Full wwPDB X-ray Structure Validation Report ⓘ

Nov 6, 2023 – 01:03 am GMT

PDB ID	:	8C0N
Title	:	Crystal structure of the red form of the mTagFT fluorescent timer
Authors	:	Boyko, K.M.; Nikolaeva, A.Y.; Vlaskina, A.V.; Agapova, Y.K.; Subach, O.M.; Popov, V.O.; Subach, F.V.
Deposited on	:	2022-12-19
Resolution	:	2.90 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:

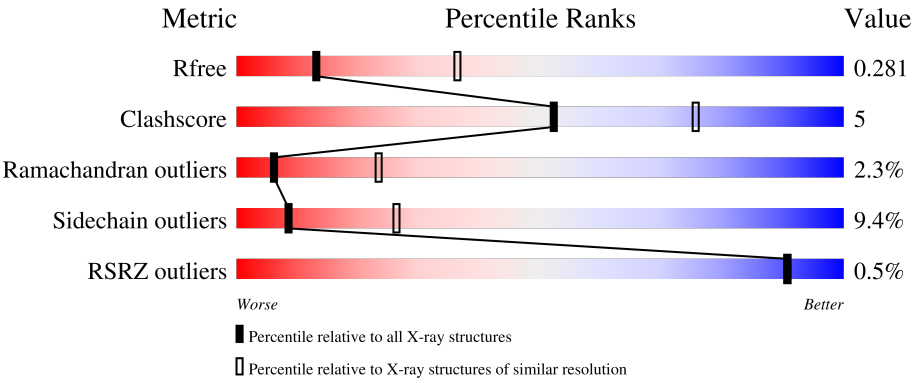
MolProbity	:	4.02b-467
Mogul	:	1.8.4, CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

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 2.90 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	1957 (2.90-2.90)
Clashscore	141614	2172 (2.90-2.90)
Ramachandran outliers	138981	2115 (2.90-2.90)
Sidechain outliers	138945	2117 (2.90-2.90)
RSRZ outliers	127900	1906 (2.90-2.90)

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 <=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	275	% 65% 13% • 20%
1	B	275	62% 16% • 20%
1	C	275	62% 16% • 20%
1	D	275	65% 13% • 20%

2 Entry composition (i)

There are 2 unique types of molecules in this entry. The entry contains 6814 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 Blue-to-red TagFT fluorescent timer.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	220	Total	C	N	O	S	0	0	0
			1683	1073	282	319	9			
1	B	220	Total	C	N	O	S	0	1	0
			1708	1087	291	321	9			
1	C	219	Total	C	N	O	S	0	0	0
			1690	1076	287	318	9			
1	D	219	Total	C	N	O	S	0	0	0
			1693	1076	287	321	9			

There are 468 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-41	MET	-	initiating methionine	UNP Q8ISF8
A	-40	GLY	-	expression tag	UNP Q8ISF8
A	-39	GLY	-	expression tag	UNP Q8ISF8
A	-38	SER	-	expression tag	UNP Q8ISF8
A	-37	HIS	-	expression tag	UNP Q8ISF8
A	-36	HIS	-	expression tag	UNP Q8ISF8
A	-35	HIS	-	expression tag	UNP Q8ISF8
A	-34	HIS	-	expression tag	UNP Q8ISF8
A	-33	HIS	-	expression tag	UNP Q8ISF8
A	-32	HIS	-	expression tag	UNP Q8ISF8
A	-31	GLY	-	expression tag	UNP Q8ISF8
A	-30	MET	-	expression tag	UNP Q8ISF8
A	-29	ALA	-	expression tag	UNP Q8ISF8
A	-28	SER	-	expression tag	UNP Q8ISF8
A	-27	MET	-	expression tag	UNP Q8ISF8
A	-26	THR	-	expression tag	UNP Q8ISF8
A	-25	GLY	-	expression tag	UNP Q8ISF8
A	-24	GLY	-	expression tag	UNP Q8ISF8
A	-23	GLN	-	expression tag	UNP Q8ISF8
A	-22	GLN	-	expression tag	UNP Q8ISF8
A	-21	MET	-	expression tag	UNP Q8ISF8

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Chain	Residue	Modelled	Actual	Comment	Reference
A	-20	GLY	-	expression tag	UNP Q8ISF8
A	-19	ARG	-	expression tag	UNP Q8ISF8
A	-18	ASP	-	expression tag	UNP Q8ISF8
A	-17	LEU	-	expression tag	UNP Q8ISF8
A	-16	TYR	-	expression tag	UNP Q8ISF8
A	-15	ASP	-	expression tag	UNP Q8ISF8
A	-14	ASP	-	expression tag	UNP Q8ISF8
A	-13	ASP	-	expression tag	UNP Q8ISF8
A	-12	ASP	-	expression tag	UNP Q8ISF8
A	-11	LYS	-	expression tag	UNP Q8ISF8
A	-10	GLU	-	expression tag	UNP Q8ISF8
A	-9	ASN	-	expression tag	UNP Q8ISF8
A	-8	LEU	-	expression tag	UNP Q8ISF8
A	-7	TYR	-	expression tag	UNP Q8ISF8
A	-6	PHE	-	expression tag	UNP Q8ISF8
A	-5	GLN	-	expression tag	UNP Q8ISF8
A	-4	GLY	-	expression tag	UNP Q8ISF8
A	-3	HIS	-	expression tag	UNP Q8ISF8
A	-2	MET	-	expression tag	UNP Q8ISF8
A	-1	ARG	-	expression tag	UNP Q8ISF8
A	0	SER	-	expression tag	UNP Q8ISF8
A	1	MET	-	expression tag	UNP Q8ISF8
A	2	VAL	-	expression tag	UNP Q8ISF8
A	3	SER	-	expression tag	UNP Q8ISF8
A	4	LYS	-	expression tag	UNP Q8ISF8
A	5	GLY	-	expression tag	UNP Q8ISF8
A	6	GLU	-	expression tag	UNP Q8ISF8
A	7	GLU	-	expression tag	UNP Q8ISF8
A	12	ILE	ASN	conflict	UNP Q8ISF8
A	14	HIS	ARG	conflict	UNP Q8ISF8
A	15	ILE	MET	conflict	UNP Q8ISF8
A	16	LYS	MET	conflict	UNP Q8ISF8
A	17	LEU	VAL	conflict	UNP Q8ISF8
A	18	TYR	VAL	conflict	UNP Q8ISF8
A	22	THR	SER	conflict	UNP Q8ISF8
A	25	ASN	GLY	conflict	UNP Q8ISF8
A	26	HIS	TYR	conflict	UNP Q8ISF8
A	27	HIS	GLN	conflict	UNP Q8ISF8
A	32	SER	GLY	conflict	UNP Q8ISF8
A	35	GLU	ASP	conflict	UNP Q8ISF8
A	37	LYS	ASN	conflict	UNP Q8ISF8
A	40	GLU	MET	conflict	UNP Q8ISF8

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Chain	Residue	Modelled	Actual	Comment	Reference
A	47	VAL	ILE	conflict	UNP Q8ISF8
A	?	-	MET	deletion	UNP Q8ISF8
A	?	-	TYR	deletion	UNP Q8ISF8
A	68	NRP	GLY	conflict	UNP Q8ISF8
A	71	ARG	LYS	conflict	UNP Q8ISF8
A	75	ASN	LYS	conflict	UNP Q8ISF8
A	78	GLN	LYS	conflict	UNP Q8ISF8
A	99	THR	ARG	conflict	UNP Q8ISF8
A	106	LEU	PHE	conflict	UNP Q8ISF8
A	108	ALA	VAL	conflict	UNP Q8ISF8
A	109	THR	MET	conflict	UNP Q8ISF8
A	115	GLN	GLU	conflict	UNP Q8ISF8
A	120	ILE	VAL	conflict	UNP Q8ISF8
A	122	ASN	HIS	conflict	UNP Q8ISF8
A	123	VAL	ALA	conflict	UNP Q8ISF8
A	125	ILE	VAL	conflict	UNP Q8ISF8
A	126	ARG	THR	conflict	UNP Q8ISF8
A	135	PRO	ALA	conflict	UNP Q8ISF8
A	142	LEU	LYS	conflict	UNP Q8ISF8
A	146	ALA	PRO	conflict	UNP Q8ISF8
A	147	SER	ASN	conflict	UNP Q8ISF8
A	150	LYS	MET	conflict	UNP Q8ISF8
A	152	LYS	TYR	conflict	UNP Q8ISF8
A	159	GLU	ARG	conflict	UNP Q8ISF8
A	161	ARG	TYR	conflict	UNP Q8ISF8
A	163	ASP	GLN	conflict	UNP Q8ISF8
A	167	LYS	ASN	conflict	UNP Q8ISF8
A	168	LEU	VAL	conflict	UNP Q8ISF8
A	169	VAL	ASP	conflict	UNP Q8ISF8
A	173	HIS	TYR	conflict	UNP Q8ISF8
A	175	ILE	SER	conflict	UNP Q8ISF8
A	177	ASN	SER	conflict	UNP Q8ISF8
A	179	LYS	GLU	conflict	UNP Q8ISF8
A	187	PRO	THR	conflict	UNP Q8ISF8
A	188	ALA	VAL	conflict	UNP Q8ISF8
A	189	LYS	GLU	conflict	UNP Q8ISF8
A	191	LEU	PHE	conflict	UNP Q8ISF8
A	196	VAL	PHE	conflict	UNP Q8ISF8
A	197	TYR	HIS	conflict	UNP Q8ISF8
A	198	TYR	PHE	conflict	UNP Q8ISF8
A	206	ILE	LEU	conflict	UNP Q8ISF8
A	207	LYS	GLU	conflict	UNP Q8ISF8

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Chain	Residue	Modelled	Actual	Comment	Reference
A	209	ALA	SER	conflict	UNP Q8ISF8
A	213	THR	MET	conflict	UNP Q8ISF8
A	214	TYR	PHE	conflict	UNP Q8ISF8
A	216	GLU	VAL	conflict	UNP Q8ISF8
A	217	LEU	GLN	conflict	UNP Q8ISF8
A	220	VAL	HIS	conflict	UNP Q8ISF8
A	221	SER	ALA	conflict	UNP Q8ISF8
A	224	ARG	LYS	conflict	UNP Q8ISF8
A	225	TYR	PHE	conflict	UNP Q8ISF8
A	226	PRO	CYS	conflict	UNP Q8ISF8
A	234	HIS	-	expression tag	UNP Q8ISF8
A	235	ARG	-	expression tag	UNP Q8ISF8
B	-41	MET	-	initiating methionine	UNP Q8ISF8
B	-40	GLY	-	expression tag	UNP Q8ISF8
B	-39	GLY	-	expression tag	UNP Q8ISF8
B	-38	SER	-	expression tag	UNP Q8ISF8
B	-37	HIS	-	expression tag	UNP Q8ISF8
B	-36	HIS	-	expression tag	UNP Q8ISF8
B	-35	HIS	-	expression tag	UNP Q8ISF8
B	-34	HIS	-	expression tag	UNP Q8ISF8
B	-33	HIS	-	expression tag	UNP Q8ISF8
B	-32	HIS	-	expression tag	UNP Q8ISF8
B	-31	GLY	-	expression tag	UNP Q8ISF8
B	-30	MET	-	expression tag	UNP Q8ISF8
B	-29	ALA	-	expression tag	UNP Q8ISF8
B	-28	SER	-	expression tag	UNP Q8ISF8
B	-27	MET	-	expression tag	UNP Q8ISF8
B	-26	THR	-	expression tag	UNP Q8ISF8
B	-25	GLY	-	expression tag	UNP Q8ISF8
B	-24	GLY	-	expression tag	UNP Q8ISF8
B	-23	GLN	-	expression tag	UNP Q8ISF8
B	-22	GLN	-	expression tag	UNP Q8ISF8
B	-21	MET	-	expression tag	UNP Q8ISF8
B	-20	GLY	-	expression tag	UNP Q8ISF8
B	-19	ARG	-	expression tag	UNP Q8ISF8
B	-18	ASP	-	expression tag	UNP Q8ISF8
B	-17	LEU	-	expression tag	UNP Q8ISF8
B	-16	TYR	-	expression tag	UNP Q8ISF8
B	-15	ASP	-	expression tag	UNP Q8ISF8
B	-14	ASP	-	expression tag	UNP Q8ISF8
B	-13	ASP	-	expression tag	UNP Q8ISF8
B	-12	ASP	-	expression tag	UNP Q8ISF8

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Chain	Residue	Modelled	Actual	Comment	Reference
B	-11	LYS	-	expression tag	UNP Q8ISF8
B	-10	GLU	-	expression tag	UNP Q8ISF8
B	-9	ASN	-	expression tag	UNP Q8ISF8
B	-8	LEU	-	expression tag	UNP Q8ISF8
B	-7	TYR	-	expression tag	UNP Q8ISF8
B	-6	PHE	-	expression tag	UNP Q8ISF8
B	-5	GLN	-	expression tag	UNP Q8ISF8
B	-4	GLY	-	expression tag	UNP Q8ISF8
B	-3	HIS	-	expression tag	UNP Q8ISF8
B	-2	MET	-	expression tag	UNP Q8ISF8
B	-1	ARG	-	expression tag	UNP Q8ISF8
B	0	SER	-	expression tag	UNP Q8ISF8
B	1	MET	-	expression tag	UNP Q8ISF8
B	2	VAL	-	expression tag	UNP Q8ISF8
B	3	SER	-	expression tag	UNP Q8ISF8
B	4	LYS	-	expression tag	UNP Q8ISF8
B	5	GLY	-	expression tag	UNP Q8ISF8
B	6	GLU	-	expression tag	UNP Q8ISF8
B	7	GLU	-	expression tag	UNP Q8ISF8
B	12	ILE	ASN	conflict	UNP Q8ISF8
B	14	HIS	ARG	conflict	UNP Q8ISF8
B	15	ILE	MET	conflict	UNP Q8ISF8
B	16	LYS	MET	conflict	UNP Q8ISF8
B	17	LEU	VAL	conflict	UNP Q8ISF8
B	18	TYR	VAL	conflict	UNP Q8ISF8
B	22	THR	SER	conflict	UNP Q8ISF8
B	25	ASN	GLY	conflict	UNP Q8ISF8
B	26	HIS	TYR	conflict	UNP Q8ISF8
B	27	HIS	GLN	conflict	UNP Q8ISF8
B	32	SER	GLY	conflict	UNP Q8ISF8
B	35	GLU	ASP	conflict	UNP Q8ISF8
B	37	LYS	ASN	conflict	UNP Q8ISF8
B	40	GLU	MET	conflict	UNP Q8ISF8
B	47	VAL	ILE	conflict	UNP Q8ISF8
B	?	-	MET	deletion	UNP Q8ISF8
B	?	-	TYR	deletion	UNP Q8ISF8
B	68	NRP	GLY	conflict	UNP Q8ISF8
B	71	ARG	LYS	conflict	UNP Q8ISF8
B	75	ASN	LYS	conflict	UNP Q8ISF8
B	78	GLN	LYS	conflict	UNP Q8ISF8
B	99	THR	ARG	conflict	UNP Q8ISF8
B	106	LEU	PHE	conflict	UNP Q8ISF8

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Chain	Residue	Modelled	Actual	Comment	Reference
B	108	ALA	VAL	conflict	UNP Q8ISF8
B	109	THR	MET	conflict	UNP Q8ISF8
B	115	GLN	GLU	conflict	UNP Q8ISF8
B	120	ILE	VAL	conflict	UNP Q8ISF8
B	122	ASN	HIS	conflict	UNP Q8ISF8
B	123	VAL	ALA	conflict	UNP Q8ISF8
B	125	ILE	VAL	conflict	UNP Q8ISF8
B	126	ARG	THR	conflict	UNP Q8ISF8
B	135	PRO	ALA	conflict	UNP Q8ISF8
B	142	LEU	LYS	conflict	UNP Q8ISF8
B	146	ALA	PRO	conflict	UNP Q8ISF8
B	147	SER	ASN	conflict	UNP Q8ISF8
B	150	LYS	MET	conflict	UNP Q8ISF8
B	152	LYS	TYR	conflict	UNP Q8ISF8
B	159	GLU	ARG	conflict	UNP Q8ISF8
B	161	ARG	TYR	conflict	UNP Q8ISF8
B	163	ASP	GLN	conflict	UNP Q8ISF8
B	167	LYS	ASN	conflict	UNP Q8ISF8
B	168	LEU	VAL	conflict	UNP Q8ISF8
B	169	VAL	ASP	conflict	UNP Q8ISF8
B	173	HIS	TYR	conflict	UNP Q8ISF8
B	175	ILE	SER	conflict	UNP Q8ISF8
B	177	ASN	SER	conflict	UNP Q8ISF8
B	179	LYS	GLU	conflict	UNP Q8ISF8
B	187	PRO	THR	conflict	UNP Q8ISF8
B	188	ALA	VAL	conflict	UNP Q8ISF8
B	189	LYS	GLU	conflict	UNP Q8ISF8
B	191	LEU	PHE	conflict	UNP Q8ISF8
B	196	VAL	PHE	conflict	UNP Q8ISF8
B	197	TYR	HIS	conflict	UNP Q8ISF8
B	198	TYR	PHE	conflict	UNP Q8ISF8
B	206	ILE	LEU	conflict	UNP Q8ISF8
B	207	LYS	GLU	conflict	UNP Q8ISF8
B	209	ALA	SER	conflict	UNP Q8ISF8
B	213	THR	MET	conflict	UNP Q8ISF8
B	214	TYR	PHE	conflict	UNP Q8ISF8
B	216	GLU	VAL	conflict	UNP Q8ISF8
B	217	LEU	GLN	conflict	UNP Q8ISF8
B	220	VAL	HIS	conflict	UNP Q8ISF8
B	221	SER	ALA	conflict	UNP Q8ISF8
B	224	ARG	LYS	conflict	UNP Q8ISF8
B	225	TYR	PHE	conflict	UNP Q8ISF8

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Chain	Residue	Modelled	Actual	Comment	Reference
B	226	PRO	CYS	conflict	UNP Q8ISF8
B	234	HIS	-	expression tag	UNP Q8ISF8
B	235	ARG	-	expression tag	UNP Q8ISF8
C	-41	MET	-	initiating methionine	UNP Q8ISF8
C	-40	GLY	-	expression tag	UNP Q8ISF8
C	-39	GLY	-	expression tag	UNP Q8ISF8
C	-38	SER	-	expression tag	UNP Q8ISF8
C	-37	HIS	-	expression tag	UNP Q8ISF8
C	-36	HIS	-	expression tag	UNP Q8ISF8
C	-35	HIS	-	expression tag	UNP Q8ISF8
C	-34	HIS	-	expression tag	UNP Q8ISF8
C	-33	HIS	-	expression tag	UNP Q8ISF8
C	-32	HIS	-	expression tag	UNP Q8ISF8
C	-31	GLY	-	expression tag	UNP Q8ISF8
C	-30	MET	-	expression tag	UNP Q8ISF8
C	-29	ALA	-	expression tag	UNP Q8ISF8
C	-28	SER	-	expression tag	UNP Q8ISF8
C	-27	MET	-	expression tag	UNP Q8ISF8
C	-26	THR	-	expression tag	UNP Q8ISF8
C	-25	GLY	-	expression tag	UNP Q8ISF8
C	-24	GLY	-	expression tag	UNP Q8ISF8
C	-23	GLN	-	expression tag	UNP Q8ISF8
C	-22	GLN	-	expression tag	UNP Q8ISF8
C	-21	MET	-	expression tag	UNP Q8ISF8
C	-20	GLY	-	expression tag	UNP Q8ISF8
C	-19	ARG	-	expression tag	UNP Q8ISF8
C	-18	ASP	-	expression tag	UNP Q8ISF8
C	-17	LEU	-	expression tag	UNP Q8ISF8
C	-16	TYR	-	expression tag	UNP Q8ISF8
C	-15	ASP	-	expression tag	UNP Q8ISF8
C	-14	ASP	-	expression tag	UNP Q8ISF8
C	-13	ASP	-	expression tag	UNP Q8ISF8
C	-12	ASP	-	expression tag	UNP Q8ISF8
C	-11	LYS	-	expression tag	UNP Q8ISF8
C	-10	GLU	-	expression tag	UNP Q8ISF8
C	-9	ASN	-	expression tag	UNP Q8ISF8
C	-8	LEU	-	expression tag	UNP Q8ISF8
C	-7	TYR	-	expression tag	UNP Q8ISF8
C	-6	PHE	-	expression tag	UNP Q8ISF8
C	-5	GLN	-	expression tag	UNP Q8ISF8
C	-4	GLY	-	expression tag	UNP Q8ISF8
C	-3	HIS	-	expression tag	UNP Q8ISF8

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Chain	Residue	Modelled	Actual	Comment	Reference
C	-2	MET	-	expression tag	UNP Q8ISF8
C	-1	ARG	-	expression tag	UNP Q8ISF8
C	0	SER	-	expression tag	UNP Q8ISF8
C	1	MET	-	expression tag	UNP Q8ISF8
C	2	VAL	-	expression tag	UNP Q8ISF8
C	3	SER	-	expression tag	UNP Q8ISF8
C	4	LYS	-	expression tag	UNP Q8ISF8
C	5	GLY	-	expression tag	UNP Q8ISF8
C	6	GLU	-	expression tag	UNP Q8ISF8
C	7	GLU	-	expression tag	UNP Q8ISF8
C	12	ILE	ASN	conflict	UNP Q8ISF8
C	14	HIS	ARG	conflict	UNP Q8ISF8
C	15	ILE	MET	conflict	UNP Q8ISF8
C	16	LYS	MET	conflict	UNP Q8ISF8
C	17	LEU	VAL	conflict	UNP Q8ISF8
C	18	TYR	VAL	conflict	UNP Q8ISF8
C	22	THR	SER	conflict	UNP Q8ISF8
C	25	ASN	GLY	conflict	UNP Q8ISF8
C	26	HIS	TYR	conflict	UNP Q8ISF8
C	27	HIS	GLN	conflict	UNP Q8ISF8
C	32	SER	GLY	conflict	UNP Q8ISF8
C	35	GLU	ASP	conflict	UNP Q8ISF8
C	37	LYS	ASN	conflict	UNP Q8ISF8
C	40	GLU	MET	conflict	UNP Q8ISF8
C	47	VAL	ILE	conflict	UNP Q8ISF8
C	?	-	MET	deletion	UNP Q8ISF8
C	?	-	TYR	deletion	UNP Q8ISF8
C	68	NRP	GLY	conflict	UNP Q8ISF8
C	71	ARG	LYS	conflict	UNP Q8ISF8
C	75	ASN	LYS	conflict	UNP Q8ISF8
C	78	GLN	LYS	conflict	UNP Q8ISF8
C	99	THR	ARG	conflict	UNP Q8ISF8
C	106	LEU	PHE	conflict	UNP Q8ISF8
C	108	ALA	VAL	conflict	UNP Q8ISF8
C	109	THR	MET	conflict	UNP Q8ISF8
C	115	GLN	GLU	conflict	UNP Q8ISF8
C	120	ILE	VAL	conflict	UNP Q8ISF8
C	122	ASN	HIS	conflict	UNP Q8ISF8
C	123	VAL	ALA	conflict	UNP Q8ISF8
C	125	ILE	VAL	conflict	UNP Q8ISF8
C	126	ARG	THR	conflict	UNP Q8ISF8
C	135	PRO	ALA	conflict	UNP Q8ISF8

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Chain	Residue	Modelled	Actual	Comment	Reference
C	142	LEU	LYS	conflict	UNP Q8ISF8
C	146	ALA	PRO	conflict	UNP Q8ISF8
C	147	SER	ASN	conflict	UNP Q8ISF8
C	150	LYS	MET	conflict	UNP Q8ISF8
C	152	LYS	TYR	conflict	UNP Q8ISF8
C	159	GLU	ARG	conflict	UNP Q8ISF8
C	161	ARG	TYR	conflict	UNP Q8ISF8
C	163	ASP	GLN	conflict	UNP Q8ISF8
C	167	LYS	ASN	conflict	UNP Q8ISF8
C	168	LEU	VAL	conflict	UNP Q8ISF8
C	169	VAL	ASP	conflict	UNP Q8ISF8
C	173	HIS	TYR	conflict	UNP Q8ISF8
C	175	ILE	SER	conflict	UNP Q8ISF8
C	177	ASN	SER	conflict	UNP Q8ISF8
C	179	LYS	GLU	conflict	UNP Q8ISF8
C	187	PRO	THR	conflict	UNP Q8ISF8
C	188	ALA	VAL	conflict	UNP Q8ISF8
C	189	LYS	GLU	conflict	UNP Q8ISF8
C	191	LEU	PHE	conflict	UNP Q8ISF8
C	196	VAL	PHE	conflict	UNP Q8ISF8
C	197	TYR	HIS	conflict	UNP Q8ISF8
C	198	TYR	PHE	conflict	UNP Q8ISF8
C	206	ILE	LEU	conflict	UNP Q8ISF8
C	207	LYS	GLU	conflict	UNP Q8ISF8
C	209	ALA	SER	conflict	UNP Q8ISF8
C	213	THR	MET	conflict	UNP Q8ISF8
C	214	TYR	PHE	conflict	UNP Q8ISF8
C	216	GLU	VAL	conflict	UNP Q8ISF8
C	217	LEU	GLN	conflict	UNP Q8ISF8
C	220	VAL	HIS	conflict	UNP Q8ISF8
C	221	SER	ALA	conflict	UNP Q8ISF8
C	224	ARG	LYS	conflict	UNP Q8ISF8
C	225	TYR	PHE	conflict	UNP Q8ISF8
C	226	PRO	CYS	conflict	UNP Q8ISF8
C	234	HIS	-	expression tag	UNP Q8ISF8
C	235	ARG	-	expression tag	UNP Q8ISF8
D	-41	MET	-	initiating methionine	UNP Q8ISF8
D	-40	GLY	-	expression tag	UNP Q8ISF8
D	-39	GLY	-	expression tag	UNP Q8ISF8
D	-38	SER	-	expression tag	UNP Q8ISF8
D	-37	HIS	-	expression tag	UNP Q8ISF8
D	-36	HIS	-	expression tag	UNP Q8ISF8

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Chain	Residue	Modelled	Actual	Comment	Reference
D	-35	HIS	-	expression tag	UNP Q8ISF8
D	-34	HIS	-	expression tag	UNP Q8ISF8
D	-33	HIS	-	expression tag	UNP Q8ISF8
D	-32	HIS	-	expression tag	UNP Q8ISF8
D	-31	GLY	-	expression tag	UNP Q8ISF8
D	-30	MET	-	expression tag	UNP Q8ISF8
D	-29	ALA	-	expression tag	UNP Q8ISF8
D	-28	SER	-	expression tag	UNP Q8ISF8
D	-27	MET	-	expression tag	UNP Q8ISF8
D	-26	THR	-	expression tag	UNP Q8ISF8
D	-25	GLY	-	expression tag	UNP Q8ISF8
D	-24	GLY	-	expression tag	UNP Q8ISF8
D	-23	GLN	-	expression tag	UNP Q8ISF8
D	-22	GLN	-	expression tag	UNP Q8ISF8
D	-21	MET	-	expression tag	UNP Q8ISF8
D	-20	GLY	-	expression tag	UNP Q8ISF8
D	-19	ARG	-	expression tag	UNP Q8ISF8
D	-18	ASP	-	expression tag	UNP Q8ISF8
D	-17	LEU	-	expression tag	UNP Q8ISF8
D	-16	TYR	-	expression tag	UNP Q8ISF8
D	-15	ASP	-	expression tag	UNP Q8ISF8
D	-14	ASP	-	expression tag	UNP Q8ISF8
D	-13	ASP	-	expression tag	UNP Q8ISF8
D	-12	ASP	-	expression tag	UNP Q8ISF8
D	-11	LYS	-	expression tag	UNP Q8ISF8
D	-10	GLU	-	expression tag	UNP Q8ISF8
D	-9	ASN	-	expression tag	UNP Q8ISF8
D	-8	LEU	-	expression tag	UNP Q8ISF8
D	-7	TYR	-	expression tag	UNP Q8ISF8
D	-6	PHE	-	expression tag	UNP Q8ISF8
D	-5	GLN	-	expression tag	UNP Q8ISF8
D	-4	GLY	-	expression tag	UNP Q8ISF8
D	-3	HIS	-	expression tag	UNP Q8ISF8
D	-2	MET	-	expression tag	UNP Q8ISF8
D	-1	ARG	-	expression tag	UNP Q8ISF8
D	0	SER	-	expression tag	UNP Q8ISF8
D	1	MET	-	expression tag	UNP Q8ISF8
D	2	VAL	-	expression tag	UNP Q8ISF8
D	3	SER	-	expression tag	UNP Q8ISF8
D	4	LYS	-	expression tag	UNP Q8ISF8
D	5	GLY	-	expression tag	UNP Q8ISF8
D	6	GLU	-	expression tag	UNP Q8ISF8

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Chain	Residue	Modelled	Actual	Comment	Reference
D	7	GLU	-	expression tag	UNP Q8ISF8
D	12	ILE	ASN	conflict	UNP Q8ISF8
D	14	HIS	ARG	conflict	UNP Q8ISF8
D	15	ILE	MET	conflict	UNP Q8ISF8
D	16	LYS	MET	conflict	UNP Q8ISF8
D	17	LEU	VAL	conflict	UNP Q8ISF8
D	18	TYR	VAL	conflict	UNP Q8ISF8
D	22	THR	SER	conflict	UNP Q8ISF8
D	25	ASN	GLY	conflict	UNP Q8ISF8
D	26	HIS	TYR	conflict	UNP Q8ISF8
D	27	HIS	GLN	conflict	UNP Q8ISF8
D	32	SER	GLY	conflict	UNP Q8ISF8
D	35	GLU	ASP	conflict	UNP Q8ISF8
D	37	LYS	ASN	conflict	UNP Q8ISF8
D	40	GLU	MET	conflict	UNP Q8ISF8
D	47	VAL	ILE	conflict	UNP Q8ISF8
D	?	-	MET	deletion	UNP Q8ISF8
D	?	-	TYR	deletion	UNP Q8ISF8
D	68	NRP	GLY	conflict	UNP Q8ISF8
D	71	ARG	LYS	conflict	UNP Q8ISF8
D	75	ASN	LYS	conflict	UNP Q8ISF8
D	78	GLN	LYS	conflict	UNP Q8ISF8
D	99	THR	ARG	conflict	UNP Q8ISF8
D	106	LEU	PHE	conflict	UNP Q8ISF8
D	108	ALA	VAL	conflict	UNP Q8ISF8
D	109	THR	MET	conflict	UNP Q8ISF8
D	115	GLN	GLU	conflict	UNP Q8ISF8
D	120	ILE	VAL	conflict	UNP Q8ISF8
D	122	ASN	HIS	conflict	UNP Q8ISF8
D	123	VAL	ALA	conflict	UNP Q8ISF8
D	125	ILE	VAL	conflict	UNP Q8ISF8
D	126	ARG	THR	conflict	UNP Q8ISF8
D	135	PRO	ALA	conflict	UNP Q8ISF8
D	142	LEU	LYS	conflict	UNP Q8ISF8
D	146	ALA	PRO	conflict	UNP Q8ISF8
D	147	SER	ASN	conflict	UNP Q8ISF8
D	150	LYS	MET	conflict	UNP Q8ISF8
D	152	LYS	TYR	conflict	UNP Q8ISF8
D	159	GLU	ARG	conflict	UNP Q8ISF8
D	161	ARG	TYR	conflict	UNP Q8ISF8
D	163	ASP	GLN	conflict	UNP Q8ISF8
D	167	LYS	ASN	conflict	UNP Q8ISF8

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Chain	Residue	Modelled	Actual	Comment	Reference
D	168	LEU	VAL	conflict	UNP Q8ISF8
D	169	VAL	ASP	conflict	UNP Q8ISF8
D	173	HIS	TYR	conflict	UNP Q8ISF8
D	175	ILE	SER	conflict	UNP Q8ISF8
D	177	ASN	SER	conflict	UNP Q8ISF8
D	179	LYS	GLU	conflict	UNP Q8ISF8
D	187	PRO	THR	conflict	UNP Q8ISF8
D	188	ALA	VAL	conflict	UNP Q8ISF8
D	189	LYS	GLU	conflict	UNP Q8ISF8
D	191	LEU	PHE	conflict	UNP Q8ISF8
D	196	VAL	PHE	conflict	UNP Q8ISF8
D	197	TYR	HIS	conflict	UNP Q8ISF8
D	198	TYR	PHE	conflict	UNP Q8ISF8
D	206	ILE	LEU	conflict	UNP Q8ISF8
D	207	LYS	GLU	conflict	UNP Q8ISF8
D	209	ALA	SER	conflict	UNP Q8ISF8
D	213	THR	MET	conflict	UNP Q8ISF8
D	214	TYR	PHE	conflict	UNP Q8ISF8
D	216	GLU	VAL	conflict	UNP Q8ISF8
D	217	LEU	GLN	conflict	UNP Q8ISF8
D	220	VAL	HIS	conflict	UNP Q8ISF8
D	221	SER	ALA	conflict	UNP Q8ISF8
D	224	ARG	LYS	conflict	UNP Q8ISF8
D	225	TYR	PHE	conflict	UNP Q8ISF8
D	226	PRO	CYS	conflict	UNP Q8ISF8
D	234	HIS	-	expression tag	UNP Q8ISF8
D	235	ARG	-	expression tag	UNP Q8ISF8

- Molecule 2 is water.

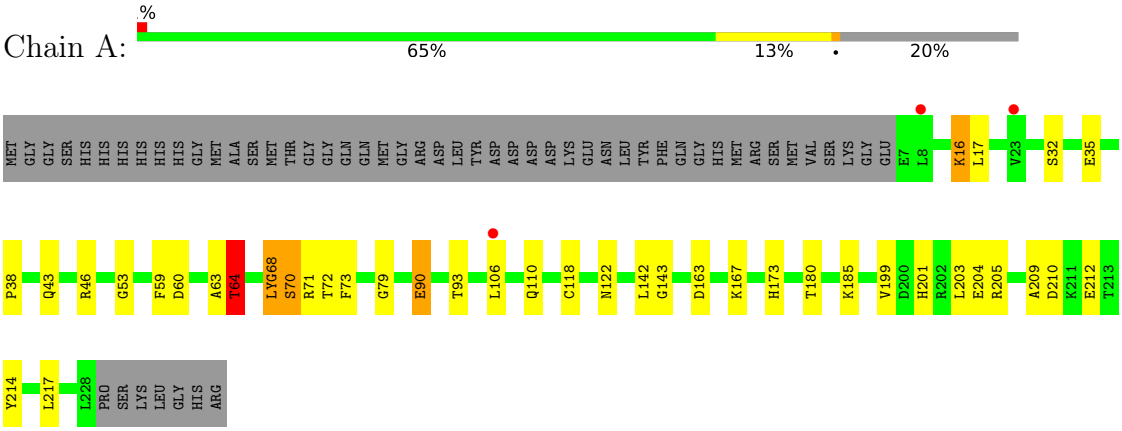
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	14	Total O 14 14	0	0
2	B	12	Total O 12 12	0	0
2	C	7	Total O 7 7	0	0
2	D	7	Total O 7 7	0	0

3 Residue-property plots (i)

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.

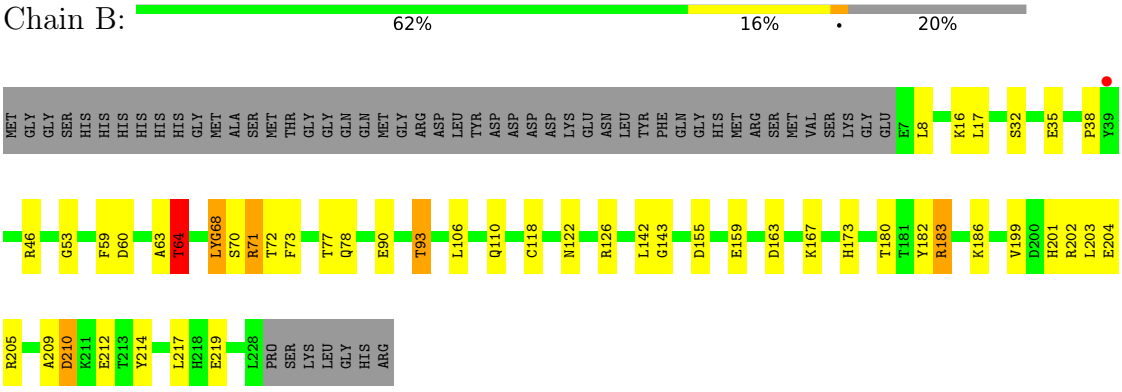
• Molecule 1: Blue-to-red TagFT fluorescent timer

Chain A:



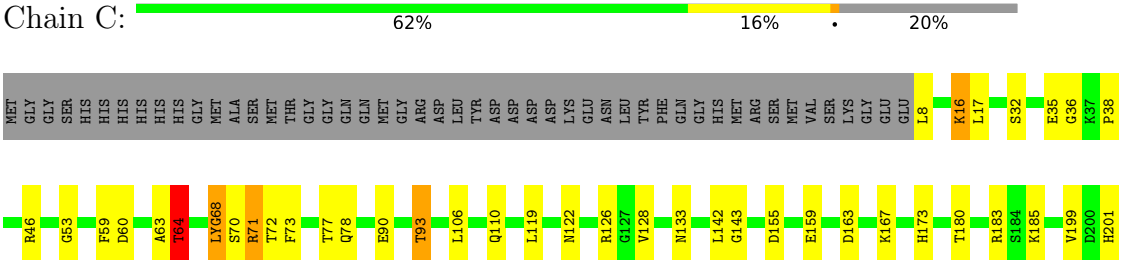
• Molecule 1: Blue-to-red TagFT fluorescent timer

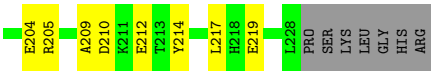
Chain B:



• Molecule 1: Blue-to-red TagFT fluorescent timer

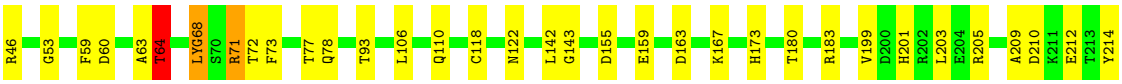
Chain C:

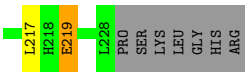




• Molecule 1: Blue-to-red TagFT fluorescent timer

Chain D:





4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 2 1	Depositor
Cell constants a, b, c, α, β, γ	60.65Å 95.32Å 95.38Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	95.32 – 2.90 95.38 – 2.90	Depositor EDS
% Data completeness (in resolution range)	96.8 (95.32-2.90) 96.7 (95.38-2.90)	Depositor EDS
R_{merge}	0.16	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.44 (at 2.91Å)	Xtriage
Refinement program	BUSTER	Depositor
R, R_{free}	0.242 , 0.277 0.240 , 0.281	Depositor DCC
R_{free} test set	1023 reflections (4.37%)	wwPDB-VP
Wilson B-factor (Å^2)	68.8	Xtriage
Anisotropy	0.312	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.34 , 54.7	EDS
L-test for twinning[2]	$< \|L\| > = 0.51$, $< L^2 > = 0.35$	Xtriage
Estimated twinning fraction	0.400 for -h,l,k 0.408 for -h,-l,-k 0.419 for h,-k,-l	Xtriage
F_o,F_c correlation	0.92	EDS
Total number of atoms	6814	wwPDB-VP
Average B, all atoms (Å^2)	73.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 6.60% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ 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

Bond lengths and bond angles in the following residue types are not validated in this section: NRP

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	0.42	0/1707	0.64	0/2318
1	B	0.43	0/1736	0.64	0/2354
1	C	0.42	0/1714	0.64	0/2325
1	D	0.42	0/1717	0.65	0/2330
All	All	0.42	0/6874	0.64	0/9327

There are no bond length outliers.

There are no bond angle outliers.

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	1683	0	1574	19	0
1	B	1708	0	1616	19	0
1	C	1690	0	1594	19	0
1	D	1693	0	1591	18	0
2	A	14	0	0	0	0
2	B	12	0	0	0	0
2	C	7	0	0	0	0
2	D	7	0	0	0	0
All	All	6814	0	6375	72	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 5.

All (72) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:68:NRP:HD3A	1:A:203:LEU:HD11	1.63	0.80
1:B:63:ALA:O	1:B:64:THR:HB	1.83	0.77
1:A:71:ARG:NH1	1:A:201:HIS:NE2	2.37	0.71
1:A:43:GLN:OE1	1:A:70:SER:HB2	1.91	0.71
1:D:63:ALA:O	1:D:64:THR:HB	1.92	0.69
1:C:63:ALA:O	1:C:64:THR:HB	1.94	0.68
1:D:71:ARG:NH1	1:D:201:HIS:NE2	2.41	0.67
1:B:17:LEU:HB3	1:B:32:SER:HB3	1.77	0.67
1:C:17:LEU:HB3	1:C:32:SER:HB3	1.78	0.66
1:D:68:NRP:HD3A	1:D:203:LEU:HD11	1.77	0.66
1:A:17:LEU:HB3	1:A:32:SER:HB3	1.77	0.65
1:D:17:LEU:HB3	1:D:32:SER:HB3	1.78	0.64
1:B:68:NRP:HD4B	1:B:219:GLU:HB3	1.82	0.61
1:C:199:VAL:HG12	1:C:201:HIS:CE1	2.35	0.60
1:C:167:LYS:HA	1:C:173:HIS:CD2	2.36	0.60
1:B:167:LYS:HA	1:B:173:HIS:CD2	2.36	0.60
1:A:199:VAL:HG12	1:A:201:HIS:CE1	2.36	0.60
1:B:199:VAL:HG12	1:B:201:HIS:CE1	2.36	0.59
1:D:167:LYS:HA	1:D:173:HIS:CD2	2.37	0.59
1:A:167:LYS:HA	1:A:173:HIS:CD2	2.37	0.58
1:B:68:NRP:HD4B	1:B:219:GLU:CB	2.34	0.57
1:A:90:GLU:HB2	1:A:185:LYS:HB2	1.88	0.56
1:A:38:PRO:HA	1:A:73:PHE:HA	1.88	0.55
1:B:93:THR:HG22	1:B:183:ARG:HB2	1.87	0.55
1:D:143:GLY:H	1:D:167:LYS:NZ	2.07	0.53
1:C:93:THR:HG22	1:C:183:ARG:HB2	1.90	0.52
1:D:199:VAL:HG12	1:D:201:HIS:CE1	2.45	0.52
1:A:16:LYS:NZ	1:D:118:CYS:SG	2.74	0.52
1:A:143:GLY:H	1:A:167:LYS:NZ	2.08	0.52
1:C:143:GLY:H	1:C:167:LYS:HZ2	1.58	0.52
1:C:90:GLU:O	1:C:185:LYS:HD2	2.10	0.51
1:A:63:ALA:O	1:A:64:THR:HB	2.08	0.51
1:B:143:GLY:H	1:B:167:LYS:HZ2	1.59	0.51
1:C:143:GLY:H	1:C:167:LYS:NZ	2.07	0.51
1:A:143:GLY:H	1:A:167:LYS:HZ2	1.58	0.50
1:B:143:GLY:H	1:B:167:LYS:NZ	2.08	0.50
1:D:143:GLY:H	1:D:167:LYS:HZ2	1.58	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:60:ASP:OD2	1:C:142:LEU:O	2.31	0.49
1:B:60:ASP:OD2	1:B:142:LEU:O	2.31	0.48
1:A:60:ASP:OD2	1:A:142:LEU:O	2.31	0.48
1:D:60:ASP:OD2	1:D:142:LEU:O	2.31	0.48
1:C:199:VAL:CG1	1:C:201:HIS:CE1	2.97	0.47
1:A:35:GLU:OE1	1:A:46:ARG:NH2	2.48	0.46
1:B:199:VAL:CG1	1:B:201:HIS:CE1	2.98	0.46
1:D:35:GLU:OE1	1:D:46:ARG:NH2	2.49	0.46
1:A:199:VAL:CG1	1:A:201:HIS:CE1	2.98	0.45
1:B:35:GLU:OE1	1:B:46:ARG:NH2	2.50	0.44
1:C:38:PRO:HA	1:C:73:PHE:HA	1.99	0.44
1:D:205:ARG:HH12	1:D:212:GLU:HG2	1.81	0.44
1:C:205:ARG:HH12	1:C:212:GLU:HG2	1.81	0.44
1:A:209:ALA:HB3	1:A:214:TYR:HB3	2.00	0.44
1:B:71:ARG:HD3	1:B:182:TYR:CE1	2.52	0.44
1:D:59:PHE:HE2	1:D:217:LEU:HD11	1.83	0.44
1:B:38:PRO:HA	1:B:73:PHE:HA	2.00	0.44
1:A:205:ARG:HH12	1:A:212:GLU:HG2	1.82	0.43
1:C:35:GLU:OE1	1:C:46:ARG:NH2	2.51	0.43
1:D:209:ALA:HB3	1:D:214:TYR:HB3	2.01	0.43
1:B:205:ARG:HH12	1:B:212:GLU:HG2	1.83	0.43
1:D:199:VAL:CG1	1:D:201:HIS:CE1	3.01	0.43
1:B:118:CYS:SG	1:C:16:LYS:NZ	2.82	0.43
1:C:59:PHE:HE2	1:C:217:LEU:HD11	1.84	0.43
1:C:68:NRP:HD4B	1:C:219:GLU:HB3	2.02	0.42
1:C:209:ALA:HB3	1:C:214:TYR:HB3	2.00	0.42
1:A:118:CYS:SG	1:D:16:LYS:NZ	2.83	0.42
1:B:59:PHE:HE2	1:B:217:LEU:HD11	1.85	0.42
1:C:71:ARG:H	1:C:71:ARG:HG2	1.54	0.42
1:C:36:GLY:O	1:C:38:PRO:HD3	2.21	0.41
1:B:203:LEU:HD13	1:B:219:GLU:HB2	2.02	0.41
1:B:209:ALA:HB3	1:B:214:TYR:HB3	2.01	0.41
1:D:68:NRP:HD4B	1:D:219:GLU:HB3	2.03	0.41
1:A:59:PHE:HE2	1:A:217:LEU:HD11	1.86	0.40
1:D:38:PRO:HA	1:D:73:PHE:HA	2.04	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	215/275 (78%)	197 (92%)	14 (6%)	4 (2%)	8	28
1	B	216/275 (78%)	201 (93%)	10 (5%)	5 (2%)	6	23
1	C	214/275 (78%)	200 (94%)	9 (4%)	5 (2%)	6	23
1	D	214/275 (78%)	200 (94%)	8 (4%)	6 (3%)	5	19
All	All	859/1100 (78%)	798 (93%)	41 (5%)	20 (2%)	6	23

All (20) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	64	THR
1	A	53	GLY
1	B	53	GLY
1	B	64	THR
1	C	53	GLY
1	C	64	THR
1	D	53	GLY
1	D	64	THR
1	D	77	THR
1	A	210	ASP
1	B	78	GLN
1	C	210	ASP
1	D	78	GLN
1	D	210	ASP
1	A	79	GLY
1	C	78	GLN
1	C	155	ASP
1	B	210	ASP
1	B	155	ASP
1	D	155	ASP

5.3.2 Protein sidechains (i)

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	171/234 (73%)	159 (93%)	12 (7%)	15 41
1	B	176/234 (75%)	155 (88%)	21 (12%)	5 15
1	C	173/234 (74%)	154 (89%)	19 (11%)	6 19
1	D	174/234 (74%)	161 (92%)	13 (8%)	13 37
All	All	694/936 (74%)	629 (91%)	65 (9%)	8 26

All (65) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	16	LYS
1	A	64	THR
1	A	70	SER
1	A	72	THR
1	A	90	GLU
1	A	93	THR
1	A	106	LEU
1	A	110	GLN
1	A	122	ASN
1	A	163	ASP
1	A	180	THR
1	A	204	GLU
1	B	8	LEU
1	B	16	LYS
1	B	64	THR
1	B	70	SER
1	B	71	ARG
1	B	72	THR
1	B	77	THR
1	B	90	GLU
1	B	93	THR
1	B	106	LEU
1	B	110	GLN
1	B	122	ASN

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Mol	Chain	Res	Type
1	B	126	ARG
1	B	159	GLU
1	B	163	ASP
1	B	180	THR
1	B	183	ARG
1	B	186	LYS
1	B	202	ARG
1	B	204	GLU
1	B	210	ASP
1	C	8	LEU
1	C	16	LYS
1	C	64	THR
1	C	70	SER
1	C	71	ARG
1	C	72	THR
1	C	77	THR
1	C	93	THR
1	C	106	LEU
1	C	110	GLN
1	C	119	LEU
1	C	122	ASN
1	C	126	ARG
1	C	128	VAL
1	C	133	ASN
1	C	159	GLU
1	C	163	ASP
1	C	180	THR
1	C	204	GLU
1	D	16	LYS
1	D	64	THR
1	D	71	ARG
1	D	72	THR
1	D	93	THR
1	D	106	LEU
1	D	110	GLN
1	D	122	ASN
1	D	159	GLU
1	D	163	ASP
1	D	180	THR
1	D	183	ARG
1	D	219	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are

no such sidechains identified.

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

4 non-standard protein/DNA/RNA residues are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. 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 $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
1	NRP	A	68	1	14,16,25	1.31	3 (21%)	13,22,35	1.96	3 (23%)
1	NRP	D	68	1	14,16,25	1.26	2 (14%)	13,22,35	2.11	4 (30%)
1	NRP	B	68	1	14,16,25	1.34	3 (21%)	13,22,35	2.35	3 (23%)
1	NRP	C	68	1	14,16,25	1.33	3 (21%)	13,22,35	2.41	3 (23%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
1	NRP	A	68	1	-	1/5/27/32	0/1/1/2
1	NRP	D	68	1	-	2/5/27/32	0/1/1/2
1	NRP	B	68	1	-	1/5/27/32	0/1/1/2
1	NRP	C	68	1	-	1/5/27/32	0/1/1/2

All (11) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	68	NRP	C1-N2	3.15	1.40	1.33
1	A	68	NRP	C1-N2	3.05	1.39	1.33
1	B	68	NRP	C1-N2	2.96	1.39	1.33
1	D	68	NRP	C1-N2	2.95	1.39	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	68	NRP	C1-N3	2.64	1.42	1.38
1	A	68	NRP	CA2-C2	2.43	1.48	1.43
1	C	68	NRP	CA2-C2	2.34	1.47	1.43
1	B	68	NRP	CA2-C2	2.30	1.47	1.43
1	C	68	NRP	C1-N3	2.19	1.42	1.38
1	D	68	NRP	CA2-C2	2.13	1.47	1.43
1	A	68	NRP	C1-N3	2.03	1.41	1.38

All (13) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	C	68	NRP	CA2-C2-N3	7.19	106.77	103.37
1	B	68	NRP	CA2-C2-N3	6.83	106.60	103.37
1	D	68	NRP	CA2-C2-N3	5.85	106.14	103.37
1	A	68	NRP	CA2-C2-N3	5.74	106.08	103.37
1	B	68	NRP	O3-C3-CA3	-3.68	115.27	126.39
1	C	68	NRP	O3-C3-CA3	-3.42	116.07	126.39
1	A	68	NRP	O3-C3-CA3	-2.97	117.41	126.39
1	D	68	NRP	O3-C3-CA3	-2.87	117.73	126.39
1	D	68	NRP	O2-C2-CA2	-2.70	129.44	130.96
1	B	68	NRP	N3-C1-N2	-2.27	110.28	113.28
1	D	68	NRP	N3-C1-N2	-2.14	110.45	113.28
1	A	68	NRP	N3-C1-N2	-2.09	110.52	113.28
1	C	68	NRP	N3-C1-N2	-2.06	110.56	113.28

There are no chirality outliers.

All (5) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	D	68	NRP	CA1-CB1-CG1-CD3
1	D	68	NRP	CA1-CB1-CG1-CD4
1	B	68	NRP	C1-CA1-CB1-CG1
1	C	68	NRP	C1-CA1-CB1-CG1
1	A	68	NRP	C3-CA3-N3-C2

There are no ring outliers.

4 monomers are involved in 6 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	A	68	NRP	1	0
1	D	68	NRP	2	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	B	68	NRP	2	0
1	C	68	NRP	1	0

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, 95^{th} 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	219/275 (79%)	0.13	3 (1%) 75 75	58, 71, 89, 96	0
1	B	219/275 (79%)	0.02	1 (0%) 91 91	58, 72, 89, 95	0
1	C	218/275 (79%)	0.10	0 100 100	60, 72, 88, 96	0
1	D	218/275 (79%)	0.07	0 100 100	58, 71, 89, 96	0
All	All	874/1100 (79%)	0.08	4 (0%) 91 91	58, 72, 89, 96	0

All (4) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	39	TYR	2.3
1	A	106	LEU	2.1
1	A	8	LEU	2.1
1	A	23	VAL	2.1

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

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
1	NRP	B	68	16/24	0.84	0.30	73,74,75,76	0
1	NRP	C	68	16/24	0.84	0.38	73,75,76,76	0
1	NRP	A	68	16/24	0.85	0.33	74,76,77,78	0
1	NRP	D	68	16/24	0.85	0.25	75,77,78,79	0

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.