wwPDB/EMDataBank EM Map/Model Validation Summary Report (i)

Mar 31, 2018 – 07:27 AM EDT

PDB ID	:	6C9K
EMDB ID:	:	EMD-7437
Title	:	Single-Particle reconstruction of DARP14 - A designed protein scaffold displaying 17kDa DARPin proteins
Authors	:	Gonen, S.; Liu, Y.; Yeates, T.O.; Gonen, T.
Deposited on	:	2018-01-26
Resolution	:	3.49 Å(reported)

This is a wwPDB/EMDataBank EM Map/Model Validation Summary Report for a publicly released PDB/EMDB entry.

We welcome your comments at *validation@mail.wwpdb.org*
A user guide is available at
https://www.wwpdb.org/validation/2017/EMValidationReportHelp
with specific help available everywhere you see the (i) symbol.

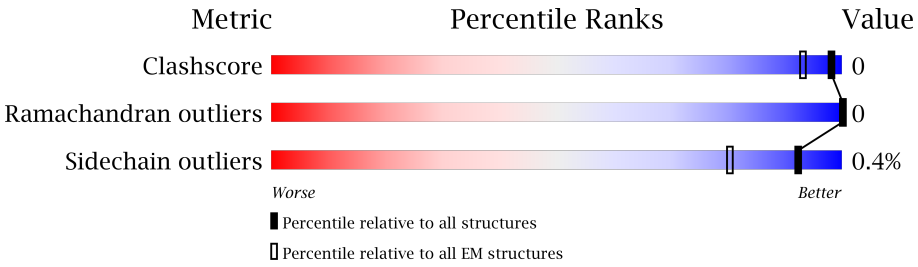
MolProbity	:	4.02b-467
Percentile statistics	:	20171227.v01 (using entries in the PDB archive December 27th 2017)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et. al. (1996)
Validation Pipeline (wwPDB-VP)	:	rb-20031021

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
ELECTRON MICROSCOPY

The reported resolution of this entry is 3.49 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)	EM structures (#Entries)
Clashscore	136327	1886
Ramachandran outliers	132723	1663
Sidechain outliers	132532	1531

The table below summarises the geometric issues observed across the polymeric chains. The red, orange, yellow and green segments on the 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 <=5%

Mol	Chain	Length	Quality of chain
1	A	319	91% · 8%
1	B	319	90% · 8%
1	C	319	91% · 9%
1	D	319	92% · 8%
1	I	319	91% · 8%
1	J	319	90% · 8%
1	K	319	91% 9%
1	L	319	92% · 8%
1	Q	319	91% · 8%

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Mol	Chain	Length	Quality of chain
1	R	319	90% 8%
1	S	319	91% 9%
1	T	319	91% 8%
2	E	131	88% 10%
2	F	131	88% 10%
2	G	131	88% 10%
2	H	131	87% 11%
2	M	131	88% 10%
2	N	131	88% 10%
2	O	131	88% 10%
2	P	131	87% 11%
2	U	131	88% 10%
2	V	131	88% 10%
2	W	131	88% 10%
2	X	131	87% 11%

2 Entry composition (i)

There are 2 unique types of molecules in this entry. The entry contains 37632 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, 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 DARP14 - Subunit A with DARPin.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	293	Total	C	N	O	S	0	0
			2255	1428	385	436	6		
1	B	292	Total	C	N	O	S	0	0
			2249	1425	384	434	6		
1	C	291	Total	C	N	O	S	0	0
			2241	1419	383	433	6		
1	D	294	Total	C	N	O	S	0	0
			2264	1434	387	437	6		
1	I	293	Total	C	N	O	S	0	0
			2255	1428	385	436	6		
1	J	292	Total	C	N	O	S	0	0
			2249	1425	384	434	6		
1	K	291	Total	C	N	O	S	0	0
			2241	1419	383	433	6		
1	L	294	Total	C	N	O	S	0	0
			2264	1434	387	437	6		
1	Q	293	Total	C	N	O	S	0	0
			2255	1428	385	436	6		
1	R	292	Total	C	N	O	S	0	0
			2249	1425	384	434	6		
1	S	291	Total	C	N	O	S	0	0
			2241	1419	383	433	6		
1	T	294	Total	C	N	O	S	0	0
			2264	1434	387	437	6		

- Molecule 2 is a protein called DARP14 - Subunit B.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	E	118	Total	C	N	O	S	0	0
			885	552	158	172	3		
2	F	118	Total	C	N	O	S	0	0
			885	552	158	172	3		
2	G	118	Total	C	N	O	S	0	0
			885	552	158	172	3		

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Mol	Chain	Residues	Atoms					AltConf	Trace
2	H	117	Total	C	N	O	S	0	0
			880	549	157	171	3		
2	M	118	Total	C	N	O	S	0	0
			885	552	158	172	3		
2	N	118	Total	C	N	O	S	0	0
			885	552	158	172	3		
2	O	118	Total	C	N	O	S	0	0
			885	552	158	172	3		
2	P	117	Total	C	N	O	S	0	0
			880	549	157	171	3		
2	U	118	Total	C	N	O	S	0	0
			885	552	158	172	3		
2	V	118	Total	C	N	O	S	0	0
			885	552	158	172	3		
2	W	118	Total	C	N	O	S	0	0
			885	552	158	172	3		
2	X	117	Total	C	N	O	S	0	0
			880	549	157	171	3		

There are 192 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
E	27	LYS	ALA	conflict	UNP Q9I2D8
E	74	ILE	ALA	conflict	UNP Q9I2D8
E	78	THR	GLN	conflict	UNP Q9I2D8
E	79	LEU	ALA	conflict	UNP Q9I2D8
E	82	ALA	GLU	conflict	UNP Q9I2D8
E	86	ALA	GLU	conflict	UNP Q9I2D8
E	90	GLU	GLY	conflict	UNP Q9I2D8
E	112	LEU	ALA	conflict	UNP Q9I2D8
E	124	LEU	-	expression tag	UNP Q9I2D8
E	125	GLU	-	expression tag	UNP Q9I2D8
E	126	HIS	-	expression tag	UNP Q9I2D8
E	127	HIS	-	expression tag	UNP Q9I2D8
E	128	HIS	-	expression tag	UNP Q9I2D8
E	129	HIS	-	expression tag	UNP Q9I2D8
E	130	HIS	-	expression tag	UNP Q9I2D8
E	131	HIS	-	expression tag	UNP Q9I2D8
F	27	LYS	ALA	conflict	UNP Q9I2D8
F	74	ILE	ALA	conflict	UNP Q9I2D8
F	78	THR	GLN	conflict	UNP Q9I2D8
F	79	LEU	ALA	conflict	UNP Q9I2D8
F	82	ALA	GLU	conflict	UNP Q9I2D8

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Chain	Residue	Modelled	Actual	Comment	Reference
F	86	ALA	GLU	conflict	UNP Q9I2D8
F	90	GLU	GLY	conflict	UNP Q9I2D8
F	112	LEU	ALA	conflict	UNP Q9I2D8
F	124	LEU	-	expression tag	UNP Q9I2D8
F	125	GLU	-	expression tag	UNP Q9I2D8
F	126	HIS	-	expression tag	UNP Q9I2D8
F	127	HIS	-	expression tag	UNP Q9I2D8
F	128	HIS	-	expression tag	UNP Q9I2D8
F	129	HIS	-	expression tag	UNP Q9I2D8
F	130	HIS	-	expression tag	UNP Q9I2D8
F	131	HIS	-	expression tag	UNP Q9I2D8
G	27	LYS	ALA	conflict	UNP Q9I2D8
G	74	ILE	ALA	conflict	UNP Q9I2D8
G	78	THR	GLN	conflict	UNP Q9I2D8
G	79	LEU	ALA	conflict	UNP Q9I2D8
G	82	ALA	GLU	conflict	UNP Q9I2D8
G	86	ALA	GLU	conflict	UNP Q9I2D8
G	90	GLU	GLY	conflict	UNP Q9I2D8
G	112	LEU	ALA	conflict	UNP Q9I2D8
G	124	LEU	-	expression tag	UNP Q9I2D8
G	125	GLU	-	expression tag	UNP Q9I2D8
G	126	HIS	-	expression tag	UNP Q9I2D8
G	127	HIS	-	expression tag	UNP Q9I2D8
G	128	HIS	-	expression tag	UNP Q9I2D8
G	129	HIS	-	expression tag	UNP Q9I2D8
G	130	HIS	-	expression tag	UNP Q9I2D8
G	131	HIS	-	expression tag	UNP Q9I2D8
H	27	LYS	ALA	conflict	UNP Q9I2D8
H	74	ILE	ALA	conflict	UNP Q9I2D8
H	78	THR	GLN	conflict	UNP Q9I2D8
H	79	LEU	ALA	conflict	UNP Q9I2D8
H	82	ALA	GLU	conflict	UNP Q9I2D8
H	86	ALA	GLU	conflict	UNP Q9I2D8
H	90	GLU	GLY	conflict	UNP Q9I2D8
H	112	LEU	ALA	conflict	UNP Q9I2D8
H	124	LEU	-	expression tag	UNP Q9I2D8
H	125	GLU	-	expression tag	UNP Q9I2D8
H	126	HIS	-	expression tag	UNP Q9I2D8
H	127	HIS	-	expression tag	UNP Q9I2D8
H	128	HIS	-	expression tag	UNP Q9I2D8
H	129	HIS	-	expression tag	UNP Q9I2D8
H	130	HIS	-	expression tag	UNP Q9I2D8

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Chain	Residue	Modelled	Actual	Comment	Reference
H	131	HIS	-	expression tag	UNP Q9I2D8
M	27	LYS	ALA	conflict	UNP Q9I2D8
M	74	ILE	ALA	conflict	UNP Q9I2D8
M	78	THR	GLN	conflict	UNP Q9I2D8
M	79	LEU	ALA	conflict	UNP Q9I2D8
M	82	ALA	GLU	conflict	UNP Q9I2D8
M	86	ALA	GLU	conflict	UNP Q9I2D8
M	90	GLU	GLY	conflict	UNP Q9I2D8
M	112	LEU	ALA	conflict	UNP Q9I2D8
M	124	LEU	-	expression tag	UNP Q9I2D8
M	125	GLU	-	expression tag	UNP Q9I2D8
M	126	HIS	-	expression tag	UNP Q9I2D8
M	127	HIS	-	expression tag	UNP Q9I2D8
M	128	HIS	-	expression tag	UNP Q9I2D8
M	129	HIS	-	expression tag	UNP Q9I2D8
M	130	HIS	-	expression tag	UNP Q9I2D8
M	131	HIS	-	expression tag	UNP Q9I2D8
N	27	LYS	ALA	conflict	UNP Q9I2D8
N	74	ILE	ALA	conflict	UNP Q9I2D8
N	78	THR	GLN	conflict	UNP Q9I2D8
N	79	LEU	ALA	conflict	UNP Q9I2D8
N	82	ALA	GLU	conflict	UNP Q9I2D8
N	86	ALA	GLU	conflict	UNP Q9I2D8
N	90	GLU	GLY	conflict	UNP Q9I2D8
N	112	LEU	ALA	conflict	UNP Q9I2D8
N	124	LEU	-	expression tag	UNP Q9I2D8
N	125	GLU	-	expression tag	UNP Q9I2D8
N	126	HIS	-	expression tag	UNP Q9I2D8
N	127	HIS	-	expression tag	UNP Q9I2D8
N	128	HIS	-	expression tag	UNP Q9I2D8
N	129	HIS	-	expression tag	UNP Q9I2D8
N	130	HIS	-	expression tag	UNP Q9I2D8
N	131	HIS	-	expression tag	UNP Q9I2D8
O	27	LYS	ALA	conflict	UNP Q9I2D8
O	74	ILE	ALA	conflict	UNP Q9I2D8
O	78	THR	GLN	conflict	UNP Q9I2D8
O	79	LEU	ALA	conflict	UNP Q9I2D8
O	82	ALA	GLU	conflict	UNP Q9I2D8
O	86	ALA	GLU	conflict	UNP Q9I2D8
O	90	GLU	GLY	conflict	UNP Q9I2D8
O	112	LEU	ALA	conflict	UNP Q9I2D8
O	124	LEU	-	expression tag	UNP Q9I2D8

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Chain	Residue	Modelled	Actual	Comment	Reference
O	125	GLU	-	expression tag	UNP Q9I2D8
O	126	HIS	-	expression tag	UNP Q9I2D8
O	127	HIS	-	expression tag	UNP Q9I2D8
O	128	HIS	-	expression tag	UNP Q9I2D8
O	129	HIS	-	expression tag	UNP Q9I2D8
O	130	HIS	-	expression tag	UNP Q9I2D8
O	131	HIS	-	expression tag	UNP Q9I2D8
P	27	LYS	ALA	conflict	UNP Q9I2D8
P	74	ILE	ALA	conflict	UNP Q9I2D8
P	78	THR	GLN	conflict	UNP Q9I2D8
P	79	LEU	ALA	conflict	UNP Q9I2D8
P	82	ALA	GLU	conflict	UNP Q9I2D8
P	86	ALA	GLU	conflict	UNP Q9I2D8
P	90	GLU	GLY	conflict	UNP Q9I2D8
P	112	LEU	ALA	conflict	UNP Q9I2D8
P	124	LEU	-	expression tag	UNP Q9I2D8
P	125	GLU	-	expression tag	UNP Q9I2D8
P	126	HIS	-	expression tag	UNP Q9I2D8
P	127	HIS	-	expression tag	UNP Q9I2D8
P	128	HIS	-	expression tag	UNP Q9I2D8
P	129	HIS	-	expression tag	UNP Q9I2D8
P	130	HIS	-	expression tag	UNP Q9I2D8
P	131	HIS	-	expression tag	UNP Q9I2D8
U	27	LYS	ALA	conflict	UNP Q9I2D8
U	74	ILE	ALA	conflict	UNP Q9I2D8
U	78	THR	GLN	conflict	UNP Q9I2D8
U	79	LEU	ALA	conflict	UNP Q9I2D8
U	82	ALA	GLU	conflict	UNP Q9I2D8
U	86	ALA	GLU	conflict	UNP Q9I2D8
U	90	GLU	GLY	conflict	UNP Q9I2D8
U	112	LEU	ALA	conflict	UNP Q9I2D8
U	124	LEU	-	expression tag	UNP Q9I2D8
U	125	GLU	-	expression tag	UNP Q9I2D8
U	126	HIS	-	expression tag	UNP Q9I2D8
U	127	HIS	-	expression tag	UNP Q9I2D8
U	128	HIS	-	expression tag	UNP Q9I2D8
U	129	HIS	-	expression tag	UNP Q9I2D8
U	130	HIS	-	expression tag	UNP Q9I2D8
U	131	HIS	-	expression tag	UNP Q9I2D8
V	27	LYS	ALA	conflict	UNP Q9I2D8
V	74	ILE	ALA	conflict	UNP Q9I2D8
V	78	THR	GLN	conflict	UNP Q9I2D8

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Chain	Residue	Modelled	Actual	Comment	Reference
V	79	LEU	ALA	conflict	UNP Q9I2D8
V	82	ALA	GLU	conflict	UNP Q9I2D8
V	86	ALA	GLU	conflict	UNP Q9I2D8
V	90	GLU	GLY	conflict	UNP Q9I2D8
V	112	LEU	ALA	conflict	UNP Q9I2D8
V	124	LEU	-	expression tag	UNP Q9I2D8
V	125	GLU	-	expression tag	UNP Q9I2D8
V	126	HIS	-	expression tag	UNP Q9I2D8
V	127	HIS	-	expression tag	UNP Q9I2D8
V	128	HIS	-	expression tag	UNP Q9I2D8
V	129	HIS	-	expression tag	UNP Q9I2D8
V	130	HIS	-	expression tag	UNP Q9I2D8
V	131	HIS	-	expression tag	UNP Q9I2D8
W	27	LYS	ALA	conflict	UNP Q9I2D8
W	74	ILE	ALA	conflict	UNP Q9I2D8
W	78	THR	GLN	conflict	UNP Q9I2D8
W	79	LEU	ALA	conflict	UNP Q9I2D8
W	82	ALA	GLU	conflict	UNP Q9I2D8
W	86	ALA	GLU	conflict	UNP Q9I2D8
W	90	GLU	GLY	conflict	UNP Q9I2D8
W	112	LEU	ALA	conflict	UNP Q9I2D8
W	124	LEU	-	expression tag	UNP Q9I2D8
W	125	GLU	-	expression tag	UNP Q9I2D8
W	126	HIS	-	expression tag	UNP Q9I2D8
W	127	HIS	-	expression tag	UNP Q9I2D8
W	128	HIS	-	expression tag	UNP Q9I2D8
W	129	HIS	-	expression tag	UNP Q9I2D8
W	130	HIS	-	expression tag	UNP Q9I2D8
W	131	HIS	-	expression tag	UNP Q9I2D8
X	27	LYS	ALA	conflict	UNP Q9I2D8
X	74	ILE	ALA	conflict	UNP Q9I2D8
X	78	THR	GLN	conflict	UNP Q9I2D8
X	79	LEU	ALA	conflict	UNP Q9I2D8
X	82	ALA	GLU	conflict	UNP Q9I2D8
X	86	ALA	GLU	conflict	UNP Q9I2D8
X	90	GLU	GLY	conflict	UNP Q9I2D8
X	112	LEU	ALA	conflict	UNP Q9I2D8
X	124	LEU	-	expression tag	UNP Q9I2D8
X	125	GLU	-	expression tag	UNP Q9I2D8
X	126	HIS	-	expression tag	UNP Q9I2D8
X	127	HIS	-	expression tag	UNP Q9I2D8
X	128	HIS	-	expression tag	UNP Q9I2D8

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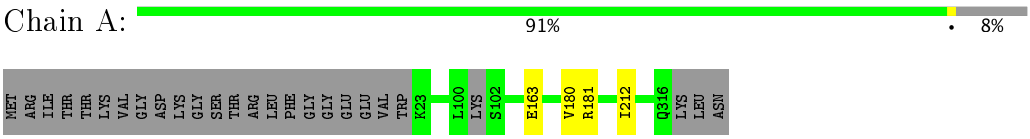
Chain	Residue	Modelled	Actual	Comment	Reference
X	129	HIS	-	expression tag	UNP Q9I2D8
X	130	HIS	-	expression tag	UNP Q9I2D8
X	131	HIS	-	expression tag	UNP Q9I2D8

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. 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. 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.

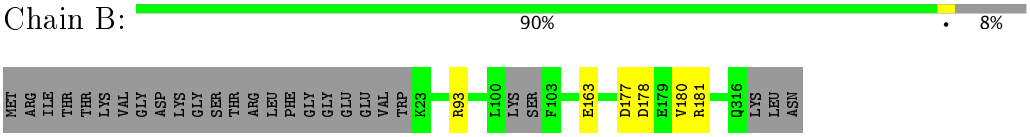
- Molecule 1: DARP14 - Subunit A with DARPin

Chain A:



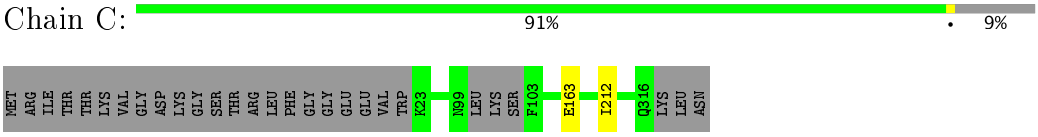
- Molecule 1: DARP14 - Subunit A with DARPin

Chain B:



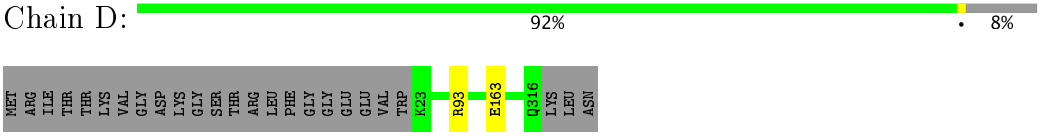
- Molecule 1: DARP14 - Subunit A with DARPin

Chain C:



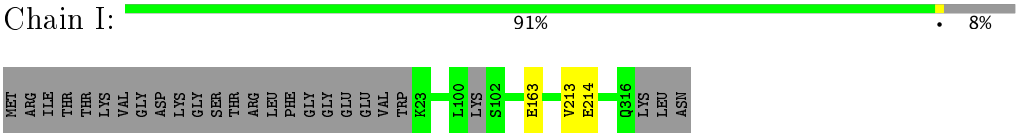
- Molecule 1: DARP14 - Subunit A with DARPin

Chain D:



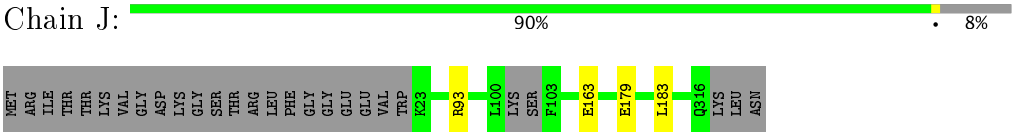
- Molecule 1: DARP14 - Subunit A with DARPin

Chain I:



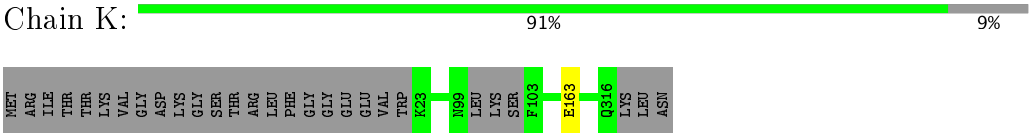
- Molecule 1: DARP14 - Subunit A with DARPin

Chain J:



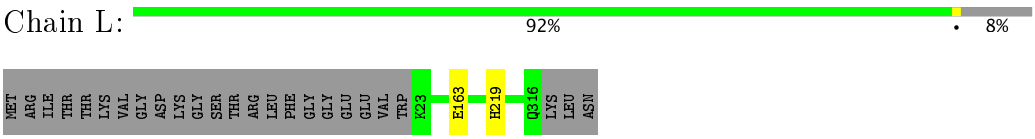
- Molecule 1: DARP14 - Subunit A with DARPin

Chain K:



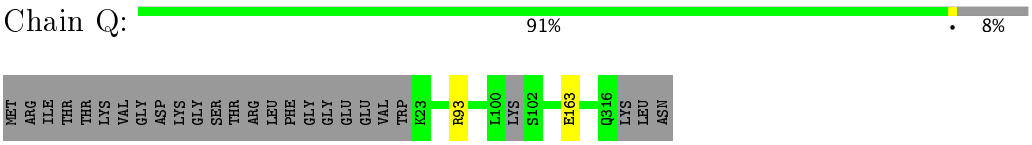
- Molecule 1: DARP14 - Subunit A with DARPin

Chain L:



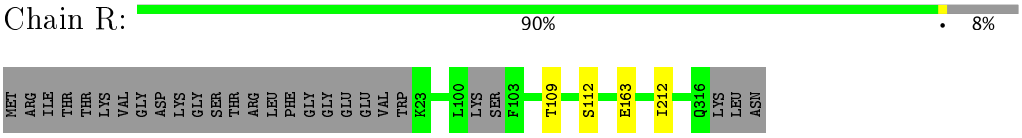
- Molecule 1: DARP14 - Subunit A with DARPin

Chain Q:



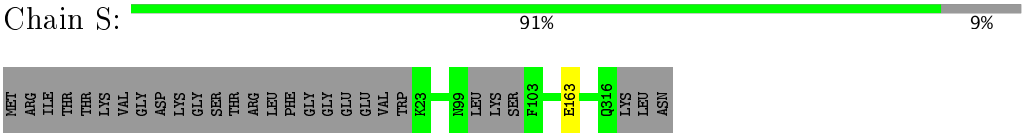
- Molecule 1: DARP14 - Subunit A with DARPin

Chain R:



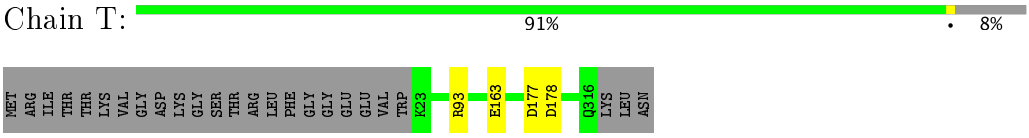
- Molecule 1: DARP14 - Subunit A with DARPin

Chain S:



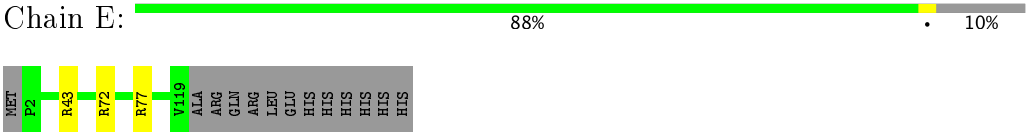
- Molecule 1: DARP14 - Subunit A with DARPin

Chain T:



- Molecule 2: DARP14 - Subunit B

Chain E:



- Molecule 2: DARP14 - Subunit B

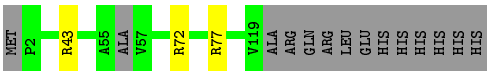
Chain F:

• Molecule 2: DARP14 - Subunit B

Chain G:

• Molecule 2: DARP14 - Subunit B

Chain H:



• Molecule 2: DARP14 - Subunit B

Chain M:

• Molecule 2: DARP14 - Subunit B

Chain N:

• Molecule 2: DARP14 - Subunit B

Chain O:

• Molecule 2: DARP14 - Subunit B

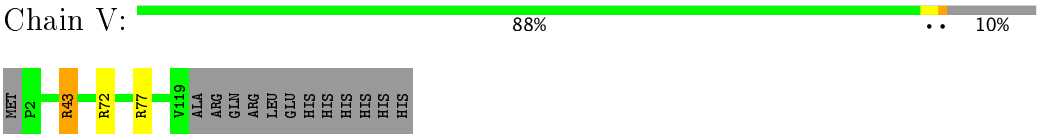
Chain P:

• Molecule 2: DARP14 - Subunit B

Chain U:

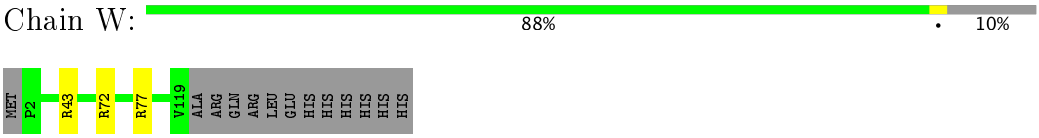
• Molecule 2: DARP14 - Subunit B

Chain V:



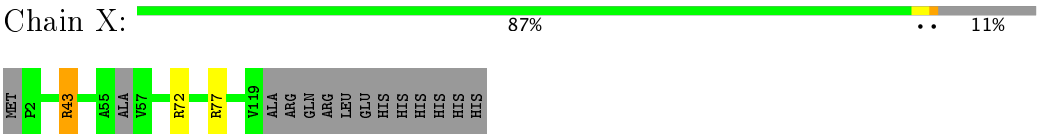
- Molecule 2: DARP14 - Subunit B

Chain W:



- Molecule 2: DARP14 - Subunit B

Chain X:



4 Experimental information (i)

Property	Value	Source
Reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, T	Depositor
Number of particles used	183753	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/Å^2$)	30	Depositor
Minimum defocus (nm)	Not provided	Depositor
Maximum defocus (nm)	Not provided	Depositor
Magnification	Not provided	Depositor
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor

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	#$\|Z\|>2$	RMSZ	#$\|Z\|>2$
1	A	0.86	1/2287 (0.0%)	0.54	0/3094
1	B	0.86	1/2281 (0.0%)	0.55	0/3086
1	C	0.87	1/2273 (0.0%)	0.54	1/3075 (0.0%)
1	D	0.85	1/2297 (0.0%)	0.54	0/3108
1	I	0.86	1/2287 (0.0%)	0.54	0/3094
1	J	0.85	1/2281 (0.0%)	0.54	0/3086
1	K	0.86	1/2273 (0.0%)	0.54	1/3075 (0.0%)
1	L	0.86	1/2297 (0.0%)	0.54	0/3108
1	Q	0.85	1/2287 (0.0%)	0.54	0/3094
1	R	0.85	1/2281 (0.0%)	0.55	0/3086
1	S	0.86	1/2273 (0.0%)	0.54	1/3075 (0.0%)
1	T	0.86	1/2297 (0.0%)	0.54	0/3108
2	E	0.73	0/894	0.43	0/1207
2	F	0.71	0/894	0.42	0/1207
2	G	0.75	0/894	0.42	0/1207
2	H	0.73	0/888	0.42	0/1197
2	M	0.73	0/894	0.43	0/1207
2	N	0.71	0/894	0.43	0/1207
2	O	0.75	0/894	0.42	0/1207
2	P	0.73	0/888	0.43	0/1197
2	U	0.71	0/894	0.44	0/1207
2	V	0.70	0/894	0.43	0/1207
2	W	0.75	0/894	0.43	0/1207
2	X	0.76	0/888	0.42	0/1197
All	All	0.82	12/38124 (0.0%)	0.51	3/51543 (0.0%)

The worst 5 of 12 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	163	GLU	C-N	9.69	1.56	1.34
1	R	163	GLU	C-N	9.69	1.56	1.34
1	J	163	GLU	C-N	9.66	1.56	1.34
1	D	163	GLU	C-N	9.06	1.54	1.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	L	163	GLU	C-N	9.06	1.54	1.34

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	S	163	GLU	C-N-CA	-5.40	108.19	121.70
1	C	163	GLU	C-N-CA	-5.38	108.25	121.70
1	K	163	GLU	C-N-CA	-5.37	108.27	121.70

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	2255	0	2269	2	0
1	B	2249	0	2264	2	0
1	C	2241	0	2253	1	0
1	D	2264	0	2283	0	0
1	I	2255	0	2269	1	0
1	J	2249	0	2264	1	0
1	K	2241	0	2253	0	0
1	L	2264	0	2283	1	0
1	Q	2255	0	2269	0	0
1	R	2249	0	2264	2	0
1	S	2241	0	2253	0	0
1	T	2264	0	2283	1	0
2	E	885	0	896	1	0
2	F	885	0	896	1	0
2	G	885	0	896	1	0
2	H	880	0	890	1	0
2	M	885	0	896	1	0
2	N	885	0	896	1	0
2	O	885	0	896	1	0
2	P	880	0	890	1	0
2	U	885	0	896	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	V	885	0	896	2	0
2	W	885	0	896	1	0
2	X	880	0	890	2	0
All	All	37632	0	37941	25	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 0.

The worst 5 of 25 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)
2:H:72:ARG:O	2:H:77:ARG:NH1	2.39	0.55
2:F:72:ARG:O	2:F:77:ARG:NH1	2.41	0.54
2:N:72:ARG:O	2:N:77:ARG:NH1	2.41	0.54
2:P:72:ARG:O	2:P:77:ARG:NH1	2.41	0.54
2:X:72:ARG:O	2:X:77:ARG:NH1	2.43	0.52

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 PDB entries followed by that with respect to all EM entries.

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	289/319 (91%)	286 (99%)	3 (1%)	0	100	100
1	B	288/319 (90%)	287 (100%)	1 (0%)	0	100	100
1	C	287/319 (90%)	285 (99%)	2 (1%)	0	100	100
1	D	292/319 (92%)	289 (99%)	3 (1%)	0	100	100
1	I	289/319 (91%)	286 (99%)	3 (1%)	0	100	100
1	J	288/319 (90%)	286 (99%)	2 (1%)	0	100	100
1	K	287/319 (90%)	285 (99%)	2 (1%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	L	292/319 (92%)	289 (99%)	3 (1%)	0	100	100
1	Q	289/319 (91%)	286 (99%)	3 (1%)	0	100	100
1	R	288/319 (90%)	286 (99%)	2 (1%)	0	100	100
1	S	287/319 (90%)	286 (100%)	1 (0%)	0	100	100
1	T	292/319 (92%)	289 (99%)	3 (1%)	0	100	100
2	E	116/131 (88%)	115 (99%)	1 (1%)	0	100	100
2	F	116/131 (88%)	116 (100%)	0	0	100	100
2	G	116/131 (88%)	116 (100%)	0	0	100	100
2	H	113/131 (86%)	113 (100%)	0	0	100	100
2	M	116/131 (88%)	115 (99%)	1 (1%)	0	100	100
2	N	116/131 (88%)	116 (100%)	0	0	100	100
2	O	116/131 (88%)	116 (100%)	0	0	100	100
2	P	113/131 (86%)	113 (100%)	0	0	100	100
2	U	116/131 (88%)	115 (99%)	1 (1%)	0	100	100
2	V	116/131 (88%)	116 (100%)	0	0	100	100
2	W	116/131 (88%)	116 (100%)	0	0	100	100
2	X	113/131 (86%)	113 (100%)	0	0	100	100
All	All	4851/5400 (90%)	4820 (99%)	31 (1%)	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 PDB entries followed by that with respect to all EM entries.

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	235/257 (91%)	235 (100%)	0	100	100
1	B	234/257 (91%)	233 (100%)	1 (0%)	92	96
1	C	233/257 (91%)	233 (100%)	0	100	100
1	D	236/257 (92%)	235 (100%)	1 (0%)	92	96

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	I	235/257 (91%)	235 (100%)	0	100	100
1	J	234/257 (91%)	233 (100%)	1 (0%)	92	96
1	K	233/257 (91%)	233 (100%)	0	100	100
1	L	236/257 (92%)	236 (100%)	0	100	100
1	Q	235/257 (91%)	234 (100%)	1 (0%)	92	96
1	R	234/257 (91%)	234 (100%)	0	100	100
1	S	233/257 (91%)	233 (100%)	0	100	100
1	T	236/257 (92%)	235 (100%)	1 (0%)	92	96
2	E	90/102 (88%)	89 (99%)	1 (1%)	76	89
2	F	90/102 (88%)	89 (99%)	1 (1%)	76	89
2	G	90/102 (88%)	89 (99%)	1 (1%)	76	89
2	H	90/102 (88%)	89 (99%)	1 (1%)	76	89
2	M	90/102 (88%)	89 (99%)	1 (1%)	76	89
2	N	90/102 (88%)	89 (99%)	1 (1%)	76	89
2	O	90/102 (88%)	89 (99%)	1 (1%)	76	89
2	P	90/102 (88%)	89 (99%)	1 (1%)	76	89
2	U	90/102 (88%)	89 (99%)	1 (1%)	76	89
2	V	90/102 (88%)	89 (99%)	1 (1%)	76	89
2	W	90/102 (88%)	89 (99%)	1 (1%)	76	89
2	X	90/102 (88%)	89 (99%)	1 (1%)	76	89
All	All	3894/4308 (90%)	3877 (100%)	17 (0%)	92	96

5 of 17 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	M	43	ARG
2	N	43	ARG
2	U	43	ARG
1	J	93	ARG
2	V	43	ARG

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (2) such sidechains are listed below:

Mol	Chain	Res	Type
2	H	3	HIS
2	V	3	HIS

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.