



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 28, 2026 – 11:05 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 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	:	4-5-2 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

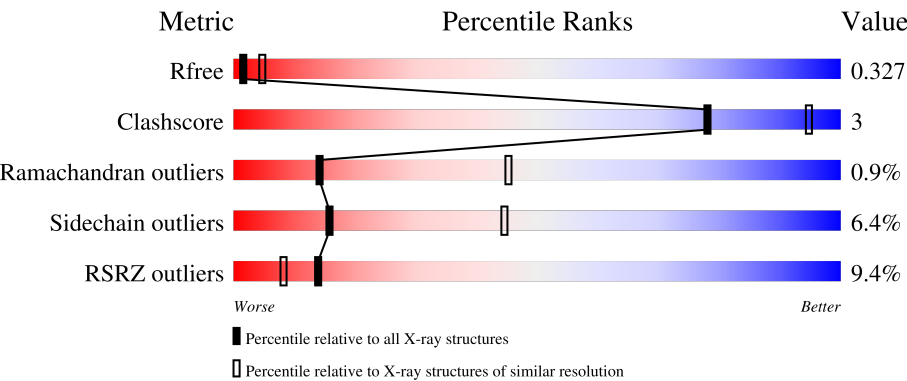
1 Overall quality at a glance i

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}	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	% 32% . 64%
1	B	514	4% 32% . 65%
1	E	514	% 31% 5% 64%
1	F	514	4% 29% . 68%
1	I	514	% 32% . 64%

Continued on next page...

Continued from previous page...

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

Continued on next page...

Continued from previous page...

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.

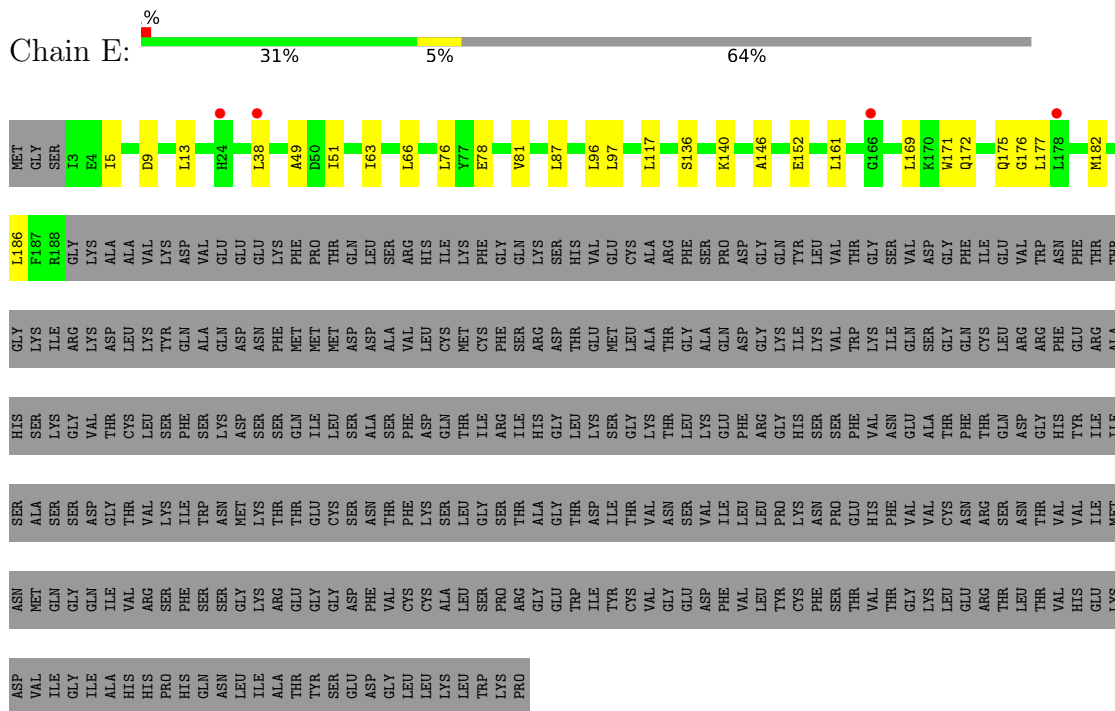
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	K	40	Total	C	N	O	S	0	0	0
			323	210	53	58	2			

There are 2 discrepancies between the modelled and reference sequences:

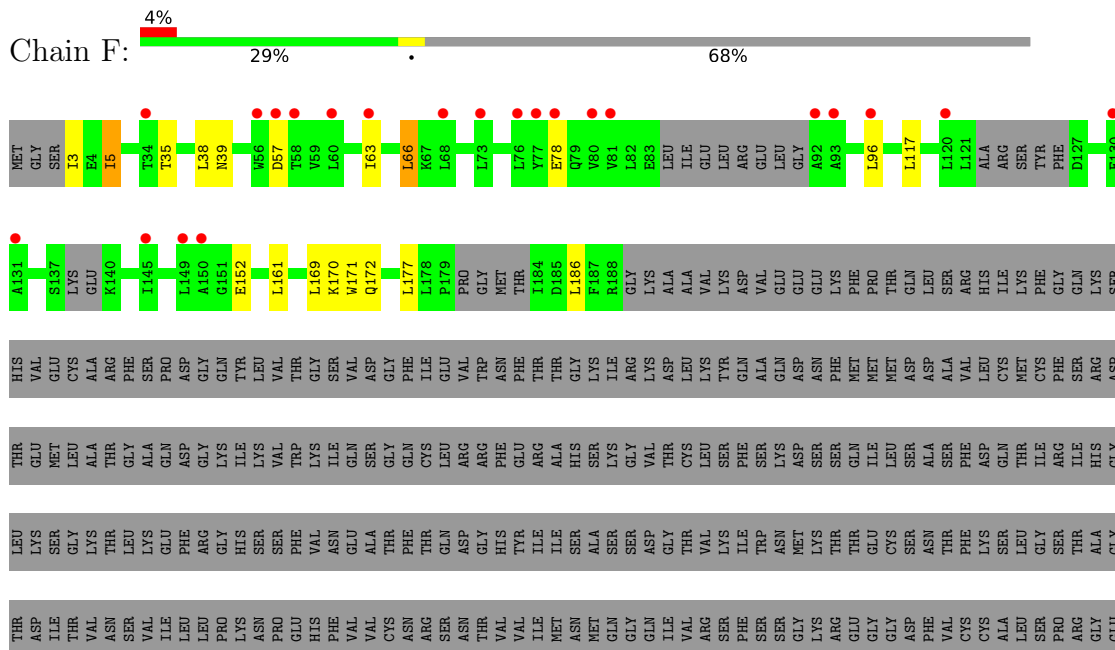
Chain	Residue	Modelled	Actual	Comment	Reference
K	2	GLY	PRO	conflict	UNP Q13123
K	257	LYS	ILE	conflict	UNP Q13123

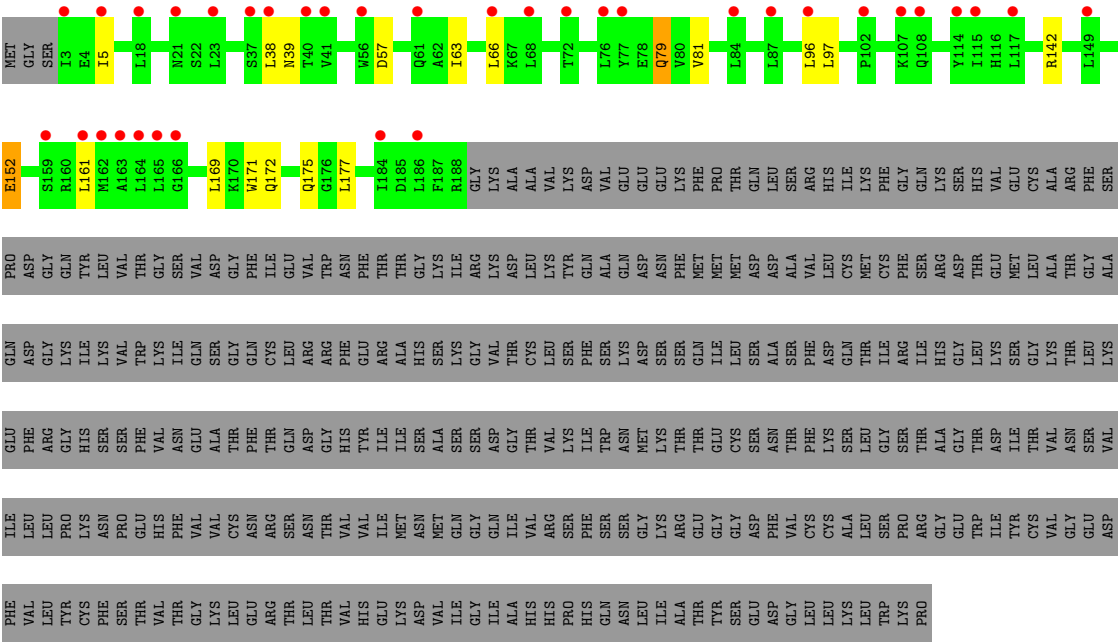
THR	LEU	THR	VAL	HIS	GLU	LYS	ASP	ASN	GLN
LEU	THR	VAL	VAL	GLU	LYS	MET	ASN	GLY	ASP
VAL	VAL	VAL	VAL	ILE	ILE	GLY	ASP	THR	HIS
GLU	GLU	VAL	VAL	GLY	GLN	GLY	ASP	THR	VAL
LYS	LYS	LYS	LYS	ILE	ILE	ILE	ILE	VAL	ILE
ASP	ASP	ASP	ASP	ALA	ALA	ALA	ALA	VAL	VAL
VAL	VAL	VAL	VAL	HIS	HIS	HIS	HIS	VAL	VAL
VAL	VAL	VAL	VAL	PRO	PRO	PRO	PRO	VAL	VAL
ILE	ILE	ILE	ILE	GLN	GLN	GLN	GLN	VAL	VAL
ILE	ILE	ILE	ILE	GLY	GLY	GLY	GLY	VAL	VAL
ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE	VAL	VAL
ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	VAL	VAL
HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	VAL	VAL
PRO	PRO	PRO	PRO	PRO	PRO	PRO	PRO	VAL	VAL
GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	VAL	VAL
ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	VAL	VAL
LEU	LEU	LEU	LEU	LEU	LEU	LEU	LEU	VAL	VAL
ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE	VAL	VAL
ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	VAL	VAL
THR	THR	THR	THR	THR	THR	THR	THR	VAL	VAL
TYR	TYR	TYR	TYR	TYR	TYR	TYR	TYR	VAL	VAL
GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	VAL	VAL
LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	VAL	VAL
ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	VAL	VAL
GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	VAL	VAL
LEU	LEU	LEU	LEU	LEU	LEU	LEU	LEU	VAL	VAL
LEU	LEU	LEU	LEU	LEU	LEU	LEU	LEU	VAL	VAL
LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	VAL	VAL
PRO	PRO	PRO	PRO	PRO	PRO	PRO	PRO	VAL	VAL
THR	THR	THR	THR	THR	THR	THR	THR	VAL	VAL
GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	VAL	VAL
LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	VAL	VAL
ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	VAL	VAL
GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	VAL	VAL
LEU	LEU	LEU	LEU	LEU	LEU	LEU	LEU	VAL	VAL
LEU	LEU	LEU	LEU	LEU	LEU	LEU	LEU	VAL	VAL
LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	VAL	VAL
PRO	PRO	PRO	PRO	PRO	PRO	PRO	PRO	VAL	VAL
THR	THR	THR	THR	THR	THR	THR	THR	VAL	VAL
GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	VAL	VAL
LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	VAL	VAL
ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	VAL	VAL
GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	VAL	VAL
LEU	LEU	LEU	LEU	LEU	LEU	LEU	LEU	VAL	VAL
LEU	LEU	LEU	LEU	LEU	LEU	LEU	LEU	VAL	VAL
LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	VAL	VAL
PRO	PRO	PRO	PRO	PRO	PRO	PRO	PRO	VAL	VAL
THR	THR	THR	THR	THR	THR	THR	THR	VAL	VAL
GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	VAL	VAL
LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	VAL	VAL
ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	VAL	VAL
GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	VAL	VAL
LEU	LEU	LEU	LEU	LEU	LEU	LEU	LEU	VAL	VAL
LEU	LEU	LEU	LEU	LEU	LEU	LEU	LEU	VAL	VAL
LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	VAL	VAL
PRO	PRO	PRO	PRO	PRO	PRO	PRO	PRO	VAL	VAL
THR	THR	THR	THR	THR	THR	THR	THR	VAL	VAL
GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	VAL	VAL
LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	VAL	VAL
ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	VAL	VAL</

- Molecule 1: WD40 repeat-containing protein SMU1

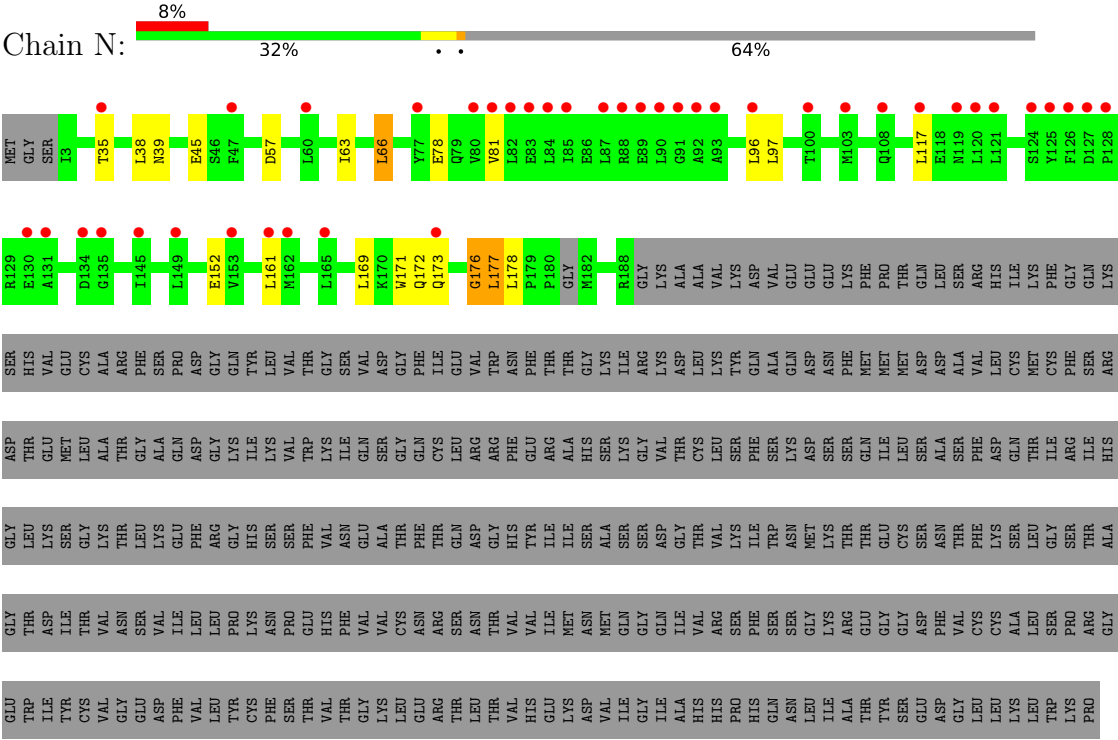


- Molecule 1: WD40 repeat-containing protein SMU1

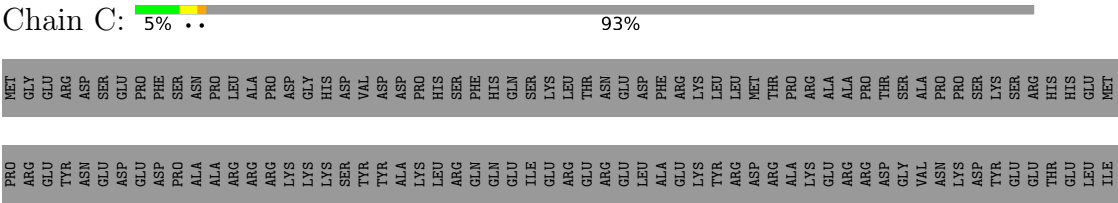




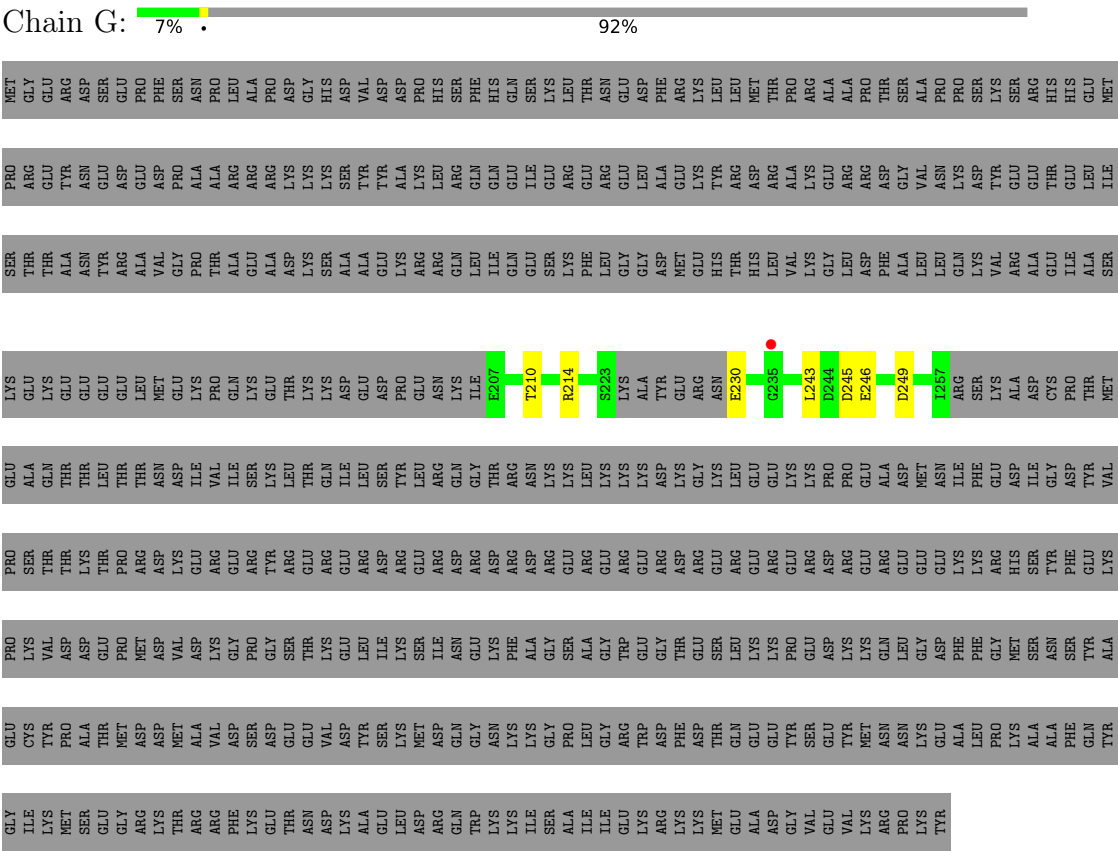
● Molecule 1: WD40 repeat-containing protein SMU1



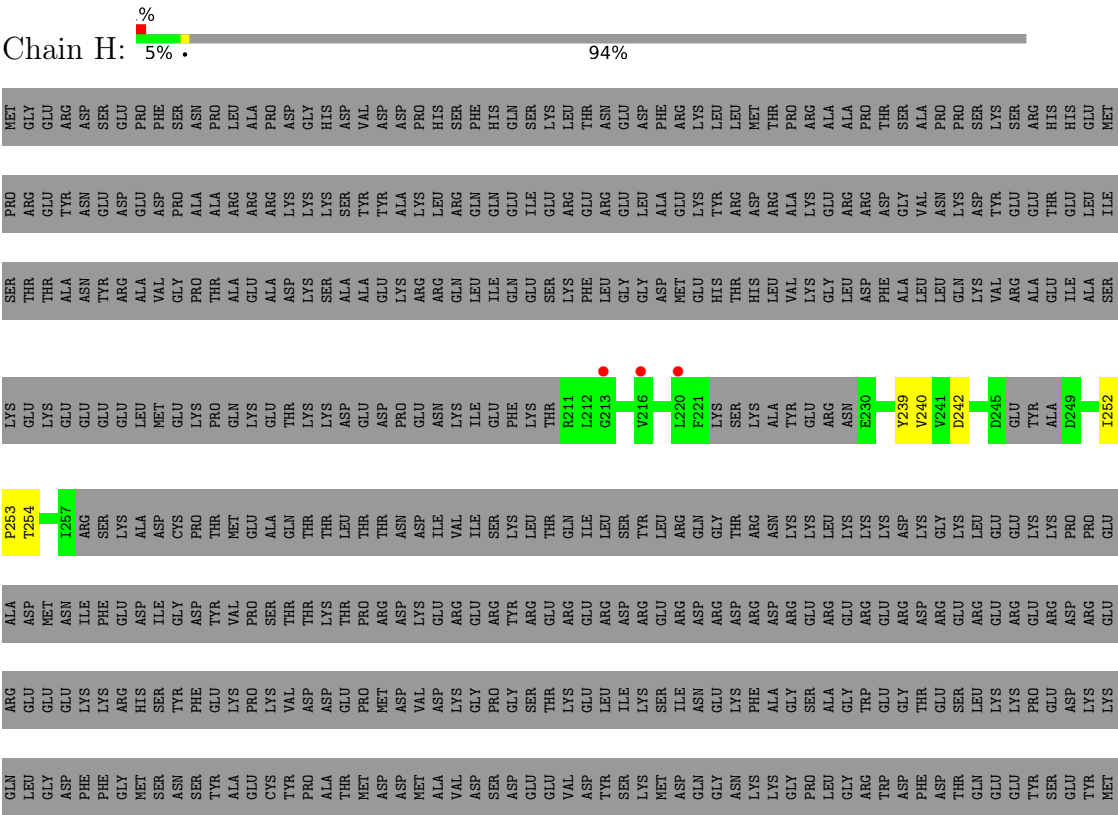
● Molecule 2: Protein Red



- Molecule 2: Protein Red



● Molecule 2: Protein Red



[illegible]

- Molecule 2: Protein Red



NET	GLY	GLU	ARG	ASP	SER	GLU	PRO	PHE	SER	ASN	PRO	LEU	ALA	ASP	GLY	ASP	HIS	ASP	VAL	ASP	PRO	HIS	SER	PHE	HIS	GLN	SER	LYS	LEU	THR	GLU	ASP	PHE	ARG	LYS	LEU	LEU	NET	MET	THR	ARG	PRO	ALA	ALA	ALA	PRO	THR	THR	SER	SER	PRO	PRO	LYS	SER	HIS	HIS	GLU	NET
-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----

PRO ARG GLU TYR ASN GLU ASP GLU ASP PRO PRO ALA ALA ARG ARG ARG LYS LYS SER TYR TYR ALA ALA LYS LEU ARG GLN GLN LEU ILE GLU ARG GLU ARG ARG GLU LEU ALA GLU LYS TYR TYR VAL ASN ASP ARG ASP GLY ASP ASP ASP ASP ASP ASP ASP ASP ASP ASP ASP ASP ASP ASP

SER	THR	THR	ALA	ASN	TYR	ARG	ALA	VAL	GLY	PRO	THR	ALA	GLU	ALA	ASP	LYS	SER	ALA	ALA	GLU	ARG	ARG	GLN	LEU	ILE	LEU	GLN	GLU	SER	LYS	PHE	LEU	LEU	GLY	GLY	ASP	ASP	MET	GLU	HIS	HIS	THR	THR	LEU	VAL	LEU	LYS	VAL	ARG	ALA	GLU	ILE	ALA	SER
-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----

LVS	LVS	LVS	GLU	GLU	GLU	GLU	GLU	LEU	MET	GLU	PRO	GLN	LVS	GLU	THR	LVS	LVS	ASP	GLU	ASP	PRO	GLU	ASN	LVS	ILE	GLU	PHE	LVS	THR	R211	R212	Y217	R218	M219	L220	S223	LVS	ALA	TYR	GLU	ARG	ASN	E230	L231	F232	L233	P234	G235	R236	V240	D245	GLU	TYR	ALA	ASP
-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	------	------	------	------	------	------	------	-----	-----	-----	-----	-----	-----	------	------	------	------	------	------	------	------	------	-----	-----	-----	-----

[illegible][illegible][illegible]

LYS
GLN
LEU
GLY
ASP
PHE
PHE
GLY
MET
MET
SER
ASN
SER
TYR
ALA
ALA
GLU
GLY
CYS
TVR
TVR
PRO
ALA
ALA
THR
MET
ASP
ASP
MET
VAL
ALA
ASP
ASP
SER
SER
ASP
ASP
GLU
GLU
VAL
ASP
ASP
TVR
SER
LYS
MET
ASP
GLN
GLN
GLY
GLY
PRO
LEU
GLY
ARG
TRP
ASP
PHE
ASP
THR
GLN
GLU
GLU
TVR
SER
GLU

TYR	MET	ASN	ASN	LYS	GLU	ALA	LEU	PRO	LYS	ALA	ALA	PHE	GLN	TYR	GLY	ILE	LYS	MET	SER	GLY	GLU	LYS	ARG	LYS	THR	ARG	ARG	PHE	LYS	GLU	THR	ASN	LYS	ALA	LEU	ASP	ASP	GLN	ARG	TRP	LYS	LYS	ILE	SER	ALA	ILE	ILE	GLU	LYS	ARG	LYS	LYS	MET	GLU	ALA	ALA	ASP	GLY	VAL	GLU
-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----

VAL
LYS
ARG
PRO
LYS
TYR

- Molecule 2: Protein Red



NET	GLY	GLY	GLU	ARG	ASP	SER	GLU	PRO	PHE	SER	ASN	LEU	ALA	PRO	ASP	GLY	HIS	ASP	VAL	ASP	ASP	PRO	HIS	SER	PHE	HIS	GLN	SER	LYS	LEU	THR	GLU	ASP	PHE	ARG	LYS	LEU	LEU	LEU	MET	THR	PRO	ARG	ALA	ALA	ALA	THR	THR	SER	PRO	PRO	PRO	SER	LYS	SER	HIS	HIS	GLU	MET
-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----

PRO	ARG	GLU	TYR	ASN	GLU	ASP	GLU	ASP	PRO	ALA	ALA	ARG	ARG	ARG	LYS	LYS	LYS	LYS	TYR	TYR	ALA	ALA	LYS	LEU	ARG	GLN	GLN	GLU	ILE	ILE	GLU	GLU	ARG	GLU	ARG	GLU	LEU	ALA	GLU	LYS	TYR	ARG	ASP	ARG	ALA	LYS	GLU	ARG	GLU	ASP	ASP	GLY	VAL	ASN	ASP	LYS	TYR	GLU	GLU	THR	GLU	LEU	ILE
-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----

SER	THR	THR	ALA	ASN	TYR	ARG	ALA	VAL	GLY	PRO	THR	ALA	GLU	ALA	ASP	LYS	SER	ALA	ALA	GLU	ARG	ARG	GLN	LEU	ILE	GLN	GLU	SER	LYS	PHE	LEU	GLY	ASP	MET	GLU	HIS	THR	HIS	LEU	VAL	LYS	GLY	LEU	ASP	PHE	ALA	LEU	GLN	LYS	VAL	ARG	ALA	GLU	ILE	ALA	SER
-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----

LVS	LVS	LVS	GLU	GLU	GLU	GLU	GLU	GLU	LEU	MET	GLU	LVS	LVS	GLN	GLN	LVS	LVS	ASP	GLU	ASP	PRO	GLU	ASN	LVS	ILE	E207	F221	LVS	SER	LVS	ALA	TYR	GLU	GLU	ASN	E230	L231	L232	L233	P234	G235	P236	M237	D245	GLU	TYR	ALA	ASP	T250	D251	L257	ARG	SER	LVS	ALA	ASP
-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	------	------	-----	-----	-----	-----	-----	-----	-----	-----	------	------	------	------	------	------	------	------	------	-----	-----	-----	-----	------	------	------	-----	-----	-----	-----	-----

[illegible]

- 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	ARG	GLU
TYR	GLU	ASP	GLU	ASN	GLU	ALA	TYR	ASN
	ALA	PHE	LYS	ILE	GLU	ARG	TYR	GLU
	LEU	PHE	LYS	PHE	GLU	SER	ARG	ASP
	PRO	GLY	ARG	GLU	LYS	GLU	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	ALA
	GLY	GLU	PRO	PRO	LYS	GLU	ARG	ARG
	ILE	CYS	LYS	SER	THR	GLN	ARG	PRO
	LYS	TYR	VAL	THR	THR	LYS	LYS	ASP
	MET	PRO	ASP	THR	THR	ASP	ASP	GLY
	SER	ALA	ASP	LYS	THR	SER	LYS	HIS
	GLU	THR	GLU	THR	LYS	ALA	SER	ASP
	ARG	ALA	VAL	GLU	ILE	ARG	LEU	PRO
	PHE	ASP	GLY	GLU	ILE	LEU	GLN	HIS
	LYS	SER	PRO	ARG	ILE	GLN	GLN	GLN
	GLU	ASP	GLY	TYR	PHE	GLY	GLU	GLY
	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	GLU	GLU	THR	LYS	ARG	ASP
	GLN	ASN	ILE	ARG	LEU	GLY	ALA	PHE
	TRP	GLY	GLU	ASP	ALA	MET	GLU	ARG
	LYS	LYS	PHE	ASP	GLU	THR	THR	LEU
	ILE	LYS	ALA	ASP	ASN	ARG	ASP	MET
	SER	GLY	GLY	ARG	LYS	VAL	ARG	THR
	ALA	PRO	SER	GLU	LYS	VAL	ALA	PRO
	ILE	LEU	ALA	ARG	LEU	GLY	GLU	ARG
	ILE	GLY	ILE	GLU	F232	LEU	ARG	ALA
	GLU	ARG	TRP	ARG	P234	ASP	ASP	PRO
	LYS	TRP	GLU	GLU	LYS	PHE	THR	SER
	ARG	ASP	GLY	ARG	W237	ALA	GLY	THR
	LYS	PHE	THR	ASP	A238	LEU	VAL	SER
	LYS	ASP	GLU	GLY	Y239	LEU	ASN	PRO
	MET	THR	SER	GLU	Y240	LYS	GLN	PRO
	GLU	GLN	LEU	ARG	Y241	LYS	ASP	SER
	ALA	GLU	LYS	GLU	GLU	VAL	TYR	LYS
	ASP	GLU	LYS	ARG	GLU	ARG	GLU	ARG
	VAL	TYR	PRO	GLU	GLU	GLY	GLU	SER
	GLY	TYR	ASP	GLU	E246	LYS	GLU	GLY
	VAL	SER	GLU	ARG	Y247	LYS	THR	HIS
	GLU	GLU	ASP	ASP	ALA	ILE	GLU	HIS
	VAL	TYR	LYS	GLU	ASP	SER	LEU	MET

- Molecule 3: Protein Red

[illegible]

ALA	ASN	TYR	GLY	CYS	LYS	SER
PHE	SER	PHE	ASP	PRO	GLU	THR
GLN	TYR	GLU	TYR	THR	LYS	THR
TYR	ALA	LYS	VAL	MET	GLU	ALA
ILE	GLU	PRO	PRO	GLU	GLU	ASN
TYR	CYS	LYS	SER	ALA	GLU	TYR
VAL	TYR	VAL	THR	GLN	GLU	ARG
MET	PRO	ASP	THR	THR	LEU	ALA
SER	ALA	ASP	LYS	THR	MET	VAL
GLU	THR	GLU	THR	LEU	GLU	GLY
GLY	MET	PRO	PRO	THR	LYS	PRO
ARG	ASP	MET	ARG	THR	PRO	THR
LYS	ASP	ASP	ASP	ASN	GLN	ALA
THR	MET	VAL	LYS	ASP	LYS	GLU
ARG	ALA	ASP	GLU	ILE	GLU	ALA
PHE	VAL	LYS	ARG	VAL	THR	ASP
ASP	ASP	GLY	GLU	ILE	LYS	LYS
LYS	SER	PRO	ARG	SER	LYS	SER
GLU	ASP	GLY	TYR	LYS	ASP	ALA
THR	GLU	SER	ARG	LEU	GLU	ALA
ASN	GLU	THR	GLU	THR	ASP	GLU
VAL	VAL	LYS	ARG	GLN	PRO	LYS
LYS	ASP	GLU	GLU	ILE	GLU	ARG
ALA	TYR	LEU	ARG	LEU	ASN	ARG
GLU	SER	ILE	ASP	SER	LYS	GLN
LEU	LYS	LYS	ARG	TYR	T206	LEU
ASP	MET	SER	GLU	LEU		ILE
ARG	ASN	ILE	ARG	ARG	T221	GLN
GLN	GLN	ASN	ASP	GLN	LYS	GLU
TRP	GLY	GLU	ARG	GLY	SER	SER
LYS	ASN	LYS	ASP	THR	LYS	LYS
ILE	LYS	PHE	ARG	ARG	ALA	PHE
LYS	LYS	ALA	ASP	ASN	TYR	LEU
SER	GLY	GLY	ARG	ASN	GLU	GLY
PRO	PRO	SER	GLU	LYS	ARG	GLY
LEU	LEU	ALA	ARG	LEU	ASN	ASP
ILE	GLY	GLY	GLU	LYS	E230	MET
ILE	GLY	TRP	ARG	LYS	T231	GLU
LYS	TRP	GLU	GLU	LYS		THR
ARG	ASP	GLY	ARG	ASP	R236	HIS
LYS	PHE	THR	ASP	LYS	T237	HIS
LYS	ASP	GLU	ARG	GLY	A238	LEU
MET	THR	SER	GLU	LYS	T239	VAL
GLU	GLN	LEU	ARG	LEU		LYS
ALA	GLU	LYS	GLU	GLU	D245	GLY
GLY	TYR	PRO	GLU	LYS	GLU	LEU
VAL	SER	GLU	ARG	LYS	TYR	ASP
GLU	GLU	ASP	ASP	PRO	ALA	PHE
VAL	TYR	LYS	ARG	PRO	ASP	ALA
LYS	MET	LYS	GLU	GLU	T250	LEU
ARG	ASN	GLN	ARG	ALA		LEU
PRO	ASN	LEU	GLU	ASP	T254	GLN
LYS	LYS	GLY	GLU	MET	T255	LYS
TYR	GLU	ASP	GLU	ASN	L256	VAL
	ALA	PHE	LYS	ILE	R257	ARG
	LEU	PHE	LYS	PHE	ARG	ALA
	PRO	GLY	ARG	GLU	LYS	ILE
	LYS	MET	HIS	ASP	LYS	GLY
	ALA	SER	SER	ILE	ASN	ALA
					ASP	SER

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

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	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.

All (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
2	O	236	ARG	C-N-CA	7.39	135.00	121.70
1	N	176	GLY	CA-C-N	6.83	133.99	121.70
1	N	176	GLY	C-N-CA	6.83	133.99	121.70
2	D	245	ASP	CA-C-N	6.31	133.05	121.70
2	D	245	ASP	C-N-CA	6.31	133.05	121.70
2	P	245	ASP	CA-C-N	6.04	132.57	121.70

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	P	245	ASP	C-N-CA	6.04	132.57	121.70
1	N	45	GLU	CB-CG-CD	5.61	122.13	112.60
1	I	157	PRO	N-CA-C	5.54	115.79	110.47
2	H	242	ASP	N-CA-C	5.23	116.79	111.14
1	A	57	ASP	CA-CB-CG	5.19	117.79	112.60
2	C	236	ARG	CA-C-N	5.16	131.39	121.54
2	C	236	ARG	C-N-CA	5.16	131.39	121.54
3	K	230	GLU	CA-C-N	5.15	130.97	121.70
3	K	230	GLU	C-N-CA	5.15	130.97	121.70
1	I	93	ALA	CA-C-N	5.07	127.08	120.28
1	I	93	ALA	C-N-CA	5.07	127.08	120.28
2	G	245	ASP	CA-C-N	5.06	131.20	121.54
2	G	245	ASP	C-N-CA	5.06	131.20	121.54
2	P	211	ARG	CA-C-N	5.04	126.99	120.44
2	P	211	ARG	C-N-CA	5.04	126.99	120.44

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	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

Continued on next page...

Continued from previous page...

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

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
All	All	1696/8568 (20%)	1599 (94%)	81 (5%)	16 (1%)	14	45

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%)	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

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
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

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

Mol	Chain	Res	Type
1	A	5	ILE
1	A	63	ILE
1	A	66	LEU
1	A	72	THR
1	A	79	GLN
1	A	96	LEU
1	A	152	GLU
1	A	175	GLN
1	B	5	ILE
1	B	35	THR
1	B	38	LEU
1	B	57	ASP
1	B	63	ILE
1	B	66	LEU
1	B	96	LEU
1	B	152	GLU
2	C	211	ARG
2	C	236	ARG
2	C	244	ASP
2	C	256	LEU
2	D	233	LEU
2	D	237	MET
2	D	256	LEU
2	D	257	ILE
1	E	5	ILE

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	E	38	LEU
1	E	63	ILE
1	E	66	LEU
1	E	76	LEU
1	E	96	LEU
1	E	152	GLU
1	E	175	GLN
1	F	3	ILE
1	F	5	ILE
1	F	35	THR
1	F	38	LEU
1	F	57	ASP
1	F	63	ILE
1	F	66	LEU
1	F	96	LEU
1	F	152	GLU
1	F	177	LEU
2	G	214	ARG
2	G	249	ASP
2	H	254	THR
1	I	5	ILE
1	I	38	LEU
1	I	57	ASP
1	I	63	ILE
1	I	66	LEU
1	I	79	GLN
1	I	96	LEU
1	I	152	GLU
1	I	156	VAL
1	I	175	GLN
1	J	2	SER
1	J	5	ILE
1	J	35	THR
1	J	38	LEU
1	J	57	ASP
1	J	63	ILE
1	J	66	LEU
1	J	96	LEU
1	J	152	GLU
1	J	186	LEU
3	K	206	ILE
3	K	236	ARG

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
3	K	237	MET
3	K	256	LEU
2	L	219	MET
2	L	220	LEU
2	L	254	THR
1	M	5	ILE
1	M	38	LEU
1	M	57	ASP
1	M	63	ILE
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	63	ILE
1	N	66	LEU
1	N	96	LEU
1	N	152	GLU
1	N	173	GLN
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 (37) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	31	GLN
1	A	110	GLN
1	B	39	ASN
1	B	79	GLN
1	B	110	GLN
1	B	119	ASN
1	B	175	GLN
1	E	21	ASN
1	E	110	GLN
1	E	119	ASN
1	F	39	ASN
1	F	79	GLN
1	F	110	GLN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	F	119	ASN
1	F	174	HIS
1	F	175	GLN
1	I	110	GLN
1	I	119	ASN
1	J	39	ASN
1	J	64	GLN
1	J	79	GLN
1	J	99	GLN
1	J	108	GLN
1	J	110	GLN
1	J	119	ASN
1	J	174	HIS
1	J	175	GLN
1	M	79	GLN
1	M	108	GLN
1	M	110	GLN
1	M	119	ASN
1	N	39	ASN
1	N	79	GLN
1	N	108	GLN
1	N	110	GLN
1	N	119	ASN
1	N	173	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

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

5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry ⓘ

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%)

All (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

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	N	120	LEU	4.1
1	N	84	LEU	4.1
1	N	131	ALA	3.9
1	E	178	LEU	3.9
1	N	96	LEU	3.9
1	M	5	ILE	3.8
1	N	87	LEU	3.8
1	N	100	THR	3.7
1	B	58	THR	3.5
2	G	235	GLY	3.5
1	N	89	GLU	3.5
1	M	108	GLN	3.5
1	F	80	VAL	3.4
1	M	117	LEU	3.3
1	M	3	ILE	3.3
1	F	63	ILE	3.3
2	D	247	TYR	3.3
1	F	60	LEU	3.2
1	F	73	LEU	3.2
1	N	134	ASP	3.2
1	M	165	LEU	3.2
1	I	38	LEU	3.1
2	P	241	VAL	3.1
1	N	117	LEU	3.1
2	O	251	ASP	3.1
1	J	97	LEU	3.1
1	M	56	TRP	3.0
1	F	56	TRP	3.0
1	B	117	LEU	3.0
1	N	80	VAL	3.0
1	I	178	LEU	2.9
1	N	93	ALA	2.9
1	F	81	VAL	2.9
1	N	126	PHE	2.9
1	N	85	ILE	2.9
1	M	161	LEU	2.9
1	N	35	THR	2.9
1	N	83	GLU	2.9
2	O	232	PHE	2.9
1	F	58	THR	2.9
1	J	135	GLY	2.9
1	N	82	LEU	2.9

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	B	97	LEU	2.9
1	M	164	LEU	2.8
1	N	165	LEU	2.8
1	M	37	SER	2.8
1	F	93	ALA	2.8
1	F	92	ALA	2.8
1	A	179	PRO	2.8
1	F	149	LEU	2.7
1	I	125	TYR	2.7
1	B	96	LEU	2.7
1	B	89	GLU	2.7
1	M	76	LEU	2.7
1	F	130	GLU	2.7
1	N	130	GLU	2.7
1	F	150	ALA	2.7
1	E	24	HIS	2.7
1	M	166	GLY	2.6
1	M	72	THR	2.6
2	D	250	THR	2.6
1	N	119	ASN	2.6
1	N	128	PRO	2.6
1	M	186	LEU	2.6
1	N	60	LEU	2.6
2	L	233	LEU	2.6
1	F	68	LEU	2.6
1	F	76	LEU	2.6
1	F	77	TYR	2.6
1	M	115	ILE	2.6
1	J	117	LEU	2.5
1	M	68	LEU	2.5
1	M	87	LEU	2.5
1	N	161	LEU	2.5
2	P	231	LEU	2.5
2	H	216	VAL	2.5
1	A	134	ASP	2.5
1	B	131	ALA	2.5
1	M	21	ASN	2.5
1	M	162	MET	2.5
1	E	38	LEU	2.5
1	N	124	SER	2.5
1	N	103	MET	2.5
1	B	68	LEU	2.5

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	N	77	TYR	2.5
1	N	125	TYR	2.5
1	J	121	LEU	2.5
1	J	151	GLY	2.5
1	B	6	GLU	2.4
2	P	256	LEU	2.4
1	B	119	ASN	2.4
1	E	166	GLY	2.4
2	P	239	TYR	2.4
1	F	145	ILE	2.4
1	J	143	ALA	2.4
1	M	84	LEU	2.4
1	N	149	LEU	2.4
1	M	40	THR	2.4
1	N	81	VAL	2.4
2	D	252	ILE	2.4
1	B	105	MET	2.4
1	N	127	ASP	2.4
1	N	90	LEU	2.3
2	P	234	PRO	2.3
1	N	88	ARG	2.3
1	M	38	LEU	2.3
2	P	232	PHE	2.3
1	F	78	GLU	2.3
1	A	3	ILE	2.3
1	B	57	ASP	2.3
1	I	163	ALA	2.3
1	B	121	LEU	2.3
2	P	233	LEU	2.3
1	M	159	SER	2.3
1	F	131	ALA	2.2
1	N	108	GLN	2.2
2	O	245	ASP	2.2
2	L	217	TYR	2.2
1	M	163	ALA	2.2
1	M	102	PRO	2.2
2	H	213	GLY	2.2
1	N	47	PHE	2.2
1	M	41	VAL	2.2
1	M	114	TYR	2.2
2	D	257	ILE	2.2
1	N	91	GLY	2.2

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
2	H	220	LEU	2.1
2	L	212	LEU	2.1
2	P	230	GLU	2.1
2	C	210	THR	2.1
1	A	178	LEU	2.1
1	B	124	SER	2.1
1	B	153	VAL	2.1
1	M	18	LEU	2.1
1	M	23	LEU	2.1
2	P	247	TYR	2.1
1	M	61	GLN	2.1
1	N	153	VAL	2.1
1	B	42	ASP	2.1
1	N	121	LEU	2.1
1	F	34	THR	2.1
1	N	173	GLN	2.1
1	N	145	ILE	2.1
2	P	257	ILE	2.1
1	N	135	GLY	2.1
1	J	90	LEU	2.0
1	M	96	LEU	2.0
1	M	184	ILE	2.0
1	A	24	HIS	2.0
1	B	132	TYR	2.0
1	B	135	GLY	2.0
1	M	107	LYS	2.0
1	F	120	LEU	2.0
1	M	66	LEU	2.0
1	B	104	ILE	2.0
1	J	65	SER	2.0
1	N	162	MET	2.0
1	J	72	THR	2.0
1	J	125	TYR	2.0
2	D	221	PHE	2.0
1	F	96	LEU	2.0

6.2 Non-standard residues in protein, DNA, RNA chains ⓘ

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.