



wwPDB X-ray Structure Validation Summary 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 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:

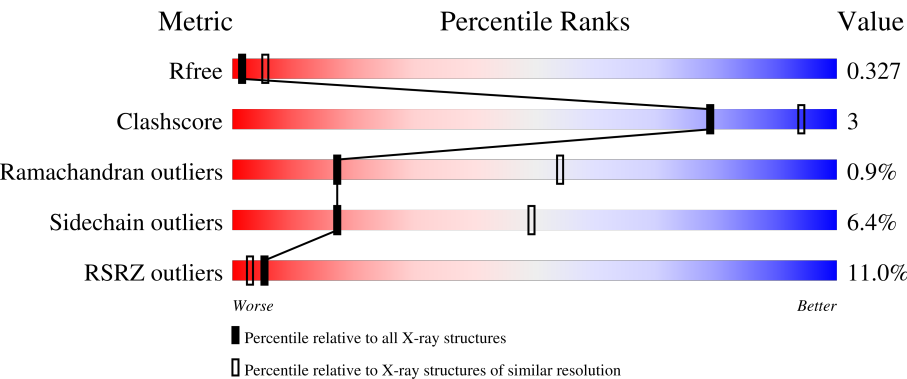
MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.20.1
EDS	:	2.37.1
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation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

1 Overall quality at a glance ⓘ

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>32% . 64%</div></div>
1	B	514	<div><div>2%</div><div>32% . 65%</div></div>
1	E	514	<div><div></div><div>31% 5% 64%</div></div>
1	F	514	<div><div>6%</div><div>29% . 68%</div></div>
1	I	514	<div><div>%</div><div>32% . 64%</div></div>

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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><div>32%</div><div>64%</div></div></div>
1	M	514	<div><div><div></div><div></div><div></div></div><div><div>15%</div><div>33%</div><div>64%</div></div></div>
1	N	514	<div><div><div></div><div></div><div></div></div><div><div>8%</div><div>32%</div><div>64%</div></div></div>
2	C	557	<div><div><div></div><div></div><div></div></div><div><div>5%</div><div>93%</div></div></div>
2	D	557	<div><div><div></div><div></div><div></div></div><div><div>5%</div><div>93%</div></div></div>
2	G	557	<div><div><div></div><div></div><div></div></div><div><div>7%</div><div>92%</div></div></div>
2	H	557	<div><div><div></div><div></div><div></div></div><div><div>%</div><div>5%</div><div>94%</div></div></div>
2	L	557	<div><div><div></div><div></div><div></div></div><div><div>5%</div><div>93%</div></div></div>
2	O	557	<div><div><div></div><div></div><div></div></div><div><div>%</div><div>6%</div><div>93%</div></div></div>
2	P	557	<div><div><div></div><div></div><div></div></div><div><div>3%</div><div>5%</div><div>93%</div></div></div>
3	K	557	<div><div><div></div><div></div><div></div></div><div><div>6%</div><div>93%</div></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

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ($RSRZ > 2$). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

- [illegible]

- Chain B:
-
- 2% 32% 65%
- Chain B:
- Met Gly Ser T35 L38 N39 D57 Q64 S65 L66 E78 W81 E89 L96 L97 I104 R113 Y114 I115 H116 L117 S124 T127 P127 D134 E152 L161 L169 K170 W171 Q172 P179 P180 M182 L186 F187 R188 G189 L190 A191

HIS	HIS	PRO	HIS	GLN	ASN	LEU	ILE	ALA	THR	TYR	SER	GLU	ASP	PHE	VAL	CYS	GLY	ASP	PHE	GLY	GLU	ARG	GLU	GLY	LYS	GLY	LYS	GLY	VAL	ASP	ARG	GLY	TRP	ILE	THR	CYS	CYS	GLY	VAL	GLY	GLU	ASP	PHE	VAL	LEU	TYR	CYS	PHE	THR	THR	VAL	THR	GLY	LYS	LEU	GLU	THR	ARG	THR	GLU	LYS	ASP	LYS	VAL	ILE	GLY	ILE	ALA
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- Molecule 1: WD40 repeat-containing protein SMU1

Chain E: 31% 5% 64%

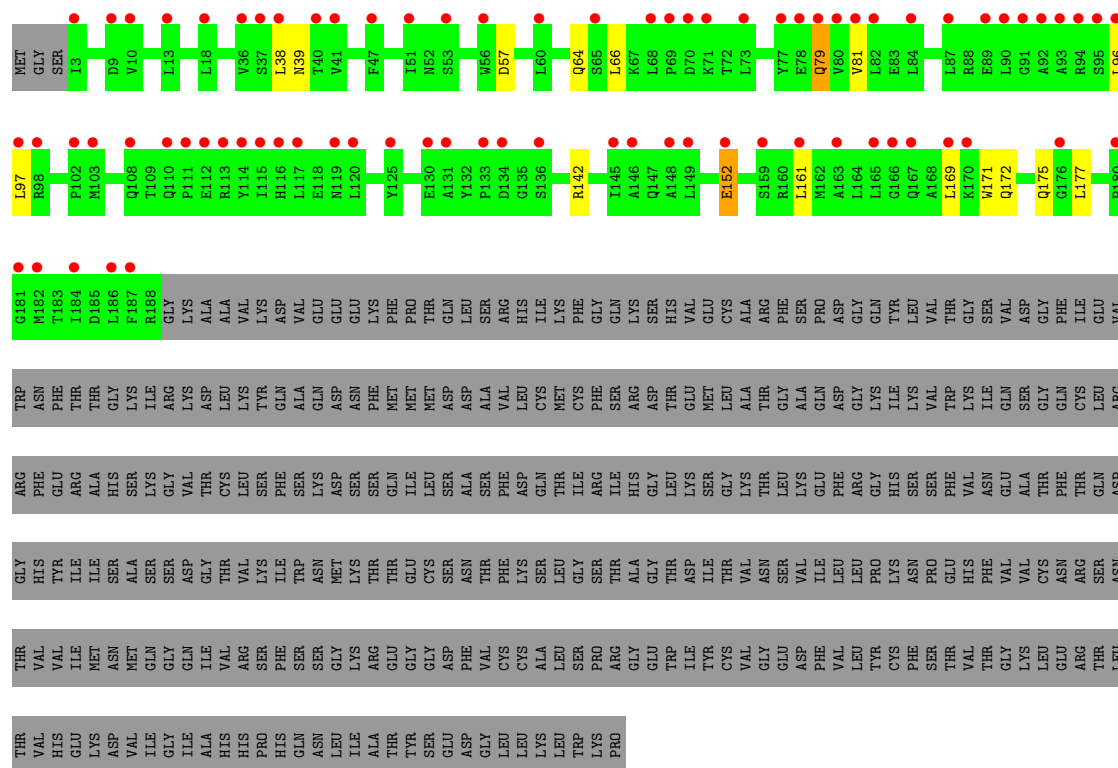
[illegible]

- Molecule 1: WD40 repeat-containing protein SMU1

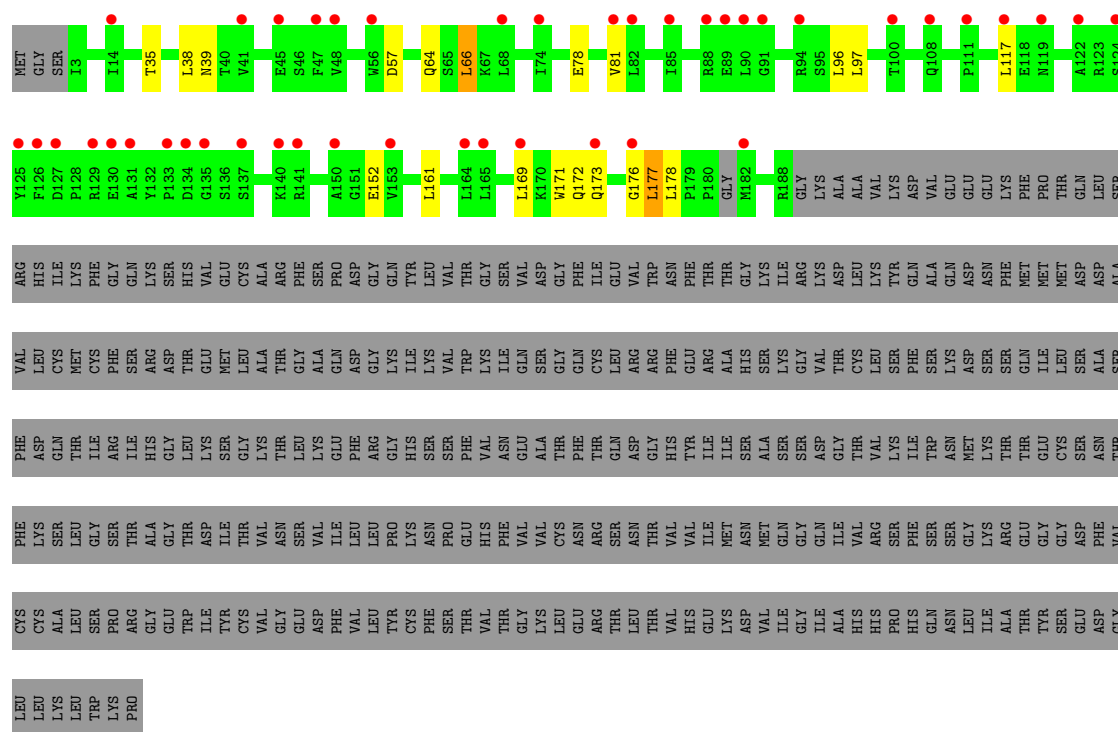
Chain F:  6% 29% 68%

[illegible]

Chain M:  15% 33% 64%



• Molecule 1: WD40 repeat-containing protein SMU1



• Molecule 2: Protein Red

93%

- Molecule 2: Protein Red

93%



[illegible]

- Molecule 2: Protein Red

Chain G: 7% . 92%

[illegible]

- Molecule 2: Protein Red

Chain H:  94%

P253	T254	I257	ARG	SER	GLU	LYS	GLU	THR	SER	PRO	MET
			GLU	THR	LYS	GLU	THR	ALA	ALA	GLU	GLY
			GLU	ASN	GLU	GLU	ASN	TYR	TYR	GLU	ASP
			GLU	THR	GLU	GLU	ARG	ALA	ALA	ASP	GLU
			LEU	ALA	LEU	ALA	VAL	VAL	GLY	PRO	PHE
			MET	CYS	GLU	GLU	GLY	GLY	PRO	ALA	ASN
			PRO	PRO	LYS	PRO	PRO	THR	THR	ALA	PRO
			THR	THR	GLN	GLN	ALA	ALA	ALA	ARG	LEU
			GLU	GLU	LYS	LYS	GLU	ALA	ALA	ARG	ALA
			THR	THR	THR	THR	GLN	ASP	ASP	LYS	PRO
			GLU	GLU	LYS	LYS	LYS	GLY	GLY	LYS	GLY
			THR	THR	LYS	LYS	SER	ALA	SER	LYS	HIS
			LEU	LEU	ASP	ASP	ALA	ALA	ALA	SER	ASP
			THR	THR	GLU	GLU	ALA	ALA	GLU	TYR	VAL
			THR	THR	ASP	ASP	GLU	GLY	GLY	TYR	ASP
			ASN	ASN	PRO	PRO	ASN	LYS	LYS	ALA	ASP
			ASP	ASP	GLU	GLU	ASN	ARG	ARG	LEU	PRO
			ILE	ILE	ASN	ASN	GLN	GLN	GLN	ARG	HIS
			VAL	VAL	LYS	LYS	ILE	LEU	LEU	ARG	SER
			SER	SER	GLU	GLU	GLU	ILE	ILE	GLN	PHE </td
			LYS	LYS	PHE	LYS	GLN	GLN	GLN	GLY	HIS
			LEU	LEU	LYS	LYS	GLU	GLU	ILE	ILE	GLY
			THR	THR	THR	THR	SER	SER	SER	GLU	MET
			GLN	GLN	R211	R211	LYS	LYS	LYS	LEU	LYS
			LEU	LEU	L212	L212	LEU	PHE	PHE	GLU	THR
			SER	SER	G213	G213	SER	LEU	LEU	ASN	GLU
			TYR	TYR	V216	V216	GLY	GLY	GLY	LEU	ASP
			ARG	ARG	Y217	Y217	ASP	ASP	ALA	ALA	PHE
			LEU	LEU	R218	R218	MET	MET	GLU	GLU	ARG
			GLN	GLN	M219	M219	GLN	LYS	LYS	LYS	LYS
			GLY	GLY	L220	L220	HIS	HIS	TYR	TYR	LEU
			THR	THR	F221	F221	THR	THR	THR	THR	LEU
			ARG	ARG	LYS	LYS	HIS	HIS	ASP	ASP	MET
			ASN	ASN	SER	SER	LEU	LEU	ARG	ARG	THR
			LYS	LYS	LYS	LYS	VAL	VAL	ALA	ALA	PRO
			LEU	LEU	GLU	GLU	LYS	LYS	GLY	GLU	ARG
			LYS	LYS	GLU	GLU	LEU	LEU	ASP	ARG	ALA
			LYS	LYS	ASN	ASN	PHE	PHE	ASP	ASP	PRO
			ASP	ASP	E290	E290	ALA	ALA	GLY	GLY	THR
			GLY	GLY	LYS	LYS	LEU	LEU	VAL	VAL	SER
			LEU	LEU	Y239	Y239	LEU	LEU	ASN	ASN	PRO
			LEU	LEU	V240	V240	LYS	LYS	GLN	LYS	PRO
			GLU	GLU	D245	D245	VAL	VAL	VAL	TYR	LYS
			GLU	GLU	GLU	GLU	ARG	ARG	GLU	GLU	ARG
			THR	THR	TYR	TYR	ALA	ALA	ALA	GLU	HIS
			PRO	PRO	D249	D249	GLU	GLU	ILE	GLU	HIS
			THR	THR	ILE	ILE	GLU	GLU	GLU	GLU	GLY
			GLU	GLU	T253	T253	SER	SER	ALA	LEU	MET

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

- Molecule 2: Protein Red

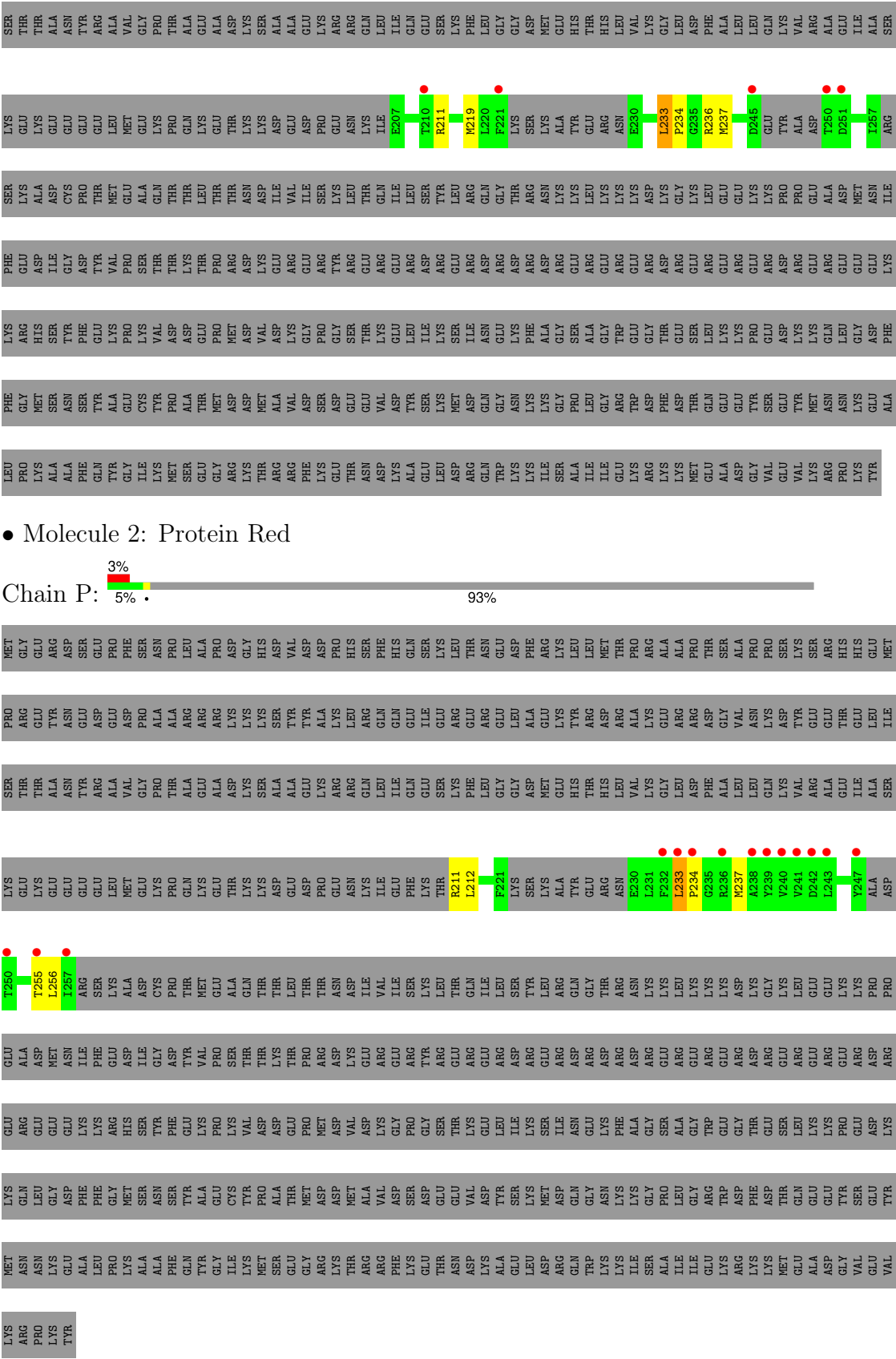
Chain L:  5% 93%

[illegible]

- Molecule 2: Protein Red

Chain O:  %

[illegible]



• Molecule 3: Protein Red

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

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.

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%)	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

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%)	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

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

Mol	Chain	Res	Type
1	J	57	ASP
1	M	38	LEU
1	J	66	LEU
3	K	237	MET
1	M	79	GLN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 17 such sidechains are listed below:

Mol	Chain	Res	Type
1	N	108	GLN
1	N	173	GLN
1	F	110	GLN
1	I	110	GLN
1	I	175	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 [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%)	-0.14	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%)

The worst 5 of 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

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.