Full wwPDB X-ray Structure Validation Report ⓘ

Jun 27, 2022 – 01:05 pm BST

PDB ID	:	7Z71
Title	:	Crystal structure of p63 DBD in complex with darpin C14
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Deposited on	:	2022-03-14
Resolution	:	1.85 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 types of validation reports are described at http://www.wwpdb.org/validation/2017/FAQs#types.

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

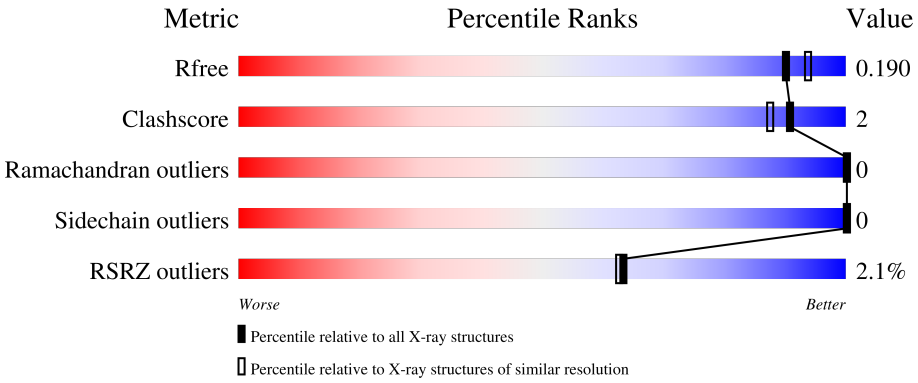
MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.13
EDS	:	2.29
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0267
CCP4	:	7.1.010 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.29

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 1.85 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	2469 (1.86-1.86)
Clashscore	141614	2625 (1.86-1.86)
Ramachandran outliers	138981	2592 (1.86-1.86)
Sidechain outliers	138945	2592 (1.86-1.86)
RSRZ outliers	127900	2436 (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 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	204	3% 91% 5%
1	C	204	2% 89% 7%
2	B	159	94% 5%
2	D	159	3% 92% 7%

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 6080 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 Isoform 4 of Tumor protein 63.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	196	Total	C	N	O	S	0	4	0
			1552	971	277	290	14			
1	C	189	Total	C	N	O	S	0	3	0
			1493	939	263	276	15			

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	121	GLY	-	expression tag	UNP Q9H3D4
A	122	SER	-	expression tag	UNP Q9H3D4
C	121	GLY	-	expression tag	UNP Q9H3D4
C	122	SER	-	expression tag	UNP Q9H3D4

- Molecule 2 is a protein called Darpin C14.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	157	Total	C	N	O	S	0	1	0
			1167	733	197	236	1			
2	D	157	Total	C	N	O	S	0	3	0
			1178	740	198	238	2			

- Molecule 3 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	1	Total	Zn	0	0
			1	1		
3	C	1	Total	Zn	0	0
			1	1		

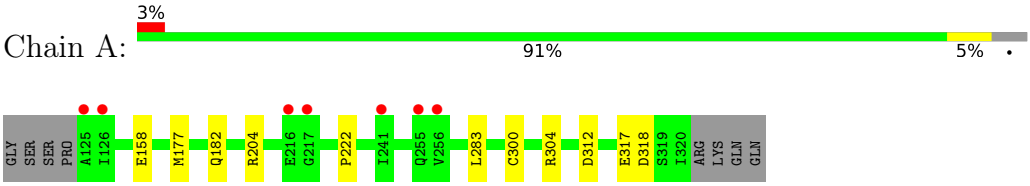
- Molecule 4 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	215	Total O 215 215	0	0
4	B	150	Total O 150 150	0	0
4	C	208	Total O 208 208	0	0
4	D	115	Total O 115 115	0	0

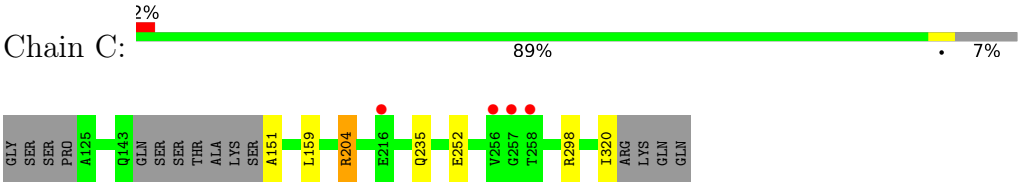
3 Residue-property plots

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.

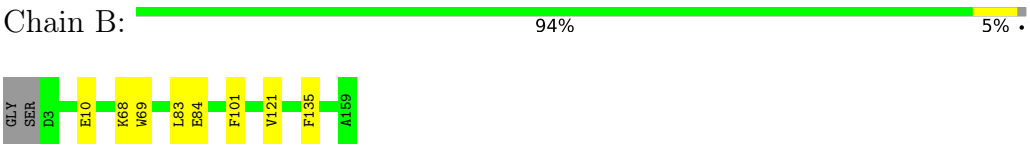
• Molecule 1: Isoform 4 of Tumor protein 63



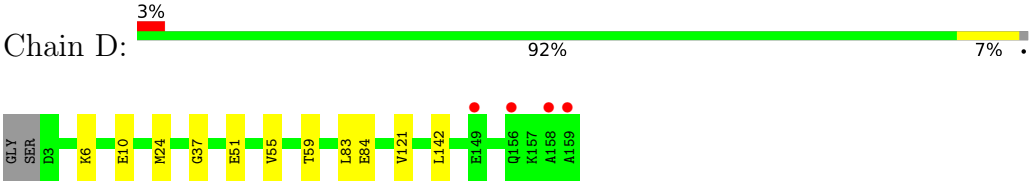
• Molecule 1: Isoform 4 of Tumor protein 63



• Molecule 2: Darpin C14



• Molecule 2: Darpin C14



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α, β, γ	53.03Å 63.93Å 65.50Å 114.46° 94.60° 104.06°	Depositor
Resolution (Å)	42.69 – 1.85 42.69 – 1.85	Depositor EDS
% Data completeness (in resolution range)	91.6 (42.69-1.85) 91.6 (42.69-1.85)	Depositor EDS
R_{merge}	0.03	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	8.58 (at 1.86Å)	Xtriage
Refinement program	REFMAC 5.8.0267	Depositor
R, R_{free}	0.142 , 0.181 0.155 , 0.190	Depositor DCC
R_{free} test set	2857 reflections (4.91%)	wwPDB-VP
Wilson B-factor (Å^2)	22.9	Xtriage
Anisotropy	0.150	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	(Not available) , (Not available)	EDS
L-test for twinning[2]	$< \|L\| > = 0.50$, $< L^2 > = 0.34$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.97	EDS
Total number of atoms	6080	wwPDB-VP
Average B, all atoms (Å^2)	27.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 7.60% 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: ZN

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	0.88	3/1597 (0.2%)	0.83	0/2170
1	C	0.95	2/1537 (0.1%)	0.84	2/2089 (0.1%)
2	B	1.00	2/1186 (0.2%)	0.75	0/1613
2	D	0.94	3/1200 (0.2%)	0.78	0/1631
All	All	0.94	10/5520 (0.2%)	0.80	2/7503 (0.0%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand.A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	C	0	1

All (10) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	84	GLU	CD-OE1	12.12	1.39	1.25
2	D	10	GLU	CD-OE1	8.62	1.35	1.25
1	C	151	ALA	C-O	7.17	1.36	1.23
2	B	10	GLU	CD-OE1	6.97	1.33	1.25
1	A	158	GLU	CD-OE2	6.38	1.32	1.25
2	D	51	GLU	CD-OE1	6.32	1.32	1.25
1	C	252	GLU	CD-OE2	5.86	1.32	1.25
2	D	84	GLU	CD-OE2	5.74	1.31	1.25
1	A	317	GLU	CD-OE1	5.34	1.31	1.25
1	A	158	GLU	CD-OE1	5.11	1.31	1.25

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	C	204	ARG	NE-CZ-NH2	-6.67	116.96	120.30
1	C	298	ARG	NE-CZ-NH2	-5.91	117.35	120.30

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	C	204	ARG	Sidechain

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	1552	0	1541	7	0
1	C	1493	0	1484	2	0
2	B	1167	0	1159	4	0
2	D	1178	0	1172	7	0
3	A	1	0	0	0	0
3	C	1	0	0	0	0
4	A	215	0	0	1	0
4	B	150	0	0	0	0
4	C	208	0	0	1	0
4	D	115	0	0	2	0
All	All	6080	0	5356	18	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 (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:C:235:GLN:OE1	4:C:501:HOH:O	2.01	0.77
1:A:304[B]:ARG:CZ	1:A:312:ASP:OD2	2.34	0.76
1:A:304[B]:ARG:NH2	1:A:312:ASP:OD2	2.25	0.69
1:A:182:GLN:OE1	4:A:501:HOH:O	2.14	0.65
2:D:24[A]:MET:HE1	2:D:55:VAL:HG12	1.78	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:6:LYS:NZ	4:D:201:HOH:O	2.31	0.60
2:B:68:LYS:HE2	2:B:69:TRP:CZ2	2.40	0.57
2:D:24[A]:MET:CE	2:D:55:VAL:HG12	2.39	0.52
2:D:142:LEU:HD11	4:D:203:HOH:O	2.11	0.49
1:A:318:ASP:HA	2:B:135:PHE:HE2	1.77	0.49
2:B:83:LEU:HD11	2:B:121:VAL:HG21	1.98	0.44
2:D:83:LEU:HD11	2:D:121:VAL:HG21	2.00	0.44
1:A:177:MET:HE3	1:A:177:MET:HA	1.99	0.44
1:A:283:LEU:HB3	1:A:300[A]:CYS:SG	2.57	0.44
2:D:59:THR:O	2:D:59:THR:HG22	2.18	0.43
1:A:204:ARG:HD3	1:A:222:PRO:O	2.18	0.43
2:B:101:PHE:CD1	2:D:37:GLY:HA2	2.55	0.41
1:C:159:LEU:HD21	1:C:320:ILE:HD11	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	198/204 (97%)	195 (98%)	3 (2%)	0	100	100
1	C	188/204 (92%)	186 (99%)	2 (1%)	0	100	100
2	B	156/159 (98%)	154 (99%)	2 (1%)	0	100	100
2	D	158/159 (99%)	156 (99%)	2 (1%)	0	100	100
All	All	700/726 (96%)	691 (99%)	9 (1%)	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	177/180 (98%)	177 (100%)	0	100	100
1	C	170/180 (94%)	170 (100%)	0	100	100
2	B	121/121 (100%)	121 (100%)	0	100	100
2	D	123/121 (102%)	123 (100%)	0	100	100
All	All	591/602 (98%)	591 (100%)	0	100	100

There are no protein residues with a non-rotameric sidechain to report.

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

There are no non-standard protein/DNA/RNA residues in this entry.

5.5 Carbohydrates

There are no monosaccharides in this entry.

5.6 Ligand geometry

Of 2 ligands modelled in this entry, 2 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 (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^{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	196/204 (96%)	-0.19	7 (3%) 42 40	16, 23, 51, 73	0
1	C	189/204 (92%)	-0.31	4 (2%) 63 63	16, 23, 44, 64	0
2	B	157/159 (98%)	-0.30	0 100 100	16, 22, 38, 46	0
2	D	157/159 (98%)	-0.16	4 (2%) 57 56	17, 25, 43, 55	0
All	All	699/726 (96%)	-0.24	15 (2%) 63 63	16, 23, 44, 73	0

All (15) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	125	ALA	4.9
1	C	257	GLY	4.6
1	A	256	VAL	4.3
1	C	216	GLU	3.8
1	A	217	GLY	3.8
1	C	256	VAL	3.3
2	D	159	ALA	3.1
1	A	126	ILE	2.9
2	D	156	GLN	2.9
2	D	158	ALA	2.7
1	A	241	ILE	2.3
1	A	216	GLU	2.3
1	C	258	THR	2.2
2	D	149	GLU	2.2
1	A	255	GLN	2.1

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

There are no non-standard protein/DNA/RNA residues in this entry.

6.3 Carbohydrates (i)

There are no monosaccharides 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^{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	ZN	A	401	1/1	0.99	0.06	26,26,26,26	0
3	ZN	C	401	1/1	1.00	0.04	21,21,21,21	0

6.5 Other polymers (i)

There are no such residues in this entry.