



wwPDB X-ray Structure Validation Summary Report ⓘ

Jun 7, 2021 – 10:11 AM EDT

PDB ID : 7N1L
Title : Crystal Structure of Ribosomal-protein-alanine N-acetyltransferase from *Brucella melitensis* biovar Abortus 2308
Authors : Seattle Structural Genomics Center for Infectious Disease; Seattle Structural Genomics Center for Infectious Disease (SSGCID)
Deposited on : 2021-05-27
Resolution : 2.30 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 following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.13
EDS	:	2.20
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)	:	2.20

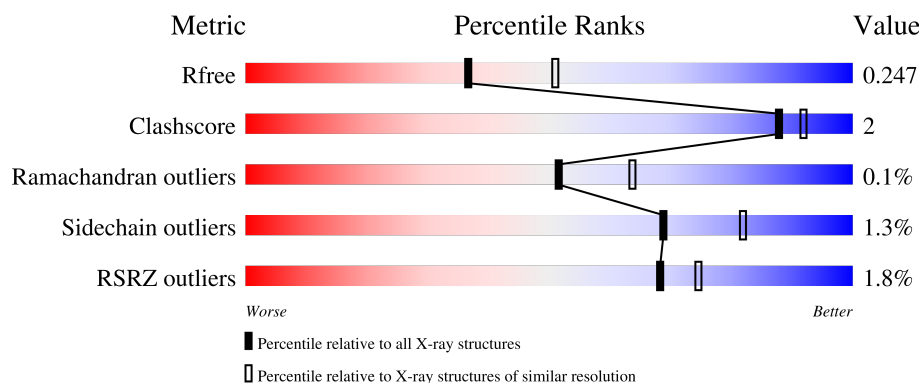
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.30 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	5042 (2.30-2.30)
Clashscore	141614	5643 (2.30-2.30)
Ramachandran outliers	138981	5575 (2.30-2.30)
Sidechain outliers	138945	5575 (2.30-2.30)
RSRZ outliers	127900	4938 (2.30-2.30)

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	173	<div> <div>2%</div> <div>80%</div> <div>17%</div> </div>
1	B	173	<div> <div>%</div> <div>77%</div> <div>5%</div> <div>17%</div> </div>
1	C	173	<div> <div>76%</div> <div>21%</div> </div>
1	D	173	<div> <div>%</div> <div>76%</div> <div>5%</div> <div>18%</div> </div>
1	E	173	<div> <div>75%</div> <div>6%</div> <div>18%</div> </div>

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Mol	Chain	Length	Quality of chain
1	F	173	 73% 8% 18%
1	G	173	 74% 7% 19%
1	H	173	 79% 5% 17%
1	I	173	 77% 6% 17%
1	J	173	 73% 23%
1	K	173	 79% 6% 14%
1	L	173	 83% 14%
1	M	173	 75% 6% 20%
1	N	173	 74% 6% 19%
1	O	173	 74% 23%
1	P	173	 75% 5% 20%

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 18064 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 GCN5-related N-acetyltransferase.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
1	A	143	Total	C	N	O	0	0	0
			1113	712	199	202			
1	B	143	Total	C	N	O	0	0	0
			1116	715	199	202			
1	C	137	Total	C	N	O	0	0	0
			1071	687	190	194			
1	D	141	Total	C	N	O	0	0	0
			1087	695	194	198			
1	E	141	Total	C	N	O	0	0	0
			1101	704	197	200			
1	F	141	Total	C	N	O	0	2	0
			1113	712	197	204			
1	G	140	Total	C	N	O	0	0	0
			1078	692	193	193			
1	H	144	Total	C	N	O	0	0	0
			1113	711	199	203			
1	I	143	Total	C	N	O	0	0	0
			1112	712	198	202			
1	J	134	Total	C	N	O	0	0	0
			1024	656	181	187			
1	K	148	Total	C	N	O	0	0	0
			1117	715	200	202			
1	L	148	Total	C	N	O	0	0	0
			1130	722	203	205			
1	M	139	Total	C	N	O	0	0	0
			1049	673	187	189			
1	N	140	Total	C	N	O	0	0	0
			1006	641	179	186			
1	O	134	Total	C	N	O	0	0	0
			949	604	168	177			
1	P	138	Total	C	N	O	0	0	0
			1041	666	186	189			

There are 336 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-20	MET	-	initiating methionine	UNP Q2YLP8
A	-19	ALA	-	expression tag	UNP Q2YLP8
A	-18	HIS	-	expression tag	UNP Q2YLP8
A	-17	HIS	-	expression tag	UNP Q2YLP8
A	-16	HIS	-	expression tag	UNP Q2YLP8
A	-15	HIS	-	expression tag	UNP Q2YLP8
A	-14	HIS	-	expression tag	UNP Q2YLP8
A	-13	HIS	-	expression tag	UNP Q2YLP8
A	-12	MET	-	expression tag	UNP Q2YLP8
A	-11	GLY	-	expression tag	UNP Q2YLP8
A	-10	THR	-	expression tag	UNP Q2YLP8
A	-9	LEU	-	expression tag	UNP Q2YLP8
A	-8	GLU	-	expression tag	UNP Q2YLP8
A	-7	ALA	-	expression tag	UNP Q2YLP8
A	-6	GLN	-	expression tag	UNP Q2YLP8
A	-5	THR	-	expression tag	UNP Q2YLP8
A	-4	GLN	-	expression tag	UNP Q2YLP8
A	-3	GLY	-	expression tag	UNP Q2YLP8
A	-2	PRO	-	expression tag	UNP Q2YLP8
A	-1	GLY	-	expression tag	UNP Q2YLP8
A	0	SER	-	expression tag	UNP Q2YLP8
B	-20	MET	-	initiating methionine	UNP Q2YLP8
B	-19	ALA	-	expression tag	UNP Q2YLP8
B	-18	HIS	-	expression tag	UNP Q2YLP8
B	-17	HIS	-	expression tag	UNP Q2YLP8
B	-16	HIS	-	expression tag	UNP Q2YLP8
B	-15	HIS	-	expression tag	UNP Q2YLP8
B	-14	HIS	-	expression tag	UNP Q2YLP8
B	-13	HIS	-	expression tag	UNP Q2YLP8
B	-12	MET	-	expression tag	UNP Q2YLP8
B	-11	GLY	-	expression tag	UNP Q2YLP8
B	-10	THR	-	expression tag	UNP Q2YLP8
B	-9	LEU	-	expression tag	UNP Q2YLP8
B	-8	GLU	-	expression tag	UNP Q2YLP8
B	-7	ALA	-	expression tag	UNP Q2YLP8
B	-6	GLN	-	expression tag	UNP Q2YLP8
B	-5	THR	-	expression tag	UNP Q2YLP8
B	-4	GLN	-	expression tag	UNP Q2YLP8
B	-3	GLY	-	expression tag	UNP Q2YLP8
B	-2	PRO	-	expression tag	UNP Q2YLP8
B	-1	GLY	-	expression tag	UNP Q2YLP8
B	0	SER	-	expression tag	UNP Q2YLP8

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Chain	Residue	Modelled	Actual	Comment	Reference
C	-20	MET	-	initiating methionine	UNP Q2YLP8
C	-19	ALA	-	expression tag	UNP Q2YLP8
C	-18	HIS	-	expression tag	UNP Q2YLP8
C	-17	HIS	-	expression tag	UNP Q2YLP8
C	-16	HIS	-	expression tag	UNP Q2YLP8
C	-15	HIS	-	expression tag	UNP Q2YLP8
C	-14	HIS	-	expression tag	UNP Q2YLP8
C	-13	HIS	-	expression tag	UNP Q2YLP8
C	-12	MET	-	expression tag	UNP Q2YLP8
C	-11	GLY	-	expression tag	UNP Q2YLP8
C	-10	THR	-	expression tag	UNP Q2YLP8
C	-9	LEU	-	expression tag	UNP Q2YLP8
C	-8	GLU	-	expression tag	UNP Q2YLP8
C	-7	ALA	-	expression tag	UNP Q2YLP8
C	-6	GLN	-	expression tag	UNP Q2YLP8
C	-5	THR	-	expression tag	UNP Q2YLP8
C	-4	GLN	-	expression tag	UNP Q2YLP8
C	-3	GLY	-	expression tag	UNP Q2YLP8
C	-2	PRO	-	expression tag	UNP Q2YLP8
C	-1	GLY	-	expression tag	UNP Q2YLP8
C	0	SER	-	expression tag	UNP Q2YLP8
D	-20	MET	-	initiating methionine	UNP Q2YLP8
D	-19	ALA	-	expression tag	UNP Q2YLP8
D	-18	HIS	-	expression tag	UNP Q2YLP8
D	-17	HIS	-	expression tag	UNP Q2YLP8
D	-16	HIS	-	expression tag	UNP Q2YLP8
D	-15	HIS	-	expression tag	UNP Q2YLP8
D	-14	HIS	-	expression tag	UNP Q2YLP8
D	-13	HIS	-	expression tag	UNP Q2YLP8
D	-12	MET	-	expression tag	UNP Q2YLP8
D	-11	GLY	-	expression tag	UNP Q2YLP8
D	-10	THR	-	expression tag	UNP Q2YLP8
D	-9	LEU	-	expression tag	UNP Q2YLP8
D	-8	GLU	-	expression tag	UNP Q2YLP8
D	-7	ALA	-	expression tag	UNP Q2YLP8
D	-6	GLN	-	expression tag	UNP Q2YLP8
D	-5	THR	-	expression tag	UNP Q2YLP8
D	-4	GLN	-	expression tag	UNP Q2YLP8
D	-3	GLY	-	expression tag	UNP Q2YLP8
D	-2	PRO	-	expression tag	UNP Q2YLP8
D	-1	GLY	-	expression tag	UNP Q2YLP8
D	0	SER	-	expression tag	UNP Q2YLP8

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Chain	Residue	Modelled	Actual	Comment	Reference
E	-20	MET	-	initiating methionine	UNP Q2YLP8
E	-19	ALA	-	expression tag	UNP Q2YLP8
E	-18	HIS	-	expression tag	UNP Q2YLP8
E	-17	HIS	-	expression tag	UNP Q2YLP8
E	-16	HIS	-	expression tag	UNP Q2YLP8
E	-15	HIS	-	expression tag	UNP Q2YLP8
E	-14	HIS	-	expression tag	UNP Q2YLP8
E	-13	HIS	-	expression tag	UNP Q2YLP8
E	-12	MET	-	expression tag	UNP Q2YLP8
E	-11	GLY	-	expression tag	UNP Q2YLP8
E	-10	THR	-	expression tag	UNP Q2YLP8
E	-9	LEU	-	expression tag	UNP Q2YLP8
E	-8	GLU	-	expression tag	UNP Q2YLP8
E	-7	ALA	-	expression tag	UNP Q2YLP8
E	-6	GLN	-	expression tag	UNP Q2YLP8
E	-5	THR	-	expression tag	UNP Q2YLP8
E	-4	GLN	-	expression tag	UNP Q2YLP8
E	-3	GLY	-	expression tag	UNP Q2YLP8
E	-2	PRO	-	expression tag	UNP Q2YLP8
E	-1	GLY	-	expression tag	UNP Q2YLP8
E	0	SER	-	expression tag	UNP Q2YLP8
F	-20	MET	-	initiating methionine	UNP Q2YLP8
F	-19	ALA	-	expression tag	UNP Q2YLP8
F	-18	HIS	-	expression tag	UNP Q2YLP8
F	-17	HIS	-	expression tag	UNP Q2YLP8
F	-16	HIS	-	expression tag	UNP Q2YLP8
F	-15	HIS	-	expression tag	UNP Q2YLP8
F	-14	HIS	-	expression tag	UNP Q2YLP8
F	-13	HIS	-	expression tag	UNP Q2YLP8
F	-12	MET	-	expression tag	UNP Q2YLP8
F	-11	GLY	-	expression tag	UNP Q2YLP8
F	-10	THR	-	expression tag	UNP Q2YLP8
F	-9	LEU	-	expression tag	UNP Q2YLP8
F	-8	GLU	-	expression tag	UNP Q2YLP8
F	-7	ALA	-	expression tag	UNP Q2YLP8
F	-6	GLN	-	expression tag	UNP Q2YLP8
F	-5	THR	-	expression tag	UNP Q2YLP8
F	-4	GLN	-	expression tag	UNP Q2YLP8
F	-3	GLY	-	expression tag	UNP Q2YLP8
F	-2	PRO	-	expression tag	UNP Q2YLP8
F	-1	GLY	-	expression tag	UNP Q2YLP8
F	0	SER	-	expression tag	UNP Q2YLP8

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Chain	Residue	Modelled	Actual	Comment	Reference
G	-20	MET	-	initiating methionine	UNP Q2YLP8
G	-19	ALA	-	expression tag	UNP Q2YLP8
G	-18	HIS	-	expression tag	UNP Q2YLP8
G	-17	HIS	-	expression tag	UNP Q2YLP8
G	-16	HIS	-	expression tag	UNP Q2YLP8
G	-15	HIS	-	expression tag	UNP Q2YLP8
G	-14	HIS	-	expression tag	UNP Q2YLP8
G	-13	HIS	-	expression tag	UNP Q2YLP8
G	-12	MET	-	expression tag	UNP Q2YLP8
G	-11	GLY	-	expression tag	UNP Q2YLP8
G	-10	THR	-	expression tag	UNP Q2YLP8
G	-9	LEU	-	expression tag	UNP Q2YLP8
G	-8	GLU	-	expression tag	UNP Q2YLP8
G	-7	ALA	-	expression tag	UNP Q2YLP8
G	-6	GLN	-	expression tag	UNP Q2YLP8
G	-5	THR	-	expression tag	UNP Q2YLP8
G	-4	GLN	-	expression tag	UNP Q2YLP8
G	-3	GLY	-	expression tag	UNP Q2YLP8
G	-2	PRO	-	expression tag	UNP Q2YLP8
G	-1	GLY	-	expression tag	UNP Q2YLP8
G	0	SER	-	expression tag	UNP Q2YLP8
H	-20	MET	-	initiating methionine	UNP Q2YLP8
H	-19	ALA	-	expression tag	UNP Q2YLP8
H	-18	HIS	-	expression tag	UNP Q2YLP8
H	-17	HIS	-	expression tag	UNP Q2YLP8
H	-16	HIS	-	expression tag	UNP Q2YLP8
H	-15	HIS	-	expression tag	UNP Q2YLP8
H	-14	HIS	-	expression tag	UNP Q2YLP8
H	-13	HIS	-	expression tag	UNP Q2YLP8
H	-12	MET	-	expression tag	UNP Q2YLP8
H	-11	GLY	-	expression tag	UNP Q2YLP8
H	-10	THR	-	expression tag	UNP Q2YLP8
H	-9	LEU	-	expression tag	UNP Q2YLP8
H	-8	GLU	-	expression tag	UNP Q2YLP8
H	-7	ALA	-	expression tag	UNP Q2YLP8
H	-6	GLN	-	expression tag	UNP Q2YLP8
H	-5	THR	-	expression tag	UNP Q2YLP8
H	-4	GLN	-	expression tag	UNP Q2YLP8
H	-3	GLY	-	expression tag	UNP Q2YLP8
H	-2	PRO	-	expression tag	UNP Q2YLP8
H	-1	GLY	-	expression tag	UNP Q2YLP8
H	0	SER	-	expression tag	UNP Q2YLP8

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Chain	Residue	Modelled	Actual	Comment	Reference
I	-20	MET	-	initiating methionine	UNP Q2YLP8
I	-19	ALA	-	expression tag	UNP Q2YLP8
I	-18	HIS	-	expression tag	UNP Q2YLP8
I	-17	HIS	-	expression tag	UNP Q2YLP8
I	-16	HIS	-	expression tag	UNP Q2YLP8
I	-15	HIS	-	expression tag	UNP Q2YLP8
I	-14	HIS	-	expression tag	UNP Q2YLP8
I	-13	HIS	-	expression tag	UNP Q2YLP8
I	-12	MET	-	expression tag	UNP Q2YLP8
I	-11	GLY	-	expression tag	UNP Q2YLP8
I	-10	THR	-	expression tag	UNP Q2YLP8
I	-9	LEU	-	expression tag	UNP Q2YLP8
I	-8	GLU	-	expression tag	UNP Q2YLP8
I	-7	ALA	-	expression tag	UNP Q2YLP8
I	-6	GLN	-	expression tag	UNP Q2YLP8
I	-5	THR	-	expression tag	UNP Q2YLP8
I	-4	GLN	-	expression tag	UNP Q2YLP8
I	-3	GLY	-	expression tag	UNP Q2YLP8
I	-2	PRO	-	expression tag	UNP Q2YLP8
I	-1	GLY	-	expression tag	UNP Q2YLP8
I	0	SER	-	expression tag	UNP Q2YLP8
J	-20	MET	-	initiating methionine	UNP Q2YLP8
J	-19	ALA	-	expression tag	UNP Q2YLP8
J	-18	HIS	-	expression tag	UNP Q2YLP8
J	-17	HIS	-	expression tag	UNP Q2YLP8
J	-16	HIS	-	expression tag	UNP Q2YLP8
J	-15	HIS	-	expression tag	UNP Q2YLP8
J	-14	HIS	-	expression tag	UNP Q2YLP8
J	-13	HIS	-	expression tag	UNP Q2YLP8
J	-12	MET	-	expression tag	UNP Q2YLP8
J	-11	GLY	-	expression tag	UNP Q2YLP8
J	-10	THR	-	expression tag	UNP Q2YLP8
J	-9	LEU	-	expression tag	UNP Q2YLP8
J	-8	GLU	-	expression tag	UNP Q2YLP8
J	-7	ALA	-	expression tag	UNP Q2YLP8
J	-6	GLN	-	expression tag	UNP Q2YLP8
J	-5	THR	-	expression tag	UNP Q2YLP8
J	-4	GLN	-	expression tag	UNP Q2YLP8
J	-3	GLY	-	expression tag	UNP Q2YLP8
J	-2	PRO	-	expression tag	UNP Q2YLP8
J	-1	GLY	-	expression tag	UNP Q2YLP8
J	0	SER	-	expression tag	UNP Q2YLP8

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Chain	Residue	Modelled	Actual	Comment	Reference
K	-20	MET	-	initiating methionine	UNP Q2YLP8
K	-19	ALA	-	expression tag	UNP Q2YLP8
K	-18	HIS	-	expression tag	UNP Q2YLP8
K	-17	HIS	-	expression tag	UNP Q2YLP8
K	-16	HIS	-	expression tag	UNP Q2YLP8
K	-15	HIS	-	expression tag	UNP Q2YLP8
K	-14	HIS	-	expression tag	UNP Q2YLP8
K	-13	HIS	-	expression tag	UNP Q2YLP8
K	-12	MET	-	expression tag	UNP Q2YLP8
K	-11	GLY	-	expression tag	UNP Q2YLP8
K	-10	THR	-	expression tag	UNP Q2YLP8
K	-9	LEU	-	expression tag	UNP Q2YLP8
K	-8	GLU	-	expression tag	UNP Q2YLP8
K	-7	ALA	-	expression tag	UNP Q2YLP8
K	-6	GLN	-	expression tag	UNP Q2YLP8
K	-5	THR	-	expression tag	UNP Q2YLP8
K	-4	GLN	-	expression tag	UNP Q2YLP8
K	-3	GLY	-	expression tag	UNP Q2YLP8
K	-2	PRO	-	expression tag	UNP Q2YLP8
K	-1	GLY	-	expression tag	UNP Q2YLP8
K	0	SER	-	expression tag	UNP Q2YLP8
L	-20	MET	-	initiating methionine	UNP Q2YLP8
L	-19	ALA	-	expression tag	UNP Q2YLP8
L	-18	HIS	-	expression tag	UNP Q2YLP8
L	-17	HIS	-	expression tag	UNP Q2YLP8
L	-16	HIS	-	expression tag	UNP Q2YLP8
L	-15	HIS	-	expression tag	UNP Q2YLP8
L	-14	HIS	-	expression tag	UNP Q2YLP8
L	-13	HIS	-	expression tag	UNP Q2YLP8
L	-12	MET	-	expression tag	UNP Q2YLP8
L	-11	GLY	-	expression tag	UNP Q2YLP8
L	-10	THR	-	expression tag	UNP Q2YLP8
L	-9	LEU	-	expression tag	UNP Q2YLP8
L	-8	GLU	-	expression tag	UNP Q2YLP8
L	-7	ALA	-	expression tag	UNP Q2YLP8
L	-6	GLN	-	expression tag	UNP Q2YLP8
L	-5	THR	-	expression tag	UNP Q2YLP8
L	-4	GLN	-	expression tag	UNP Q2YLP8
L	-3	GLY	-	expression tag	UNP Q2YLP8
L	-2	PRO	-	expression tag	UNP Q2YLP8
L	-1	GLY	-	expression tag	UNP Q2YLP8
L	0	SER	-	expression tag	UNP Q2YLP8

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Chain	Residue	Modelled	Actual	Comment	Reference
M	-20	MET	-	initiating methionine	UNP Q2YLP8
M	-19	ALA	-	expression tag	UNP Q2YLP8
M	-18	HIS	-	expression tag	UNP Q2YLP8
M	-17	HIS	-	expression tag	UNP Q2YLP8
M	-16	HIS	-	expression tag	UNP Q2YLP8
M	-15	HIS	-	expression tag	UNP Q2YLP8
M	-14	HIS	-	expression tag	UNP Q2YLP8
M	-13	HIS	-	expression tag	UNP Q2YLP8
M	-12	MET	-	expression tag	UNP Q2YLP8
M	-11	GLY	-	expression tag	UNP Q2YLP8
M	-10	THR	-	expression tag	UNP Q2YLP8
M	-9	LEU	-	expression tag	UNP Q2YLP8
M	-8	GLU	-	expression tag	UNP Q2YLP8
M	-7	ALA	-	expression tag	UNP Q2YLP8
M	-6	GLN	-	expression tag	UNP Q2YLP8
M	-5	THR	-	expression tag	UNP Q2YLP8
M	-4	GLN	-	expression tag	UNP Q2YLP8
M	-3	GLY	-	expression tag	UNP Q2YLP8
M	-2	PRO	-	expression tag	UNP Q2YLP8
M	-1	GLY	-	expression tag	UNP Q2YLP8
M	0	SER	-	expression tag	UNP Q2YLP8
N	-20	MET	-	initiating methionine	UNP Q2YLP8
N	-19	ALA	-	expression tag	UNP Q2YLP8
N	-18	HIS	-	expression tag	UNP Q2YLP8
N	-17	HIS	-	expression tag	UNP Q2YLP8
N	-16	HIS	-	expression tag	UNP Q2YLP8
N	-15	HIS	-	expression tag	UNP Q2YLP8
N	-14	HIS	-	expression tag	UNP Q2YLP8
N	-13	HIS	-	expression tag	UNP Q2YLP8
N	-12	MET	-	expression tag	UNP Q2YLP8
N	-11	GLY	-	expression tag	UNP Q2YLP8
N	-10	THR	-	expression tag	UNP Q2YLP8
N	-9	LEU	-	expression tag	UNP Q2YLP8
N	-8	GLU	-	expression tag	UNP Q2YLP8
N	-7	ALA	-	expression tag	UNP Q2YLP8
N	-6	GLN	-	expression tag	UNP Q2YLP8
N	-5	THR	-	expression tag	UNP Q2YLP8
N	-4	GLN	-	expression tag	UNP Q2YLP8
N	-3	GLY	-	expression tag	UNP Q2YLP8
N	-2	PRO	-	expression tag	UNP Q2YLP8
N	-1	GLY	-	expression tag	UNP Q2YLP8
N	0	SER	-	expression tag	UNP Q2YLP8

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Chain	Residue	Modelled	Actual	Comment	Reference
O	-20	MET	-	initiating methionine	UNP Q2YLP8
O	-19	ALA	-	expression tag	UNP Q2YLP8
O	-18	HIS	-	expression tag	UNP Q2YLP8
O	-17	HIS	-	expression tag	UNP Q2YLP8
O	-16	HIS	-	expression tag	UNP Q2YLP8
O	-15	HIS	-	expression tag	UNP Q2YLP8
O	-14	HIS	-	expression tag	UNP Q2YLP8
O	-13	HIS	-	expression tag	UNP Q2YLP8
O	-12	MET	-	expression tag	UNP Q2YLP8
O	-11	GLY	-	expression tag	UNP Q2YLP8
O	-10	THR	-	expression tag	UNP Q2YLP8
O	-9	LEU	-	expression tag	UNP Q2YLP8
O	-8	GLU	-	expression tag	UNP Q2YLP8
O	-7	ALA	-	expression tag	UNP Q2YLP8
O	-6	GLN	-	expression tag	UNP Q2YLP8
O	-5	THR	-	expression tag	UNP Q2YLP8
O	-4	GLN	-	expression tag	UNP Q2YLP8
O	-3	GLY	-	expression tag	UNP Q2YLP8
O	-2	PRO	-	expression tag	UNP Q2YLP8
O	-1	GLY	-	expression tag	UNP Q2YLP8
O	0	SER	-	expression tag	UNP Q2YLP8
P	-20	MET	-	initiating methionine	UNP Q2YLP8
P	-19	ALA	-	expression tag	UNP Q2YLP8
P	-18	HIS	-	expression tag	UNP Q2YLP8
P	-17	HIS	-	expression tag	UNP Q2YLP8
P	-16	HIS	-	expression tag	UNP Q2YLP8
P	-15	HIS	-	expression tag	UNP Q2YLP8
P	-14	HIS	-	expression tag	UNP Q2YLP8
P	-13	HIS	-	expression tag	UNP Q2YLP8
P	-12	MET	-	expression tag	UNP Q2YLP8
P	-11	GLY	-	expression tag	UNP Q2YLP8
P	-10	THR	-	expression tag	UNP Q2YLP8
P	-9	LEU	-	expression tag	UNP Q2YLP8
P	-8	GLU	-	expression tag	UNP Q2YLP8
P	-7	ALA	-	expression tag	UNP Q2YLP8
P	-6	GLN	-	expression tag	UNP Q2YLP8
P	-5	THR	-	expression tag	UNP Q2YLP8
P	-4	GLN	-	expression tag	UNP Q2YLP8
P	-3	GLY	-	expression tag	UNP Q2YLP8
P	-2	PRO	-	expression tag	UNP Q2YLP8
P	-1	GLY	-	expression tag	UNP Q2YLP8
P	0	SER	-	expression tag	UNP Q2YLP8

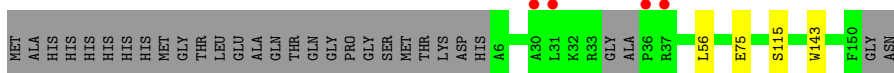
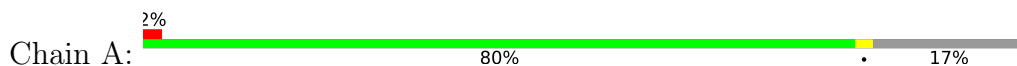
- Molecule 2 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	90	Total 90	O 90	0	0
2	B	100	Total 100	O 100	0	0
2	C	74	Total 74	O 74	0	0
2	D	78	Total 79	O 79	0	1
2	E	84	Total 85	O 85	0	1
2	F	59	Total 59	O 59	0	0
2	G	72	Total 72	O 72	0	0
2	H	58	Total 58	O 58	0	0
2	I	53	Total 53	O 53	0	0
2	J	42	Total 42	O 42	0	0
2	K	40	Total 40	O 40	0	0
2	L	46	Total 46	O 46	0	0
2	M	12	Total 12	O 12	0	0
2	N	5	Total 5	O 5	0	0
2	O	11	Total 11	O 11	0	0
2	P	18	Total 18	O 18	0	0

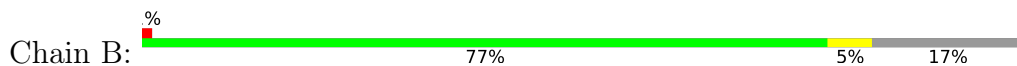
3 Residue-property plots [i](#)

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.

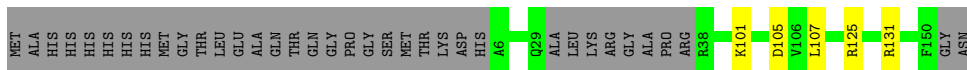
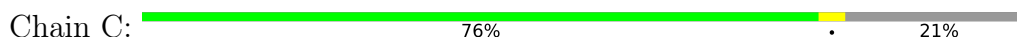
- Molecule 1: GCN5-related N-acetyltransferase



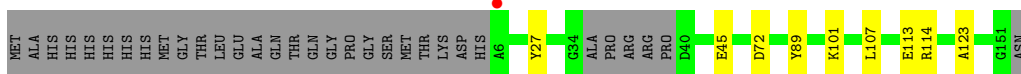
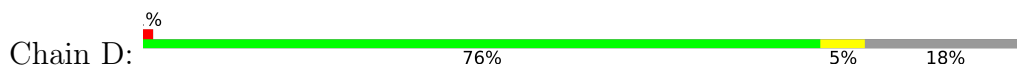
- Molecule 1: GCN5-related N-acetyltransferase



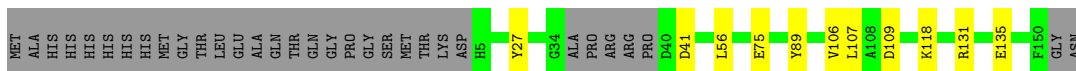
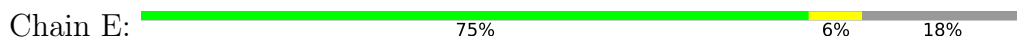
- Molecule 1: GCN5-related N-acetyltransferase



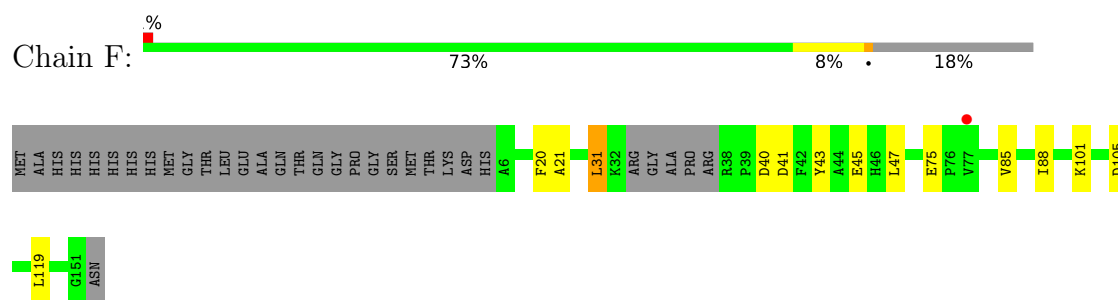
- Molecule 1: GCN5-related N-acetyltransferase



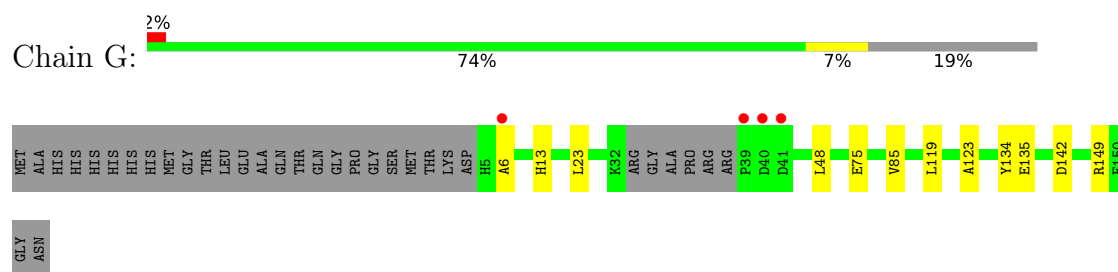
- Molecule 1: GCN5-related N-acetyltransferase



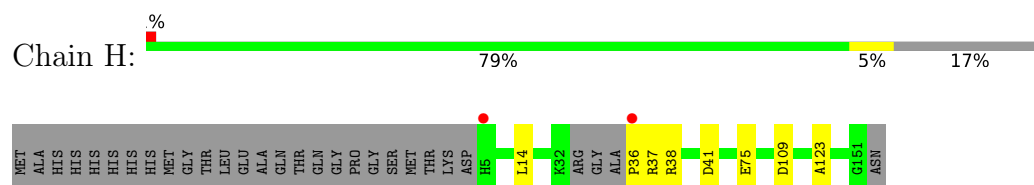
- Molecule 1: GCN5-related N-acetyltransferase



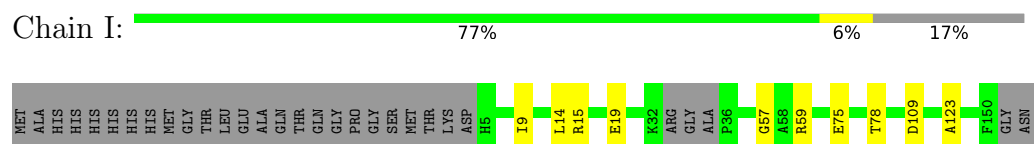
- Molecule 1: GCN5-related N-acetyltransferase



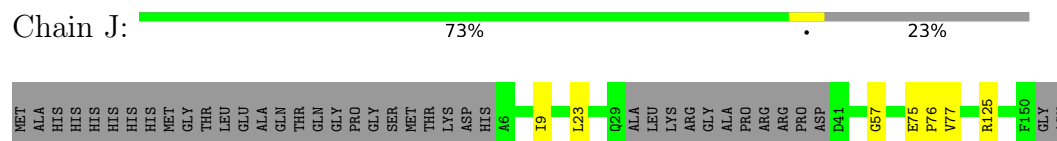
- Molecule 1: GCN5-related N-acetyltransferase



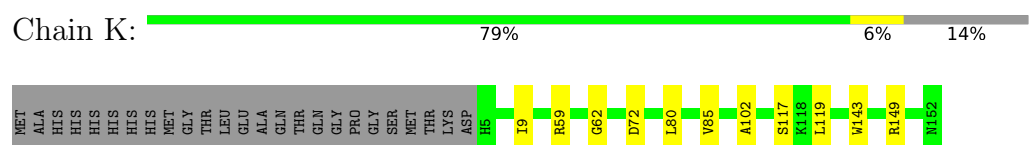
- Molecule 1: GCN5-related N-acetyltransferase



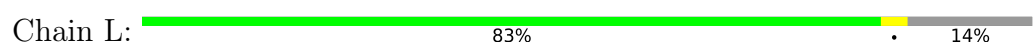
- Molecule 1: GCN5-related N-acetyltransferase

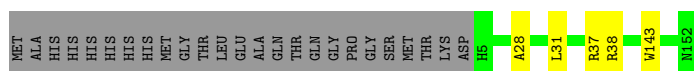


- Molecule 1: GCN5-related N-acetyltransferase

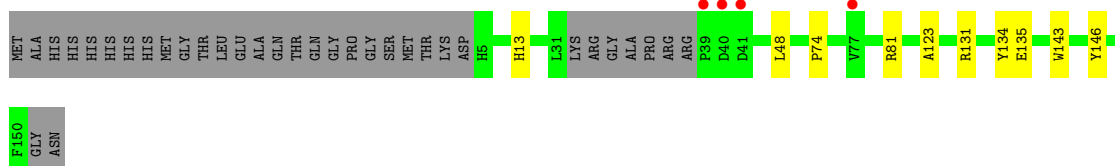
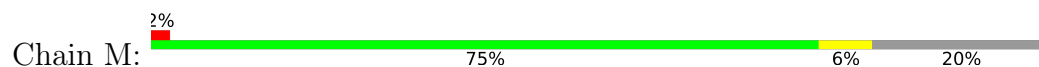


- Molecule 1: GCN5-related N-acetyltransferase

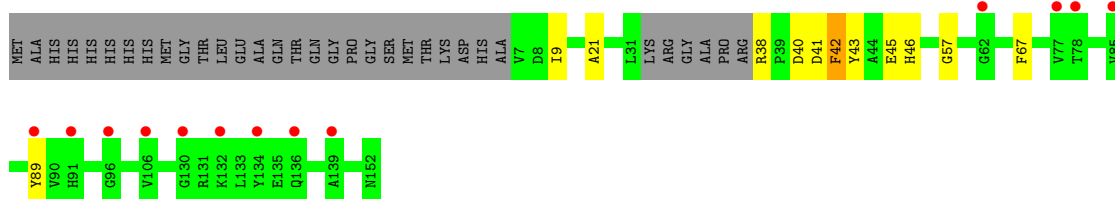




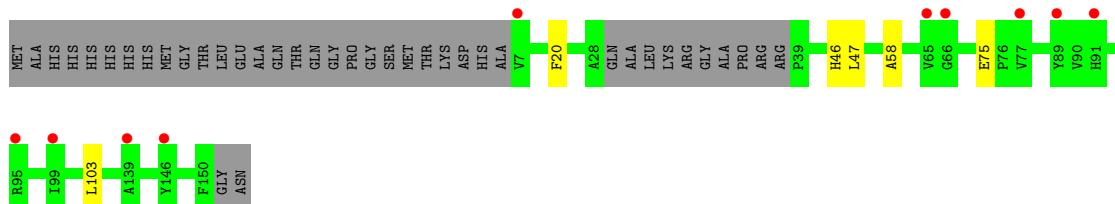
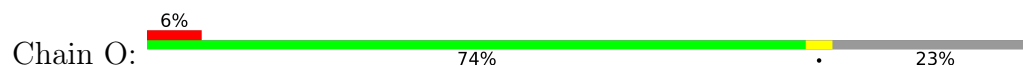
- Molecule 1: GCN5-related N-acetyltransferase



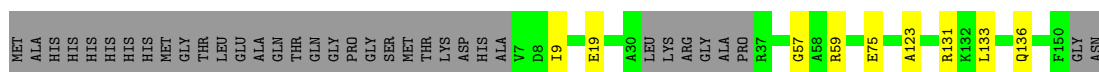
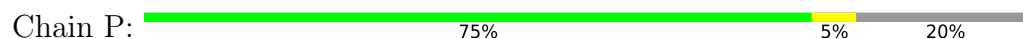
- Molecule 1: GCN5-related N-acetyltransferase



- Molecule 1: GCN5-related N-acetyltransferase



- Molecule 1: GCN5-related N-acetyltransferase



4 Data and refinement statistics

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α , β , γ	67.02Å 114.90Å 122.00Å 87.12° 76.27° 73.14°	Depositor
Resolution (Å)	48.73 – 2.30 48.73 – 2.30	Depositor EDS
% Data completeness (in resolution range)	98.4 (48.73-2.30) 98.4 (48.73-2.30)	Depositor EDS
R_{merge}	0.08	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.70 (at 2.29Å)	Xtriage
Refinement program	PHENIX 1.19 dev 4224	Depositor
R, R_{free}	0.209 , 0.248 0.208 , 0.247	Depositor DCC
R_{free} test set	1756 reflections (1.19%)	wwPDB-VP
Wilson B-factor (Å ²)	33.8	Xtriage
Anisotropy	0.618	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.30 , 31.4	EDS
L-test for twinning ²	$\langle L \rangle = 0.46$, $\langle L^2 \rangle = 0.28$	Xtriage
Estimated twinning fraction	0.115 for h,h-k,h-l 0.028 for -h,-h+k,-l 0.027 for -h,-k,-h+l	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	18064	wwPDB-VP
Average B, all atoms (Å ²)	52.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.82% 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	0.48	0/1140	0.68	1/1550 (0.1%)
1	B	0.47	0/1143	0.69	0/1554
1	C	0.44	0/1097	0.65	0/1492
1	D	0.46	0/1112	0.66	0/1511
1	E	0.49	0/1126	0.68	0/1529
1	F	0.43	0/1145	0.63	0/1556
1	G	0.42	0/1103	0.65	0/1500
1	H	0.38	0/1140	0.61	0/1551
1	I	0.34	0/1139	0.61	0/1550
1	J	0.41	0/1046	0.62	0/1423
1	K	0.40	0/1145	0.63	0/1561
1	L	0.40	0/1158	0.64	0/1576
1	M	0.29	0/1074	0.55	0/1464
1	N	0.27	0/1032	0.52	0/1412
1	O	0.27	0/970	0.53	0/1329
1	P	0.28	0/1067	0.54	0/1456
All	All	0.40	0/17637	0.62	1/24014 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	56	LEU	CB-CG-CD2	-6.30	100.29	111.00

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen

atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	1113	0	1075	2	0
1	B	1116	0	1084	3	0
1	C	1071	0	1039	5	0
1	D	1087	0	1047	7	0
1	E	1101	0	1070	5	0
1	F	1113	0	1083	7	0
1	G	1078	0	1049	7	0
1	H	1113	0	1067	4	0
1	I	1112	0	1073	6	0
1	J	1024	0	992	5	0
1	K	1117	0	1060	6	0
1	L	1130	0	1082	3	0
1	M	1049	0	997	6	0
1	N	1006	0	877	6	0
1	O	949	0	840	2	0
1	P	1041	0	966	6	0
2	A	90	0	0	0	0
2	B	100	0	0	0	0
2	C	74	0	0	2	0
2	D	79	0	0	1	0
2	E	85	0	0	0	0
2	F	59	0	0	0	0
2	G	72	0	0	3	0
2	H	58	0	0	0	0
2	I	53	0	0	1	0
2	J	42	0	0	1	0
2	K	40	0	0	1	0
2	L	46	0	0	0	0
2	M	12	0	0	0	0
2	N	5	0	0	0	0
2	O	11	0	0	0	0
2	P	18	0	0	0	0
All	All	18064	0	16401	68	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 2.

The worst 5 of 68 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:G:135:GLU:OE1	2:G:201:HOH:O	2.06	0.73
1:F:31:LEU:HD13	1:J:77:VAL:HG22	1.73	0.69
1:J:125:ARG:NH1	2:J:202:HOH:O	2.24	0.69
1:G:142:ASP:OD1	2:G:202:HOH:O	2.11	0.68
1:D:45:GLU:OE1	1:H:38:ARG:NH1	2.28	0.63

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	139/173 (80%)	137 (99%)	2 (1%)	0	100	100
1	B	139/173 (80%)	136 (98%)	2 (1%)	1 (1%)	22	26
1	C	133/173 (77%)	132 (99%)	1 (1%)	0	100	100
1	D	137/173 (79%)	136 (99%)	1 (1%)	0	100	100
1	E	137/173 (79%)	135 (98%)	2 (2%)	0	100	100
1	F	139/173 (80%)	138 (99%)	1 (1%)	0	100	100
1	G	136/173 (79%)	134 (98%)	1 (1%)	1 (1%)	22	26
1	H	140/173 (81%)	138 (99%)	2 (1%)	0	100	100
1	I	139/173 (80%)	136 (98%)	3 (2%)	0	100	100
1	J	130/173 (75%)	129 (99%)	1 (1%)	0	100	100
1	K	146/173 (84%)	142 (97%)	4 (3%)	0	100	100
1	L	146/173 (84%)	144 (99%)	2 (1%)	0	100	100
1	M	135/173 (78%)	134 (99%)	1 (1%)	0	100	100
1	N	136/173 (79%)	134 (98%)	2 (2%)	0	100	100
1	O	130/173 (75%)	129 (99%)	1 (1%)	0	100	100
1	P	134/173 (78%)	133 (99%)	1 (1%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
All	All	2196/2768 (79%)	2167 (99%)	27 (1%)	2 (0%)	51 64

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	G	6	ALA
1	B	31	LEU

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	108/135 (80%)	107 (99%)	1 (1%)	78 89
1	B	109/135 (81%)	106 (97%)	3 (3%)	43 60
1	C	105/135 (78%)	105 (100%)	0	100 100
1	D	104/135 (77%)	104 (100%)	0	100 100
1	E	107/135 (79%)	106 (99%)	1 (1%)	78 89
1	F	110/135 (82%)	107 (97%)	3 (3%)	44 61
1	G	103/135 (76%)	102 (99%)	1 (1%)	76 87
1	H	107/135 (79%)	104 (97%)	3 (3%)	43 60
1	I	108/135 (80%)	106 (98%)	2 (2%)	57 73
1	J	98/135 (73%)	97 (99%)	1 (1%)	76 87
1	K	103/135 (76%)	102 (99%)	1 (1%)	76 87
1	L	106/135 (78%)	105 (99%)	1 (1%)	78 89
1	M	97/135 (72%)	97 (100%)	0	100 100
1	N	83/135 (62%)	82 (99%)	1 (1%)	71 84
1	O	79/135 (58%)	77 (98%)	2 (2%)	47 65
1	P	95/135 (70%)	94 (99%)	1 (1%)	73 86
All	All	1622/2160 (75%)	1601 (99%)	21 (1%)	69 82

5 of 21 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	J	75	GLU
1	N	42	PHE
1	P	75	GLU
1	O	46	HIS
1	L	38	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (2) such sidechains are listed below:

Mol	Chain	Res	Type
1	L	49	GLN
1	M	92	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 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 [i](#)

6.1 Protein, DNA and RNA chains [i](#)

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	143/173 (82%)	-0.44	4 (2%) 53 60	24, 33, 61, 99	0
1	B	143/173 (82%)	-0.43	2 (1%) 75 80	21, 32, 56, 99	0
1	C	137/173 (79%)	-0.46	0 100 100	23, 40, 63, 97	0
1	D	141/173 (81%)	-0.46	1 (0%) 87 91	24, 35, 63, 93	0
1	E	141/173 (81%)	-0.48	0 100 100	21, 35, 58, 88	0
1	F	141/173 (81%)	-0.35	1 (0%) 87 91	22, 44, 71, 92	0
1	G	140/173 (80%)	-0.37	4 (2%) 51 58	23, 41, 73, 130	0
1	H	144/173 (83%)	-0.44	2 (1%) 75 80	30, 48, 83, 99	0
1	I	143/173 (82%)	-0.39	0 100 100	33, 51, 84, 104	0
1	J	134/173 (77%)	-0.17	0 100 100	23, 57, 84, 101	0
1	K	148/173 (85%)	-0.46	0 100 100	31, 47, 61, 71	0
1	L	148/173 (85%)	-0.45	0 100 100	31, 50, 66, 81	0
1	M	139/173 (80%)	-0.12	4 (2%) 51 58	45, 69, 99, 134	0
1	N	140/173 (80%)	0.40	13 (9%) 8 11	65, 90, 116, 126	0
1	O	134/173 (77%)	0.33	10 (7%) 14 19	58, 90, 119, 134	0
1	P	138/173 (79%)	-0.11	0 100 100	48, 75, 104, 112	0
All	All	2254/2768 (81%)	-0.28	41 (1%) 68 74	21, 48, 100, 134	0

The worst 5 of 41 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	G	40	ASP	5.3
1	O	65	VAL	4.6
1	B	36	PRO	4.5
1	N	134	TYR	4.5
1	M	41	ASP	4.3

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

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

6.3 Carbohydrates [i](#)

There are no 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.