



wwPDB/EMDatabank EM Map/Model Validation Summary Report ⓘ

Mar 12, 2018 – 03:08 PM EDT

PDB ID : 6C9I
EMDB ID: : EMD-7436
Title : Single-Particle reconstruction of DARP14 - A designed protein scaffold displaying 17kDa DARPin proteins - Scaffold
Authors : Gonen, S.; Liu, Y.; Yeates, T.O.; Gonen, T.
Deposited on : 2018-01-26
Resolution : 3.09 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
<http://wwpdb.org/validation/2016/EMValidationReportHelp>
with specific help available everywhere you see the ⓘ symbol.

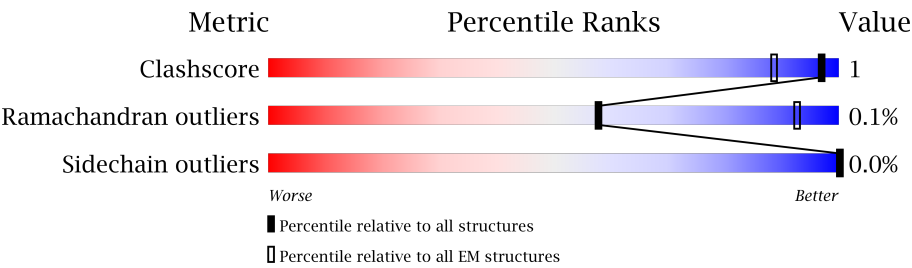
MolProbity : 4.02b-467
Percentile statistics : 20161228.v01 (using entries in the PDB archive December 28th 2016)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et. al. (1996)
Validation Pipeline (wwPDB-VP) : rb-20030736

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 3.09 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	125131	1336
Ramachandran outliers	121729	1120
Sidechain outliers	121581	1026

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 $\leq 5\%$

Mol	Chain	Length	Quality of chain
1	A	163	80% 6% 14%
1	B	163	78% 7% 15%
1	C	163	78% 7% 15%
1	D	163	78% 8% 13%
1	I	163	79% 7% 14%
1	J	163	75% 10% 15%
1	K	163	78% 7% 15%
1	L	163	79% 7% 13%
1	Q	163	79% 7% 14%

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
1	R	163	
1	S	163	
1	T	163	
2	E	131	
2	F	131	
2	G	131	
2	H	131	
2	M	131	
2	N	131	
2	O	131	
2	P	131	
2	U	131	
2	V	131	
2	W	131	
2	X	131	

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 23700 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	140	Total	C	N	O	S	0	0
			1096	704	180	207	5		
1	B	139	Total	C	N	O	S	0	0
			1090	701	179	205	5		
1	C	138	Total	C	N	O	S	0	0
			1082	695	178	204	5		
1	D	141	Total	C	N	O	S	0	0
			1099	704	182	208	5		
1	I	140	Total	C	N	O	S	0	0
			1096	704	180	207	5		
1	J	139	Total	C	N	O	S	0	0
			1090	701	179	205	5		
1	K	138	Total	C	N	O	S	0	0
			1082	695	178	204	5		
1	L	141	Total	C	N	O	S	0	0
			1099	704	182	208	5		
1	Q	140	Total	C	N	O	S	0	0
			1096	704	180	207	5		
1	R	139	Total	C	N	O	S	0	0
			1084	695	179	205	5		
1	S	138	Total	C	N	O	S	0	0
			1082	695	178	204	5		
1	T	141	Total	C	N	O	S	0	0
			1099	704	182	208	5		

There are 156 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	85	ALA	LYS	conflict	UNP O58404
A	88	LEU	GLU	conflict	UNP O58404
A	89	LYS	GLY	conflict	UNP O58404
A	92	LEU	SER	conflict	UNP O58404
A	95	MET	GLU	conflict	UNP O58404
A	126	LEU	GLU	conflict	UNP O58404

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
A	130	LEU	ALA	conflict	UNP O58404
A	133	THR	LEU	conflict	UNP O58404
A	140	ALA	LYS	conflict	UNP O58404
A	143	ALA	LEU	conflict	UNP O58404
A	144	ALA	VAL	conflict	UNP O58404
A	147	LEU	ASN	conflict	UNP O58404
A	148	ALA	ARG	conflict	UNP O58404
B	85	ALA	LYS	conflict	UNP O58404
B	88	LEU	GLU	conflict	UNP O58404
B	89	LYS	GLY	conflict	UNP O58404
B	92	LEU	SER	conflict	UNP O58404
B	95	MET	GLU	conflict	UNP O58404
B	126	LEU	GLU	conflict	UNP O58404
B	130	LEU	ALA	conflict	UNP O58404
B	133	THR	LEU	conflict	UNP O58404
B	140	ALA	LYS	conflict	UNP O58404
B	143	ALA	LEU	conflict	UNP O58404
B	144	ALA	VAL	conflict	UNP O58404
B	147	LEU	ASN	conflict	UNP O58404
B	148	ALA	ARG	conflict	UNP O58404
C	85	ALA	LYS	conflict	UNP O58404
C	88	LEU	GLU	conflict	UNP O58404
C	89	LYS	GLY	conflict	UNP O58404
C	92	LEU	SER	conflict	UNP O58404
C	95	MET	GLU	conflict	UNP O58404
C	126	LEU	GLU	conflict	UNP O58404
C	130	LEU	ALA	conflict	UNP O58404
C	133	THR	LEU	conflict	UNP O58404
C	140	ALA	LYS	conflict	UNP O58404
C	143	ALA	LEU	conflict	UNP O58404
C	144	ALA	VAL	conflict	UNP O58404
C	147	LEU	ASN	conflict	UNP O58404
C	148	ALA	ARG	conflict	UNP O58404
D	85	ALA	LYS	conflict	UNP O58404
D	88	LEU	GLU	conflict	UNP O58404
D	89	LYS	GLY	conflict	UNP O58404
D	92	LEU	SER	conflict	UNP O58404
D	95	MET	GLU	conflict	UNP O58404
D	126	LEU	GLU	conflict	UNP O58404
D	130	LEU	ALA	conflict	UNP O58404
D	133	THR	LEU	conflict	UNP O58404
D	140	ALA	LYS	conflict	UNP O58404

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
D	143	ALA	LEU	conflict	UNP O58404
D	144	ALA	VAL	conflict	UNP O58404
D	147	LEU	ASN	conflict	UNP O58404
D	148	ALA	ARG	conflict	UNP O58404
I	85	ALA	LYS	conflict	UNP O58404
I	88	LEU	GLU	conflict	UNP O58404
I	89	LYS	GLY	conflict	UNP O58404
I	92	LEU	SER	conflict	UNP O58404
I	95	MET	GLU	conflict	UNP O58404
I	126	LEU	GLU	conflict	UNP O58404
I	130	LEU	ALA	conflict	UNP O58404
I	133	THR	LEU	conflict	UNP O58404
I	140	ALA	LYS	conflict	UNP O58404
I	143	ALA	LEU	conflict	UNP O58404
I	144	ALA	VAL	conflict	UNP O58404
I	147	LEU	ASN	conflict	UNP O58404
I	148	ALA	ARG	conflict	UNP O58404
J	85	ALA	LYS	conflict	UNP O58404
J	88	LEU	GLU	conflict	UNP O58404
J	89	LYS	GLY	conflict	UNP O58404
J	92	LEU	SER	conflict	UNP O58404
J	95	MET	GLU	conflict	UNP O58404
J	126	LEU	GLU	conflict	UNP O58404
J	130	LEU	ALA	conflict	UNP O58404
J	133	THR	LEU	conflict	UNP O58404
J	140	ALA	LYS	conflict	UNP O58404
J	143	ALA	LEU	conflict	UNP O58404
J	144	ALA	VAL	conflict	UNP O58404
J	147	LEU	ASN	conflict	UNP O58404
J	148	ALA	ARG	conflict	UNP O58404
K	85	ALA	LYS	conflict	UNP O58404
K	88	LEU	GLU	conflict	UNP O58404
K	89	LYS	GLY	conflict	UNP O58404
K	92	LEU	SER	conflict	UNP O58404
K	95	MET	GLU	conflict	UNP O58404
K	126	LEU	GLU	conflict	UNP O58404
K	130	LEU	ALA	conflict	UNP O58404
K	133	THR	LEU	conflict	UNP O58404
K	140	ALA	LYS	conflict	UNP O58404
K	143	ALA	LEU	conflict	UNP O58404
K	144	ALA	VAL	conflict	UNP O58404
K	147	LEU	ASN	conflict	UNP O58404

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
K	148	ALA	ARG	conflict	UNP O58404
L	85	ALA	LYS	conflict	UNP O58404
L	88	LEU	GLU	conflict	UNP O58404
L	89	LYS	GLY	conflict	UNP O58404
L	92	LEU	SER	conflict	UNP O58404
L	95	MET	GLU	conflict	UNP O58404
L	126	LEU	GLU	conflict	UNP O58404
L	130	LEU	ALA	conflict	UNP O58404
L	133	THR	LEU	conflict	UNP O58404
L	140	ALA	LYS	conflict	UNP O58404
L	143	ALA	LEU	conflict	UNP O58404
L	144	ALA	VAL	conflict	UNP O58404
L	147	LEU	ASN	conflict	UNP O58404
L	148	ALA	ARG	conflict	UNP O58404
Q	85	ALA	LYS	conflict	UNP O58404
Q	88	LEU	GLU	conflict	UNP O58404
Q	89	LYS	GLY	conflict	UNP O58404
Q	92	LEU	SER	conflict	UNP O58404
Q	95	MET	GLU	conflict	UNP O58404
Q	126	LEU	GLU	conflict	UNP O58404
Q	130	LEU	ALA	conflict	UNP O58404
Q	133	THR	LEU	conflict	UNP O58404
Q	140	ALA	LYS	conflict	UNP O58404
Q	143	ALA	LEU	conflict	UNP O58404
Q	144	ALA	VAL	conflict	UNP O58404
Q	147	LEU	ASN	conflict	UNP O58404
Q	148	ALA	ARG	conflict	UNP O58404
R	85	ALA	LYS	conflict	UNP O58404
R	88	LEU	GLU	conflict	UNP O58404
R	89	LYS	GLY	conflict	UNP O58404
R	92	LEU	SER	conflict	UNP O58404
R	95	MET	GLU	conflict	UNP O58404
R	126	LEU	GLU	conflict	UNP O58404
R	130	LEU	ALA	conflict	UNP O58404
R	133	THR	LEU	conflict	UNP O58404
R	140	ALA	LYS	conflict	UNP O58404
R	143	ALA	LEU	conflict	UNP O58404
R	144	ALA	VAL	conflict	UNP O58404
R	147	LEU	ASN	conflict	UNP O58404
R	148	ALA	ARG	conflict	UNP O58404
S	85	ALA	LYS	conflict	UNP O58404
S	88	LEU	GLU	conflict	UNP O58404

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
S	89	LYS	GLY	conflict	UNP O58404
S	92	LEU	SER	conflict	UNP O58404
S	95	MET	GLU	conflict	UNP O58404
S	126	LEU	GLU	conflict	UNP O58404
S	130	LEU	ALA	conflict	UNP O58404
S	133	THR	LEU	conflict	UNP O58404
S	140	ALA	LYS	conflict	UNP O58404
S	143	ALA	LEU	conflict	UNP O58404
S	144	ALA	VAL	conflict	UNP O58404
S	147	LEU	ASN	conflict	UNP O58404
S	148	ALA	ARG	conflict	UNP O58404
T	85	ALA	LYS	conflict	UNP O58404
T	88	LEU	GLU	conflict	UNP O58404
T	89	LYS	GLY	conflict	UNP O58404
T	92	LEU	SER	conflict	UNP O58404
T	95	MET	GLU	conflict	UNP O58404
T	126	LEU	GLU	conflict	UNP O58404
T	130	LEU	ALA	conflict	UNP O58404
T	133	THR	LEU	conflict	UNP O58404
T	140	ALA	LYS	conflict	UNP O58404
T	143	ALA	LEU	conflict	UNP O58404
T	144	ALA	VAL	conflict	UNP O58404
T	147	LEU	ASN	conflict	UNP O58404
T	148	ALA	ARG	conflict	UNP O58404

- 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		
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		

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms					AltConf	Trace
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
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

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
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
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

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
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
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

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
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
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

Continued on next page...


Continued from previous page...

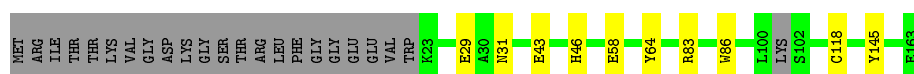
Chain	Residue	Modelled	Actual	Comment	Reference
V	127	HIS	-	expression tag	UNP Q9I2D8
V	128	HIS	-	expression tag	UNP Q9I2D8
V	129	HIS	-	expression tag	UNP Q9I2D8
V	130	HIS	-	expression tag	UNP Q9I2D8
V	131	HIS	-	expression tag	UNP Q9I2D8
W	27	LYS	ALA	conflict	UNP Q9I2D8
W	74	ILE	ALA	conflict	UNP Q9I2D8
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
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


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.

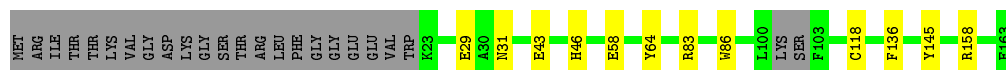
- Molecule 1: DARP14 - Subunit A with DARPin

Chain A: 




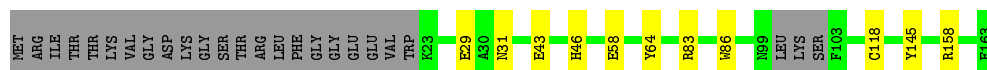
- Molecule 1: DARP14 - Subunit A with DARPin

Chain B: 




- Molecule 1: DARP14 - Subunit A with DARPin

Chain C: 




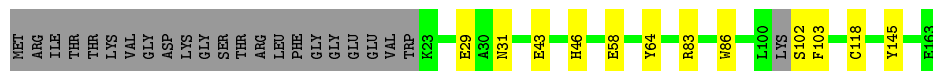
- Molecule 1: DARP14 - Subunit A with DARPin

Chain D: 



- Molecule 1: DARP14 - Subunit A with DARPin

Chain I: 




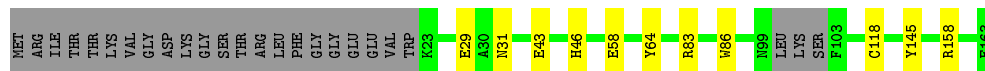
- Molecule 1: DARP14 - Subunit A with DARPin

Chain J: 




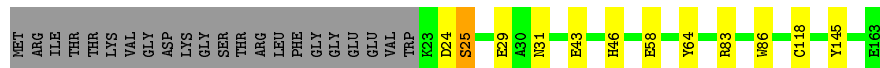
- Molecule 1: DARPin14 - Subunit A with DARPin

Chain K:  78% 7% 15%




- Molecule 1: DARPin14 - Subunit A with DARPin

Chain L:  79% 7% 13%




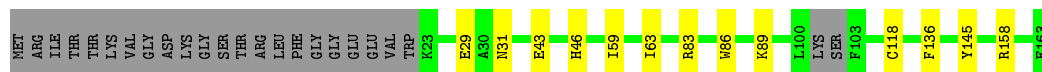
- Molecule 1: DARPin14 - Subunit A with DARPin

Chain Q:  79% 7% 14%



- Molecule 1: DARPin14 - Subunit A with DARPin

Chain R:  77% 8% 15%




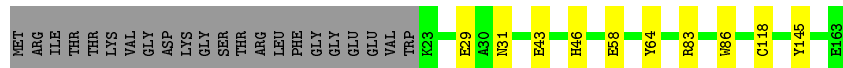
- Molecule 1: DARPin14 - Subunit A with DARPin

Chain S:  75% 10% 15%




- Molecule 1: DARPin14 - Subunit A with DARPin

Chain T:  80% 6% 13%




- Molecule 2: DARPin14 - Subunit B

Chain E:  84% 6% 10%

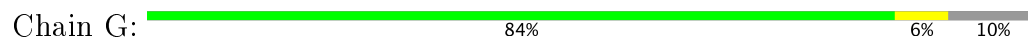


- Molecule 2: DARPin14 - Subunit B

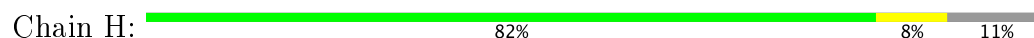
Chain F:  83% 7% 10%



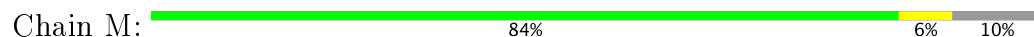
- Molecule 2: DARP14 - Subunit B



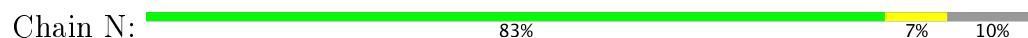
- Molecule 2: DARP14 - Subunit B



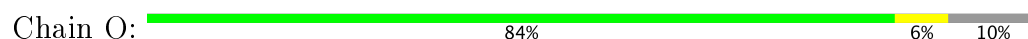
- Molecule 2: DARP14 - Subunit B



- Molecule 2: DARP14 - Subunit B



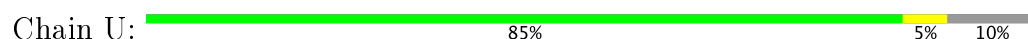
- Molecule 2: DARP14 - Subunit B



- Molecule 2: DARP14 - Subunit B



- Molecule 2: DARP14 - Subunit B



- Molecule 2: DARP14 - Subunit B

Chain V:

84%

6%

10%



• Molecule 2: DARP14 - Subunit B

Chain W:

82%

8%

10%



• Molecule 2: DARP14 - Subunit B

Chain X:

82%

7%

11%



4 Experimental information

Property	Value	Source
Reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, T	Depositor
Number of particles used	34650	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 ($e^-/\text{\AA}^2$)	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	1.51	11/1107 (1.0%)	0.85	1/1487 (0.1%)
1	B	1.47	11/1101 (1.0%)	0.84	2/1479 (0.1%)
1	C	1.52	11/1093 (1.0%)	0.85	3/1468 (0.2%)
1	D	1.49	10/1110 (0.9%)	0.84	2/1492 (0.1%)
1	I	1.51	10/1107 (0.9%)	0.85	1/1487 (0.1%)
1	J	1.45	10/1101 (0.9%)	0.84	2/1479 (0.1%)
1	K	1.51	11/1093 (1.0%)	0.84	3/1468 (0.2%)
1	L	1.50	11/1110 (1.0%)	0.84	1/1492 (0.1%)
1	Q	1.51	11/1107 (1.0%)	0.84	1/1487 (0.1%)
1	R	1.45	9/1094 (0.8%)	0.85	3/1470 (0.2%)
1	S	1.46	11/1093 (1.0%)	0.82	2/1468 (0.1%)
1	T	1.50	11/1110 (1.0%)	0.83	1/1492 (0.1%)
2	E	1.55	5/894 (0.6%)	0.88	2/1207 (0.2%)
2	F	1.57	4/894 (0.4%)	0.87	2/1207 (0.2%)
2	G	1.55	3/894 (0.3%)	0.86	2/1207 (0.2%)
2	H	1.56	5/888 (0.6%)	0.89	4/1197 (0.3%)
2	M	1.55	6/894 (0.7%)	0.88	2/1207 (0.2%)
2	N	1.56	3/894 (0.3%)	0.87	2/1207 (0.2%)
2	O	1.55	3/894 (0.3%)	0.86	2/1207 (0.2%)
2	P	1.56	3/888 (0.3%)	0.89	4/1197 (0.3%)
2	U	1.55	6/894 (0.7%)	0.88	2/1207 (0.2%)
2	V	1.56	4/894 (0.4%)	0.87	2/1207 (0.2%)
2	W	1.57	5/894 (0.6%)	0.86	2/1207 (0.2%)
2	X	1.56	4/888 (0.5%)	0.90	4/1197 (0.3%)
All	All	1.52	178/23936 (0.7%)	0.86	52/32223 (0.2%)

The worst 5 of 178 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	G	85	CYS	CB-SG	-8.39	1.68	1.82
2	W	85	CYS	CB-SG	-8.36	1.68	1.82
2	O	85	CYS	CB-SG	-8.22	1.68	1.82
2	F	85	CYS	CB-SG	-7.99	1.68	1.82

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	V	85	CYS	CB-SG	-7.99	1.68	1.82

The worst 5 of 52 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	J	83	ARG	NE-CZ-NH2	-9.33	115.63	120.30
1	R	83	ARG	NE-CZ-NH2	-9.29	115.66	120.30
1	B	83	ARG	NE-CZ-NH2	-9.29	115.66	120.30
1	I	83	ARG	NE-CZ-NH2	-9.17	115.71	120.30
1	Q	83	ARG	NE-CZ-NH2	-9.12	115.74	120.30

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	1096	0	1144	0	0
1	B	1090	0	1139	1	0
1	C	1082	0	1128	0	0
1	D	1099	0	1151	2	0
1	I	1096	0	1144	1	0
1	J	1090	0	1139	5	0
1	K	1082	0	1128	0	0
1	L	1099	0	1151	1	0
1	Q	1096	0	1144	1	0
1	R	1084	0	1132	3	0
1	S	1082	0	1128	3	0
1	T	1099	0	1151	0	0
2	E	885	0	896	1	0
2	F	885	0	896	2	0
2	G	885	0	896	2	0
2	H	880	0	890	2	0
2	M	885	0	896	1	0
2	N	885	0	896	3	0
2	O	885	0	896	2	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	P	880	0	890	2	0
2	U	885	0	896	0	0
2	V	885	0	896	2	0
2	W	885	0	896	2	0
2	X	880	0	890	2	0
All	All	23700	0	24413	36	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 1.

The worst 5 of 36 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:J:59:ILE:O	1:J:63:ILE:HG13	1.99	0.63
1:J:64:TYR:CD1	1:J:67:MET:HE3	2.40	0.57
1:R:59:ILE:O	1:R:63:ILE:HG13	2.04	0.57
1:B:64:TYR:OH	1:D:106:PRO:HD3	2.05	0.57
1:S:59:ILE:O	1:S:63:ILE:HG13	2.07	0.54

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	136/163 (83%)	135 (99%)	1 (1%)	0	100	100
1	B	135/163 (83%)	134 (99%)	1 (1%)	0	100	100
1	C	134/163 (82%)	133 (99%)	1 (1%)	0	100	100
1	D	139/163 (85%)	138 (99%)	0	1 (1%)	25	64
1	I	136/163 (83%)	135 (99%)	1 (1%)	0	100	100

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	J	135/163 (83%)	134 (99%)	1 (1%)	0	100	100
1	K	134/163 (82%)	134 (100%)	0	0	100	100
1	L	139/163 (85%)	138 (99%)	0	1 (1%)	25	64
1	Q	136/163 (83%)	135 (99%)	1 (1%)	0	100	100
1	R	135/163 (83%)	134 (99%)	1 (1%)	0	100	100
1	S	134/163 (82%)	133 (99%)	1 (1%)	0	100	100
1	T	139/163 (85%)	138 (99%)	1 (1%)	0	100	100
2	E	116/131 (88%)	116 (100%)	0	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%)	116 (100%)	0	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%)	116 (100%)	0	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	3015/3528 (86%)	3004 (100%)	9 (0%)	2 (0%)	58	88

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	D	25	SER
1	L	25	SER

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 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	117/136 (86%)	117 (100%)	0	100	100
1	B	116/136 (85%)	116 (100%)	0	100	100
1	C	115/136 (85%)	115 (100%)	0	100	100
1	D	117/136 (86%)	117 (100%)	0	100	100
1	I	117/136 (86%)	117 (100%)	0	100	100
1	J	116/136 (85%)	116 (100%)	0	100	100
1	K	115/136 (85%)	115 (100%)	0	100	100
1	L	117/136 (86%)	117 (100%)	0	100	100
1	Q	117/136 (86%)	117 (100%)	0	100	100
1	R	115/136 (85%)	115 (100%)	0	100	100
1	S	115/136 (85%)	114 (99%)	1 (1%)	82	93
1	T	117/136 (86%)	117 (100%)	0	100	100
2	E	90/102 (88%)	90 (100%)	0	100	100
2	F	90/102 (88%)	90 (100%)	0	100	100
2	G	90/102 (88%)	90 (100%)	0	100	100
2	H	90/102 (88%)	90 (100%)	0	100	100
2	M	90/102 (88%)	90 (100%)	0	100	100
2	N	90/102 (88%)	90 (100%)	0	100	100
2	O	90/102 (88%)	90 (100%)	0	100	100
2	P	90/102 (88%)	90 (100%)	0	100	100
2	U	90/102 (88%)	90 (100%)	0	100	100
2	V	90/102 (88%)	90 (100%)	0	100	100
2	W	90/102 (88%)	90 (100%)	0	100	100
2	X	90/102 (88%)	90 (100%)	0	100	100
All	All	2474/2856 (87%)	2473 (100%)	1 (0%)	100	100

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

Mol	Chain	Res	Type
1	S	65	LYS

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.