



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 09:48 AM UTC

PDB ID : 4ZWT / pdb_00004zwt
Title : Crystal Structure of the Bacteriophage T4 recombination mediator protein
UvsY, Lattice Type IV
Authors : Gajewski, S.; White, S.W.
Deposited on : 2015-05-19
Resolution : 4.20 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

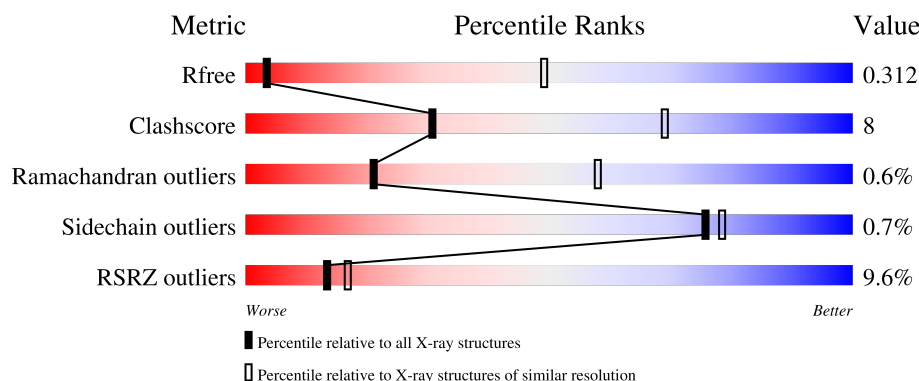
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 4.20 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.



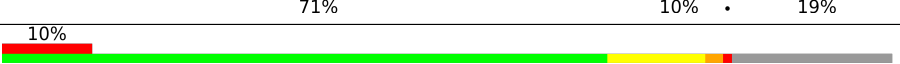
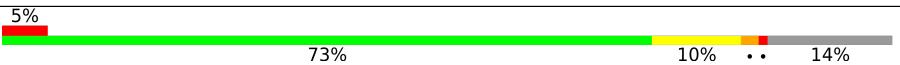
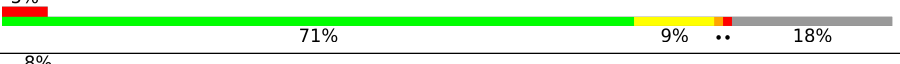
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	1004 (4.52-3.88)
Clashscore	190562	1019 (4.50-3.90)
Ramachandran outliers	187476	1020 (4.56-3.84)
Sidechain outliers	187428	1006 (4.56-3.84)
RSRZ outliers	180081	1001 (4.52-3.88)

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	157	8% 62% 12% •• 23%
1	B	157	8% 70% 8% •• 20%
1	C	157	10% 71% 11% •• 15%
1	D	157	7% 61% 17% •• 18%
1	E	157	10% 67% 10% •• 20%

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Mol	Chain	Length	Quality of chain
1	F	157	
1	G	157	
1	H	157	
1	I	157	
1	J	157	
1	K	157	
1	L	157	
1	M	157	
1	N	157	

2 Entry composition

There is only 1 type of molecule in this entry. The entry contains 11717 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 Recombination protein uvsY.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	121	Total	C	N	O	S	0	0	0
			798	496	135	166	1			
1	B	126	Total	C	N	O	S	0	0	0
			826	513	143	169	1			
1	C	134	Total	C	N	O	S	0	0	0
			848	528	145	174	1			
1	D	128	Total	C	N	O	S	0	0	0
			833	519	142	171	1			
1	E	126	Total	C	N	O	S	0	0	0
			837	519	145	172	1			
1	F	125	Total	C	N	O	S	0	0	0
			812	501	140	170	1			
1	G	127	Total	C	N	O	S	0	0	0
			866	551	143	170	2			
1	H	127	Total	C	N	O	S	0	0	0
			838	522	144	171	1			
1	I	128	Total	C	N	O	S	0	0	0
			843	522	146	174	1			
1	J	135	Total	C	N	O	S	0	0	0
			886	550	154	181	1			
1	K	128	Total	C	N	O	S	0	0	0
			847	525	147	174	1			
1	L	126	Total	C	N	O	S	0	0	0
			825	514	145	165	1			
1	M	123	Total	C	N	O	S	0	0	0
			811	501	141	168	1			
1	N	125	Total	C	N	O	S	0	0	0
			847	535	146	163	3			

There are 322 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-19	MET	-	expression tag	UNP P04537

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Chain	Residue	Modelled	Actual	Comment	Reference
A	-18	GLY	-	expression tag	UNP P04537
A	-17	SER	-	expression tag	UNP P04537
A	-16	SER	-	expression tag	UNP P04537
A	-15	HIS	-	expression tag	UNP P04537
A	-14	HIS	-	expression tag	UNP P04537
A	-13	HIS	-	expression tag	UNP P04537
A	-12	HIS	-	expression tag	UNP P04537
A	-11	HIS	-	expression tag	UNP P04537
A	-10	HIS	-	expression tag	UNP P04537
A	-9	SER	-	expression tag	UNP P04537
A	-8	SER	-	expression tag	UNP P04537
A	-7	GLY	-	expression tag	UNP P04537
A	-6	LEU	-	expression tag	UNP P04537
A	-5	VAL	-	expression tag	UNP P04537
A	-4	PRO	-	expression tag	UNP P04537
A	-3	ARG	-	expression tag	UNP P04537
A	-2	GLY	-	expression tag	UNP P04537
A	-1	SER	-	expression tag	UNP P04537
A	0	HIS	-	expression tag	UNP P04537
A	79	ALA	GLU	engineered mutation	UNP P04537
A	80	ALA	LYS	engineered mutation	UNP P04537
A	81	ALA	SER	engineered mutation	UNP P04537
B	-19	MET	-	expression tag	UNP P04537
B	-18	GLY	-	expression tag	UNP P04537
B	-17	SER	-	expression tag	UNP P04537
B	-16	SER	-	expression tag	UNP P04537
B	-15	HIS	-	expression tag	UNP P04537
B	-14	HIS	-	expression tag	UNP P04537
B	-13	HIS	-	expression tag	UNP P04537
B	-12	HIS	-	expression tag	UNP P04537
B	-11	HIS	-	expression tag	UNP P04537
B	-10	HIS	-	expression tag	UNP P04537
B	-9	SER	-	expression tag	UNP P04537
B	-8	SER	-	expression tag	UNP P04537
B	-7	GLY	-	expression tag	UNP P04537
B	-6	LEU	-	expression tag	UNP P04537
B	-5	VAL	-	expression tag	UNP P04537
B	-4	PRO	-	expression tag	UNP P04537
B	-3	ARG	-	expression tag	UNP P04537
B	-2	GLY	-	expression tag	UNP P04537
B	-1	SER	-	expression tag	UNP P04537
B	0	HIS	-	expression tag	UNP P04537

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Chain	Residue	Modelled	Actual	Comment	Reference
B	79	ALA	GLU	engineered mutation	UNP P04537
B	80	ALA	LYS	engineered mutation	UNP P04537
B	81	ALA	SER	engineered mutation	UNP P04537
C	-19	MET	-	expression tag	UNP P04537
C	-18	GLY	-	expression tag	UNP P04537
C	-17	SER	-	expression tag	UNP P04537
C	-16	SER	-	expression tag	UNP P04537
C	-15	HIS	-	expression tag	UNP P04537
C	-14	HIS	-	expression tag	UNP P04537
C	-13	HIS	-	expression tag	UNP P04537
C	-12	HIS	-	expression tag	UNP P04537
C	-11	HIS	-	expression tag	UNP P04537
C	-10	HIS	-	expression tag	UNP P04537
C	-9	SER	-	expression tag	UNP P04537
C	-8	SER	-	expression tag	UNP P04537
C	-7	GLY	-	expression tag	UNP P04537
C	-6	LEU	-	expression tag	UNP P04537
C	-5	VAL	-	expression tag	UNP P04537
C	-4	PRO	-	expression tag	UNP P04537
C	-3	ARG	-	expression tag	UNP P04537
C	-2	GLY	-	expression tag	UNP P04537
C	-1	SER	-	expression tag	UNP P04537
C	0	HIS	-	expression tag	UNP P04537
C	79	ALA	GLU	engineered mutation	UNP P04537
C	80	ALA	LYS	engineered mutation	UNP P04537
C	81	ALA	SER	engineered mutation	UNP P04537
D	-19	MET	-	expression tag	UNP P04537
D	-18	GLY	-	expression tag	UNP P04537
D	-17	SER	-	expression tag	UNP P04537
D	-16	SER	-	expression tag	UNP P04537
D	-15	HIS	-	expression tag	UNP P04537
D	-14	HIS	-	expression tag	UNP P04537
D	-13	HIS	-	expression tag	UNP P04537
D	-12	HIS	-	expression tag	UNP P04537
D	-11	HIS	-	expression tag	UNP P04537
D	-10	HIS	-	expression tag	UNP P04537
D	-9	SER	-	expression tag	UNP P04537
D	-8	SER	-	expression tag	UNP P04537
D	-7	GLY	-	expression tag	UNP P04537
D	-6	LEU	-	expression tag	UNP P04537
D	-5	VAL	-	expression tag	UNP P04537
D	-4	PRO	-	expression tag	UNP P04537

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Chain	Residue	Modelled	Actual	Comment	Reference
D	-3	ARG	-	expression tag	UNP P04537
D	-2	GLY	-	expression tag	UNP P04537
D	-1	SER	-	expression tag	UNP P04537
D	0	HIS	-	expression tag	UNP P04537
D	79	ALA	GLU	engineered mutation	UNP P04537
D	80	ALA	LYS	engineered mutation	UNP P04537
D	81	ALA	SER	engineered mutation	UNP P04537
E	-19	MET	-	expression tag	UNP P04537
E	-18	GLY	-	expression tag	UNP P04537
E	-17	SER	-	expression tag	UNP P04537
E	-16	SER	-	expression tag	UNP P04537
E	-15	HIS	-	expression tag	UNP P04537
E	-14	HIS	-	expression tag	UNP P04537
E	-13	HIS	-	expression tag	UNP P04537
E	-12	HIS	-	expression tag	UNP P04537
E	-11	HIS	-	expression tag	UNP P04537
E	-10	HIS	-	expression tag	UNP P04537
E	-9	SER	-	expression tag	UNP P04537
E	-8	SER	-	expression tag	UNP P04537
E	-7	GLY	-	expression tag	UNP P04537
E	-6	LEU	-	expression tag	UNP P04537
E	-5	VAL	-	expression tag	UNP P04537
E	-4	PRO	-	expression tag	UNP P04537
E	-3	ARG	-	expression tag	UNP P04537
E	-2	GLY	-	expression tag	UNP P04537
E	-1	SER	-	expression tag	UNP P04537
E	0	HIS	-	expression tag	UNP P04537
E	79	ALA	GLU	engineered mutation	UNP P04537
E	80	ALA	LYS	engineered mutation	UNP P04537
E	81	ALA	SER	engineered mutation	UNP P04537
F	-19	MET	-	expression tag	UNP P04537
F	-18	GLY	-	expression tag	UNP P04537
F	-17	SER	-	expression tag	UNP P04537
F	-16	SER	-	expression tag	UNP P04537
F	-15	HIS	-	expression tag	UNP P04537
F	-14	HIS	-	expression tag	UNP P04537
F	-13	HIS	-	expression tag	UNP P04537
F	-12	HIS	-	expression tag	UNP P04537
F	-11	HIS	-	expression tag	UNP P04537
F	-10	HIS	-	expression tag	UNP P04537
F	-9	SER	-	expression tag	UNP P04537
F	-8	SER	-	expression tag	UNP P04537

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Chain	Residue	Modelled	Actual	Comment	Reference
F	-7	GLY	-	expression tag	UNP P04537
F	-6	LEU	-	expression tag	UNP P04537
F	-5	VAL	-	expression tag	UNP P04537
F	-4	PRO	-	expression tag	UNP P04537
F	-3	ARG	-	expression tag	UNP P04537
F	-2	GLY	-	expression tag	UNP P04537
F	-1	SER	-	expression tag	UNP P04537
F	0	HIS	-	expression tag	UNP P04537
F	79	ALA	GLU	engineered mutation	UNP P04537
F	80	ALA	LYS	engineered mutation	UNP P04537
F	81	ALA	SER	engineered mutation	UNP P04537
G	-19	MET	-	expression tag	UNP P04537
G	-18	GLY	-	expression tag	UNP P04537
G	-17	SER	-	expression tag	UNP P04537
G	-16	SER	-	expression tag	UNP P04537
G	-15	HIS	-	expression tag	UNP P04537
G	-14	HIS	-	expression tag	UNP P04537
G	-13	HIS	-	expression tag	UNP P04537
G	-12	HIS	-	expression tag	UNP P04537
G	-11	HIS	-	expression tag	UNP P04537
G	-10	HIS	-	expression tag	UNP P04537
G	-9	SER	-	expression tag	UNP P04537
G	-8	SER	-	expression tag	UNP P04537
G	-7	GLY	-	expression tag	UNP P04537
G	-6	LEU	-	expression tag	UNP P04537
G	-5	VAL	-	expression tag	UNP P04537
G	-4	PRO	-	expression tag	UNP P04537
G	-3	ARG	-	expression tag	UNP P04537
G	-2	GLY	-	expression tag	UNP P04537
G	-1	SER	-	expression tag	UNP P04537
G	0	HIS	-	expression tag	UNP P04537
G	79	ALA	GLU	engineered mutation	UNP P04537
G	80	ALA	LYS	engineered mutation	UNP P04537
G	81	ALA	SER	engineered mutation	UNP P04537
H	-19	MET	-	expression tag	UNP P04537
H	-18	GLY	-	expression tag	UNP P04537
H	-17	SER	-	expression tag	UNP P04537
H	-16	SER	-	expression tag	UNP P04537
H	-15	HIS	-	expression tag	UNP P04537
H	-14	HIS	-	expression tag	UNP P04537
H	-13	HIS	-	expression tag	UNP P04537
H	-12	HIS	-	expression tag	UNP P04537

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Chain	Residue	Modelled	Actual	Comment	Reference
H	-11	HIS	-	expression tag	UNP P04537
H	-10	HIS	-	expression tag	UNP P04537
H	-9	SER	-	expression tag	UNP P04537
H	-8	SER	-	expression tag	UNP P04537
H	-7	GLY	-	expression tag	UNP P04537
H	-6	LEU	-	expression tag	UNP P04537
H	-5	VAL	-	expression tag	UNP P04537
H	-4	PRO	-	expression tag	UNP P04537
H	-3	ARG	-	expression tag	UNP P04537
H	-2	GLY	-	expression tag	UNP P04537
H	-1	SER	-	expression tag	UNP P04537
H	0	HIS	-	expression tag	UNP P04537
H	79	ALA	GLU	engineered mutation	UNP P04537
H	80	ALA	LYS	engineered mutation	UNP P04537
H	81	ALA	SER	engineered mutation	UNP P04537
I	-19	MET	-	expression tag	UNP P04537
I	-18	GLY	-	expression tag	UNP P04537
I	-17	SER	-	expression tag	UNP P04537
I	-16	SER	-	expression tag	UNP P04537
I	-15	HIS	-	expression tag	UNP P04537
I	-14	HIS	-	expression tag	UNP P04537
I	-13	HIS	-	expression tag	UNP P04537
I	-12	HIS	-	expression tag	UNP P04537
I	-11	HIS	-	expression tag	UNP P04537
I	-10	HIS	-	expression tag	UNP P04537
I	-9	SER	-	expression tag	UNP P04537
I	-8	SER	-	expression tag	UNP P04537
I	-7	GLY	-	expression tag	UNP P04537
I	-6	LEU	-	expression tag	UNP P04537
I	-5	VAL	-	expression tag	UNP P04537
I	-4	PRO	-	expression tag	UNP P04537
I	-3	ARG	-	expression tag	UNP P04537
I	-2	GLY	-	expression tag	UNP P04537
I	-1	SER	-	expression tag	UNP P04537
I	0	HIS	-	expression tag	UNP P04537
I	79	ALA	GLU	engineered mutation	UNP P04537
I	80	ALA	LYS	engineered mutation	UNP P04537
I	81	ALA	SER	engineered mutation	UNP P04537
J	-19	MET	-	expression tag	UNP P04537
J	-18	GLY	-	expression tag	UNP P04537
J	-17	SER	-	expression tag	UNP P04537
J	-16	SER	-	expression tag	UNP P04537

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Chain	Residue	Modelled	Actual	Comment	Reference
J	-15	HIS	-	expression tag	UNP P04537
J	-14	HIS	-	expression tag	UNP P04537
J	-13	HIS	-	expression tag	UNP P04537
J	-12	HIS	-	expression tag	UNP P04537
J	-11	HIS	-	expression tag	UNP P04537
J	-10	HIS	-	expression tag	UNP P04537
J	-9	SER	-	expression tag	UNP P04537
J	-8	SER	-	expression tag	UNP P04537
J	-7	GLY	-	expression tag	UNP P04537
J	-6	LEU	-	expression tag	UNP P04537
J	-5	VAL	-	expression tag	UNP P04537
J	-4	PRO	-	expression tag	UNP P04537
J	-3	ARG	-	expression tag	UNP P04537
J	-2	GLY	-	expression tag	UNP P04537
J	-1	SER	-	expression tag	UNP P04537
J	0	HIS	-	expression tag	UNP P04537
J	79	ALA	GLU	engineered mutation	UNP P04537
J	80	ALA	LYS	engineered mutation	UNP P04537
J	81	ALA	SER	engineered mutation	UNP P04537
K	-19	MET	-	expression tag	UNP P04537
K	-18	GLY	-	expression tag	UNP P04537
K	-17	SER	-	expression tag	UNP P04537
K	-16	SER	-	expression tag	UNP P04537
K	-15	HIS	-	expression tag	UNP P04537
K	-14	HIS	-	expression tag	UNP P04537
K	-13	HIS	-	expression tag	UNP P04537
K	-12	HIS	-	expression tag	UNP P04537
K	-11	HIS	-	expression tag	UNP P04537
K	-10	HIS	-	expression tag	UNP P04537
K	-9	SER	-	expression tag	UNP P04537
K	-8	SER	-	expression tag	UNP P04537
K	-7	GLY	-	expression tag	UNP P04537
K	-6	LEU	-	expression tag	UNP P04537
K	-5	VAL	-	expression tag	UNP P04537
K	-4	PRO	-	expression tag	UNP P04537
K	-3	ARG	-	expression tag	UNP P04537
K	-2	GLY	-	expression tag	UNP P04537
K	-1	SER	-	expression tag	UNP P04537
K	0	HIS	-	expression tag	UNP P04537
K	79	ALA	GLU	engineered mutation	UNP P04537
K	80	ALA	LYS	engineered mutation	UNP P04537
K	81	ALA	SER	engineered mutation	UNP P04537

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Chain	Residue	Modelled	Actual	Comment	Reference
L	-19	MET	-	expression tag	UNP P04537
L	-18	GLY	-	expression tag	UNP P04537
L	-17	SER	-	expression tag	UNP P04537
L	-16	SER	-	expression tag	UNP P04537
L	-15	HIS	-	expression tag	UNP P04537
L	-14	HIS	-	expression tag	UNP P04537
L	-13	HIS	-	expression tag	UNP P04537
L	-12	HIS	-	expression tag	UNP P04537
L	-11	HIS	-	expression tag	UNP P04537
L	-10	HIS	-	expression tag	UNP P04537
L	-9	SER	-	expression tag	UNP P04537
L	-8	SER	-	expression tag	UNP P04537
L	-7	GLY	-	expression tag	UNP P04537
L	-6	LEU	-	expression tag	UNP P04537
L	-5	VAL	-	expression tag	UNP P04537
L	-4	PRO	-	expression tag	UNP P04537
L	-3	ARG	-	expression tag	UNP P04537
L	-2	GLY	-	expression tag	UNP P04537
L	-1	SER	-	expression tag	UNP P04537
L	0	HIS	-	expression tag	UNP P04537
L	79	ALA	GLU	engineered mutation	UNP P04537
L	80	ALA	LYS	engineered mutation	UNP P04537
L	81	ALA	SER	engineered mutation	UNP P04537
M	-19	MET	-	expression tag	UNP P04537
M	-18	GLY	-	expression tag	UNP P04537
M	-17	SER	-	expression tag	UNP P04537
M	-16	SER	-	expression tag	UNP P04537
M	-15	HIS	-	expression tag	UNP P04537
M	-14	HIS	-	expression tag	UNP P04537
M	-13	HIS	-	expression tag	UNP P04537
M	-12	HIS	-	expression tag	UNP P04537
M	-11	HIS	-	expression tag	UNP P04537
M	-10	HIS	-	expression tag	UNP P04537
M	-9	SER	-	expression tag	UNP P04537
M	-8	SER	-	expression tag	UNP P04537
M	-7	GLY	-	expression tag	UNP P04537
M	-6	LEU	-	expression tag	UNP P04537
M	-5	VAL	-	expression tag	UNP P04537
M	-4	PRO	-	expression tag	UNP P04537
M	-3	ARG	-	expression tag	UNP P04537
M	-2	GLY	-	expression tag	UNP P04537
M	-1	SER	-	expression tag	UNP P04537

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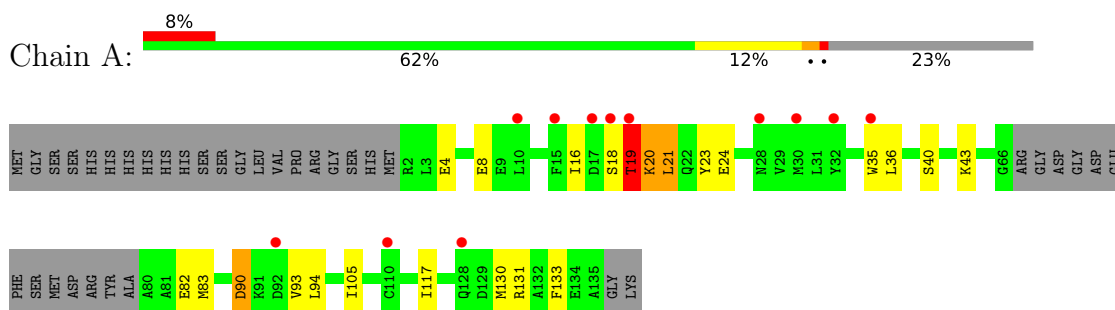
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Chain	Residue	Modelled	Actual	Comment	Reference
M	0	HIS	-	expression tag	UNP P04537
M	79	ALA	GLU	engineered mutation	UNP P04537
M	80	ALA	LYS	engineered mutation	UNP P04537
M	81	ALA	SER	engineered mutation	UNP P04537
N	-19	MET	-	expression tag	UNP P04537
N	-18	GLY	-	expression tag	UNP P04537
N	-17	SER	-	expression tag	UNP P04537
N	-16	SER	-	expression tag	UNP P04537
N	-15	HIS	-	expression tag	UNP P04537
N	-14	HIS	-	expression tag	UNP P04537
N	-13	HIS	-	expression tag	UNP P04537
N	-12	HIS	-	expression tag	UNP P04537
N	-11	HIS	-	expression tag	UNP P04537
N	-10	HIS	-	expression tag	UNP P04537
N	-9	SER	-	expression tag	UNP P04537
N	-8	SER	-	expression tag	UNP P04537
N	-7	GLY	-	expression tag	UNP P04537
N	-6	LEU	-	expression tag	UNP P04537
N	-5	VAL	-	expression tag	UNP P04537
N	-4	PRO	-	expression tag	UNP P04537
N	-3	ARG	-	expression tag	UNP P04537
N	-2	GLY	-	expression tag	UNP P04537
N	-1	SER	-	expression tag	UNP P04537
N	0	HIS	-	expression tag	UNP P04537
N	79	ALA	GLU	engineered mutation	UNP P04537
N	80	ALA	LYS	engineered mutation	UNP P04537
N	81	ALA	SER	engineered mutation	UNP P04537

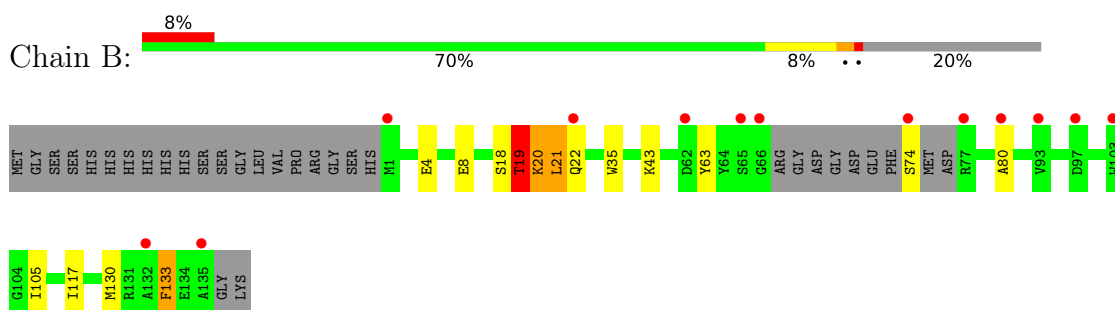
3 Residue-property plots [i](#)

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.

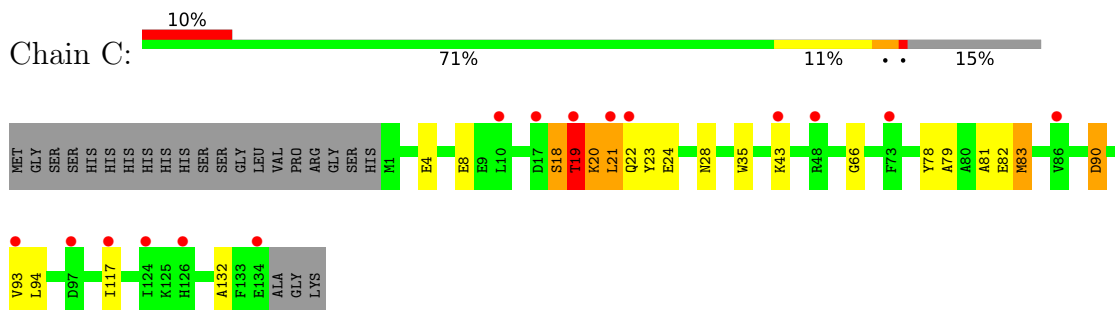
- Molecule 1: Recombination protein uvsY



- Molecule 1: Recombination protein uvsY

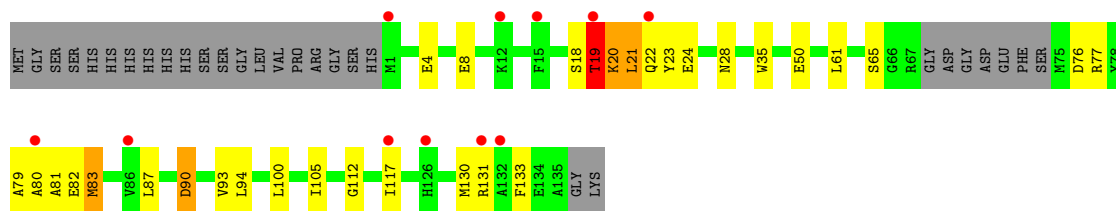


- Molecule 1: Recombination protein uvsY

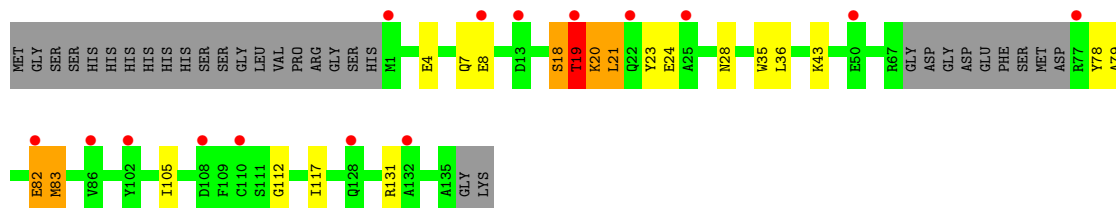


- Molecule 1: Recombination protein uvsY

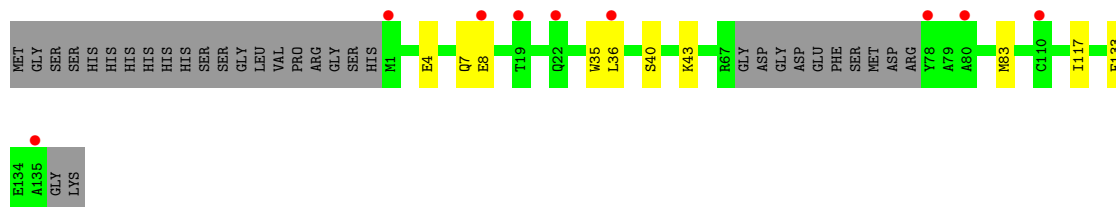
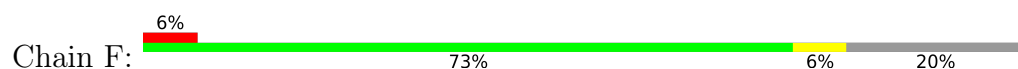




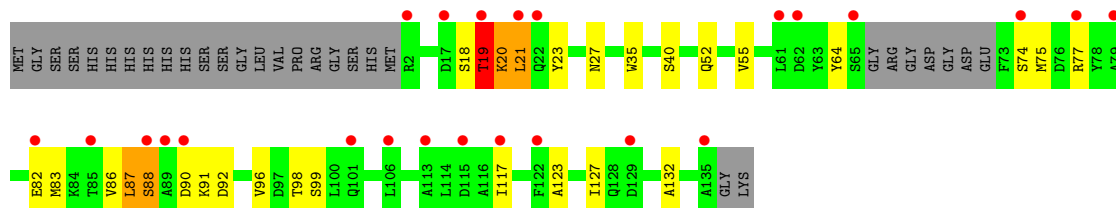
• Molecule 1: Recombination protein uvsY



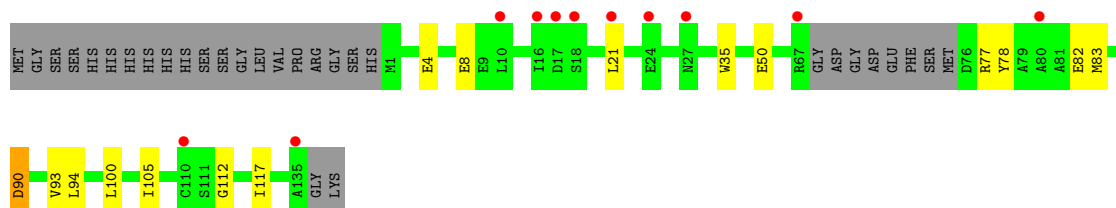
• Molecule 1: Recombination protein uvsY



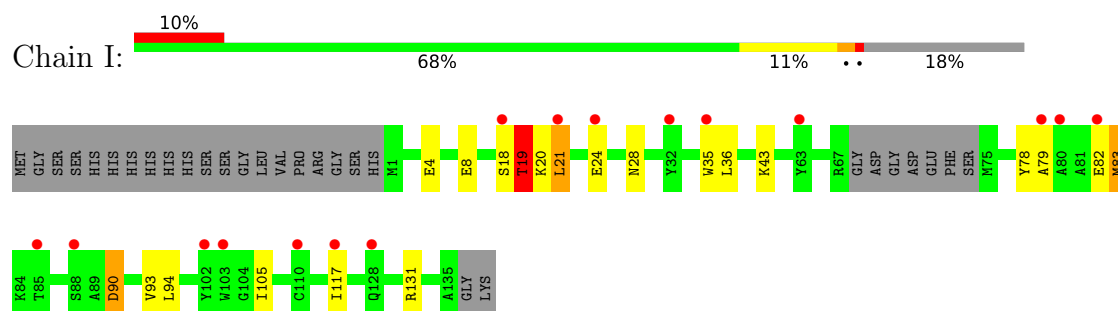
• Molecule 1: Recombination protein uvsY



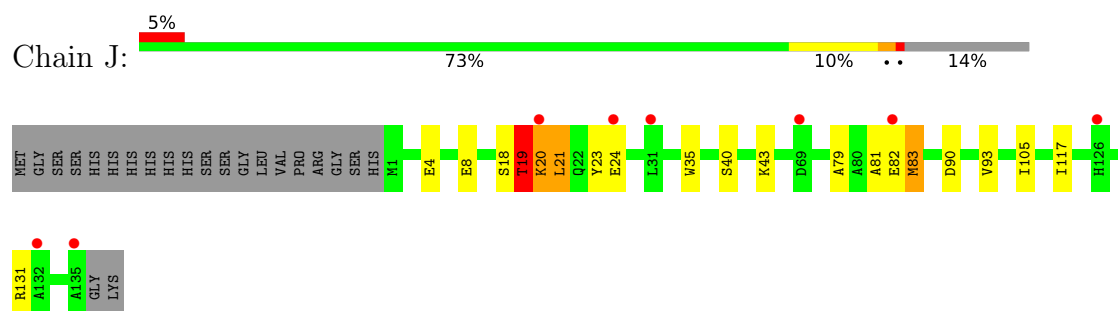
• Molecule 1: Recombination protein uvsY



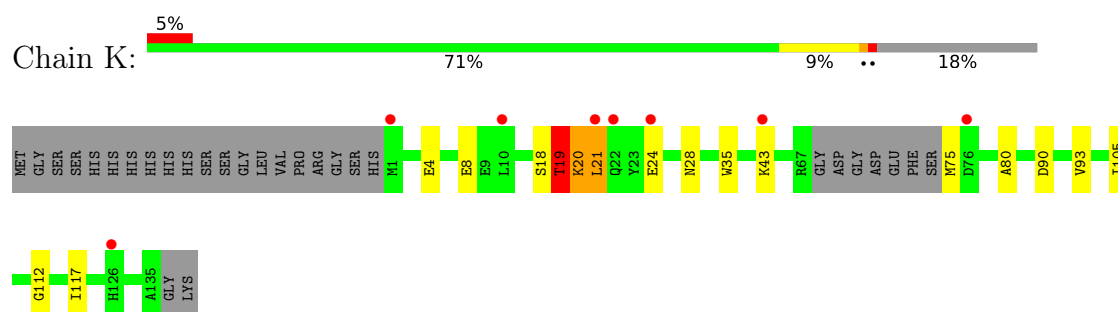
- Molecule 1: Recombination protein uvsY



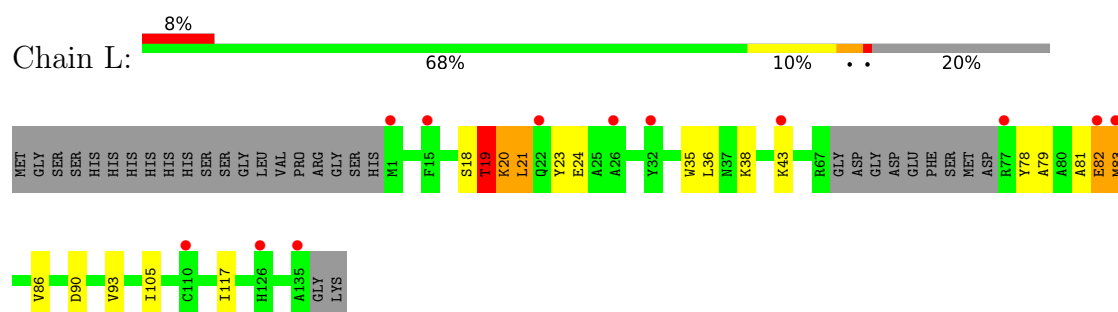
- Molecule 1: Recombination protein uvsY



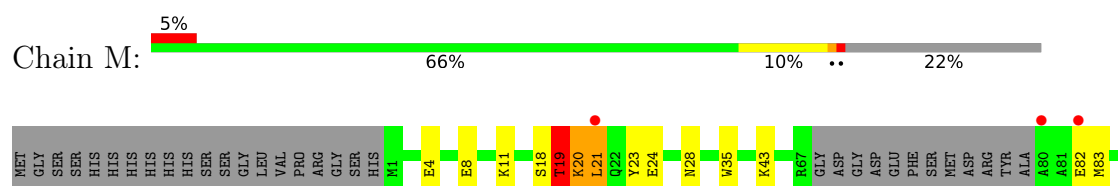
- Molecule 1: Recombination protein uvsY

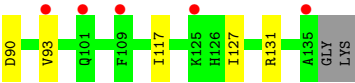


- Molecule 1: Recombination protein uvsY

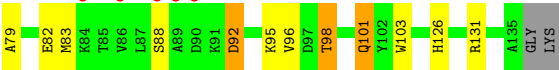


- Molecule 1: Recombination protein uvsY





● Molecule 1: Recombination protein uvsY



4 Data and refinement statistics

Property	Value	Source
Space group	I 4 2 2	Depositor
Cell constants a, b, c, α , β , γ	184.38Å 184.38Å 615.01Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	49.62 – 4.20 49.62 – 4.20	Depositor EDS
% Data completeness (in resolution range)	64.7 (49.62-4.20) 64.6 (49.62-4.20)	Depositor EDS
R_{merge}	0.20	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.62 (at 4.00Å)	Xtriage
Refinement program	PHENIX 1.9_1692	Depositor
R, R_{free}	0.274 , 0.308 0.282 , 0.312	Depositor DCC
R_{free} test set	1281 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å ²)	128.6	Xtriage
Anisotropy	0.315	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.27 , 230.9	EDS
L-test for twinning ²	$\langle L \rangle = 0.41$, $\langle L^2 \rangle = 0.24$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.87	EDS
Total number of atoms	11717	wwPDB-VP
Average B, all atoms (Å ²)	140.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.48% 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	0.62	1/807 (0.1%)	1.32	10/1107 (0.9%)
1	B	0.60	1/834 (0.1%)	1.23	8/1142 (0.7%)
1	C	0.59	0/858	1.34	13/1180 (1.1%)
1	D	0.63	1/842 (0.1%)	1.39	16/1156 (1.4%)
1	E	0.58	1/846 (0.1%)	1.29	11/1158 (0.9%)
1	F	0.49	0/820	0.94	1/1125 (0.1%)
1	G	0.62	1/878 (0.1%)	1.37	13/1202 (1.1%)
1	H	0.51	0/848	1.15	6/1163 (0.5%)
1	I	0.65	1/852 (0.1%)	1.32	9/1168 (0.8%)
1	J	0.61	1/897 (0.1%)	1.29	9/1229 (0.7%)
1	K	0.62	1/856 (0.1%)	1.27	7/1172 (0.6%)
1	L	0.61	1/834 (0.1%)	1.34	11/1143 (1.0%)
1	M	0.61	1/819 (0.1%)	1.25	8/1122 (0.7%)
1	N	0.63	1/858 (0.1%)	1.34	9/1173 (0.8%)
All	All	0.60	11/11849 (0.1%)	1.28	131/16240 (0.8%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	1
1	B	0	1
1	C	0	1
1	D	0	1
1	E	0	1
1	G	0	1
1	I	0	1
1	J	0	1
1	K	0	2
1	L	0	1
1	M	0	1

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Mol	Chain	#Chirality outliers	#Planarity outliers
1	N	0	1
All	All	0	13

All (11) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	M	20	LYS	CA-C	-6.23	1.44	1.52
1	K	20	LYS	CA-C	-6.22	1.44	1.52
1	I	20	LYS	CA-C	-6.20	1.44	1.52
1	A	20	LYS	CA-C	-6.16	1.44	1.52
1	L	20	LYS	CA-C	-6.07	1.44	1.52
1	J	20	LYS	CA-C	-6.00	1.44	1.52
1	B	20	LYS	CA-C	-5.96	1.44	1.52
1	E	20	LYS	CA-C	-5.75	1.45	1.52
1	D	20	LYS	CA-C	-5.57	1.45	1.52
1	G	20	LYS	CA-C	-5.41	1.45	1.52
1	N	20	LYS	CA-C	-5.30	1.45	1.52

All (131) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	E	21	LEU	N-CA-C	-17.39	92.40	111.36
1	D	21	LEU	N-CA-C	-17.29	92.51	111.36
1	C	21	LEU	N-CA-C	-17.25	92.55	111.36
1	G	21	LEU	N-CA-C	-16.41	93.48	111.36
1	B	21	LEU	N-CA-C	-16.28	93.61	111.36
1	A	21	LEU	N-CA-C	-16.20	93.70	111.36
1	N	21	LEU	N-CA-C	-16.18	93.72	111.36
1	L	21	LEU	N-CA-C	-16.11	93.80	111.36
1	K	21	LEU	N-CA-C	-15.86	94.07	111.36
1	J	21	LEU	N-CA-C	-15.85	94.08	111.36
1	M	21	LEU	N-CA-C	-15.85	94.08	111.36
1	I	21	LEU	N-CA-C	-15.65	94.30	111.36
1	H	83	MET	N-CA-C	-11.08	99.18	111.14
1	I	83	MET	N-CA-C	-10.90	99.37	111.14
1	A	83	MET	N-CA-C	-10.59	99.71	111.14
1	E	83	MET	N-CA-C	-10.36	99.95	111.14
1	C	83	MET	N-CA-C	-10.20	100.12	111.14
1	J	83	MET	N-CA-C	-10.08	100.26	111.14
1	D	83	MET	N-CA-C	-10.04	100.42	111.36
1	L	83	MET	N-CA-C	-10.02	100.32	111.14
1	M	83	MET	N-CA-C	-9.85	100.50	111.14

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	N	83	MET	N-CA-C	-9.79	100.57	111.14
1	D	82	GLU	N-CA-C	-9.13	101.57	112.89
1	C	20	LYS	N-CA-C	-9.00	98.43	111.30
1	I	82	GLU	N-CA-C	-8.74	102.06	112.89
1	G	83	MET	N-CA-C	-8.72	101.72	111.14
1	L	82	GLU	N-CA-C	-8.71	102.09	112.89
1	H	82	GLU	N-CA-C	-8.39	102.49	112.89
1	J	82	GLU	N-CA-C	-8.27	102.63	112.89
1	G	87	LEU	N-CA-C	8.27	120.29	111.28
1	A	82	GLU	N-CA-C	-8.07	102.89	112.89
1	E	82	GLU	N-CA-C	-7.94	103.04	112.89
1	C	82	GLU	N-CA-C	-7.88	103.12	112.89
1	K	21	LEU	CA-C-N	-7.71	109.95	120.44
1	K	21	LEU	C-N-CA	-7.71	109.95	120.44
1	I	21	LEU	CA-C-N	-7.64	109.44	120.29
1	I	21	LEU	C-N-CA	-7.64	109.44	120.29
1	C	19	THR	CA-C-N	-7.62	110.37	123.25
1	C	19	THR	C-N-CA	-7.62	110.37	123.25
1	M	21	LEU	CA-C-N	-7.62	110.08	120.44
1	M	21	LEU	C-N-CA	-7.62	110.08	120.44
1	N	18	SER	N-CA-C	7.59	120.44	111.71
1	J	21	LEU	CA-C-N	-7.55	110.18	120.44
1	J	21	LEU	C-N-CA	-7.55	110.18	120.44
1	M	82	GLU	N-CA-C	-7.49	103.61	112.89
1	H	77	ARG	CA-C-N	7.40	133.04	122.09
1	H	77	ARG	C-N-CA	7.40	133.04	122.09
1	G	64	TYR	N-CA-C	7.21	120.19	111.82
1	G	18	SER	N-CA-C	7.10	119.88	111.71
1	L	21	LEU	CA-C-N	-7.09	110.23	120.29
1	L	21	LEU	C-N-CA	-7.09	110.23	120.29
1	G	19	THR	N-CA-C	-7.03	104.71	113.28
1	C	19	THR	N-CA-C	-6.99	104.75	113.28
1	D	80	ALA	N-CA-C	6.87	118.76	111.28
1	N	19	THR	N-CA-C	-6.85	104.92	113.28
1	G	19	THR	CA-C-N	-6.80	108.55	121.54
1	G	19	THR	C-N-CA	-6.80	108.55	121.54
1	H	21	LEU	N-CA-C	6.75	118.64	111.28
1	E	19	THR	N-CA-C	-6.65	105.17	113.28
1	A	131	ARG	N-CA-C	-6.65	103.96	111.14
1	I	20	LYS	N-CA-C	-6.63	96.68	110.80
1	L	78	TYR	N-CA-C	6.58	120.39	109.46
1	I	78	TYR	N-CA-C	6.54	120.32	109.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	19	THR	N-CA-C	-6.51	105.34	113.28
1	B	19	THR	CA-C-N	-6.49	109.14	121.54
1	B	19	THR	C-N-CA	-6.49	109.14	121.54
1	C	78	TYR	N-CA-C	6.49	120.23	109.46
1	B	21	LEU	CA-C-N	-6.47	111.64	120.44
1	B	21	LEU	C-N-CA	-6.47	111.64	120.44
1	E	78	TYR	N-CA-C	6.47	120.20	109.46
1	G	90	ASP	N-CA-C	-6.43	102.94	111.24
1	M	19	THR	CA-C-N	-6.43	109.27	121.54
1	M	19	THR	C-N-CA	-6.43	109.27	121.54
1	A	19	THR	CA-C-N	-6.41	109.30	121.54
1	A	19	THR	C-N-CA	-6.41	109.30	121.54
1	D	19	THR	CA-C-N	-6.38	109.36	121.54
1	D	19	THR	C-N-CA	-6.38	109.36	121.54
1	A	21	LEU	CA-C-N	-6.35	111.80	120.44
1	A	21	LEU	C-N-CA	-6.35	111.80	120.44
1	N	19	THR	CA-C-N	-6.34	109.44	121.54
1	N	19	THR	C-N-CA	-6.34	109.44	121.54
1	D	131	ARG	N-CA-C	-6.32	104.31	111.14
1	N	82	GLU	N-CA-C	-6.30	105.08	112.89
1	K	20	LYS	N-CA-C	-6.23	97.53	110.80
1	J	20	LYS	N-CA-C	-6.18	97.63	110.80
1	E	19	THR	CA-C-N	-6.18	109.75	121.54
1	E	19	THR	C-N-CA	-6.18	109.75	121.54
1	L	19	THR	CA-C-N	-6.16	109.78	121.54
1	L	19	THR	C-N-CA	-6.16	109.78	121.54
1	A	20	LYS	N-CA-C	-6.12	97.75	110.80
1	G	86	VAL	N-CA-C	6.10	116.26	110.53
1	B	20	LYS	N-CA-C	-6.07	97.87	110.80
1	L	20	LYS	N-CA-C	-6.02	97.98	110.80
1	J	19	THR	CA-C-N	-6.02	110.05	121.54
1	J	19	THR	C-N-CA	-6.02	110.05	121.54
1	G	20	LYS	N-CA-C	-6.00	98.01	110.80
1	K	19	THR	CA-C-N	-5.98	110.12	121.54
1	K	19	THR	C-N-CA	-5.98	110.12	121.54
1	I	19	THR	CA-C-N	-5.94	110.20	121.54
1	I	19	THR	C-N-CA	-5.94	110.20	121.54
1	H	78	TYR	N-CA-C	5.93	119.93	109.96
1	B	133	PHE	N-CA-C	5.93	117.82	111.36
1	D	20	LYS	N-CA-C	-5.91	98.21	110.80
1	B	80	ALA	N-CA-C	5.79	117.59	111.28
1	D	77	ARG	N-CA-C	5.71	118.88	107.62

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	G	82	GLU	N-CA-C	-5.69	105.83	112.89
1	K	80	ALA	N-CA-C	5.69	117.48	111.28
1	M	20	LYS	N-CA-C	-5.61	98.85	110.80
1	E	21	LEU	CA-C-N	-5.57	112.87	120.44
1	E	21	LEU	C-N-CA	-5.57	112.87	120.44
1	N	20	LYS	N-CA-C	-5.55	98.98	110.80
1	E	18	SER	N-CA-C	5.51	118.05	111.71
1	E	20	LYS	N-CA-C	-5.50	99.09	110.80
1	D	87	LEU	N-CA-C	-5.42	105.38	111.28
1	C	66	GLY	N-CA-C	-5.41	107.80	115.43
1	F	83	MET	N-CA-C	-5.38	105.33	111.14
1	C	21	LEU	CA-C-N	-5.33	113.19	120.44
1	C	21	LEU	C-N-CA	-5.33	113.19	120.44
1	L	81	ALA	N-CA-C	-5.29	105.68	111.82
1	D	76	ASP	CA-C-N	-5.29	115.32	123.14
1	D	76	ASP	C-N-CA	-5.29	115.32	123.14
1	G	77	ARG	N-CA-C	5.28	118.03	107.62
1	D	21	LEU	CA-C-N	-5.25	113.29	120.44
1	D	21	LEU	C-N-CA	-5.25	113.29	120.44
1	C	18	SER	N-CA-C	5.24	117.74	111.71
1	D	81	ALA	N-CA-C	-5.21	105.78	111.82
1	N	31	LEU	N-CA-C	-5.19	105.70	111.36
1	A	16	ILE	N-CA-C	5.11	115.32	108.17
1	C	81	ALA	N-CA-C	-5.10	105.90	111.82
1	L	38	LYS	N-CA-C	-5.09	105.62	111.07
1	J	81	ALA	N-CA-C	-5.06	105.95	111.82

There are no chirality outliers.

All (13) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	19	THR	Mainchain
1	B	19	THR	Mainchain
1	C	19	THR	Mainchain
1	D	19	THR	Mainchain
1	E	19	THR	Mainchain
1	G	19	THR	Mainchain
1	I	19	THR	Mainchain
1	J	19	THR	Mainchain
1	K	19	THR	Mainchain
1	K	75	MET	Mainchain
1	L	19	THR	Mainchain

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Mol	Chain	Res	Type	Group
1	M	19	THR	Mainchain
1	N	19	THR	Mainchain

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	798	0	625	16	0
1	B	826	0	649	12	0
1	C	848	0	642	15	0
1	D	833	0	652	17	0
1	E	837	0	669	19	0
1	F	812	0	629	7	0
1	G	866	0	719	11	0
1	H	838	0	659	10	0
1	I	843	0	662	16	0
1	J	886	0	697	15	0
1	K	847	0	673	11	0
1	L	825	0	656	13	0
1	M	811	0	642	15	0
1	N	847	0	705	17	0
All	All	11717	0	9279	175	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 8.

All (175) 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:K:35:TRP:CD1	1:K:117:ILE:HD11	2.29	0.67
1:A:90:ASP:OD2	1:A:93:VAL:N	2.17	0.64
1:J:79:ALA:O	1:J:83:MET:N	2.31	0.63
1:K:105:ILE:HG23	1:L:43:LYS:HD2	1.81	0.62
1:B:63:TYR:O	1:B:74:SER:N	2.33	0.61
1:H:35:TRP:HD1	1:H:117:ILE:HD11	1.66	0.61
1:A:90:ASP:HB3	1:A:93:VAL:HB	1.82	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:35:TRP:CD1	1:I:117:ILE:HD11	2.36	0.60
1:C:90:ASP:O	1:C:94:LEU:N	2.23	0.60
1:I:90:ASP:HB3	1:I:93:VAL:HB	1.84	0.59
1:J:35:TRP:HD1	1:J:117:ILE:HD11	1.66	0.59
1:E:35:TRP:CD1	1:E:117:ILE:HD11	2.38	0.59
1:L:79:ALA:O	1:L:83:MET:N	2.36	0.58
1:E:105:ILE:HG23	1:F:43:LYS:HD2	1.84	0.58
1:L:35:TRP:CD1	1:L:117:ILE:HD11	2.38	0.58
1:I:105:ILE:HG23	1:J:43:LYS:HD2	1.84	0.57
1:F:35:TRP:CD1	1:F:117:ILE:HD11	2.38	0.57
1:D:35:TRP:CD1	1:D:117:ILE:HD11	2.39	0.57
1:L:105:ILE:HG23	1:M:43:LYS:HD2	1.87	0.57
1:C:35:TRP:CD1	1:C:117:ILE:HD11	2.39	0.57
1:D:18:SER:HA	1:D:21:LEU:HD13	1.86	0.57
1:A:18:SER:O	1:A:21:LEU:HB2	2.05	0.57
1:I:79:ALA:O	1:I:83:MET:N	2.38	0.57
1:E:112:GLY:HA3	1:F:36:LEU:HD21	1.86	0.56
1:B:35:TRP:CD1	1:B:117:ILE:HD11	2.41	0.55
1:G:35:TRP:CD1	1:G:117:ILE:HD11	2.41	0.55
1:J:18:SER:HB3	1:J:131:ARG:HH21	1.71	0.55
1:F:4:GLU:O	1:F:8:GLU:HG3	2.07	0.55
1:A:18:SER:HA	1:A:21:LEU:HD13	1.88	0.55
1:I:4:GLU:O	1:I:8:GLU:HG3	2.07	0.55
1:N:95:LYS:O	1:N:98:THR:HG22	2.07	0.55
1:A:35:TRP:CD1	1:A:117:ILE:HD11	2.41	0.54
1:H:112:GLY:HA3	1:I:36:LEU:HD21	1.90	0.54
1:I:18:SER:O	1:I:21:LEU:HB2	2.07	0.54
1:N:49:ILE:HG22	1:N:96:VAL:HG13	1.90	0.54
1:B:4:GLU:O	1:B:8:GLU:HG3	2.07	0.54
1:N:18:SER:HB3	1:N:131:ARG:NH2	2.22	0.54
1:M:4:GLU:O	1:M:8:GLU:HG3	2.07	0.54
1:E:79:ALA:O	1:E:83:MET:N	2.41	0.53
1:K:18:SER:HA	1:K:21:LEU:HD13	1.89	0.53
1:C:18:SER:O	1:C:21:LEU:HB2	2.08	0.53
1:I:18:SER:HB3	1:I:131:ARG:HH21	1.73	0.53
1:A:105:ILE:HG23	1:B:43:LYS:HD2	1.89	0.53
1:K:18:SER:O	1:K:21:LEU:HB2	2.08	0.53
1:B:105:ILE:HG23	1:C:43:LYS:HD2	1.89	0.53
1:B:130:MET:O	1:B:133:PHE:HB3	2.09	0.53
1:E:18:SER:O	1:E:21:LEU:HB2	2.09	0.53
1:J:4:GLU:O	1:J:8:GLU:HG3	2.09	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:79:ALA:O	1:C:83:MET:N	2.42	0.53
1:D:18:SER:O	1:D:21:LEU:HB2	2.09	0.52
1:C:4:GLU:O	1:C:8:GLU:HG3	2.09	0.52
1:D:24:GLU:O	1:D:28:ASN:N	2.41	0.52
1:E:18:SER:HA	1:E:21:LEU:HD13	1.91	0.52
1:M:21:LEU:HD22	1:M:131:ARG:CZ	2.39	0.52
1:M:35:TRP:CD1	1:M:117:ILE:HD11	2.44	0.52
1:N:20:LYS:CB	1:N:23:TYR:HB3	2.40	0.52
1:A:4:GLU:O	1:A:8:GLU:HG3	2.09	0.51
1:E:4:GLU:O	1:E:8:GLU:HG3	2.10	0.51
1:H:105:ILE:HG23	1:I:43:LYS:HD2	1.93	0.51
1:E:20:LYS:CB	1:E:23:TYR:HB3	2.40	0.51
1:K:4:GLU:O	1:K:8:GLU:HG3	2.10	0.51
1:H:4:GLU:O	1:H:8:GLU:HG3	2.11	0.51
1:D:4:GLU:O	1:D:8:GLU:HG3	2.10	0.51
1:H:90:ASP:O	1:H:94:LEU:N	2.24	0.51
1:I:18:SER:HA	1:I:21:LEU:HD13	1.93	0.51
1:L:20:LYS:O	1:L:24:GLU:N	2.27	0.51
1:N:49:ILE:CG2	1:N:96:VAL:HG13	2.41	0.51
1:D:61:LEU:O	1:D:65:SER:N	2.38	0.50
1:G:20:LYS:CB	1:G:23:TYR:HB3	2.42	0.50
1:A:20:LYS:O	1:A:24:GLU:N	2.27	0.50
1:A:130:MET:O	1:A:133:PHE:HB3	2.09	0.50
1:K:20:LYS:O	1:K:24:GLU:N	2.27	0.50
1:J:18:SER:O	1:J:21:LEU:HB2	2.11	0.50
1:N:52:GLN:O	1:N:55:VAL:HG12	2.12	0.50
1:J:35:TRP:CD1	1:J:117:ILE:HD11	2.45	0.49
1:L:18:SER:O	1:L:21:LEU:HB2	2.11	0.49
1:M:11:LYS:O	1:N:30:MET:HE1	2.12	0.49
1:F:7:GLN:HE21	1:G:40:SER:HB2	1.78	0.49
1:M:20:LYS:O	1:M:24:GLU:N	2.25	0.49
1:M:18:SER:C	1:M:131:ARG:HH22	2.19	0.49
1:C:24:GLU:O	1:C:28:ASN:N	2.42	0.49
1:G:52:GLN:O	1:G:55:VAL:HG12	2.13	0.49
1:N:49:ILE:HG13	1:N:103:TRP:HZ3	1.77	0.49
1:A:90:ASP:O	1:A:94:LEU:N	2.27	0.48
1:D:79:ALA:O	1:D:83:MET:N	2.47	0.48
1:I:19:THR:C	1:I:21:LEU:H	2.21	0.48
1:C:18:SER:HA	1:C:21:LEU:HD13	1.95	0.48
1:D:112:GLY:HA3	1:E:36:LEU:HD21	1.95	0.47
1:N:49:ILE:HG13	1:N:103:TRP:CZ3	2.49	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:24:GLU:O	1:E:28:ASN:N	2.47	0.47
1:H:35:TRP:HA	1:H:35:TRP:CE3	2.50	0.47
1:J:105:ILE:HG23	1:K:43:LYS:HD2	1.95	0.47
1:B:18:SER:O	1:B:21:LEU:HB2	2.14	0.47
1:E:4:GLU:CD	1:E:4:GLU:H	2.23	0.47
1:G:87:LEU:O	1:G:88:SER:C	2.58	0.46
1:N:26:ALA:O	1:N:29:VAL:HG12	2.15	0.46
1:E:7:GLN:NE2	1:F:40:SER:OG	2.41	0.46
1:G:92:ASP:O	1:G:96:VAL:HG23	2.15	0.46
1:D:20:LYS:CB	1:D:23:TYR:HB3	2.46	0.46
1:N:92:ASP:O	1:N:96:VAL:HG23	2.16	0.46
1:D:90:ASP:O	1:D:94:LEU:N	2.26	0.46
1:J:90:ASP:HB3	1:J:93:VAL:HB	1.98	0.46
1:M:24:GLU:O	1:M:28:ASN:N	2.49	0.46
1:A:19:THR:C	1:A:21:LEU:H	2.24	0.45
1:B:4:GLU:H	1:B:4:GLU:CD	2.24	0.45
1:D:4:GLU:H	1:D:4:GLU:CD	2.25	0.45
1:G:123:ALA:O	1:G:127:ILE:HD13	2.15	0.45
1:N:18:SER:HB3	1:N:131:ARG:HH21	1.80	0.45
1:B:20:LYS:C	1:B:22:GLN:N	2.71	0.45
1:J:19:THR:C	1:J:21:LEU:H	2.24	0.45
1:N:20:LYS:O	1:N:24:GLU:N	2.38	0.45
1:I:4:GLU:CD	1:I:4:GLU:H	2.24	0.45
1:G:19:THR:C	1:G:21:LEU:H	2.24	0.45
1:G:96:VAL:O	1:G:99:SER:HB3	2.17	0.45
1:B:19:THR:C	1:B:21:LEU:H	2.25	0.45
1:C:35:TRP:HD1	1:C:117:ILE:HD11	1.80	0.45
1:H:90:ASP:CB	1:H:93:VAL:HB	2.47	0.45
1:K:19:THR:C	1:K:21:LEU:H	2.24	0.45
1:L:18:SER:HA	1:L:21:LEU:HD13	1.99	0.45
1:E:18:SER:HB3	1:E:131:ARG:HH21	1.81	0.44
1:E:35:TRP:HD1	1:E:117:ILE:HD11	1.81	0.44
1:A:40:SER:O	1:A:43:LYS:HG2	2.17	0.44
1:J:4:GLU:H	1:J:4:GLU:CD	2.25	0.44
1:J:20:LYS:O	1:J:24:GLU:N	2.28	0.44
1:D:90:ASP:CB	1:D:93:VAL:HB	2.47	0.44
1:K:24:GLU:O	1:K:28:ASN:N	2.51	0.44
1:L:90:ASP:HB3	1:L:93:VAL:HB	2.00	0.44
1:N:2:ARG:O	1:N:6:LEU:HD13	2.18	0.44
1:C:4:GLU:H	1:C:4:GLU:CD	2.26	0.44
1:H:4:GLU:H	1:H:4:GLU:CD	2.25	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:19:THR:C	1:L:21:LEU:H	2.26	0.44
1:A:36:LEU:HD12	1:A:36:LEU:HA	1.92	0.43
1:I:90:ASP:O	1:I:94:LEU:N	2.29	0.43
1:K:90:ASP:HB3	1:K:93:VAL:HB	2.00	0.43
1:M:4:GLU:CD	1:M:4:GLU:H	2.27	0.43
1:C:20:LYS:C	1:C:22:GLN:N	2.69	0.43
1:D:130:MET:O	1:D:133:PHE:HB3	2.19	0.43
1:A:20:LYS:CB	1:A:23:TYR:HB3	2.49	0.43
1:A:90:ASP:OD2	1:A:93:VAL:HG23	2.19	0.42
1:C:90:ASP:CB	1:C:93:VAL:HB	2.49	0.42
1:I:35:TRP:HD1	1:I:117:ILE:HD11	1.81	0.42
1:A:4:GLU:H	1:A:4:GLU:CD	2.28	0.42
1:E:18:SER:O	1:E:131:ARG:NH2	2.50	0.42
1:C:20:LYS:CB	1:C:23:TYR:HB3	2.50	0.42
1:E:79:ALA:HB3	1:E:82:GLU:CB	2.50	0.42
1:I:90:ASP:OD1	1:I:90:ASP:C	2.62	0.42
1:M:18:SER:HB3	1:M:131:ARG:HH21	1.84	0.42
1:D:19:THR:C	1:D:21:LEU:H	2.27	0.42
1:M:90:ASP:HB3	1:M:93:VAL:HB	2.02	0.42
1:N:19:THR:C	1:N:21:LEU:H	2.25	0.42
1:N:78:TYR:O	1:N:79:ALA:HB3	2.19	0.41
1:I:24:GLU:O	1:I:28:ASN:N	2.49	0.41
1:M:18:SER:O	1:M:21:LEU:HB2	2.21	0.41
1:B:18:SER:HA	1:B:21:LEU:HD13	2.03	0.41
1:C:19:THR:C	1:C:21:LEU:H	2.27	0.41
1:M:19:THR:C	1:M:21:LEU:H	2.28	0.41
1:E:19:THR:C	1:E:21:LEU:H	2.28	0.41
1:L:20:LYS:CB	1:L:23:TYR:HB3	2.50	0.41
1:L:79:ALA:HB3	1:L:82:GLU:CB	2.50	0.41
1:L:82:GLU:O	1:L:86:VAL:HG23	2.21	0.41
1:D:20:LYS:C	1:D:22:GLN:N	2.71	0.41
1:D:50:GLU:HG3	1:D:100:LEU:HD21	2.03	0.41
1:M:20:LYS:CB	1:M:23:TYR:HB3	2.51	0.41
1:F:133:PHE:CE1	1:G:132:ALA:HA	2.55	0.40
1:G:91:LYS:HA	1:N:101:GLN:OE1	2.21	0.40
1:H:35:TRP:CD1	1:H:117:ILE:HD11	2.51	0.40
1:J:20:LYS:CB	1:J:23:TYR:HB3	2.52	0.40
1:J:40:SER:O	1:J:43:LYS:HG2	2.21	0.40
1:M:127:ILE:O	1:M:131:ARG:HG3	2.21	0.40
1:B:133:PHE:CE1	1:C:132:ALA:HA	2.57	0.40
1:E:18:SER:C	1:E:131:ARG:HH22	2.29	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:50:GLU:HG3	1:H:100:LEU:HD21	2.02	0.40
1:J:18:SER:HA	1:J:21:LEU:HD13	2.03	0.40
1:D:105:ILE:HG23	1:E:43:LYS:HD2	2.04	0.40
1:K:112:GLY:HA3	1:L:36:LEU:HD21	2.02	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	117/157 (74%)	116 (99%)	0	1 (1%)	14	49
1	B	121/157 (77%)	120 (99%)	1 (1%)	0	100	100
1	C	132/157 (84%)	130 (98%)	1 (1%)	1 (1%)	16	52
1	D	124/157 (79%)	123 (99%)	0	1 (1%)	16	52
1	E	122/157 (78%)	122 (100%)	0	0	100	100
1	F	121/157 (77%)	121 (100%)	0	0	100	100
1	G	123/157 (78%)	118 (96%)	2 (2%)	3 (2%)	4	28
1	H	123/157 (78%)	122 (99%)	0	1 (1%)	16	52
1	I	124/157 (79%)	122 (98%)	1 (1%)	1 (1%)	16	52
1	J	133/157 (85%)	129 (97%)	4 (3%)	0	100	100
1	K	124/157 (79%)	124 (100%)	0	0	100	100
1	L	122/157 (78%)	122 (100%)	0	0	100	100
1	M	119/157 (76%)	118 (99%)	1 (1%)	0	100	100
1	N	121/157 (77%)	117 (97%)	2 (2%)	2 (2%)	7	35
All	All	1726/2198 (78%)	1704 (99%)	12 (1%)	10 (1%)	21	58

All (10) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	G	74	SER
1	G	75	MET
1	N	92	ASP
1	C	90	ASP
1	G	88	SER
1	A	90	ASP
1	D	90	ASP
1	H	90	ASP
1	I	90	ASP
1	N	88	SER

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	59/133 (44%)	59 (100%)	0	100	100
1	B	59/133 (44%)	59 (100%)	0	100	100
1	C	56/133 (42%)	56 (100%)	0	100	100
1	D	59/133 (44%)	59 (100%)	0	100	100
1	E	62/133 (47%)	62 (100%)	0	100	100
1	F	58/133 (44%)	58 (100%)	0	100	100
1	G	68/133 (51%)	66 (97%)	2 (3%)	37	58
1	H	60/133 (45%)	60 (100%)	0	100	100
1	I	61/133 (46%)	61 (100%)	0	100	100
1	J	63/133 (47%)	63 (100%)	0	100	100
1	K	62/133 (47%)	62 (100%)	0	100	100
1	L	58/133 (44%)	58 (100%)	0	100	100
1	M	60/133 (45%)	60 (100%)	0	100	100
1	N	65/133 (49%)	61 (94%)	4 (6%)	16	39
All	All	850/1862 (46%)	844 (99%)	6 (1%)	76	78

All (6) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	G	27	ASN
1	G	98	THR
1	N	27	ASN
1	N	98	THR
1	N	101	GLN
1	N	126	HIS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (8) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	128	GLN
1	E	22	GLN
1	F	7	GLN
1	G	27	ASN
1	I	39	HIS
1	L	39	HIS
1	N	27	ASN
1	N	39	HIS

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

There are no ligands in this entry.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

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	121/157 (77%)	0.69	12 (9%) 13 16	147, 180, 217, 231	0
1	B	126/157 (80%)	0.88	13 (10%) 12 15	114, 148, 204, 230	0
1	C	134/157 (85%)	0.77	15 (11%) 10 14	99, 134, 184, 199	0
1	D	128/157 (81%)	0.67	11 (8%) 16 19	89, 134, 195, 216	0
1	E	126/157 (80%)	0.69	15 (11%) 9 12	92, 140, 206, 218	0
1	F	125/157 (79%)	0.76	9 (7%) 21 23	111, 151, 201, 221	0
1	G	127/157 (80%)	0.97	24 (18%) 3 7	133, 178, 223, 241	0
1	H	127/157 (80%)	0.64	11 (8%) 16 19	93, 127, 175, 207	0
1	I	128/157 (81%)	0.74	16 (12%) 8 12	78, 111, 150, 182	0
1	J	135/157 (85%)	0.58	8 (5%) 28 27	68, 104, 149, 179	0
1	K	128/157 (81%)	0.65	8 (6%) 26 26	68, 109, 169, 186	0
1	L	126/157 (80%)	0.62	12 (9%) 14 17	78, 117, 177, 192	0
1	M	123/157 (78%)	0.75	8 (6%) 25 25	100, 135, 171, 193	0
1	N	125/157 (79%)	0.67	9 (7%) 21 23	100, 132, 216, 261	0
All	All	1779/2198 (80%)	0.72	171 (9%) 13 17	68, 136, 202, 261	0

All (171) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	N	86	VAL	5.4
1	G	62	ASP	4.9
1	I	82	GLU	4.3
1	B	77	ARG	4.1
1	J	135	ALA	4.0
1	N	90	ASP	4.0
1	F	78	TYR	4.0
1	E	77	ARG	4.0

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Mol	Chain	Res	Type	RSRZ
1	I	18	SER	3.8
1	L	82	GLU	3.7
1	H	17	ASP	3.7
1	L	135	ALA	3.7
1	F	135	ALA	3.6
1	B	74	SER	3.6
1	E	22	GLN	3.6
1	N	75	MET	3.6
1	C	134	GLU	3.5
1	K	22	GLN	3.5
1	L	77	ARG	3.4
1	E	1	MET	3.4
1	K	1	MET	3.3
1	H	21	LEU	3.3
1	H	80	ALA	3.3
1	C	93	VAL	3.3
1	I	103	TRP	3.3
1	G	89	ALA	3.2
1	M	21	LEU	3.2
1	N	19	THR	3.2
1	D	1	MET	3.2
1	E	82	GLU	3.2
1	J	126	HIS	3.1
1	A	19	THR	3.1
1	D	126	HIS	3.1
1	M	101	GLN	3.1
1	G	90	ASP	3.1
1	G	122	PHE	3.1
1	B	22	GLN	3.1
1	L	1	MET	3.1
1	H	24	GLU	3.1
1	G	65	SER	3.0
1	A	110	CYS	3.0
1	N	89	ALA	3.0
1	I	21	LEU	3.0
1	G	88	SER	3.0
1	B	135	ALA	3.0
1	I	32	TYR	3.0
1	D	15	PHE	2.9
1	G	22	GLN	2.9
1	K	126	HIS	2.9
1	I	110	CYS	2.8

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Mol	Chain	Res	Type	RSRZ
1	F	8	GLU	2.8
1	G	74	SER	2.8
1	L	83	MET	2.8
1	C	10	LEU	2.8
1	J	82	GLU	2.8
1	N	88	SER	2.8
1	C	17	ASP	2.8
1	G	129	ASP	2.8
1	K	21	LEU	2.7
1	L	32	TYR	2.7
1	F	22	GLN	2.7
1	L	22	GLN	2.7
1	G	19	THR	2.7
1	G	2	ARG	2.7
1	C	126	HIS	2.7
1	I	117	ILE	2.7
1	I	79	ALA	2.7
1	J	69	ASP	2.6
1	D	132	ALA	2.6
1	K	24	GLU	2.6
1	L	126	HIS	2.6
1	J	31	LEU	2.6
1	G	85	THR	2.6
1	M	82	GLU	2.6
1	I	80	ALA	2.6
1	A	18	SER	2.6
1	C	43	LYS	2.5
1	C	117	ILE	2.5
1	G	115	ASP	2.5
1	D	22	GLN	2.5
1	B	1	MET	2.5
1	E	19	THR	2.5
1	B	103	TRP	2.5
1	K	76	ASP	2.5
1	L	43	LYS	2.5
1	N	84	LYS	2.5
1	F	1	MET	2.5
1	H	10	LEU	2.5
1	A	35	TRP	2.5
1	G	77	ARG	2.4
1	I	85	THR	2.4
1	E	128	GLN	2.4

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Mol	Chain	Res	Type	RSRZ
1	A	10	LEU	2.4
1	G	21	LEU	2.4
1	G	113	ALA	2.4
1	I	88	SER	2.4
1	G	61	LEU	2.4
1	M	125	LYS	2.4
1	B	80	ALA	2.4
1	C	124	ILE	2.4
1	E	110	CYS	2.4
1	C	21	LEU	2.4
1	C	22	GLN	2.3
1	G	101	GLN	2.3
1	E	108	ASP	2.3
1	G	117	ILE	2.3
1	E	25	ALA	2.3
1	E	13	ASP	2.3
1	L	15	PHE	2.3
1	M	80	ALA	2.3
1	B	97	ASP	2.3
1	F	80	ALA	2.3
1	A	30	MET	2.3
1	C	73	PHE	2.3
1	G	135	ALA	2.3
1	J	20	LYS	2.3
1	F	19	THR	2.3
1	D	80	ALA	2.3
1	J	132	ALA	2.3
1	A	92	ASP	2.3
1	C	48	ARG	2.3
1	E	8	GLU	2.2
1	A	28	ASN	2.2
1	H	110	CYS	2.2
1	E	86	VAL	2.2
1	E	132	ALA	2.2
1	H	27	ASN	2.2
1	G	82	GLU	2.2
1	H	67	ARG	2.2
1	H	18	SER	2.2
1	N	18	SER	2.2
1	J	24	GLU	2.2
1	K	10	LEU	2.2
1	C	86	VAL	2.2

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Mol	Chain	Res	Type	RSRZ
1	A	15	PHE	2.2
1	M	109	PHE	2.2
1	B	132	ALA	2.2
1	H	135	ALA	2.2
1	D	19	THR	2.2
1	E	102	TYR	2.2
1	N	1	MET	2.2
1	L	26	ALA	2.2
1	D	117	ILE	2.2
1	I	128	GLN	2.2
1	I	24	GLU	2.2
1	I	35	TRP	2.2
1	D	12	LYS	2.1
1	A	32	TYR	2.1
1	I	102	TYR	2.1
1	E	50	GLU	2.1
1	H	16	ILE	2.1
1	K	43	LYS	2.1
1	D	131	ARG	2.1
1	F	110	CYS	2.1
1	A	128	GLN	2.1
1	A	17	ASP	2.1
1	B	93	VAL	2.1
1	D	86	VAL	2.1
1	B	62	ASP	2.1
1	G	17	ASP	2.1
1	G	106	LEU	2.1
1	C	97	ASP	2.0
1	F	36	LEU	2.0
1	I	63	TYR	2.0
1	G	79	ALA	2.0
1	M	135	ALA	2.0
1	L	110	CYS	2.0
1	B	66	GLY	2.0
1	M	93	VAL	2.0
1	C	19	THR	2.0
1	B	65	SER	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.