20	0

6.3 Carbohydrates

There are no monosaccharides in this entry.

6.4 Ligands

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^{th} 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(Å^2)	Q<0.9
3	CL	A	201	1/1	0.98	0.04	23,23,23,23	0
4	MG	C	203	1/1	0.98	0.07	23,23,23,23	1
4	MG	B	101	1/1	0.98	0.10	18,18,18,18	1
3	CL	A	203	1/1	0.99	0.04	23,23,23,23	0
3	CL	C	202	1/1	0.99	0.05	23,23,23,23	0
4	MG	C	204	1/1	0.99	0.07	14,14,14,14	1
4	MG	A	204	1/1	0.99	0.05	13,13,13,13	1
3	CL	C	201	1/1	0.99	0.04	20,20,20,20	0
3	CL	A	202	1/1	1.00	0.08	16,16,16,16	0

6.5 Other polymers (i)

There are no such residues in this entry.