



wwPDB X-ray Structure Validation Summary Report ⓘ

Feb 28, 2026 – 11:02 PM UTC

PDB ID : 6Q8I / pdb_00006q8i
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 wwPDB X-ray Structure Validation Summary 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 : 4-5-2 with Phenix2.0
Xtriage (Phenix) : 2.0
EDS : 3.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4 : 9.0.010 (Gargrove)
Density-Fitness : 1.0.12
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

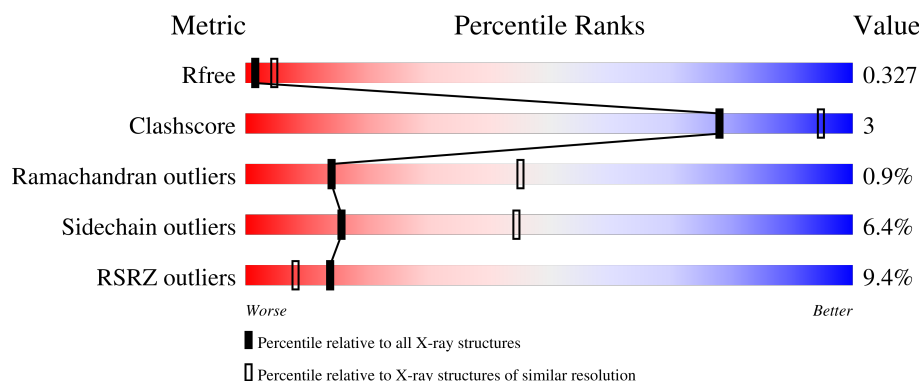
1 Overall quality at a glance

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}	180053	2001 (3.20-3.16)
Clashscore	190562	2119 (3.20-3.16)
Ramachandran outliers	187476	2070 (3.20-3.16)
Sidechain outliers	187428	2069 (3.20-3.16)
RSRZ outliers	180081	2001 (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	
1	B	514	
1	E	514	
1	F	514	
1	I	514	

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

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.

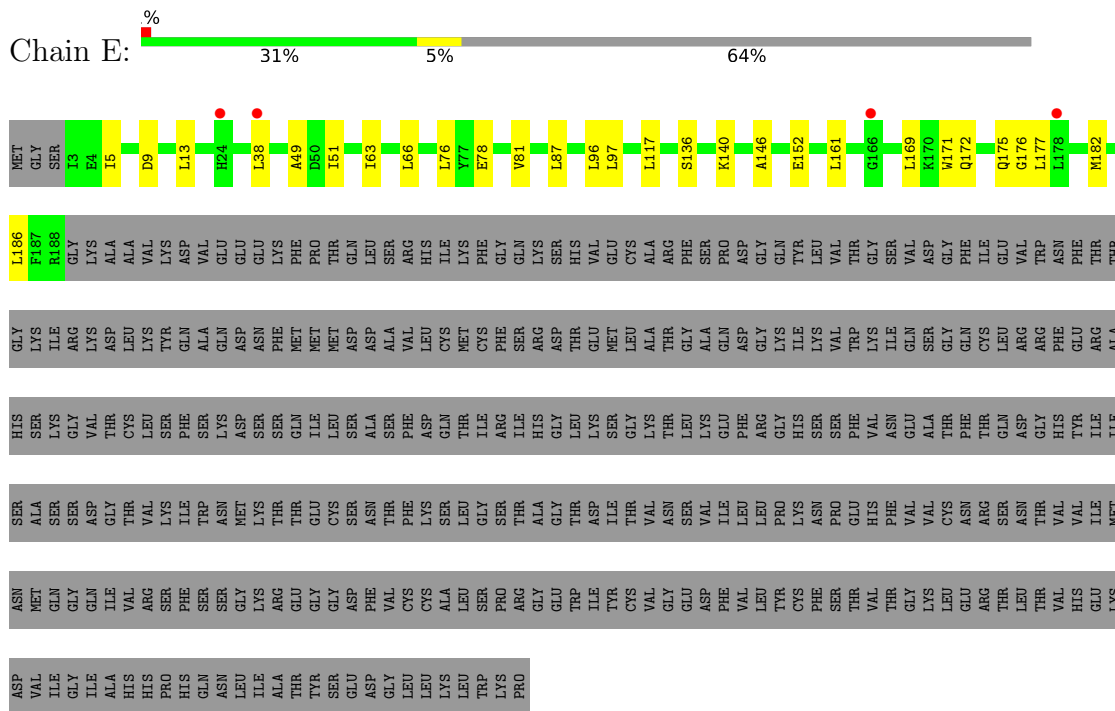
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	K	40	Total	C	N	O	S	0	0	0
			323	210	53	58	2			

There are 2 discrepancies between the modelled and reference sequences:

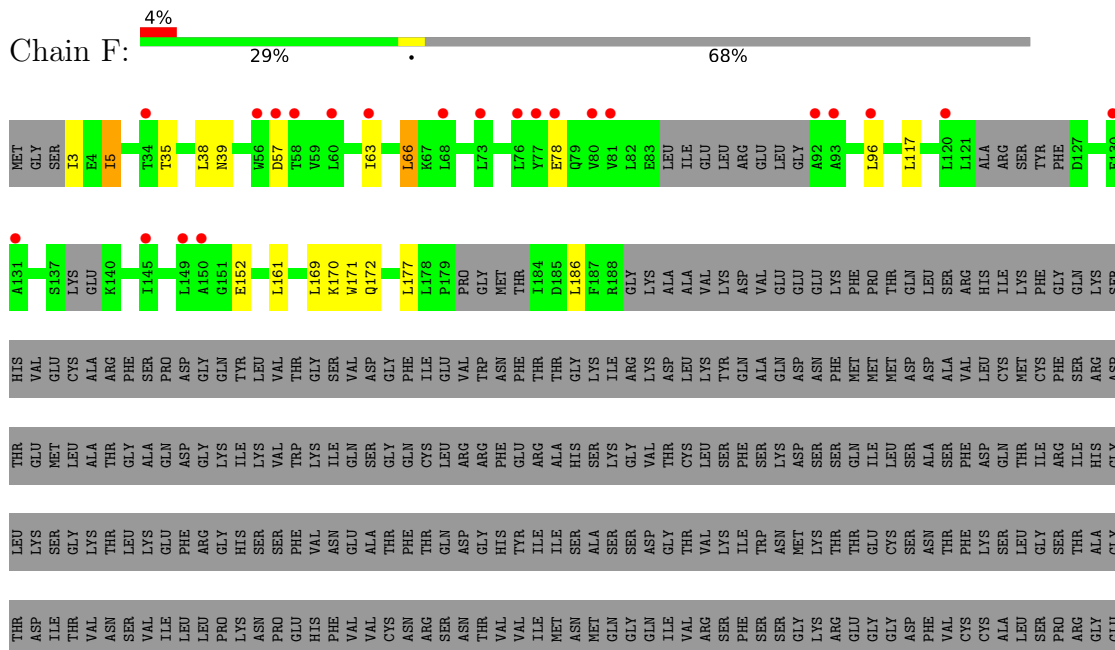
Chain	Residue	Modelled	Actual	Comment	Reference
K	2	GLY	PRO	conflict	UNP Q13123
K	257	LYS	ILE	conflict	UNP Q13123

[illegible]

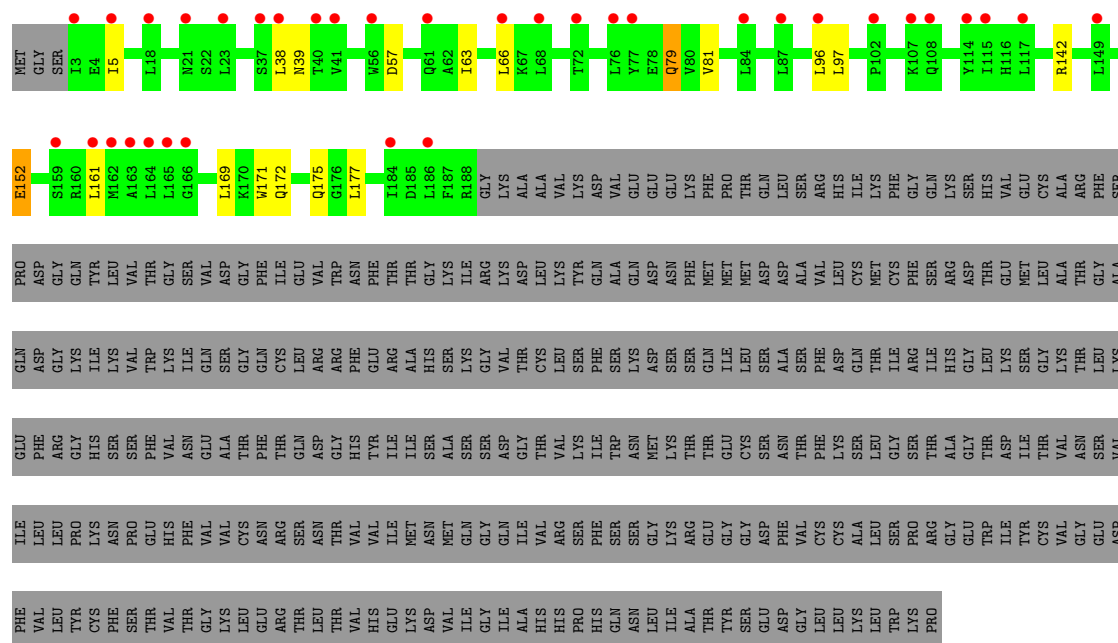
- Molecule 1: WD40 repeat-containing protein SMU1



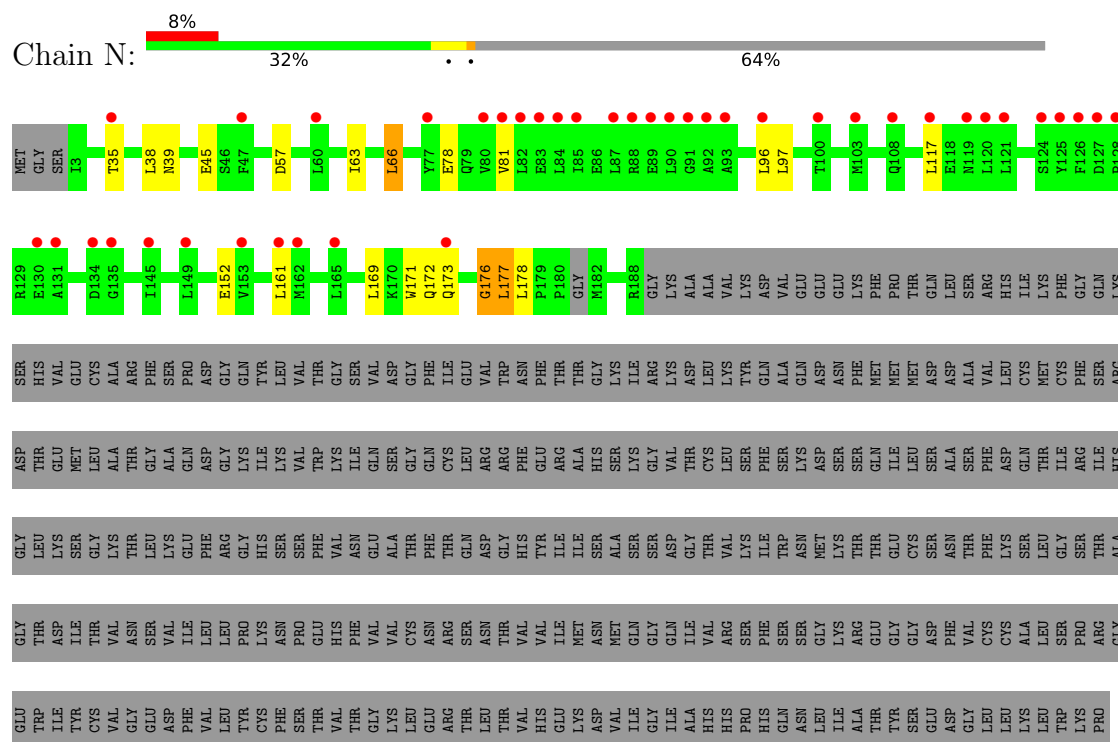
- Molecule 1: WD40 repeat-containing protein SMU1



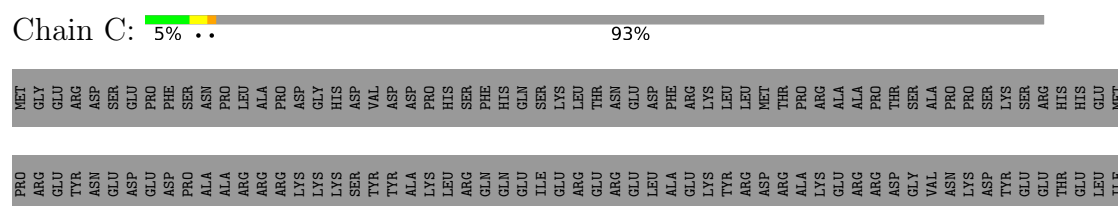




• Molecule 1: WD40 repeat-containing protein SMU1



• Molecule 2: Protein Red



- Molecule 2: Protein Red

92%

- Molecule 2: Protein Red

94%



[illegible]

- Molecule 2: Protein Red



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

- Molecule 2: Protein Red



MET	GLY	GLU	ARG	ASP	SER	GLU	PRO	PHE	SER	ASN	PRO	LEU	ALA	ASP	GLY	HIS	ASP	VAL	ASP	PRO	HIS	SER	LYS	LEU	THR	GLN	ASN	GLU	ASP	PHE	ARG	LYS	LEU	LEU	MET	THR	PRO	ARG	ALA	ALA	PRO	THR	SER	LYS	SER	ARG	HIS	HIS	GLU	MET
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PRO	ARG	GLU	TYR	ASN	GLU	ASP	GLU	ASP	PRO	ALA	ALA	ARG	ARG	ARG	LYS	LYS	SER	TYR	TYR	LYS	LEU	ARG	GLN	GLN	ILE	ILE	GLU	ARG	GLU	ARG	GLU	LEU	ALA	ALA	ARG	ASP	ASP	ARG	ALA	LYS	GLU	ARG	GLY	VAL	ASN	ASP	LYS	TYR	GLU	GLU	THR	GLU	LEU	ILE
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SER	THR	THR	ALA	ASN	TYR	ARG	ALA	VAL	GLY	PRO	THR	ALA	GLU	ALA	ASP	LYS	SER	ALA	ALA	GLU	GLY	ARG	ARG	GLN	LEU	ILE	LEU	GLN	GLU	SER	LYS	PHE	LEU	GLY	GLY	GLY	ASP	ASP	NET	GLU	GLU	HIS	HIS	THR	THR	LEU	VAL	LEU	LYS	GLY	GLN	LEU	LEU	ASP	PHE	ALA	ALA	ARG	ALA	GLU	ILE	LEU	ALA	SER
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LYS	GLU	LYS	GLU	GLU	GLU	GLU	LEU	MET	GLU	LYS	PRO	GLN	LYS	GLU	THR	LYS	LYS	ASP	GLU	ASP	PRO	GLU	ASN	LYS	ILE	E207	F221	LYS	SER	ALA	TYR	GLU	ARG	ASN	E230	E231	L233	P234	G236	R235	M237	D245	GLU	TYR	ALA	ASP	T250	D251	T257	ARG	SER	LYS	ALA	ASP
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- Molecule 2: Protein Red



ARG	ASN	GLN	ARG	ALA	LYS	SER	PRO	MET
PRO	ASN	LEU	GLU	ASP	GLU	THR	ARG	GLY
LYS	LYS	GLY	GLU	MET	LYS	THR	GLU	GLU
TYR	GLU	ASP	GLU	ASN	GLU	ALA	TYR	ASN
	ALA	PHE	LYS	ILE	ARG	ARG	GLU	SER
	LEU	PHE	ARG	PHE	SER	TYR	GLU	GLY
	PRO	GLY	ARG	GLU	LYS	ARG	ASP	GLU
	LYS	MET	HIS	ASP	ALA	ALA	GLU	PRO
	ALA	SER	SER	ILE	MET	VAL	ASP	PHE
	ALA	ASN	TYR	GLY	CYS	GLY	PRO	SER
	PHE	SER	PHE	ASP	LYS	GLY	ALA	ASN
	GLN	TYR	GLU	TYR	PRO	THR	THR	PRO
	TYR	ALA	LYS	VAL	GLN	ALA	ALA	ARG
	GLY	GLU	PRO	PRO	LYS	GLU	ARG	ARG
	ILE	CYS	LYS	SER	THR	ALA	ALA	PRO
	LYS	TYR	VAL	THR	GLN	LYS	LYS	ASP
	MET	PRO	ASP	THR	LYS	ASP	LYS	GLY
	SER	ALA	ASP	LYS	THR	SER	LYS	HIS
	GLU	THR	GLU	THR	LYS	ALA	ALA	LEU
	GLY	MET	GLY	THR	ASP	GLU	ARG	ASP
	ARG	MET	PRO	PRO	GLU	ALA	TYR	VAL
	ASP	ASP	MET	ARG	ASP	GLU	TYR	ASP
	LYS	ASP	ASP	ASP	PRO	LYS	LYS	ASP
	THR	MET	VAL	LYS	GLU	ARG	LYS	PRO
	ALA	ASP	VAL	GLU	ILE	ARG	LEU	HIS
	ARG	VAL	LYS	ARG	LYS	GLN	LEU	SER
	PHE	ASP	GLY	GLU	ILE	LEU	GLN	PHE
	LYS	SER	PRO	ARG	ILE	GLN	GLN	HIS
	GLU	ASP	GLY	TYR	PHE	GLY	GLU	GLN
	THR	GLU	SER	ARG	LYS	GLU	ILE	SER
	ASN	GLU	THR	GLU	THR	SER	GLU	LYS
	LYS	VAL	LYS	ARG	THR	LYS	ARG	LEU
	ASP	ASP	ILE	GLU	LEU	ASP	ALA	ASP
	GLN	ARG	ILE	ARG	SER	MET	GLU	PHE
	TRP	GLY	GLU	ARG	TYR	GLU	LYS	LYS
	LYS	LYS	PHE	ARG	ARG	THR	ASP	LEU
	ILE	LYS	ALA	ASP	ASN	ARG	ASP	MET
	SER	GLY	GLY	ARG	LYS	LEU	VAL	THR
	ALA	PRO	SER	GLU	LYS	VAL	ALA	PRO
	ILE	LEU	ALA	ARG	LYS	GLY	GLU	ARG
	ILE	GLY	ILE	GLU	F232	GLY	ALA	ALA
	GLU	ARG	TRP	ARG	P234	ASP	ARG	PRO
	LYS	TRP	GLU	GLU	LYS	PHE	THR	SER
	ARG	ASP	GLY	ARG	W237	ALA	GLY	THR
	LYS	PHE	THR	ASP	A238	LEU	VAL	THR
	LYS	ASP	GLU	ARG	Y239	GLY	ASN	PRO
	MET	THR	SER	GLU	V240	LYS	GLN	PRO
	GLU	GLN	LEU	ARG	V241	LYS	ASP	SER
	ALA	GLU	LYS	GLU	GLU	VAL	TYR	LYS
	ASP	GLU	LYS	ARG	GLU	ARG	GLU	ARG
	GLY	TYR	PRO	GLU	E246	LYS	GLU	SER
	VAL	SER	GLU	ARG	Y247	LYS	THR	HIS
	GLU	GLU	ASP	ASP	ALA	ILE	GLU	HIS
	VAL	TYR	LYS	GLU	ASP	SER	LEU	MET
	TYR	MET	THR	GLU	W249	THR	LEU	GLY

- Molecule 3: Protein Red

[illegible]

[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 – 3.17	Depositor EDS
% Data completeness (in resolution range)	90.8 (49.00-3.17) 90.7 (49.00-3.17)	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)	0.30 , 112.3	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	0.75	0/1497	1.38	1/2032 (0.0%)
1	B	0.73	0/1407	1.39	0/1912
1	E	0.75	0/1499	1.40	0/2034
1	F	0.73	0/1301	1.36	0/1766
1	I	0.75	0/1499	1.39	3/2034 (0.1%)
1	J	0.73	0/1429	1.39	0/1942
1	M	0.75	0/1494	1.37	0/2028
1	N	0.74	0/1419	1.42	3/1931 (0.2%)
2	C	0.76	0/317	1.46	4/428 (0.9%)
2	D	0.78	0/277	1.26	2/375 (0.5%)
2	G	0.76	0/336	1.29	2/456 (0.4%)
2	H	0.76	0/259	1.28	1/352 (0.3%)
2	L	0.78	0/278	1.14	0/376
2	O	0.81	0/274	1.27	2/371 (0.5%)
2	P	0.74	0/289	1.24	4/389 (1.0%)
3	K	0.81	0/327	1.34	4/440 (0.9%)
All	All	0.75	0/13902	1.37	26/18866 (0.1%)

There are no bond length outliers.

The worst 5 of 26 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	249	ASP	CA-C-N	9.79	139.31	121.70
2	C	249	ASP	C-N-CA	9.79	139.31	121.70
3	K	236	ARG	CA-C-N	7.62	135.41	121.70
3	K	236	ARG	C-N-CA	7.62	135.41	121.70
2	O	236	ARG	CA-C-N	7.39	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.

The worst 5 of 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

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 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
1	B	176/514 (34%)	170 (97%)	6 (3%)	0	100	100
1	E	184/514 (36%)	176 (96%)	6 (3%)	2 (1%)	11	41
1	F	157/514 (30%)	152 (97%)	5 (3%)	0	100	100
1	I	184/514 (36%)	177 (96%)	6 (3%)	1 (0%)	24	57
1	J	179/514 (35%)	174 (97%)	4 (2%)	1 (1%)	21	53
1	M	184/514 (36%)	177 (96%)	7 (4%)	0	100	100
1	N	181/514 (35%)	173 (96%)	6 (3%)	2 (1%)	11	41
2	C	35/557 (6%)	27 (77%)	5 (14%)	3 (9%)	0	3
2	D	31/557 (6%)	27 (87%)	3 (10%)	1 (3%)	3	19
2	G	41/557 (7%)	30 (73%)	10 (24%)	1 (2%)	4	25
2	H	30/557 (5%)	27 (90%)	3 (10%)	0	100	100
2	L	31/557 (6%)	26 (84%)	4 (13%)	1 (3%)	3	19
2	O	33/557 (6%)	27 (82%)	4 (12%)	2 (6%)	1	8
2	P	31/557 (6%)	28 (90%)	2 (6%)	1 (3%)	3	19
3	K	34/557 (6%)	30 (88%)	3 (9%)	1 (3%)	3	21
All	All	1696/8568 (20%)	1599 (94%)	81 (5%)	16 (1%)	14	45

5 of 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

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%)	22	52
1	B	146/450 (32%)	138 (94%)	8 (6%)	19	49
1	E	163/450 (36%)	155 (95%)	8 (5%)	22	52
1	F	138/450 (31%)	128 (93%)	10 (7%)	13	40
1	I	163/450 (36%)	153 (94%)	10 (6%)	17	46
1	J	150/450 (33%)	140 (93%)	10 (7%)	15	43
1	M	161/450 (36%)	152 (94%)	9 (6%)	19	48
1	N	145/450 (32%)	137 (94%)	8 (6%)	19	49
2	C	30/497 (6%)	26 (87%)	4 (13%)	4	17
2	D	26/497 (5%)	22 (85%)	4 (15%)	2	13
2	G	30/497 (6%)	28 (93%)	2 (7%)	15	43
2	H	24/497 (5%)	23 (96%)	1 (4%)	26	56
2	L	27/497 (5%)	24 (89%)	3 (11%)	6	23
2	O	21/497 (4%)	21 (100%)	0	100	100
2	P	28/497 (6%)	25 (89%)	3 (11%)	6	25
3	K	34/497 (7%)	30 (88%)	4 (12%)	5	21
All	All	1448/7576 (19%)	1356 (94%)	92 (6%)	16	44

5 of 92 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	J	35	THR
2	L	254	THR
1	J	57	ASP
3	K	206	ILE
1	M	63	ILE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 37 such sidechains are listed below:

Mol	Chain	Res	Type
1	M	108	GLN
1	N	119	ASN
1	M	110	GLN
1	N	79	GLN
1	F	110	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 oligosaccharides 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 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%)	0.36	5 (2%) 56 35	40, 70, 104, 118	0
1	B	182/514 (35%)	0.89	19 (10%) 11 7	52, 116, 215, 236	1 (0%)
1	E	186/514 (36%)	0.32	4 (2%) 62 41	44, 70, 106, 135	0
1	F	167/514 (32%)	0.93	22 (13%) 7 5	68, 176, 238, 250	1 (0%)
1	I	186/514 (36%)	0.47	4 (2%) 62 41	57, 89, 131, 149	0
1	J	183/514 (35%)	0.74	10 (5%) 30 18	62, 100, 174, 198	1 (0%)
1	M	186/514 (36%)	1.31	35 (18%) 3 2	167, 239, 278, 288	0
1	N	185/514 (35%)	1.37	41 (22%) 2 2	106, 219, 269, 283	1 (0%)
2	C	41/557 (7%)	0.60	1 (2%) 59 39	59, 72, 100, 124	0
2	D	37/557 (6%)	0.91	5 (13%) 7 5	49, 79, 129, 153	0
2	G	45/557 (8%)	0.55	1 (2%) 62 41	39, 81, 100, 104	0
2	H	36/557 (6%)	0.73	3 (8%) 17 10	56, 75, 248, 253	0
2	L	37/557 (6%)	0.78	3 (8%) 18 10	78, 100, 126, 152	0
2	O	39/557 (7%)	1.05	3 (7%) 19 11	142, 192, 248, 261	0
2	P	37/557 (6%)	1.22	10 (27%) 1 1	89, 232, 251, 256	0
3	K	40/557 (7%)	0.49	0 100 100	68, 85, 110, 142	0
All	All	1774/8568 (20%)	0.79	166 (9%) 14 8	39, 102, 252, 288	4 (0%)

The worst 5 of 166 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	M	149	LEU	6.5
1	F	57	ASP	5.9
1	N	92	ALA	5.5
1	B	150	ALA	4.4
1	M	77	TYR	4.3

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 oligosaccharides 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.