



Full wwPDB X-ray Structure Validation Report ⓘ

Jun 23, 2024 – 10:06 PM EDT

PDB ID : 6Q8I
Title : Nterminal domain of human SMU1 in complex with human REDmid
Authors : Tengo, L.; Le Corre, L.; Fournier, G.; Ashraf, U.; Busca, P.; Rameix-Welti, M.-A.; Gravier-Pelletier, C.; Ruigrok, R.W.H.; Jacob, Y.; Vidalain, P.-O.; Pietrancosta, N.; Naffakh, N.; McCarthy, A.A.; Crepin, T.
Deposited on : 2018-12-14
Resolution : 3.17 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

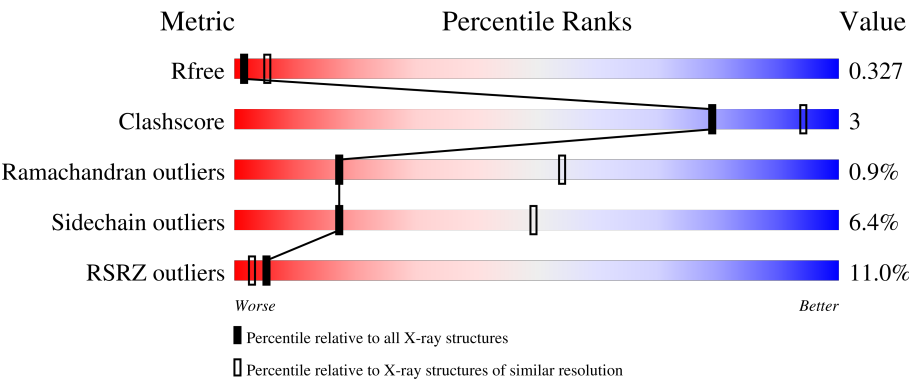
MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.20.1
EDS	:	2.37.1
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.37.1

1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 3.17 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	1467 (3.20-3.16)
Clashscore	141614	1599 (3.20-3.16)
Ramachandran outliers	138981	1574 (3.20-3.16)
Sidechain outliers	138945	1573 (3.20-3.16)
RSRZ outliers	127900	1423 (3.20-3.16)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	514	<div><div></div><div></div><div></div><div></div><div></div></div> <div>32% . 64%</div>
1	B	514	<div>2%</div> <div></div> <div></div> <div></div> <div></div>

32% . 65%

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Mol	Chain	Length	Quality of chain
1	J	514	<div><div><div></div><div></div><div></div></div><div>%</div><div>32%64%</div><div>••</div></div>
1	M	514	<div><div><div></div><div></div><div></div></div><div>15%</div><div>33%64%</div><div>•</div></div>
1	N	514	<div><div><div></div><div></div><div></div></div><div>8%</div><div>32%64%</div><div>•</div></div>
2	C	557	<div><div><div></div><div></div><div></div></div><div>5%••</div><div>93%</div></div>
2	D	557	<div><div><div></div><div></div><div></div></div><div>5%•</div><div>93%</div></div>
2	G	557	<div><div><div></div><div></div><div></div></div><div>7%•</div><div>92%</div></div>
2	H	557	<div><div><div></div><div></div><div></div></div><div>%</div><div>5%•</div><div>94%</div></div>
2	L	557	<div><div><div></div><div></div><div></div></div><div>5%•</div><div>93%</div></div>
2	O	557	<div><div><div></div><div></div><div></div></div><div>%</div><div>6%•</div><div>93%</div></div>
2	P	557	<div><div><div></div><div></div><div></div></div><div>3%</div><div>5%•</div><div>93%</div></div>
3	K	557	<div><div><div></div><div></div><div></div></div><div>6%•</div><div>93%</div></div>

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 13701 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called WD40 repeat-containing protein SMU1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	187	Total	C	N	O	S	0	0	0
			1473	933	253	282	5			
1	B	182	Total	C	N	O	S	0	0	0
			1388	877	243	264	4			
1	E	186	Total	C	N	O	S	0	0	0
			1475	934	255	281	5			
1	F	167	Total	C	N	O	S	0	0	0
			1284	814	222	244	4			
1	I	186	Total	C	N	O	S	0	0	0
			1475	934	255	281	5			
1	J	183	Total	C	N	O	S	0	0	0
			1408	890	245	269	4			
1	M	186	Total	C	N	O	S	0	0	0
			1470	931	255	280	4			
1	N	185	Total	C	N	O	S	0	0	0
			1398	882	246	265	5			

There are 16 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	0	MET	-	initiating methionine	UNP Q2TAY7
A	1	GLY	-	expression tag	UNP Q2TAY7
B	0	MET	-	initiating methionine	UNP Q2TAY7
B	1	GLY	-	expression tag	UNP Q2TAY7
E	0	MET	-	initiating methionine	UNP Q2TAY7
E	1	GLY	-	expression tag	UNP Q2TAY7
F	0	MET	-	initiating methionine	UNP Q2TAY7
F	1	GLY	-	expression tag	UNP Q2TAY7
I	0	MET	-	initiating methionine	UNP Q2TAY7
I	1	GLY	-	expression tag	UNP Q2TAY7
J	0	MET	-	initiating methionine	UNP Q2TAY7
J	1	GLY	-	expression tag	UNP Q2TAY7
M	0	MET	-	initiating methionine	UNP Q2TAY7

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Chain	Residue	Modelled	Actual	Comment	Reference
M	1	GLY	-	expression tag	UNP Q2TAY7
N	0	MET	-	initiating methionine	UNP Q2TAY7
N	1	GLY	-	expression tag	UNP Q2TAY7

- Molecule 2 is a protein called Protein Red.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	C	41	Total	C	N	O	S	0	0	0
			313	201	54	56	2			
2	D	37	Total	C	N	O	S	0	0	0
			274	179	44	49	2			
2	G	45	Total	C	N	O	S	0	0	0
			331	210	55	64	2			
2	H	36	Total	C	N	O	S	0	0	0
			257	165	40	50	2			
2	L	37	Total	C	N	O	S	0	0	0
			275	177	44	52	2			
2	O	39	Total	C	N	O	S	0	0	0
			271	175	49	45	2			
2	P	37	Total	C	N	O	S	0	0	0
			286	185	50	49	2			

There are 7 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
C	2	GLY	PRO	conflict	UNP Q13123
D	2	GLY	PRO	conflict	UNP Q13123
G	2	GLY	PRO	conflict	UNP Q13123
H	2	GLY	PRO	conflict	UNP Q13123
L	2	GLY	PRO	conflict	UNP Q13123
O	2	GLY	PRO	conflict	UNP Q13123
P	2	GLY	PRO	conflict	UNP Q13123

- Molecule 3 is a protein called Protein Red.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	K	40	Total	C	N	O	S	0	0	0
			323	210	53	58	2			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
K	2	GLY	PRO	conflict	UNP Q13123
K	257	LYS	ILE	conflict	UNP Q13123

VAL	ARG	ARG	PHE	SER	SER	GLY	LYS	ARG	GLY	GLY	ASP	PHE	VAL	CYS	CYS	ALA	LEU	SER	PRO	ARG	GLY	GLY	TRP	ILE	TYR	CYS	VAL	GLY	GLY	ASP	PHE	VAL	LEU	TYR	CYS	THR	PHE	SER	THR	VAL	HIS	GLY	LYS	ASP	VAL	ILE	GLY	ILE	ALA
HIS	PRO	HIS	GLN	ASN	LEU	ILE	ALA	THR	TYR	SER	GLY	ASP	GLY	VAL	LYS	LEU	LEU	TRP	LYS	PRO																													

● Molecule 1: WD40 repeat-containing protein SMU1

Chain E:  31% 5% 64%

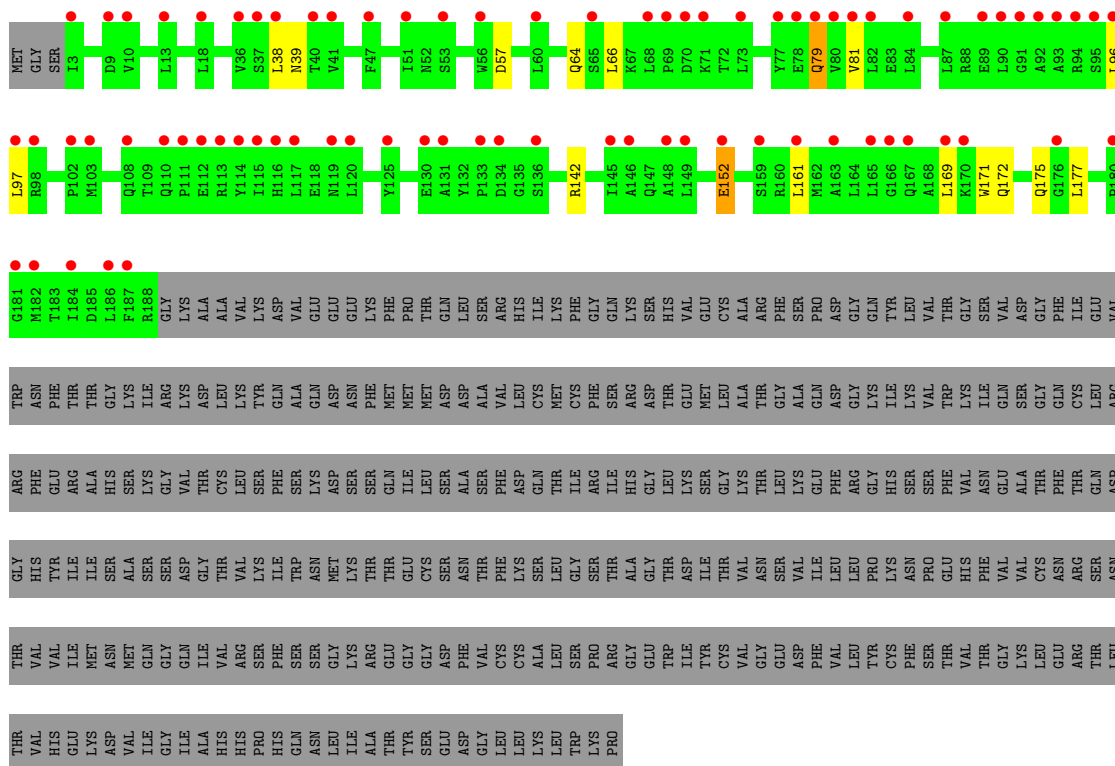
HIS	GLN	ASN	LEU	ILE	ALA	THR	THR	GLY	SER	GLY	ASP	PHE	VAL	CYS	LEU	LEU	LEU	TRP	LYS	PRO																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																									
PHE	SER	SER	GLY	LYS	ARG	GLY	GLY	ASP	PHE	VAL	GLY	THR	THR	VAL	CYS	LEU	LEU	PRO	SER	THR	ILE	THR	TYR	ILE	THR	CYS	VAL	GLY	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	

● Molecule 1: WD40 repeat-containing protein SMU1

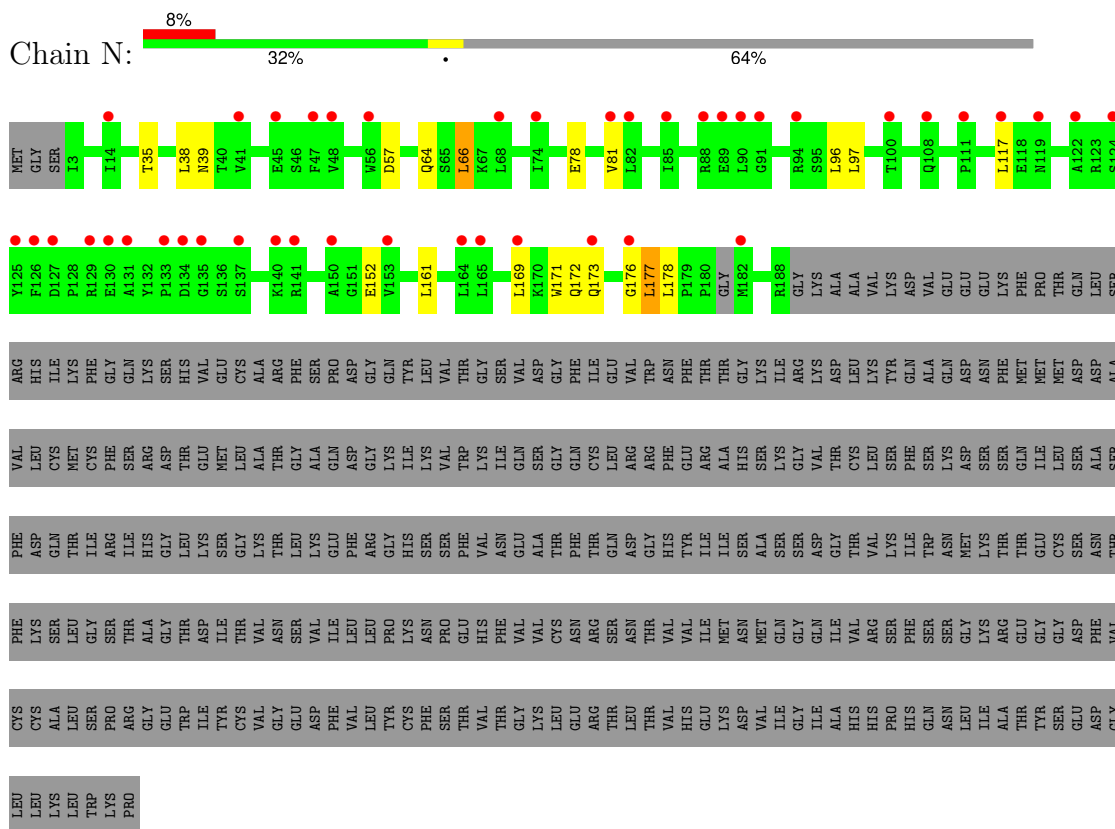
Chain F:  6% 29% 68%

GLY	ASP	ASP	GLN	THR	SER	THR	GLY	MET	THR	GLN	THR	GLY	ASP	ASP	ASP	GLN	THR	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY</
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Chain M:  15% 33% 64%



- Molecule 1: WD40 repeat-containing protein SMU1



- Molecule 2: Protein Red

93%

- Molecule 2: Protein Red

93%



- Molecule 2: Protein Red

Chain G: 7% 92%

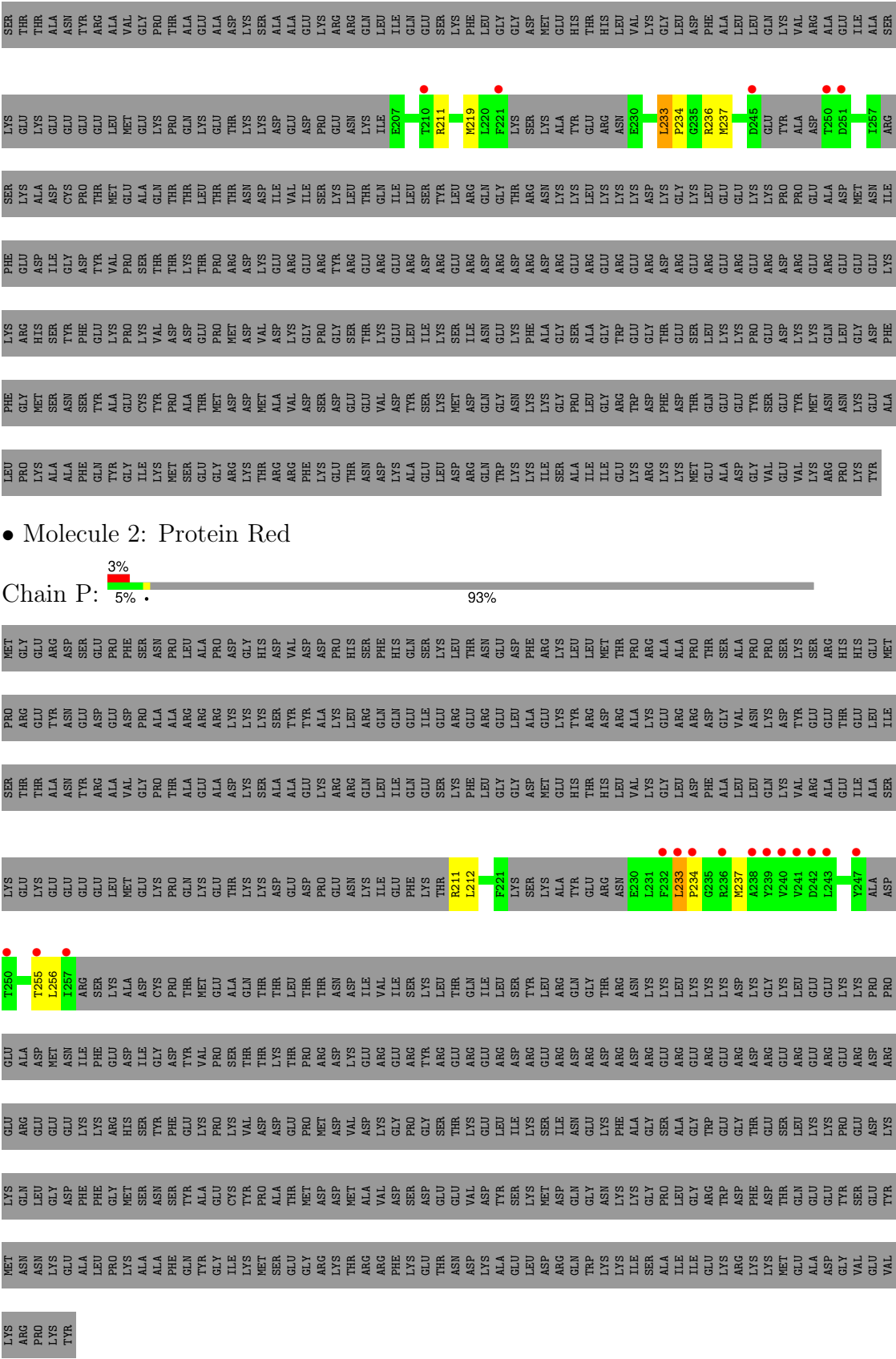
[illegible]

- Molecule 2: Protein Red

Chain H:  %

[illegible]





Chain K: 6% 93%

[illegible]

4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	127.98Å 68.16Å 145.30Å 90.00° 109.40° 90.00°	Depositor
Resolution (Å)	49.00 – 3.17 49.00 – 3.10	Depositor EDS
% Data completeness (in resolution range)	90.8 (49.00-3.17) 90.8 (49.00-3.10)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.44 (at 3.12Å)	Xtriage
Refinement program	BUSTER 2.10.2	Depositor
R, R_{free}	0.256 , 0.277 0.299 , 0.327	Depositor DCC
R_{free} test set	1940 reflections (4.92%)	wwPDB-VP
Wilson B-factor (Å ²)	66.5	Xtriage
Anisotropy	0.749	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.29 , 71.1	EDS
L-test for twinning ²	$\langle L \rangle = 0.43$, $\langle L^2 \rangle = 0.26$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.86	EDS
Total number of atoms	13701	wwPDB-VP
Average B, all atoms (Å ²)	132.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 7.40% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality [i](#)

5.1 Standard geometry [i](#)

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
1	A	0.39	0/1497	0.58	0/2032
1	B	0.39	0/1407	0.57	0/1912
1	E	0.39	0/1499	0.59	0/2034
1	F	0.38	0/1301	0.56	0/1766
1	I	0.39	0/1499	0.57	0/2034
1	J	0.39	0/1429	0.56	0/1942
1	M	0.38	0/1494	0.56	0/2028
1	N	0.39	0/1419	0.58	0/1931
2	C	0.44	0/317	0.80	1/428 (0.2%)
2	D	0.42	0/277	0.65	0/375
2	G	0.40	0/336	0.66	0/456
2	H	0.41	0/259	0.60	0/352
2	L	0.42	0/278	0.63	0/376
2	O	0.42	0/274	0.63	1/371 (0.3%)
2	P	0.41	0/289	0.61	0/389
3	K	0.43	0/327	0.69	1/440 (0.2%)
All	All	0.39	0/13902	0.59	3/18866 (0.0%)

There are no bond length outliers.

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	249	ASP	C-N-CA	7.05	139.31	121.70
3	K	236	ARG	C-N-CA	5.49	135.41	121.70
2	O	236	ARG	C-N-CA	5.32	135.00	121.70

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	1473	0	1494	12	0
1	B	1388	0	1376	6	0
1	E	1475	0	1502	13	0
1	F	1284	0	1280	10	0
1	I	1475	0	1502	8	0
1	J	1408	0	1399	9	0
1	M	1470	0	1490	7	0
1	N	1398	0	1373	7	0
2	C	313	0	288	4	0
2	D	274	0	252	3	0
2	G	331	0	283	3	0
2	H	257	0	225	2	0
2	L	275	0	248	4	0
2	O	271	0	232	1	0
2	P	286	0	274	3	0
3	K	323	0	313	3	0
All	All	13701	0	13531	76	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 3.

All (76) 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:D:233:LEU:HB3	2:D:234:PRO:HD3	1.54	0.88
2:D:233:LEU:HB3	2:D:234:PRO:CD	2.07	0.85
1:A:25:ARG:HD3	1:J:122:ALA:HB1	1.69	0.74
1:N:39:ASN:HA	1:N:66:LEU:HB3	1.67	0.73
2:P:233:LEU:HB3	2:P:234:PRO:CD	2.18	0.73
1:A:25:ARG:HD3	1:J:122:ALA:CB	2.21	0.70
1:B:39:ASN:HA	1:B:66:LEU:HB3	1.73	0.70
1:F:39:ASN:HA	1:F:66:LEU:HB3	1.74	0.68
1:J:186:LEU:H	1:J:186:LEU:HD23	1.61	0.66
1:J:39:ASN:HA	1:J:66:LEU:HB3	1.78	0.64
1:M:171:TRP:HB2	1:N:171:TRP:HB2	1.82	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:171:TRP:HB2	1:F:171:TRP:HB2	1.83	0.60
1:A:13:LEU:HD11	1:B:186:LEU:HD13	1.83	0.60
1:I:171:TRP:HB2	1:J:171:TRP:HB2	1.83	0.59
2:P:233:LEU:HB3	2:P:234:PRO:HD2	1.83	0.58
1:A:39:ASN:HA	1:A:66:LEU:HB3	1.87	0.57
1:M:161:LEU:HD11	1:N:161:LEU:HD11	1.88	0.56
1:A:171:TRP:HB2	1:B:171:TRP:HB2	1.89	0.55
2:P:211:ARG:HG3	2:P:212:LEU:H	1.73	0.54
2:D:221:PHE:HD1	1:J:99:GLN:HE21	1.57	0.53
1:E:161:LEU:HD11	1:F:161:LEU:HD11	1.90	0.52
3:K:236:ARG:HB2	3:K:238:ALA:HB2	1.93	0.51
2:C:249:ASP:CB	2:C:250:THR:HB	2.41	0.51
1:E:81:VAL:HG11	1:E:97:LEU:HD13	1.94	0.50
2:H:239:TYR:HB3	2:H:252:ILE:HG21	1.94	0.49
2:O:233:LEU:CB	2:O:234:PRO:HD2	2.43	0.48
1:I:81:VAL:HG11	1:I:97:LEU:HD13	1.96	0.48
1:N:81:VAL:HG11	1:N:97:LEU:HD13	1.96	0.48
1:E:13:LEU:HD11	1:F:186:LEU:HD13	1.96	0.48
1:A:81:VAL:HG11	1:A:97:LEU:HD13	1.96	0.47
1:E:49:ALA:HB1	2:L:236:ARG:HH12	1.79	0.47
1:E:87:LEU:HD22	2:G:210:THR:HG21	1.95	0.47
1:M:79:GLN:HE22	1:M:142:ARG:HG3	1.80	0.47
1:B:81:VAL:HG11	1:B:97:LEU:HD13	1.97	0.47
1:J:81:VAL:HG11	1:J:97:LEU:HD13	1.96	0.47
1:A:161:LEU:HD11	1:B:161:LEU:HD11	1.97	0.47
1:M:81:VAL:HG11	1:M:97:LEU:HD13	1.96	0.46
2:H:240:VAL:O	2:H:253:PRO:HD2	2.16	0.45
1:E:9:ASP:HB3	1:F:186:LEU:HD12	1.97	0.45
1:E:136:SER:HA	1:E:140:LYS:HD3	1.99	0.45
1:N:176:GLY:HA2	1:N:177:LEU:CB	2.46	0.45
1:M:39:ASN:HB3	1:M:152:GLU:O	2.17	0.45
1:A:16:GLN:HA	1:A:38:LEU:HD11	1.98	0.45
1:A:157:PRO:HB2	1:A:160:ARG:HD3	1.98	0.44
2:L:234:PRO:HA	2:L:235:GLY:HA2	1.83	0.44
2:C:248:ALA:HA	2:C:249:ASP:HA	1.70	0.43
1:I:157:PRO:HB2	1:I:160:ARG:HD3	2.01	0.42
1:B:169:LEU:HA	1:B:172:GLN:HB2	2.02	0.42
1:F:78:GLU:HG3	1:F:117:LEU:HD11	2.01	0.42
1:I:169:LEU:HA	1:I:172:GLN:HB2	2.01	0.42
1:M:172:GLN:HB3	1:M:177:LEU:HD12	2.01	0.42
1:A:169:LEU:HA	1:A:172:GLN:HB2	2.02	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:169:LEU:HA	1:F:172:GLN:HB2	2.01	0.42
1:E:51:ILE:HD13	1:E:146:ALA:HA	2.02	0.42
1:I:172:GLN:HB3	1:I:177:LEU:HD12	2.02	0.42
3:K:231:LEU:HG	3:K:237:MET:HG2	2.02	0.42
1:M:169:LEU:HA	1:M:172:GLN:HB2	2.02	0.41
1:E:169:LEU:HA	1:E:172:GLN:HB2	2.01	0.41
1:J:169:LEU:HA	1:J:172:GLN:HB2	2.01	0.41
2:C:239:TYR:CE1	2:C:254:THR:HG22	2.56	0.41
1:F:170:LYS:HG2	2:G:243:LEU:HA	2.02	0.41
1:N:169:LEU:HA	1:N:172:GLN:HB2	2.02	0.41
2:C:250:THR:HA	2:C:251:ASP:HA	1.67	0.41
1:F:66:LEU:H	1:F:66:LEU:HG	1.76	0.41
1:A:109:THR:HG22	2:G:230:GLU:HB2	2.02	0.41
1:E:186:LEU:HD12	1:F:5:ILE:HG21	2.02	0.41
1:I:66:LEU:H	1:I:66:LEU:HG	1.76	0.41
2:L:232:PHE:O	2:L:234:PRO:HA	2.21	0.41
1:N:78:GLU:HG3	1:N:117:LEU:HD11	2.03	0.41
1:I:94:ARG:HG2	1:I:121:LEU:HD21	2.02	0.40
1:I:161:LEU:HD11	1:J:161:LEU:HD11	2.03	0.40
1:A:172:GLN:HB3	1:A:177:LEU:HD12	2.03	0.40
1:E:78:GLU:HG3	1:E:117:LEU:HD11	2.04	0.40
3:K:239:TYR:CE1	3:K:254:THR:HG22	2.56	0.40
1:E:172:GLN:HB3	1:E:177:LEU:HD12	2.02	0.40
2:L:240:VAL:O	2:L:253:PRO:HD2	2.20	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	A	185/514 (36%)	178 (96%)	7 (4%)	0	100 100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	B	176/514 (34%)	170 (97%)	6 (3%)	0	100	100
1	E	184/514 (36%)	176 (96%)	6 (3%)	2 (1%)	14	50
1	F	157/514 (30%)	152 (97%)	5 (3%)	0	100	100
1	I	184/514 (36%)	177 (96%)	6 (3%)	1 (0%)	29	66
1	J	179/514 (35%)	174 (97%)	4 (2%)	1 (1%)	25	63
1	M	184/514 (36%)	177 (96%)	7 (4%)	0	100	100
1	N	181/514 (35%)	173 (96%)	6 (3%)	2 (1%)	14	50
2	C	35/557 (6%)	27 (77%)	5 (14%)	3 (9%)	1	4
2	D	31/557 (6%)	27 (87%)	3 (10%)	1 (3%)	4	23
2	G	41/557 (7%)	30 (73%)	10 (24%)	1 (2%)	6	31
2	H	30/557 (5%)	27 (90%)	3 (10%)	0	100	100
2	L	31/557 (6%)	26 (84%)	4 (13%)	1 (3%)	4	23
2	O	33/557 (6%)	27 (82%)	4 (12%)	2 (6%)	1	10
2	P	31/557 (6%)	28 (90%)	2 (6%)	1 (3%)	4	23
3	K	34/557 (6%)	30 (88%)	3 (9%)	1 (3%)	4	26
All	All	1696/8568 (20%)	1599 (94%)	81 (5%)	16 (1%)	17	54

All (16) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	D	233	LEU
2	G	246	GLU
2	L	233	LEU
2	C	234	PRO
2	C	237	MET
1	E	182	MET
2	P	233	LEU
2	C	250	THR
1	N	178	LEU
2	O	237	MET
3	K	237	MET
1	N	177	LEU
1	I	182	MET
1	J	39	ASN
2	O	233	LEU
1	E	176	GLY

5.3.2 Protein sidechains ⓘ

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	162/450 (36%)	154 (95%)	8 (5%)	25	59
1	B	146/450 (32%)	139 (95%)	7 (5%)	25	60
1	E	163/450 (36%)	157 (96%)	6 (4%)	34	67
1	F	138/450 (31%)	130 (94%)	8 (6%)	20	53
1	I	163/450 (36%)	155 (95%)	8 (5%)	25	59
1	J	150/450 (33%)	141 (94%)	9 (6%)	19	51
1	M	161/450 (36%)	153 (95%)	8 (5%)	24	58
1	N	145/450 (32%)	137 (94%)	8 (6%)	21	55
2	C	30/497 (6%)	24 (80%)	6 (20%)	1	6
2	D	26/497 (5%)	21 (81%)	5 (19%)	1	7
2	G	30/497 (6%)	26 (87%)	4 (13%)	4	17
2	H	24/497 (5%)	22 (92%)	2 (8%)	11	38
2	L	27/497 (5%)	24 (89%)	3 (11%)	6	24
2	O	21/497 (4%)	19 (90%)	2 (10%)	8	30
2	P	28/497 (6%)	25 (89%)	3 (11%)	6	25
3	K	34/497 (7%)	29 (85%)	5 (15%)	3	14
All	All	1448/7576 (19%)	1356 (94%)	92 (6%)	17	49

All (92) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	38	LEU
1	A	64	GLN
1	A	66	LEU
1	A	72	THR
1	A	79	GLN
1	A	96	LEU
1	A	152	GLU
1	A	175	GLN

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Mol	Chain	Res	Type
1	B	35	THR
1	B	38	LEU
1	B	57	ASP
1	B	64	GLN
1	B	66	LEU
1	B	96	LEU
1	B	152	GLU
2	C	211	ARG
2	C	219	MET
2	C	236	ARG
2	C	244	ASP
2	C	251	ASP
2	C	256	LEU
2	D	219	MET
2	D	233	LEU
2	D	237	MET
2	D	256	LEU
2	D	257	ILE
1	E	38	LEU
1	E	64	GLN
1	E	66	LEU
1	E	96	LEU
1	E	152	GLU
1	E	175	GLN
1	F	35	THR
1	F	38	LEU
1	F	57	ASP
1	F	64	GLN
1	F	66	LEU
1	F	96	LEU
1	F	152	GLU
1	F	177	LEU
2	G	211	ARG
2	G	214	ARG
2	G	219	MET
2	G	249	ASP
2	H	219	MET
2	H	254	THR
1	I	38	LEU
1	I	57	ASP
1	I	64	GLN
1	I	66	LEU

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Mol	Chain	Res	Type
1	I	79	GLN
1	I	96	LEU
1	I	152	GLU
1	I	175	GLN
1	J	2	SER
1	J	35	THR
1	J	38	LEU
1	J	57	ASP
1	J	64	GLN
1	J	66	LEU
1	J	96	LEU
1	J	152	GLU
1	J	186	LEU
3	K	219	MET
3	K	236	ARG
3	K	237	MET
3	K	251	ASP
3	K	256	LEU
2	L	219	MET
2	L	220	LEU
2	L	254	THR
1	M	38	LEU
1	M	57	ASP
1	M	64	GLN
1	M	66	LEU
1	M	79	GLN
1	M	96	LEU
1	M	152	GLU
1	M	175	GLN
1	N	35	THR
1	N	38	LEU
1	N	57	ASP
1	N	64	GLN
1	N	66	LEU
1	N	96	LEU
1	N	152	GLU
1	N	173	GLN
2	O	211	ARG
2	O	219	MET
2	P	237	MET
2	P	255	THR
2	P	256	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (17) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	110	GLN
1	A	175	GLN
1	B	110	GLN
1	E	110	GLN
1	E	175	GLN
1	F	21	ASN
1	F	79	GLN
1	F	110	GLN
1	I	110	GLN
1	I	175	GLN
1	J	108	GLN
1	M	39	ASN
1	M	64	GLN
1	M	79	GLN
1	N	108	GLN
1	N	110	GLN
1	N	173	GLN

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 ⓘ

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

In the following table, the column labelled ‘#RSRZ > 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q < 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	187/514 (36%)	-0.14	1 (0%) 91 86	40, 70, 104, 118	0
1	B	182/514 (35%)	0.33	9 (4%) 29 16	52, 116, 215, 236	1 (0%)
1	E	186/514 (36%)	-0.14	0 100 100	44, 70, 106, 135	0
1	F	167/514 (32%)	0.86	31 (18%) 1 0	68, 176, 238, 250	1 (0%)
1	I	186/514 (36%)	0.12	4 (2%) 62 48	57, 89, 131, 149	0
1	J	183/514 (35%)	0.10	3 (1%) 72 59	62, 100, 174, 198	1 (0%)
1	M	186/514 (36%)	1.92	78 (41%) 0 0	167, 239, 278, 288	0
1	N	185/514 (35%)	1.23	43 (23%) 0 0	128, 219, 269, 283	1 (0%)
2	C	41/557 (7%)	-0.11	0 100 100	59, 72, 100, 124	0
2	D	37/557 (6%)	-0.12	1 (2%) 54 39	49, 79, 129, 153	0
2	G	45/557 (8%)	-0.20	0 100 100	39, 81, 100, 104	0
2	H	36/557 (6%)	0.28	6 (16%) 1 1	56, 75, 248, 253	0
2	L	37/557 (6%)	0.04	0 100 100	78, 100, 126, 152	0
2	O	39/557 (7%)	0.78	5 (12%) 3 2	142, 192, 248, 261	0
2	P	37/557 (6%)	1.23	14 (37%) 0 0	89, 232, 251, 256	0
3	K	40/557 (7%)	-0.24	0 100 100	68, 85, 110, 142	0
All	All	1774/8568 (20%)	0.47	195 (10%) 5 3	39, 102, 252, 288	4 (0%)

All (195) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	N	134	ASP	11.4
1	M	149	LEU	9.5
1	M	41	VAL	7.2
1	N	90	LEU	6.8
1	M	92	ALA	6.6

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Mol	Chain	Res	Type	RSRZ
1	M	68	LEU	6.5
1	M	115	ILE	6.5
1	N	130	GLU	5.9
1	N	108	GLN	5.8
1	N	135	GLY	5.6
2	P	257	ILE	5.3
1	F	81	VAL	5.2
1	M	182	MET	4.9
1	N	137	SER	4.9
1	M	37	SER	4.9
1	M	51	ILE	4.9
1	M	134	ASP	4.9
1	F	147	GLN	4.8
1	M	120	LEU	4.8
1	M	110	GLN	4.7
1	F	63	ILE	4.6
1	F	145	ILE	4.6
1	M	117	LEU	4.6
1	N	111	PRO	4.5
1	M	96	LEU	4.5
2	P	239	TYR	4.5
1	M	145	ILE	4.4
1	M	40	THR	4.4
1	N	85	ILE	4.4
1	M	77	TYR	4.4
1	N	125	TYR	4.3
1	M	184	ILE	4.3
1	M	94	ARG	4.3
1	M	36	VAL	4.3
1	N	119	ASN	4.3
1	F	57	ASP	4.1
1	M	165	LEU	4.0
1	M	180	PRO	4.0
1	M	170	LYS	4.0
1	M	90	LEU	4.0
1	F	144	ALA	3.9
1	M	181	GLY	3.9
1	F	153	VAL	3.8
1	M	113	ARG	3.7
1	F	127	ASP	3.7
1	M	108	GLN	3.7
1	M	38	LEU	3.7

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Mol	Chain	Res	Type	RSRZ
1	M	102	PRO	3.7
2	O	251	ASP	3.7
1	N	133	PRO	3.6
1	N	182	MET	3.6
1	N	82	LEU	3.6
1	M	70	ASP	3.5
1	M	148	ALA	3.5
1	M	136	SER	3.5
1	B	134	ASP	3.5
1	M	89	GLU	3.5
1	N	153	VAL	3.5
1	M	146	ALA	3.4
1	M	112	GLU	3.4
2	O	245	ASP	3.4
1	M	95	SER	3.4
1	F	99	GLN	3.4
2	H	213	GLY	3.4
2	P	240	VAL	3.4
1	B	113	ARG	3.4
1	M	82	LEU	3.4
1	M	3	ILE	3.3
1	F	56	TRP	3.3
1	N	173	GLN	3.3
1	B	104	ILE	3.3
1	M	73	LEU	3.3
1	M	56	TRP	3.2
1	F	67	LYS	3.2
1	F	83	GLU	3.2
1	I	134	ASP	3.2
1	M	131	ALA	3.1
1	F	141	ARG	3.1
1	N	94	ARG	3.1
1	N	165	LEU	3.1
2	P	247	TYR	3.0
1	F	60	LEU	3.0
1	F	120	LEU	3.0
1	N	74	ILE	3.0
2	H	216	VAL	3.0
2	P	238	ALA	3.0
1	N	140	LYS	3.0
2	O	221	PHE	2.9
2	H	211	ARG	2.9

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Mol	Chain	Res	Type	RSRZ
1	N	164	LEU	2.9
1	N	176	GLY	2.9
1	B	124	SER	2.9
2	P	242	ASP	2.9
1	N	150	ALA	2.9
1	F	131	ALA	2.8
1	M	163	ALA	2.8
2	P	255	THR	2.8
1	M	125	TYR	2.8
1	M	87	LEU	2.8
1	M	91	GLY	2.8
1	F	102	PRO	2.8
1	N	41	VAL	2.8
1	F	104	ILE	2.8
1	M	13	LEU	2.7
1	M	47	PHE	2.7
1	M	133	PRO	2.7
1	M	152	GLU	2.7
2	H	212	LEU	2.7
2	P	241	VAL	2.7
1	M	119	ASN	2.7
1	N	68	LEU	2.7
1	M	169	LEU	2.7
1	F	117	LEU	2.7
1	B	117	LEU	2.6
1	I	125	TYR	2.6
2	P	233	LEU	2.6
1	M	81	VAL	2.6
1	M	130	GLU	2.6
1	M	60	LEU	2.6
1	N	131	ALA	2.6
1	N	141	ARG	2.6
1	F	62	ALA	2.6
1	M	98	ARG	2.6
1	M	53	SER	2.6
1	F	150	ALA	2.5
1	M	10	VAL	2.5
1	N	91	GLY	2.5
1	M	97	LEU	2.5
1	N	100	THR	2.5
1	M	78	GLU	2.5
1	N	81	VAL	2.5

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Mol	Chain	Res	Type	RSRZ
1	F	68	LEU	2.5
1	M	71	LYS	2.5
1	B	115	ILE	2.5
1	J	104	ILE	2.5
1	B	89	GLU	2.4
1	F	92	ALA	2.4
1	M	9	ASP	2.4
1	F	135	GLY	2.4
1	N	122	ALA	2.4
1	J	112	GLU	2.4
1	M	187	PHE	2.4
2	O	250	THR	2.4
2	P	234	PRO	2.4
1	N	14	ILE	2.4
1	M	18	LEU	2.4
1	N	129	ARG	2.4
1	M	69	PRO	2.4
1	F	105	MET	2.3
2	P	236	ARG	2.3
1	F	133	PRO	2.3
1	M	84	LEU	2.3
1	N	124	SER	2.3
1	M	176	GLY	2.3
1	M	111	PRO	2.3
1	F	110	GLN	2.3
1	M	114	TYR	2.3
1	M	65	SER	2.3
1	M	159	SER	2.3
1	M	166	GLY	2.3
1	N	56	TRP	2.3
1	N	127	ASP	2.2
1	B	81	VAL	2.2
1	F	55	HIS	2.2
1	F	98	ARG	2.2
1	F	116	HIS	2.2
2	P	243	LEU	2.2
2	D	221	PHE	2.2
1	M	103	MET	2.2
1	N	169	LEU	2.2
2	O	210	THR	2.2
1	M	186	LEU	2.2
1	M	167	GLN	2.2

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Mol	Chain	Res	Type	RSRZ
1	F	132	TYR	2.1
1	I	178	LEU	2.1
1	I	181	GLY	2.1
1	M	116	HIS	2.1
1	N	47	PHE	2.1
1	J	117	LEU	2.1
1	M	80	VAL	2.1
1	M	161	LEU	2.1
1	N	126	PHE	2.1
2	H	218	ARG	2.1
2	P	250	THR	2.1
1	N	88	ARG	2.1
1	A	178	LEU	2.1
1	N	48	VAL	2.1
1	M	93	ALA	2.0
1	B	78	GLU	2.0
2	H	219	MET	2.0
1	N	45	GLU	2.0
1	N	89	GLU	2.0
1	N	117	LEU	2.0
2	P	232	PHE	2.0
1	M	79	GLN	2.0

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

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

6.3 Carbohydrates [i](#)

There are no monosaccharides in this entry.

6.4 Ligands [i](#)

There are no ligands in this entry.

6.5 Other polymers [i](#)

There are no such residues in this entry.