



Full wwPDB EM Validation Report ⓘ

Nov 6, 2022 – 09:24 AM EST

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 Full wwPDB EM 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/EMValidationReportHelp>
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:

EMDB validation analysis : 0.0.1.dev43
MolProbity : 4.02b-467
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ : 1.9.9
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.31.2

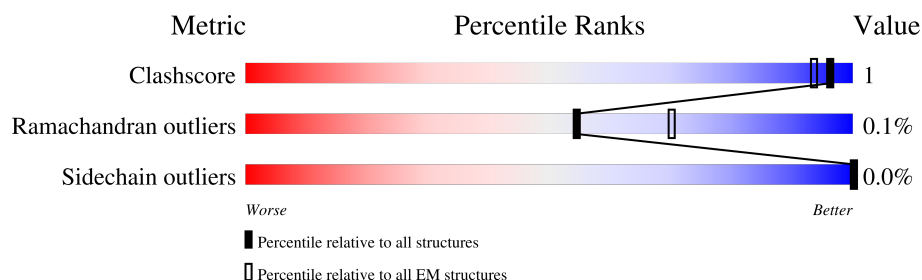
1 Overall quality at a glance

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	158937	4297
Ramachandran outliers	154571	4023
Sidechain outliers	154315	3826

The table below summarises the geometric issues observed across the polymeric chains and their fit to the map. The red, orange, yellow and green segments of the 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 $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the EM map (all-atom inclusion $< 40\%$). The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	163	
1	B	163	
1	C	163	
1	D	163	
1	I	163	
1	J	163	
1	K	163	
1	L	163	

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Mol	Chain	Length	Quality of chain
1	Q	163	
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 [i](#)

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

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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

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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

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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

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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		

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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

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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

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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

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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

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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, 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 atom inclusion in map 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 diamond above a residue indicates a poor fit to the EM map for this residue (all-atom inclusion < 40%). 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: 




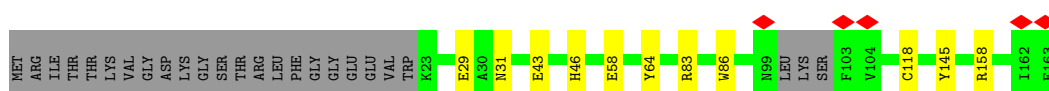
- Molecule 1: DARP14 - Subunit A with DARPin

Chain B: 




- Molecule 1: DARP14 - Subunit A with DARPin

Chain C: 




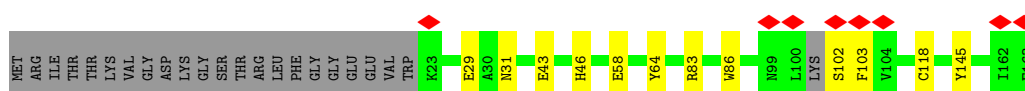
- Molecule 1: DARP14 - Subunit A with DARPin

Chain D: 




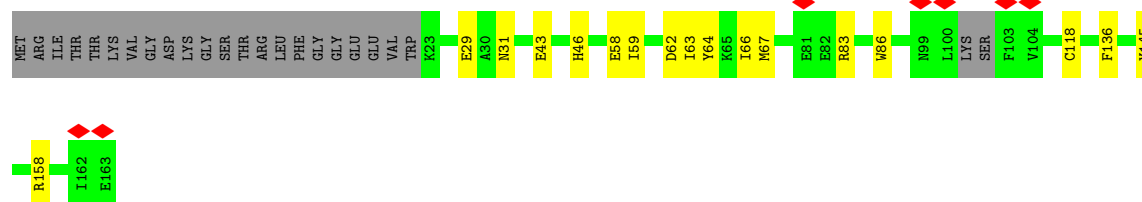
- Molecule 1: DARP14 - Subunit A with DARPin

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: 




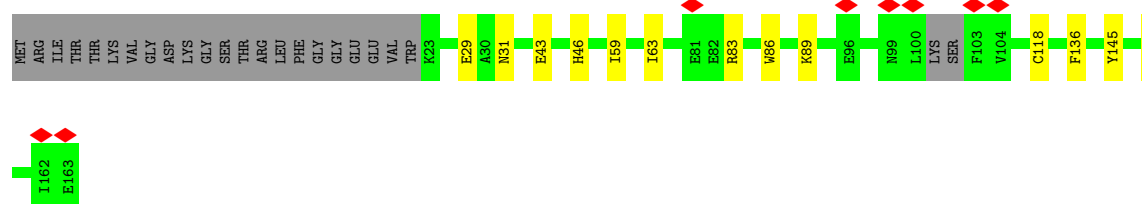
- Molecule 1: DARP14 - Subunit A with DARPin

Chain Q: 



- Molecule 1: DARP14 - Subunit A with DARPin

Chain R: 



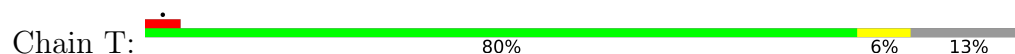
- Molecule 1: DARP14 - Subunit A with DARPin

Chain S: 

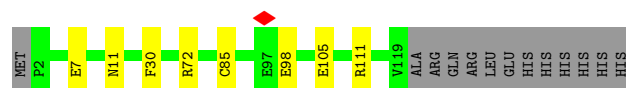
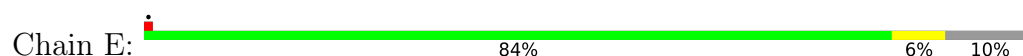




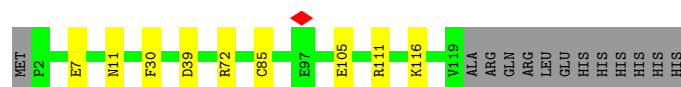
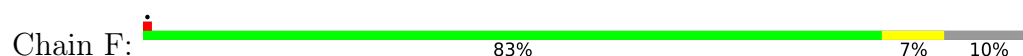
- Molecule 1: DARP14 - Subunit A with DARPin



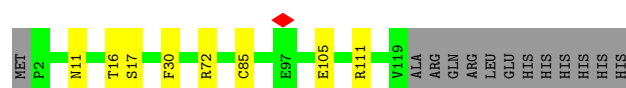
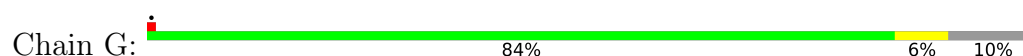
- Molecule 2: DARP14 - Subunit B



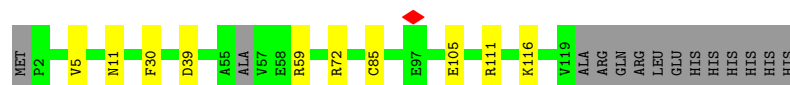
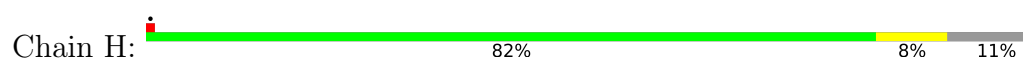
- Molecule 2: DARP14 - Subunit B



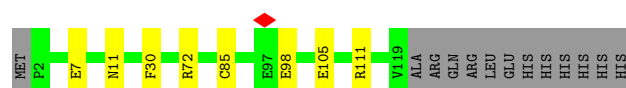
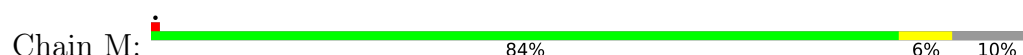
- Molecule 2: DARP14 - Subunit B



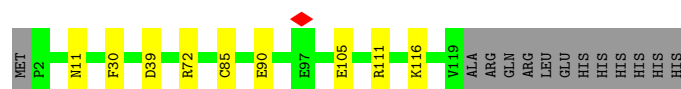
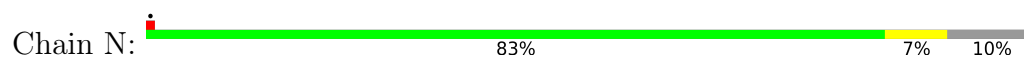
- Molecule 2: DARP14 - Subunit B



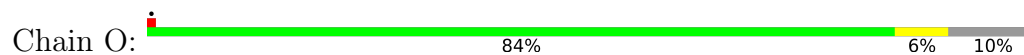
- Molecule 2: DARP14 - Subunit B



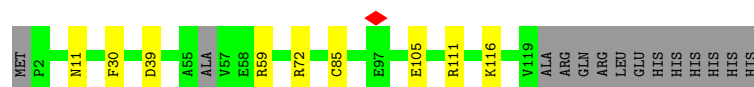
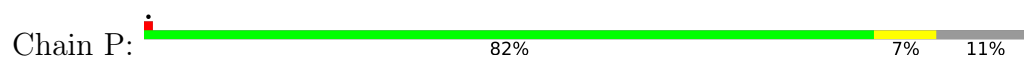
- Molecule 2: DARP14 - Subunit B



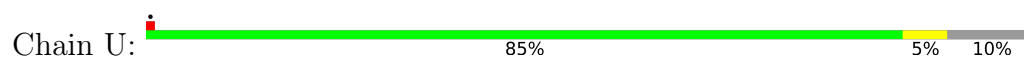
• Molecule 2: DARP14 - Subunit B



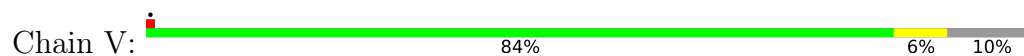
• Molecule 2: DARP14 - Subunit B



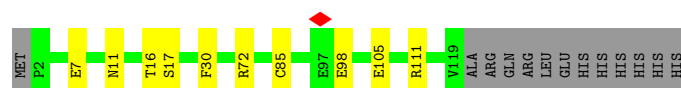
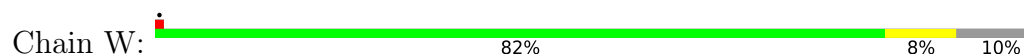
• Molecule 2: DARP14 - Subunit B



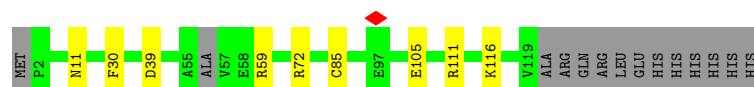
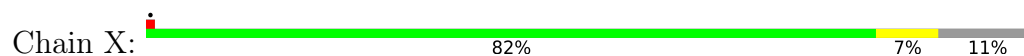
• Molecule 2: DARP14 - Subunit B



• Molecule 2: DARP14 - Subunit B



• Molecule 2: DARP14 - Subunit B



4 Experimental information

Property	Value	Source
EM 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	
Maximum defocus (nm)	Not provided	
Magnification	Not provided	
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor
Maximum map value	0.150	Depositor
Minimum map value	-0.112	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.006	Depositor
Recommended contour level	0.0164	Depositor
Map size (Å)	241.04, 241.04, 241.04	wwPDB
Map dimensions	368, 368, 368	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	0.655, 0.655, 0.655	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	$\# Z > 5$	RMSZ	$\# Z > 5$
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%)

All (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

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	V	85	CYS	CB-SG	-7.99	1.68	1.82
2	N	85	CYS	CB-SG	-7.98	1.68	1.82
2	E	85	CYS	CB-SG	-7.74	1.69	1.82
2	M	85	CYS	CB-SG	-7.71	1.69	1.82
2	U	85	CYS	CB-SG	-7.69	1.69	1.82
2	P	85	CYS	CB-SG	-7.62	1.69	1.82
2	H	85	CYS	CB-SG	-7.61	1.69	1.82
2	X	85	CYS	CB-SG	-7.58	1.69	1.82
1	L	118	CYS	CB-SG	-7.15	1.70	1.82
1	A	118	CYS	CB-SG	-7.13	1.70	1.82
1	T	118	CYS	CB-SG	-7.10	1.70	1.82
1	D	118	CYS	CB-SG	-7.08	1.70	1.82
1	C	118	CYS	CB-SG	-7.07	1.70	1.82
1	Q	118	CYS	CB-SG	-7.03	1.70	1.82
1	B	118	CYS	CB-SG	-7.01	1.70	1.82
1	I	118	CYS	CB-SG	-7.00	1.70	1.82
1	S	118	CYS	CB-SG	-6.97	1.70	1.82
1	J	118	CYS	CB-SG	-6.95	1.70	1.82
1	R	118	CYS	CB-SG	-6.95	1.70	1.82
1	K	118	CYS	CB-SG	-6.94	1.70	1.82
1	C	64	TYR	CB-CG	-6.71	1.41	1.51
1	K	64	TYR	CB-CG	-6.62	1.41	1.51
1	J	86	TRP	CD2-CE2	-6.45	1.33	1.41
1	K	31	ASN	CB-CG	-6.41	1.36	1.51
1	B	86	TRP	CD2-CE2	-6.40	1.33	1.41
1	D	31	ASN	CB-CG	-6.40	1.36	1.51
1	T	31	ASN	CB-CG	-6.39	1.36	1.51
1	S	31	ASN	CB-CG	-6.38	1.36	1.51
1	R	31	ASN	CB-CG	-6.35	1.36	1.51
1	C	31	ASN	CB-CG	-6.34	1.36	1.51
1	L	31	ASN	CB-CG	-6.32	1.36	1.51
1	B	31	ASN	CB-CG	-6.31	1.36	1.51
1	I	31	ASN	CB-CG	-6.30	1.36	1.51
1	J	31	ASN	CB-CG	-6.30	1.36	1.51
2	G	30	PHE	CB-CG	-6.29	1.40	1.51
1	A	31	ASN	CB-CG	-6.27	1.36	1.51
2	W	30	PHE	CB-CG	-6.23	1.40	1.51
1	B	58	GLU	CD-OE1	-6.23	1.18	1.25
1	J	58	GLU	CD-OE1	-6.21	1.18	1.25
1	R	86	TRP	CD2-CE2	-6.20	1.33	1.41
2	V	30	PHE	CB-CG	-6.19	1.40	1.51
2	O	30	PHE	CB-CG	-6.16	1.40	1.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	Q	31	ASN	CB-CG	-6.15	1.36	1.51
2	N	30	PHE	CB-CG	-6.13	1.41	1.51
2	F	30	PHE	CB-CG	-6.12	1.41	1.51
2	U	30	PHE	CB-CG	-6.12	1.41	1.51
2	M	30	PHE	CB-CG	-6.12	1.41	1.51
2	E	30	PHE	CB-CG	-6.10	1.41	1.51
2	X	30	PHE	CB-CG	-6.04	1.41	1.51
2	H	30	PHE	CB-CG	-6.03	1.41	1.51
1	L	86	TRP	CD2-CE2	-6.01	1.34	1.41
1	T	86	TRP	CD2-CE2	-6.01	1.34	1.41
1	D	64	TYR	CB-CG	-6.00	1.42	1.51
1	A	86	TRP	CD2-CE2	-5.98	1.34	1.41
1	T	64	TYR	CB-CG	-5.98	1.42	1.51
1	I	86	TRP	CD2-CE2	-5.97	1.34	1.41
1	K	86	TRP	CD2-CE2	-5.97	1.34	1.41
1	A	64	TYR	CB-CG	-5.96	1.42	1.51
2	P	30	PHE	CB-CG	-5.95	1.41	1.51
1	C	86	TRP	CD2-CE2	-5.95	1.34	1.41
1	Q	64	TYR	CB-CG	-5.94	1.42	1.51
1	D	86	TRP	CD2-CE2	-5.92	1.34	1.41
1	I	64	TYR	CB-CG	-5.91	1.42	1.51
1	S	86	TRP	CD2-CE2	-5.91	1.34	1.41
1	L	64	TYR	CB-CG	-5.91	1.42	1.51
1	Q	86	TRP	CD2-CE2	-5.90	1.34	1.41
1	C	58	GLU	CG-CD	-5.88	1.43	1.51
1	Q	58	GLU	CG-CD	-5.84	1.43	1.51
1	I	58	GLU	CG-CD	-5.83	1.43	1.51
1	A	58	GLU	CG-CD	-5.81	1.43	1.51
1	S	58	GLU	CG-CD	-5.75	1.43	1.51
1	L	58	GLU	CG-CD	-5.68	1.43	1.51
1	T	58	GLU	CG-CD	-5.67	1.43	1.51
2	O	105	GLU	CG-CD	-5.65	1.43	1.51
1	D	58	GLU	CG-CD	-5.65	1.43	1.51
1	K	58	GLU	CG-CD	-5.65	1.43	1.51
2	N	105	GLU	CG-CD	-5.63	1.43	1.51
2	G	105	GLU	CG-CD	-5.60	1.43	1.51
1	J	43	GLU	CD-OE1	-5.60	1.19	1.25
1	I	43	GLU	CD-OE1	-5.58	1.19	1.25
1	R	46	HIS	CB-CG	-5.58	1.40	1.50
1	D	46	HIS	CB-CG	-5.56	1.40	1.50
2	H	105	GLU	CG-CD	-5.55	1.43	1.51
1	K	43	GLU	CG-CD	-5.55	1.43	1.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	P	105	GLU	CG-CD	-5.55	1.43	1.51
1	T	46	HIS	CB-CG	-5.54	1.40	1.50
1	D	43	GLU	CD-OE1	-5.54	1.19	1.25
1	Q	46	HIS	CB-CG	-5.54	1.40	1.50
1	R	43	GLU	CD-OE1	-5.53	1.19	1.25
1	C	46	HIS	CB-CG	-5.53	1.40	1.50
1	L	43	GLU	CG-CD	-5.53	1.43	1.51
1	I	46	HIS	CB-CG	-5.52	1.40	1.50
1	J	46	HIS	CB-CG	-5.52	1.40	1.50
1	S	43	GLU	CG-CD	-5.51	1.43	1.51
2	X	105	GLU	CG-CD	-5.51	1.43	1.51
1	B	46	HIS	CB-CG	-5.51	1.40	1.50
1	A	46	HIS	CB-CG	-5.50	1.40	1.50
1	B	43	GLU	CG-CD	-5.50	1.43	1.51
1	K	46	HIS	CB-CG	-5.50	1.40	1.50
1	Q	43	GLU	CG-CD	-5.50	1.43	1.51
2	F	105	GLU	CG-CD	-5.49	1.43	1.51
2	W	105	GLU	CG-CD	-5.49	1.43	1.51
1	L	46	HIS	CB-CG	-5.49	1.40	1.50
2	V	105	GLU	CG-CD	-5.47	1.43	1.51
1	T	43	GLU	CG-CD	-5.46	1.43	1.51
1	C	43	GLU	CG-CD	-5.45	1.43	1.51
1	S	43	GLU	CD-OE1	-5.44	1.19	1.25
1	S	46	HIS	CB-CG	-5.43	1.40	1.50
1	B	43	GLU	CD-OE1	-5.42	1.19	1.25
2	E	105	GLU	CG-CD	-5.39	1.43	1.51
1	A	43	GLU	CG-CD	-5.39	1.43	1.51
2	M	105	GLU	CG-CD	-5.35	1.44	1.51
2	U	105	GLU	CG-CD	-5.35	1.44	1.51
1	K	43	GLU	CD-OE1	-5.33	1.19	1.25
1	Q	43	GLU	CD-OE1	-5.33	1.19	1.25
1	T	43	GLU	CD-OE1	-5.33	1.19	1.25
1	I	29	GLU	CD-OE1	-5.29	1.19	1.25
1	A	43	GLU	CD-OE1	-5.28	1.19	1.25
1	L	43	GLU	CD-OE1	-5.27	1.19	1.25
1	L	145	TYR	CE2-CZ	-5.26	1.31	1.38
1	S	145	TYR	CE2-CZ	-5.26	1.31	1.38
1	T	145	TYR	CE2-CZ	-5.26	1.31	1.38
1	C	43	GLU	CD-OE1	-5.24	1.19	1.25
1	K	145	TYR	CE2-CZ	-5.24	1.31	1.38
1	Q	29	GLU	CD-OE1	-5.22	1.20	1.25
1	A	29	GLU	CD-OE1	-5.21	1.20	1.25

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	Q	145	TYR	CE2-CZ	-5.21	1.31	1.38
1	J	86	TRP	CZ3-CH2	-5.20	1.31	1.40
1	C	145	TYR	CE2-CZ	-5.20	1.31	1.38
1	S	29	GLU	CD-OE1	-5.17	1.20	1.25
1	B	86	TRP	CZ3-CH2	-5.17	1.31	1.40
2	M	98	GLU	CD-OE1	-5.16	1.20	1.25
1	I	145	TYR	CE2-CZ	-5.16	1.31	1.38
1	K	29	GLU	CD-OE1	-5.15	1.20	1.25
1	S	136	PHE	CG-CD1	-5.15	1.31	1.38
2	F	7	GLU	CD-OE1	-5.15	1.20	1.25
1	J	29	GLU	CD-OE1	-5.15	1.20	1.25
1	K	86	TRP	CZ3-CH2	-5.14	1.31	1.40
1	R	86	TRP	CZ3-CH2	-5.14	1.31	1.40
1	Q	86	TRP	CZ3-CH2	-5.13	1.31	1.40
1	B	29	GLU	CD-OE1	-5.13	1.20	1.25
1	B	136	PHE	CB-CG	-5.13	1.42	1.51
2	U	98	GLU	CD-OE1	-5.12	1.20	1.25
1	D	29	GLU	CD-OE1	-5.12	1.20	1.25
1	R	29	GLU	CD-OE1	-5.11	1.20	1.25
1	A	145	TYR	CE2-CZ	-5.11	1.31	1.38
1	L	29	GLU	CD-OE1	-5.10	1.20	1.25
1	C	29	GLU	CD-OE1	-5.10	1.20	1.25
1	T	86	TRP	CZ3-CH2	-5.10	1.31	1.40
1	J	136	PHE	CB-CG	-5.10	1.42	1.51
2	W	7	GLU	CD-OE1	-5.10	1.20	1.25
2	E	7	GLU	CD-OE1	-5.10	1.20	1.25
1	D	145	TYR	CE2-CZ	-5.10	1.31	1.38
1	R	145	TYR	CE2-CZ	-5.09	1.31	1.38
1	R	136	PHE	CB-CG	-5.09	1.42	1.51
1	S	86	TRP	CZ3-CH2	-5.09	1.31	1.40
1	D	86	TRP	CZ3-CH2	-5.08	1.31	1.40
2	U	7	GLU	CD-OE1	-5.08	1.20	1.25
1	B	145	TYR	CE2-CZ	-5.08	1.31	1.38
2	E	98	GLU	CD-OE1	-5.07	1.20	1.25
1	L	86	TRP	CZ3-CH2	-5.07	1.31	1.40
1	A	86	TRP	CZ3-CH2	-5.06	1.31	1.40
1	I	86	TRP	CZ3-CH2	-5.06	1.31	1.40
2	U	105	GLU	CD-OE2	-5.06	1.20	1.25
2	V	105	GLU	CD-OE2	-5.06	1.20	1.25
1	J	145	TYR	CE2-CZ	-5.06	1.31	1.38
1	C	86	TRP	CZ3-CH2	-5.05	1.31	1.40
2	X	105	GLU	CD-OE1	-5.05	1.20	1.25

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	M	7	GLU	CD-OE1	-5.04	1.20	1.25
1	T	29	GLU	CD-OE1	-5.04	1.20	1.25
2	M	105	GLU	CD-OE1	-5.03	1.20	1.25
2	W	98	GLU	CD-OE1	-5.02	1.20	1.25
2	H	105	GLU	CD-OE1	-5.01	1.20	1.25
2	H	5	VAL	CB-CG2	-5.01	1.42	1.52

All (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
1	A	83	ARG	NE-CZ-NH2	-9.03	115.78	120.30
1	K	83	ARG	NE-CZ-NH2	-9.02	115.79	120.30
1	C	83	ARG	NE-CZ-NH2	-8.89	115.85	120.30
1	S	83	ARG	NE-CZ-NH2	-8.89	115.86	120.30
1	T	83	ARG	NE-CZ-NH2	-8.81	115.90	120.30
1	L	83	ARG	NE-CZ-NH2	-8.79	115.91	120.30
1	D	83	ARG	NE-CZ-NH2	-8.50	116.05	120.30
2	P	59	ARG	NE-CZ-NH2	-7.04	116.78	120.30
2	X	59	ARG	NE-CZ-NH2	-7.04	116.78	120.30
2	H	59	ARG	NE-CZ-NH2	-6.93	116.84	120.30
2	P	111	ARG	NE-CZ-NH2	-6.36	117.12	120.30
2	N	111	ARG	NE-CZ-NH2	-6.34	117.13	120.30
2	V	111	ARG	NE-CZ-NH2	-6.31	117.14	120.30
2	X	111	ARG	NE-CZ-NH2	-6.29	117.16	120.30
2	W	111	ARG	NE-CZ-NH2	-6.26	117.17	120.30
2	F	111	ARG	NE-CZ-NH2	-6.22	117.19	120.30
2	M	111	ARG	NE-CZ-NH2	-6.20	117.20	120.30
2	E	111	ARG	NE-CZ-NH2	-6.20	117.20	120.30
2	G	111	ARG	NE-CZ-NH2	-6.19	117.20	120.30
2	O	111	ARG	NE-CZ-NH2	-6.18	117.21	120.30
2	U	111	ARG	NE-CZ-NH2	-6.18	117.21	120.30
2	H	111	ARG	NE-CZ-NH2	-6.18	117.21	120.30
2	N	72	ARG	NE-CZ-NH1	6.16	123.38	120.30
2	U	72	ARG	NE-CZ-NH1	6.11	123.35	120.30
2	F	72	ARG	NE-CZ-NH1	6.11	123.35	120.30
2	V	72	ARG	NE-CZ-NH1	6.07	123.33	120.30
2	M	72	ARG	NE-CZ-NH1	6.03	123.32	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	H	72	ARG	NE-CZ-NH1	6.01	123.31	120.30
2	O	72	ARG	NE-CZ-NH1	5.98	123.29	120.30
2	E	72	ARG	NE-CZ-NH1	5.93	123.27	120.30
2	G	72	ARG	NE-CZ-NH1	5.93	123.27	120.30
2	W	72	ARG	NE-CZ-NH1	5.93	123.26	120.30
2	P	72	ARG	NE-CZ-NH1	5.92	123.26	120.30
2	X	72	ARG	NE-CZ-NH1	5.90	123.25	120.30
1	C	64	TYR	CB-CG-CD2	-5.38	117.77	121.00
1	K	64	TYR	CB-CG-CD2	-5.34	117.80	121.00
1	S	158	ARG	NE-CZ-NH1	5.33	122.96	120.30
1	C	158	ARG	NE-CZ-NH1	5.30	122.95	120.30
1	R	158	ARG	NE-CZ-NH1	5.28	122.94	120.30
2	P	59	ARG	NE-CZ-NH1	5.27	122.94	120.30
2	H	59	ARG	NE-CZ-NH1	5.25	122.93	120.30
1	K	158	ARG	NE-CZ-NH1	5.22	122.91	120.30
1	B	158	ARG	NE-CZ-NH1	5.19	122.90	120.30
1	J	158	ARG	NE-CZ-NH1	5.19	122.90	120.30
2	X	59	ARG	NE-CZ-NH1	5.19	122.90	120.30
1	D	158	ARG	NE-CZ-NH1	5.13	122.86	120.30
1	R	83	ARG	NE-CZ-NH1	5.12	122.86	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

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
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
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.

All (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
2:O:11:ASN:OD1	2:O:11:ASN:N	2.42	0.53
1:J:63:ILE:O	1:J:63:ILE:HG22	2.08	0.52
1:S:63:ILE:HG22	1:S:63:ILE:O	2.11	0.49
1:R:63:ILE:O	1:R:63:ILE:HG22	2.12	0.49
2:N:11:ASN:N	2:N:11:ASN:OD1	2.43	0.48
2:V:11:ASN:N	2:V:11:ASN:OD1	2.43	0.48
2:H:11:ASN:N	2:H:11:ASN:OD1	2.44	0.48
2:P:11:ASN:N	2:P:11:ASN:OD1	2.44	0.47
2:V:39:ASP:OD1	2:V:116:LYS:NZ	2.48	0.47
2:X:39:ASP:OD1	2:X:116:LYS:NZ	2.48	0.46
2:H:39:ASP:OD1	2:H:116:LYS:NZ	2.48	0.46
2:F:11:ASN:N	2:F:11:ASN:OD1	2.43	0.46
2:G:11:ASN:N	2:G:11:ASN:OD1	2.43	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:N:39:ASP:OD1	2:N:116:LYS:NZ	2.49	0.46
2:F:39:ASP:OD1	2:F:116:LYS:NZ	2.48	0.45
2:W:11:ASN:OD1	2:W:11:ASN:N	2.43	0.45
2:X:11:ASN:N	2:X:11:ASN:OD1	2.44	0.45
2:P:39:ASP:OD1	2:P:116:LYS:NZ	2.49	0.45
1:J:64:TYR:CD1	1:J:67:MET:CE	3.01	0.43
1:I:102:SER:OG	1:I:103:PHE:N	2.50	0.42
1:J:62:ASP:O	1:J:66:ILE:HG13	2.18	0.42
1:Q:102:SER:OG	1:Q:103:PHE:N	2.50	0.42
2:E:11:ASN:N	2:E:11:ASN:OD1	2.52	0.42
1:S:62:ASP:C	1:S:64:TYR:N	2.73	0.42
2:O:16:THR:OG1	2:O:17:SER:N	2.54	0.41
2:W:16:THR:OG1	2:W:17:SER:N	2.54	0.41
1:L:24:ASP:O	1:L:25:SER:C	2.59	0.41
2:M:11:ASN:N	2:M:11:ASN:OD1	2.52	0.40
2:N:90:GLU:OE2	1:R:89:LYS:NZ	2.52	0.40
1:D:24:ASP:O	1:D:25:SER:C	2.59	0.40
2:G:16:THR:OG1	2:G:17:SER:N	2.54	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

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%)	22	57
1	I	136/163 (83%)	135 (99%)	1 (1%)	0	100	100
1	J	135/163 (83%)	134 (99%)	1 (1%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	K	134/163 (82%)	134 (100%)	0	0	100	100
1	L	139/163 (85%)	138 (99%)	0	1 (1%)	22	57
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%)	54	83

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%)	78	91
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

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

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains [i](#)

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

5.5 Carbohydrates [i](#)

There are no monosaccharides in this entry.

5.6 Ligand geometry [i](#)

There are no ligands in this entry.

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.

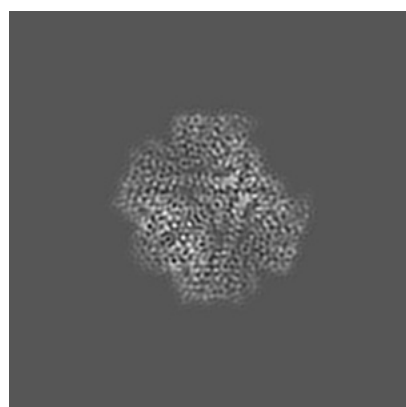
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-7436. These allow visual inspection of the internal detail of the map and identification of artifacts.

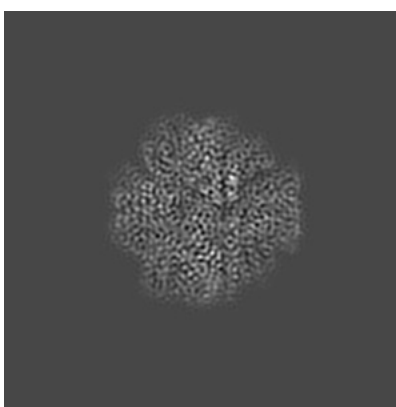
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

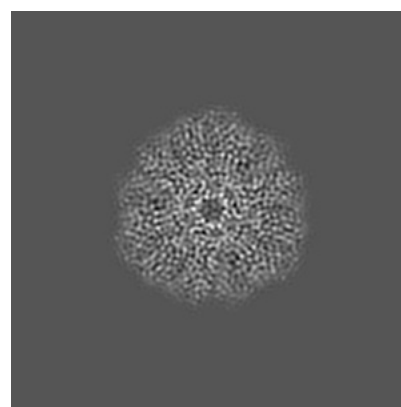
6.1.1 Primary map



X



Y

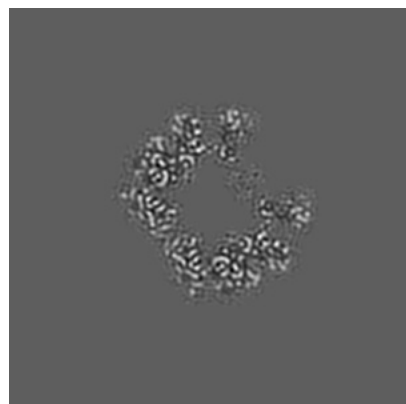


Z

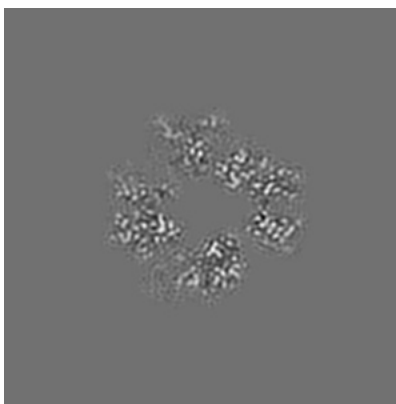
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

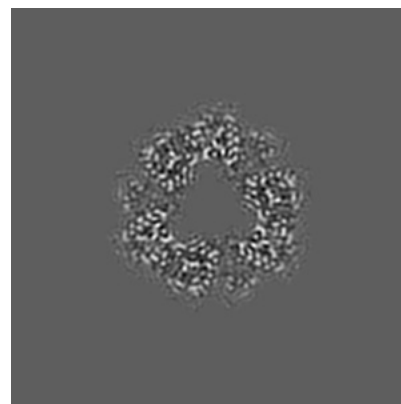
6.2.1 Primary map



X Index: 184



Y Index: 184



Z Index: 184

The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

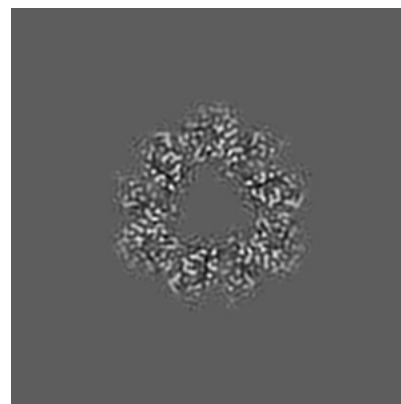
6.3.1 Primary map



X Index: 194



Y Index: 167

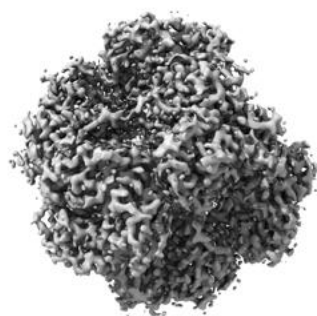


Z Index: 186

The images above show the largest variance slices of the map in three orthogonal directions.

6.4 Orthogonal surface views [i](#)

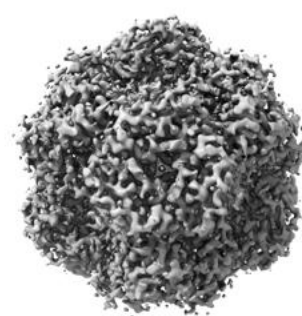
6.4.1 Primary map



X



Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.0164. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

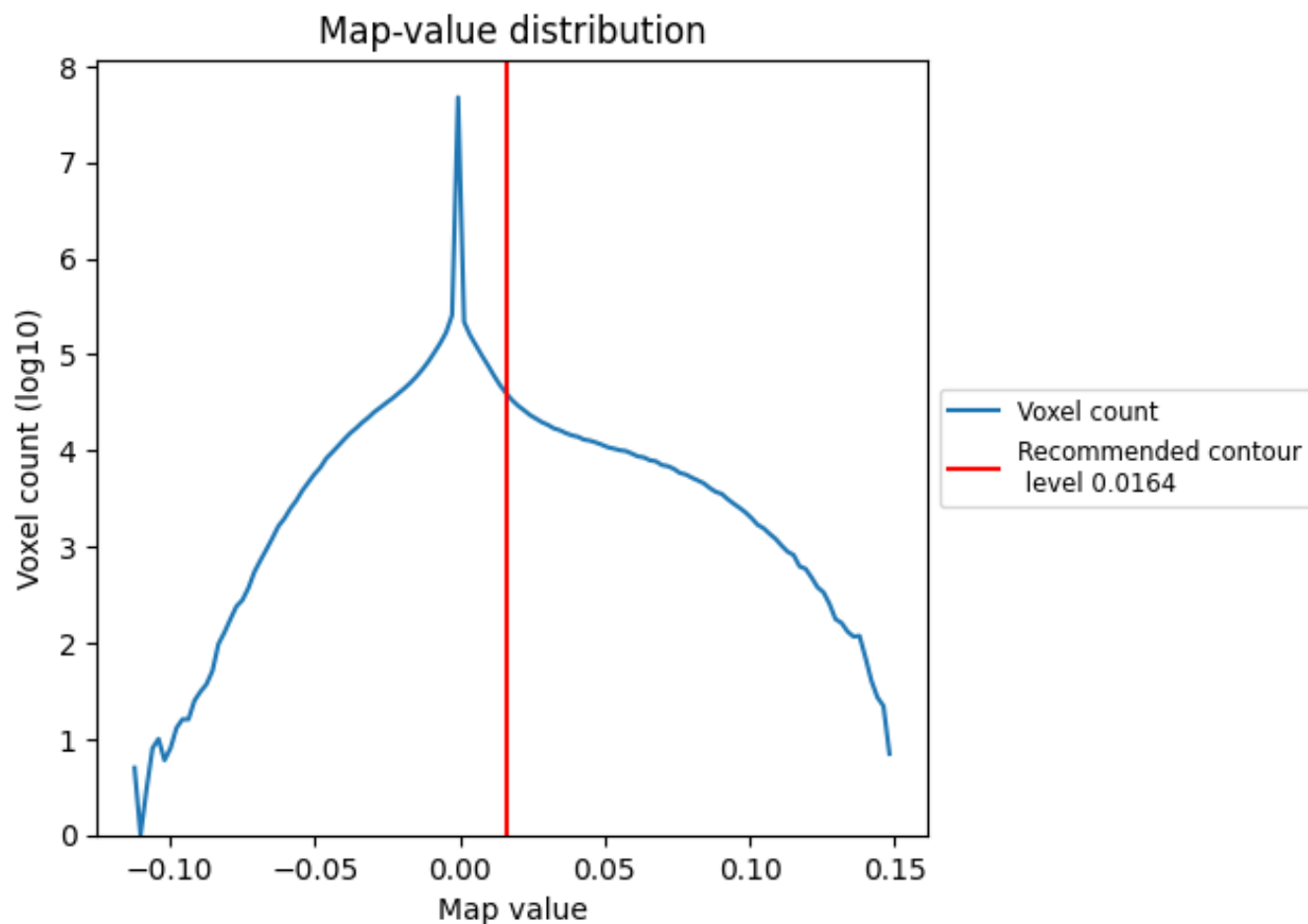
6.5 Mask visualisation

This section was not generated. No masks/segmentation were deposited.

7 Map analysis [i](#)

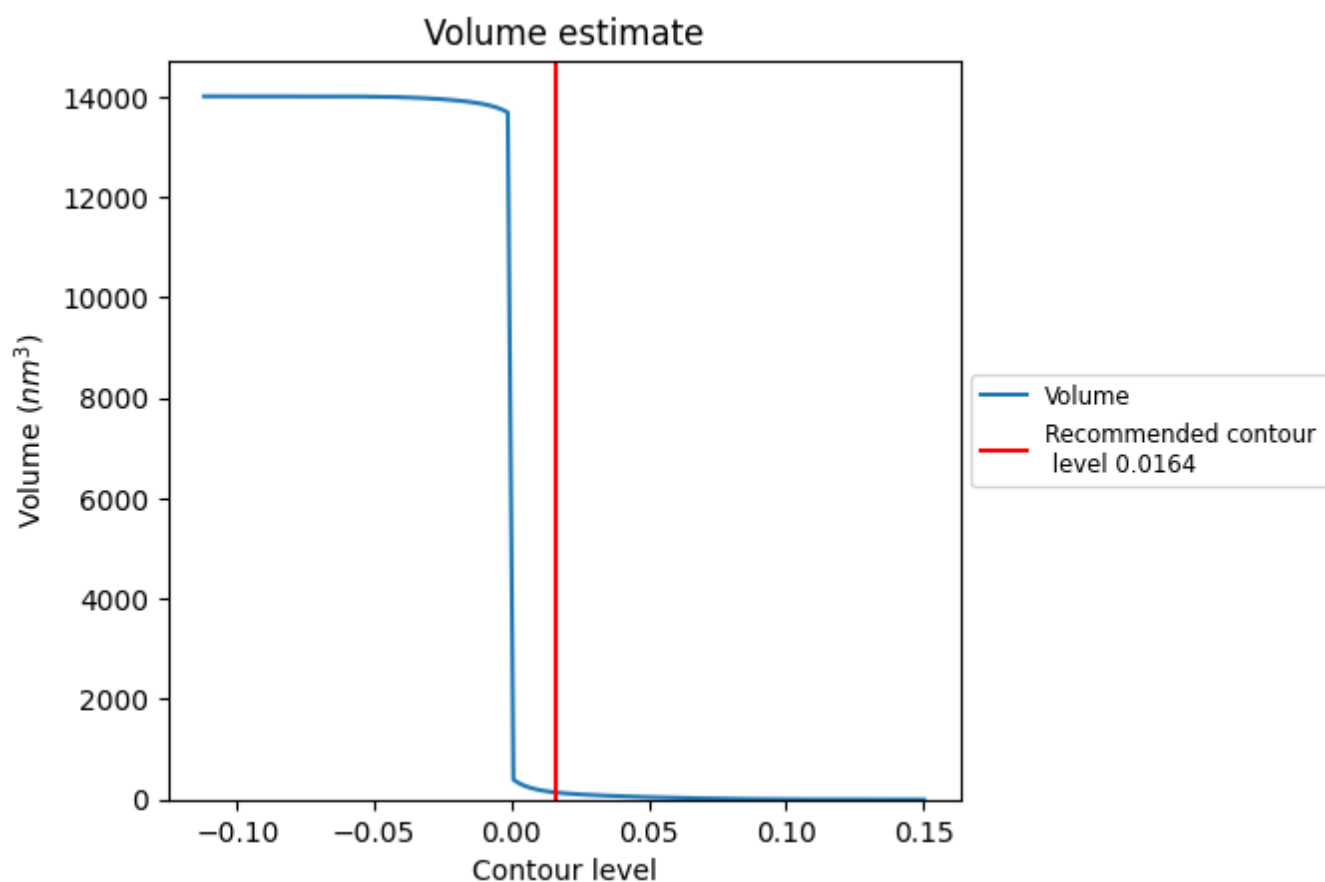
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution [i](#)



The map-value distribution is plotted in 128 intervals along the x-axis. The y-axis is logarithmic. A spike in this graph at zero usually indicates that the volume has been masked.

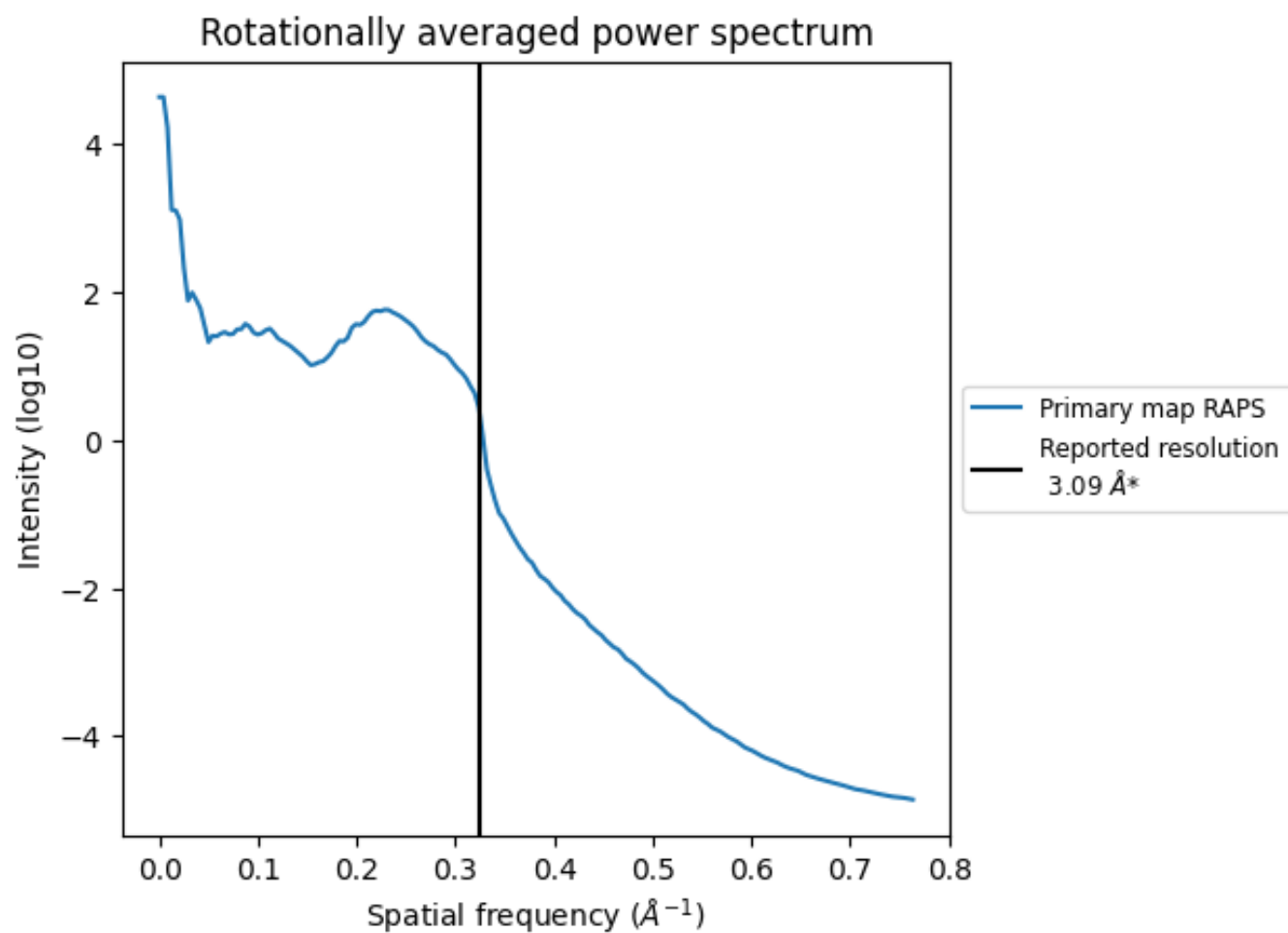
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 140 nm³; this corresponds to an approximate mass of 126 kDa.

The volume estimate graph shows how the enclosed volume varies with the contour level. The recommended contour level is shown as a vertical line and the intersection between the line and the curve gives the volume of the enclosed surface at the given level.

7.3 Rotationally averaged power spectrum ⓘ



*Reported resolution corresponds to spatial frequency of 0.324 Å⁻¹

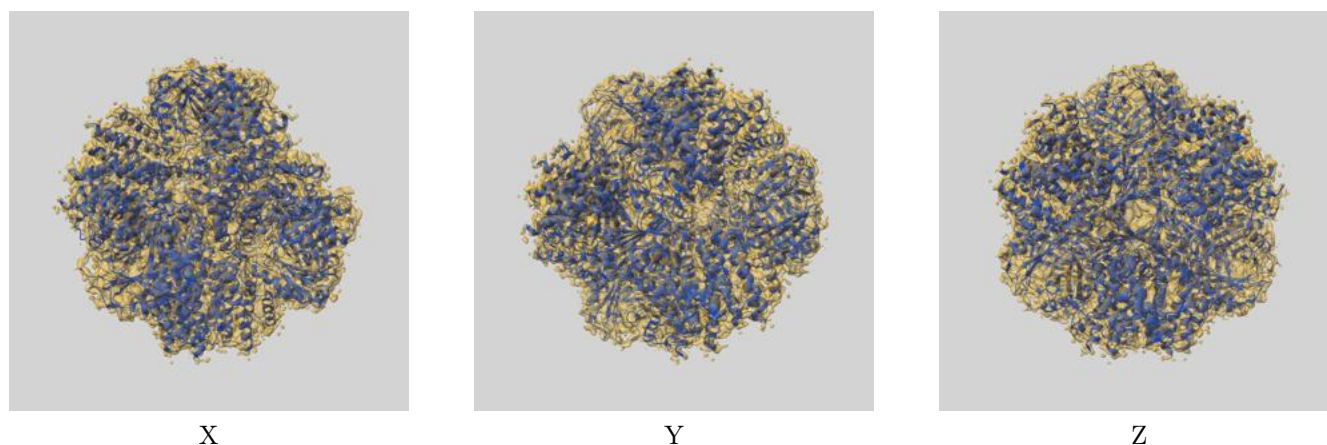
8 Fourier-Shell correlation ⓘ

This section was not generated. No FSC curve or half-maps provided.

9 Map-model fit [i](#)

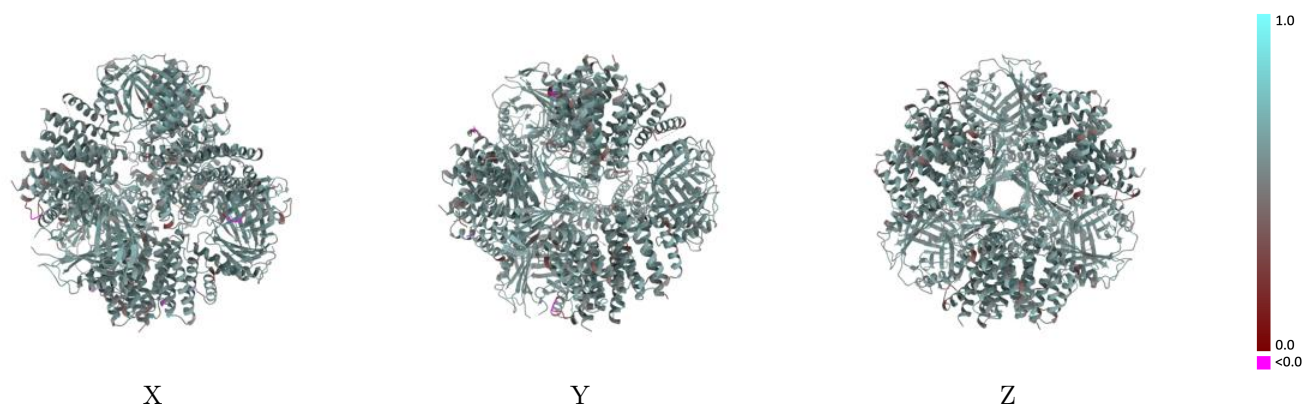
This section contains information regarding the fit between EMDB map EMD-7436 and PDB model 6C9I. Per-residue inclusion information can be found in section 3 on page 14.

9.1 Map-model overlay [i](#)



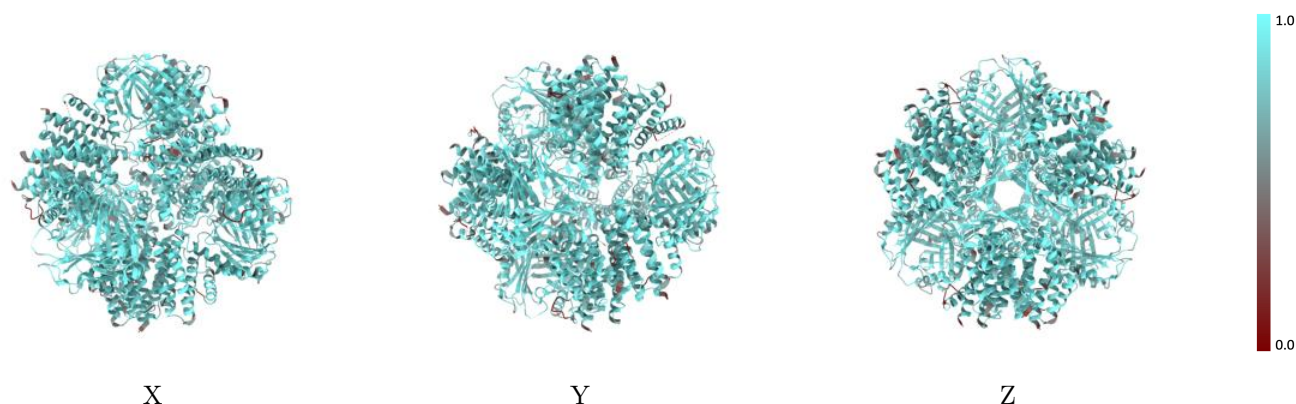
The images above show the 3D surface view of the map at the recommended contour level 0.0164 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

9.2 Q-score mapped to coordinate model [i](#)



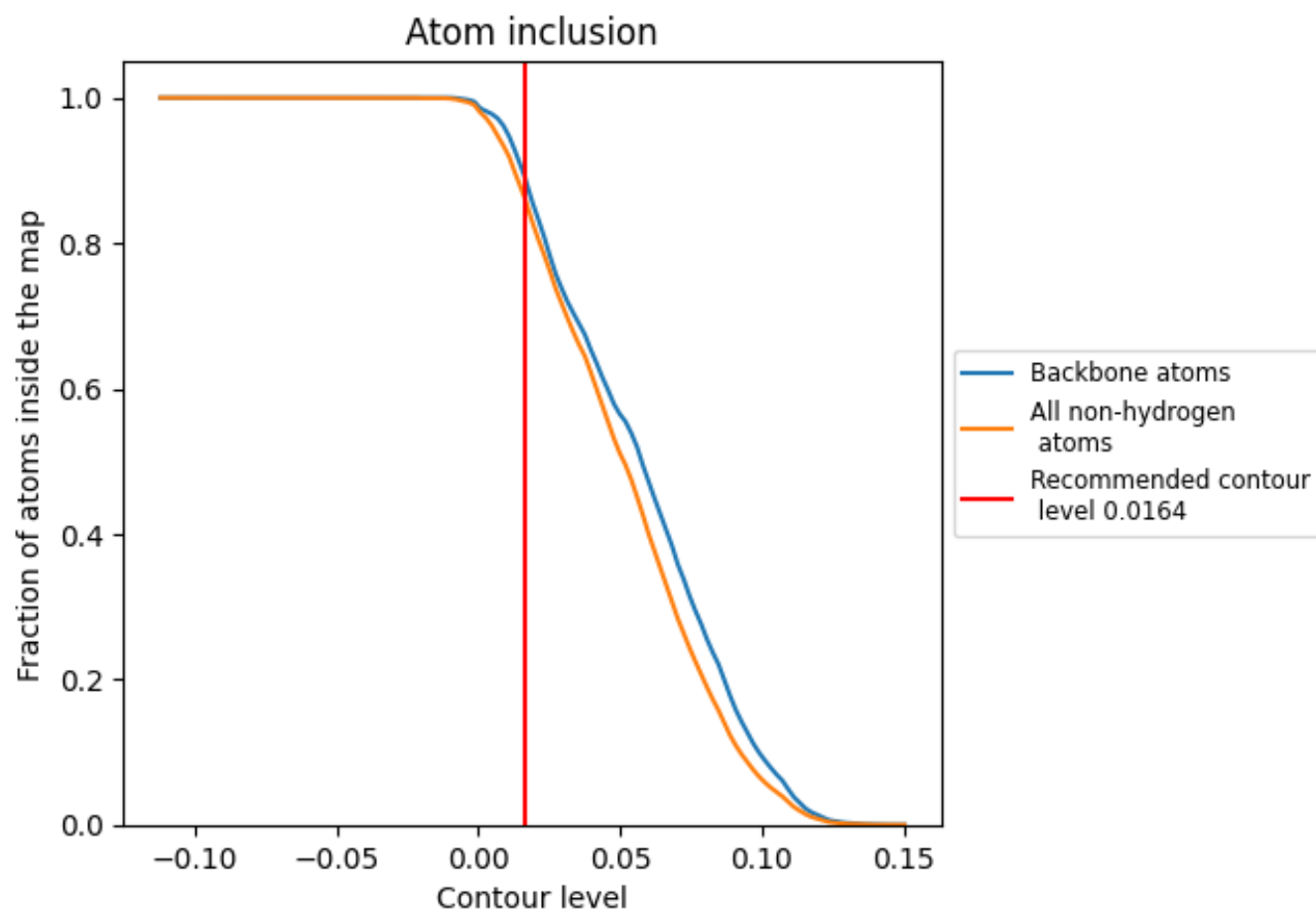
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions at which atoms can be resolved. Low Q-score values may therefore be expected for many entries.

9.3 Atom inclusion mapped to coordinate model [i](#)



The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.0164).



















































9.4 Atom inclusion [i](#)



At the recommended contour level, 89% of all backbone atoms, 86% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary ⓘ

The table lists the average atom inclusion at the recommended contour level (0.0164) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.8620	 0.5700
A	 0.8363	 0.5550
B	 0.8354	 0.5590
C	 0.8388	 0.5620
D	 0.8293	 0.5530
E	 0.8958	 0.5830
F	 0.8912	 0.5840
G	 0.8947	 0.5840
H	 0.8987	 0.5850
I	 0.8335	 0.5570
J	 0.8326	 0.5580
K	 0.8445	 0.5640
L	 0.8293	 0.5520
M	 0.8935	 0.5840
N	 0.8935	 0.5830
O	 0.8900	 0.5870
P	 0.8987	 0.5870
Q	 0.8326	 0.5560
R	 0.8410	 0.5600
S	 0.8426	 0.5650
T	 0.8312	 0.5530
U	 0.8970	 0.5840
V	 0.8947	 0.5860
W	 0.8947	 0.5860
X	 0.8941	 0.5870

