



# wwPDB X-ray Structure Validation Summary Report ⓘ

Jun 11, 2024 – 10:13 PM EDT

PDB ID : 6NAY  
Title : Crystal structure of Neisseria meningitidis ClpP protease E31A+E58A activated double mutant  
Authors : Mabanglo, M.F.; Houry, W.A.  
Deposited on : 2018-12-06  
Resolution : 2.20 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](mailto: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>.

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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 : 2.36.2  
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) : 2.36.2

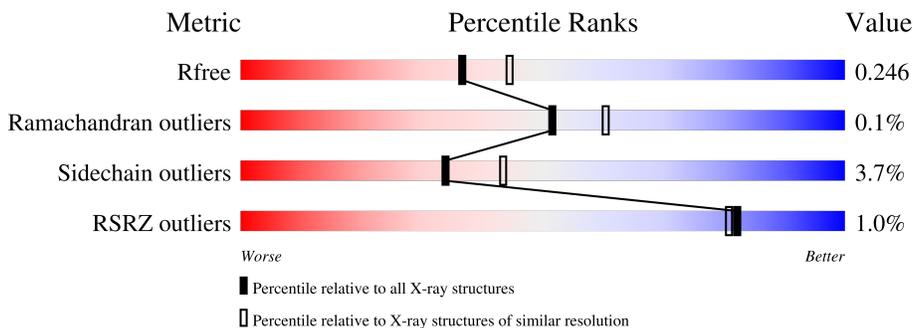
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.20 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))
$R_{free}$	130704	4898 (2.20-2.20)
Ramachandran outliers	138981	5503 (2.20-2.20)
Sidechain outliers	138945	5504 (2.20-2.20)
RSRZ outliers	127900	4800 (2.20-2.20)

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  $\geq 3$ , 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	217	
1	B	217	
1	C	217	
1	D	217	
1	E	217	
1	F	217	

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Mol	Chain	Length	Quality of chain
1	G	217	 80% 18%
1	H	217	 77% 19%
1	I	217	 76% 20%
1	J	217	 77% 19%
1	K	217	 78% 19%
1	L	217	 78% 19%
1	M	217	 76% 21%
1	N	217	 77% 18%
1	O	217	 77% 20%
1	P	217	 78% 18%
1	Q	217	 78% 19%
1	R	217	 76% 20%
1	S	217	 76% 21%
1	T	217	 79% 19%
1	U	217	 78% 19%
1	V	217	 78% 19%
1	W	217	 76% 20%
1	X	217	 78% 19%
1	Y	217	 79% 18%
1	Z	217	 78% 19%
1	a	217	 78% 20%
1	b	217	 78% 19%

## 2 Entry composition [i](#)

There are 2 unique types of molecules in this entry. The entry contains 39500 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 ATP-dependent Clp protease proteolytic subunit.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	174	1355	855	233	259	8	0	0	0
1	B	174	1355	855	233	259	8	0	0	0
1	C	175	1359	857	234	260	8	0	0	0
1	D	175	1364	863	234	259	8	0	0	0
1	E	173	1348	851	232	257	8	0	0	0
1	F	178	1386	875	240	263	8	0	0	0
1	G	178	1377	868	237	264	8	0	0	0
1	H	175	1359	857	234	260	8	0	0	0
1	I	174	1353	854	233	258	8	0	0	0
1	J	176	1367	863	235	261	8	0	0	0
1	K	176	1367	863	235	261	8	0	0	0
1	L	175	1359	857	234	260	8	0	0	0
1	M	172	1344	849	231	256	8	0	0	0
1	N	177	1373	866	236	263	8	0	0	0
1	O	174	1355	855	233	259	8	0	0	0
1	P	177	1371	865	236	262	8	0	0	0

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	Q	175	1359	857	234	260	8	0	0	0
1	R	174	1353	854	233	258	8	0	0	0
1	S	172	1337	845	228	256	8	0	0	0
1	T	176	1367	863	235	261	8	0	0	0
1	U	176	1365	860	235	262	8	0	0	0
1	V	175	1359	857	234	260	8	0	0	0
1	W	174	1353	854	233	258	8	0	0	0
1	X	176	1367	863	235	261	8	0	0	0
1	Y	179	1381	870	238	265	8	0	0	0
1	Z	175	1359	857	234	260	8	0	0	0
1	a	174	1355	855	233	259	8	0	0	0
1	b	176	1367	863	235	261	8	0	0	0

There are 420 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-12	HIS	-	expression tag	UNP A0A0H5Q9L9
A	-11	HIS	-	expression tag	UNP A0A0H5Q9L9
A	-10	HIS	-	expression tag	UNP A0A0H5Q9L9
A	-9	HIS	-	expression tag	UNP A0A0H5Q9L9
A	-8	HIS	-	expression tag	UNP A0A0H5Q9L9
A	-7	HIS	-	expression tag	UNP A0A0H5Q9L9
A	-6	GLU	-	expression tag	UNP A0A0H5Q9L9
A	-5	ASN	-	expression tag	UNP A0A0H5Q9L9
A	-4	LEU	-	expression tag	UNP A0A0H5Q9L9
A	-3	TYR	-	expression tag	UNP A0A0H5Q9L9
A	-2	PHE	-	expression tag	UNP A0A0H5Q9L9
A	-1	GLN	-	expression tag	UNP A0A0H5Q9L9
A	0	GLY	-	expression tag	UNP A0A0H5Q9L9
A	31	ALA	GLU	engineered mutation	UNP A0A0H5Q9L9
A	58	ALA	GLU	engineered mutation	UNP A0A0H5Q9L9

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Chain	Residue	Modelled	Actual	Comment	Reference
B	-12	HIS	-	expression tag	UNP A0A0H5Q9L9
B	-11	HIS	-	expression tag	UNP A0A0H5Q9L9
B	-10	HIS	-	expression tag	UNP A0A0H5Q9L9
B	-9	HIS	-	expression tag	UNP A0A0H5Q9L9
B	-8	HIS	-	expression tag	UNP A0A0H5Q9L9
B	-7	HIS	-	expression tag	UNP A0A0H5Q9L9
B	-6	GLU	-	expression tag	UNP A0A0H5Q9L9
B	-5	ASN	-	expression tag	UNP A0A0H5Q9L9
B	-4	LEU	-	expression tag	UNP A0A0H5Q9L9
B	-3	TYR	-	expression tag	UNP A0A0H5Q9L9
B	-2	PHE	-	expression tag	UNP A0A0H5Q9L9
B	-1	GLN	-	expression tag	UNP A0A0H5Q9L9
B	0	GLY	-	expression tag	UNP A0A0H5Q9L9
B	31	ALA	GLU	engineered mutation	UNP A0A0H5Q9L9
B	58	ALA	GLU	engineered mutation	UNP A0A0H5Q9L9
C	-12	HIS	-	expression tag	UNP A0A0H5Q9L9
C	-11	HIS	-	expression tag	UNP A0A0H5Q9L9
C	-10	HIS	-	expression tag	UNP A0A0H5Q9L9
C	-9	HIS	-	expression tag	UNP A0A0H5Q9L9
C	-8	HIS	-	expression tag	UNP A0A0H5Q9L9
C	-7	HIS	-	expression tag	UNP A0A0H5Q9L9
C	-6	GLU	-	expression tag	UNP A0A0H5Q9L9
C	-5	ASN	-	expression tag	UNP A0A0H5Q9L9
C	-4	LEU	-	expression tag	UNP A0A0H5Q9L9
C	-3	TYR	-	expression tag	UNP A0A0H5Q9L9
C	-2	PHE	-	expression tag	UNP A0A0H5Q9L9
C	-1	GLN	-	expression tag	UNP A0A0H5Q9L9
C	0	GLY	-	expression tag	UNP A0A0H5Q9L9
C	31	ALA	GLU	engineered mutation	UNP A0A0H5Q9L9
C	58	ALA	GLU	engineered mutation	UNP A0A0H5Q9L9
D	-12	HIS	-	expression tag	UNP A0A0H5Q9L9
D	-11	HIS	-	expression tag	UNP A0A0H5Q9L9
D	-10	HIS	-	expression tag	UNP A0A0H5Q9L9
D	-9	HIS	-	expression tag	UNP A0A0H5Q9L9
D	-8	HIS	-	expression tag	UNP A0A0H5Q9L9
D	-7	HIS	-	expression tag	UNP A0A0H5Q9L9
D	-6	GLU	-	expression tag	UNP A0A0H5Q9L9
D	-5	ASN	-	expression tag	UNP A0A0H5Q9L9
D	-4	LEU	-	expression tag	UNP A0A0H5Q9L9
D	-3	TYR	-	expression tag	UNP A0A0H5Q9L9
D	-2	PHE	-	expression tag	UNP A0A0H5Q9L9
D	-1	GLN	-	expression tag	UNP A0A0H5Q9L9

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Chain	Residue	Modelled	Actual	Comment	Reference
D	0	GLY	-	expression tag	UNP A0A0H5Q9L9
D	31	ALA	GLU	engineered mutation	UNP A0A0H5Q9L9
D	58	ALA	GLU	engineered mutation	UNP A0A0H5Q9L9
E	-12	HIS	-	expression tag	UNP A0A0H5Q9L9
E	-11	HIS	-	expression tag	UNP A0A0H5Q9L9
E	-10	HIS	-	expression tag	UNP A0A0H5Q9L9
E	-9	HIS	-	expression tag	UNP A0A0H5Q9L9
E	-8	HIS	-	expression tag	UNP A0A0H5Q9L9
E	-7	HIS	-	expression tag	UNP A0A0H5Q9L9
E	-6	GLU	-	expression tag	UNP A0A0H5Q9L9
E	-5	ASN	-	expression tag	UNP A0A0H5Q9L9
E	-4	LEU	-	expression tag	UNP A0A0H5Q9L9
E	-3	TYR	-	expression tag	UNP A0A0H5Q9L9
E	-2	PHE	-	expression tag	UNP A0A0H5Q9L9
E	-1	GLN	-	expression tag	UNP A0A0H5Q9L9
E	0	GLY	-	expression tag	UNP A0A0H5Q9L9
E	31	ALA	GLU	engineered mutation	UNP A0A0H5Q9L9
E	58	ALA	GLU	engineered mutation	UNP A0A0H5Q9L9
F	-12	HIS	-	expression tag	UNP A0A0H5Q9L9
F	-11	HIS	-	expression tag	UNP A0A0H5Q9L9
F	-10	HIS	-	expression tag	UNP A0A0H5Q9L9
F	-9	HIS	-	expression tag	UNP A0A0H5Q9L9
F	-8	HIS	-	expression tag	UNP A0A0H5Q9L9
F	-7	HIS	-	expression tag	UNP A0A0H5Q9L9
F	-6	GLU	-	expression tag	UNP A0A0H5Q9L9
F	-5	ASN	-	expression tag	UNP A0A0H5Q9L9
F	-4	LEU	-	expression tag	UNP A0A0H5Q9L9
F	-3	TYR	-	expression tag	UNP A0A0H5Q9L9
F	-2	PHE	-	expression tag	UNP A0A0H5Q9L9
F	-1	GLN	-	expression tag	UNP A0A0H5Q9L9
F	0	GLY	-	expression tag	UNP A0A0H5Q9L9
F	31	ALA	GLU	engineered mutation	UNP A0A0H5Q9L9
F	58	ALA	GLU	engineered mutation	UNP A0A0H5Q9L9
G	-12	HIS	-	expression tag	UNP A0A0H5Q9L9
G	-11	HIS	-	expression tag	UNP A0A0H5Q9L9
G	-10	HIS	-	expression tag	UNP A0A0H5Q9L9
G	-9	HIS	-	expression tag	UNP A0A0H5Q9L9
G	-8	HIS	-	expression tag	UNP A0A0H5Q9L9
G	-7	HIS	-	expression tag	UNP A0A0H5Q9L9
G	-6	GLU	-	expression tag	UNP A0A0H5Q9L9
G	-5	ASN	-	expression tag	UNP A0A0H5Q9L9
G	-4	LEU	-	expression tag	UNP A0A0H5Q9L9

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Chain	Residue	Modelled	Actual	Comment	Reference
G	-3	TYR	-	expression tag	UNP A0A0H5Q9L9
G	-2	PHE	-	expression tag	UNP A0A0H5Q9L9
G	-1	GLN	-	expression tag	UNP A0A0H5Q9L9
G	0	GLY	-	expression tag	UNP A0A0H5Q9L9
G	31	ALA	GLU	engineered mutation	UNP A0A0H5Q9L9
G	58	ALA	GLU	engineered mutation	UNP A0A0H5Q9L9
H	-12	HIS	-	expression tag	UNP A0A0H5Q9L9
H	-11	HIS	-	expression tag	UNP A0A0H5Q9L9
H	-10	HIS	-	expression tag	UNP A0A0H5Q9L9
H	-9	HIS	-	expression tag	UNP A0A0H5Q9L9
H	-8	HIS	-	expression tag	UNP A0A0H5Q9L9
H	-7	HIS	-	expression tag	UNP A0A0H5Q9L9
H	-6	GLU	-	expression tag	UNP A0A0H5Q9L9
H	-5	ASN	-	expression tag	UNP A0A0H5Q9L9
H	-4	LEU	-	expression tag	UNP A0A0H5Q9L9
H	-3	TYR	-	expression tag	UNP A0A0H5Q9L9
H	-2	PHE	-	expression tag	UNP A0A0H5Q9L9
H	-1	GLN	-	expression tag	UNP A0A0H5Q9L9
H	0	GLY	-	expression tag	UNP A0A0H5Q9L9
H	31	ALA	GLU	engineered mutation	UNP A0A0H5Q9L9
H	58	ALA	GLU	engineered mutation	UNP A0A0H5Q9L9
I	-12	HIS	-	expression tag	UNP A0A0H5Q9L9
I	-11	HIS	-	expression tag	UNP A0A0H5Q9L9
I	-10	HIS	-	expression tag	UNP A0A0H5Q9L9
I	-9	HIS	-	expression tag	UNP A0A0H5Q9L9
I	-8	HIS	-	expression tag	UNP A0A0H5Q9L9
I	-7	HIS	-	expression tag	UNP A0A0H5Q9L9
I	-6	GLU	-	expression tag	UNP A0A0H5Q9L9
I	-5	ASN	-	expression tag	UNP A0A0H5Q9L9
I	-4	LEU	-	expression tag	UNP A0A0H5Q9L9
I	-3	TYR	-	expression tag	UNP A0A0H5Q9L9
I	-2	PHE	-	expression tag	UNP A0A0H5Q9L9
I	-1	GLN	-	expression tag	UNP A0A0H5Q9L9
I	0	GLY	-	expression tag	UNP A0A0H5Q9L9
I	31	ALA	GLU	engineered mutation	UNP A0A0H5Q9L9
I	58	ALA	GLU	engineered mutation	UNP A0A0H5Q9L9
J	-12	HIS	-	expression tag	UNP A0A0H5Q9L9
J	-11	HIS	-	expression tag	UNP A0A0H5Q9L9
J	-10	HIS	-	expression tag	UNP A0A0H5Q9L9
J	-9	HIS	-	expression tag	UNP A0A0H5Q9L9
J	-8	HIS	-	expression tag	UNP A0A0H5Q9L9
J	-7	HIS	-	expression tag	UNP A0A0H5Q9L9

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Chain	Residue	Modelled	Actual	Comment	Reference
J	-6	GLU	-	expression tag	UNP A0A0H5Q9L9
J	-5	ASN	-	expression tag	UNP A0A0H5Q9L9
J	-4	LEU	-	expression tag	UNP A0A0H5Q9L9
J	-3	TYR	-	expression tag	UNP A0A0H5Q9L9
J	-2	PHE	-	expression tag	UNP A0A0H5Q9L9
J	-1	GLN	-	expression tag	UNP A0A0H5Q9L9
J	0	GLY	-	expression tag	UNP A0A0H5Q9L9
J	31	ALA	GLU	engineered mutation	UNP A0A0H5Q9L9
J	58	ALA	GLU	engineered mutation	UNP A0A0H5Q9L9
K	-12	HIS	-	expression tag	UNP A0A0H5Q9L9
K	-11	HIS	-	expression tag	UNP A0A0H5Q9L9
K	-10	HIS	-	expression tag	UNP A0A0H5Q9L9
K	-9	HIS	-	expression tag	UNP A0A0H5Q9L9
K	-8	HIS	-	expression tag	UNP A0A0H5Q9L9
K	-7	HIS	-	expression tag	UNP A0A0H5Q9L9
K	-6	GLU	-	expression tag	UNP A0A0H5Q9L9
K	-5	ASN	-	expression tag	UNP A0A0H5Q9L9
K	-4	LEU	-	expression tag	UNP A0A0H5Q9L9
K	-3	TYR	-	expression tag	UNP A0A0H5Q9L9
K	-2	PHE	-	expression tag	UNP A0A0H5Q9L9
K	-1	GLN	-	expression tag	UNP A0A0H5Q9L9
K	0	GLY	-	expression tag	UNP A0A0H5Q9L9
K	31	ALA	GLU	engineered mutation	UNP A0A0H5Q9L9
K	58	ALA	GLU	engineered mutation	UNP A0A0H5Q9L9
L	-12	HIS	-	expression tag	UNP A0A0H5Q9L9
L	-11	HIS	-	expression tag	UNP A0A0H5Q9L9
L	-10	HIS	-	expression tag	UNP A0A0H5Q9L9
L	-9	HIS	-	expression tag	UNP A0A0H5Q9L9
L	-8	HIS	-	expression tag	UNP A0A0H5Q9L9
L	-7	HIS	-	expression tag	UNP A0A0H5Q9L9
L	-6	GLU	-	expression tag	UNP A0A0H5Q9L9
L	-5	ASN	-	expression tag	UNP A0A0H5Q9L9
L	-4	LEU	-	expression tag	UNP A0A0H5Q9L9
L	-3	TYR	-	expression tag	UNP A0A0H5Q9L9
L	-2	PHE	-	expression tag	UNP A0A0H5Q9L9
L	-1	GLN	-	expression tag	UNP A0A0H5Q9L9
L	0	GLY	-	expression tag	UNP A0A0H5Q9L9
L	31	ALA	GLU	engineered mutation	UNP A0A0H5Q9L9
L	58	ALA	GLU	engineered mutation	UNP A0A0H5Q9L9
M	-12	HIS	-	expression tag	UNP A0A0H5Q9L9
M	-11	HIS	-	expression tag	UNP A0A0H5Q9L9
M	-10	HIS	-	expression tag	UNP A0A0H5Q9L9

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Chain	Residue	Modelled	Actual	Comment	Reference
M	-9	HIS	-	expression tag	UNP A0A0H5Q9L9
M	-8	HIS	-	expression tag	UNP A0A0H5Q9L9
M	-7	HIS	-	expression tag	UNP A0A0H5Q9L9
M	-6	GLU	-	expression tag	UNP A0A0H5Q9L9
M	-5	ASN	-	expression tag	UNP A0A0H5Q9L9
M	-4	LEU	-	expression tag	UNP A0A0H5Q9L9
M	-3	TYR	-	expression tag	UNP A0A0H5Q9L9
M	-2	PHE	-	expression tag	UNP A0A0H5Q9L9
M	-1	GLN	-	expression tag	UNP A0A0H5Q9L9
M	0	GLY	-	expression tag	UNP A0A0H5Q9L9
M	31	ALA	GLU	engineered mutation	UNP A0A0H5Q9L9
M	58	ALA	GLU	engineered mutation	UNP A0A0H5Q9L9
N	-12	HIS	-	expression tag	UNP A0A0H5Q9L9
N	-11	HIS	-	expression tag	UNP A0A0H5Q9L9
N	-10	HIS	-	expression tag	UNP A0A0H5Q9L9
N	-9	HIS	-	expression tag	UNP A0A0H5Q9L9
N	-8	HIS	-	expression tag	UNP A0A0H5Q9L9
N	-7	HIS	-	expression tag	UNP A0A0H5Q9L9
N	-6	GLU	-	expression tag	UNP A0A0H5Q9L9
N	-5	ASN	-	expression tag	UNP A0A0H5Q9L9
N	-4	LEU	-	expression tag	UNP A0A0H5Q9L9
N	-3	TYR	-	expression tag	UNP A0A0H5Q9L9
N	-2	PHE	-	expression tag	UNP A0A0H5Q9L9
N	-1	GLN	-	expression tag	UNP A0A0H5Q9L9
N	0	GLY	-	expression tag	UNP A0A0H5Q9L9
N	31	ALA	GLU	engineered mutation	UNP A0A0H5Q9L9
N	58	ALA	GLU	engineered mutation	UNP A0A0H5Q9L9
O	-12	HIS	-	expression tag	UNP A0A0H5Q9L9
O	-11	HIS	-	expression tag	UNP A0A0H5Q9L9
O	-10	HIS	-	expression tag	UNP A0A0H5Q9L9
O	-9	HIS	-	expression tag	UNP A0A0H5Q9L9
O	-8	HIS	-	expression tag	UNP A0A0H5Q9L9
O	-7	HIS	-	expression tag	UNP A0A0H5Q9L9
O	-6	GLU	-	expression tag	UNP A0A0H5Q9L9
O	-5	ASN	-	expression tag	UNP A0A0H5Q9L9
O	-4	LEU	-	expression tag	UNP A0A0H5Q9L9
O	-3	TYR	-	expression tag	UNP A0A0H5Q9L9
O	-2	PHE	-	expression tag	UNP A0A0H5Q9L9
O	-1	GLN	-	expression tag	UNP A0A0H5Q9L9
O	0	GLY	-	expression tag	UNP A0A0H5Q9L9
O	31	ALA	GLU	engineered mutation	UNP A0A0H5Q9L9
O	58	ALA	GLU	engineered mutation	UNP A0A0H5Q9L9

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Chain	Residue	Modelled	Actual	Comment	Reference
P	-12	HIS	-	expression tag	UNP A0A0H5Q9L9
P	-11	HIS	-	expression tag	UNP A0A0H5Q9L9
P	-10	HIS	-	expression tag	UNP A0A0H5Q9L9
P	-9	HIS	-	expression tag	UNP A0A0H5Q9L9
P	-8	HIS	-	expression tag	UNP A0A0H5Q9L9
P	-7	HIS	-	expression tag	UNP A0A0H5Q9L9
P	-6	GLU	-	expression tag	UNP A0A0H5Q9L9
P	-5	ASN	-	expression tag	UNP A0A0H5Q9L9
P	-4	LEU	-	expression tag	UNP A0A0H5Q9L9
P	-3	TYR	-	expression tag	UNP A0A0H5Q9L9
P	-2	PHE	-	expression tag	UNP A0A0H5Q9L9
P	-1	GLN	-	expression tag	UNP A0A0H5Q9L9
P	0	GLY	-	expression tag	UNP A0A0H5Q9L9
P	31	ALA	GLU	engineered mutation	UNP A0A0H5Q9L9
P	58	ALA	GLU	engineered mutation	UNP A0A0H5Q9L9
Q	-12	HIS	-	expression tag	UNP A0A0H5Q9L9
Q	-11	HIS	-	expression tag	UNP A0A0H5Q9L9
Q	-10	HIS	-	expression tag	UNP A0A0H5Q9L9
Q	-9	HIS	-	expression tag	UNP A0A0H5Q9L9
Q	-8	HIS	-	expression tag	UNP A0A0H5Q9L9
Q	-7	HIS	-	expression tag	UNP A0A0H5Q9L9
Q	-6	GLU	-	expression tag	UNP A0A0H5Q9L9
Q	-5	ASN	-	expression tag	UNP A0A0H5Q9L9
Q	-4	LEU	-	expression tag	UNP A0A0H5Q9L9
Q	-3	TYR	-	expression tag	UNP A0A0H5Q9L9
Q	-2	PHE	-	expression tag	UNP A0A0H5Q9L9
Q	-1	GLN	-	expression tag	UNP A0A0H5Q9L9
Q	0	GLY	-	expression tag	UNP A0A0H5Q9L9
Q	31	ALA	GLU	engineered mutation	UNP A0A0H5Q9L9
Q	58	ALA	GLU	engineered mutation	UNP A0A0H5Q9L9
R	-12	HIS	-	expression tag	UNP A0A0H5Q9L9
R	-11	HIS	-	expression tag	UNP A0A0H5Q9L9
R	-10	HIS	-	expression tag	UNP A0A0H5Q9L9
R	-9	HIS	-	expression tag	UNP A0A0H5Q9L9
R	-8	HIS	-	expression tag	UNP A0A0H5Q9L9
R	-7	HIS	-	expression tag	UNP A0A0H5Q9L9
R	-6	GLU	-	expression tag	UNP A0A0H5Q9L9
R	-5	ASN	-	expression tag	UNP A0A0H5Q9L9
R	-4	LEU	-	expression tag	UNP A0A0H5Q9L9
R	-3	TYR	-	expression tag	UNP A0A0H5Q9L9
R	-2	PHE	-	expression tag	UNP A0A0H5Q9L9
R	-1	GLN	-	expression tag	UNP A0A0H5Q9L9

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Chain	Residue	Modelled	Actual	Comment	Reference
R	0	GLY	-	expression tag	UNP A0A0H5Q9L9
R	31	ALA	GLU	engineered mutation	UNP A0A0H5Q9L9
R	58	ALA	GLU	engineered mutation	UNP A0A0H5Q9L9
S	-12	HIS	-	expression tag	UNP A0A0H5Q9L9
S	-11	HIS	-	expression tag	UNP A0A0H5Q9L9
S	-10	HIS	-	expression tag	UNP A0A0H5Q9L9
S	-9	HIS	-	expression tag	UNP A0A0H5Q9L9
S	-8	HIS	-	expression tag	UNP A0A0H5Q9L9
S	-7	HIS	-	expression tag	UNP A0A0H5Q9L9
S	-6	GLU	-	expression tag	UNP A0A0H5Q9L9
S	-5	ASN	-	expression tag	UNP A0A0H5Q9L9
S	-4	LEU	-	expression tag	UNP A0A0H5Q9L9
S	-3	TYR	-	expression tag	UNP A0A0H5Q9L9
S	-2	PHE	-	expression tag	UNP A0A0H5Q9L9
S	-1	GLN	-	expression tag	UNP A0A0H5Q9L9
S	0	GLY	-	expression tag	UNP A0A0H5Q9L9
S	31	ALA	GLU	engineered mutation	UNP A0A0H5Q9L9
S	58	ALA	GLU	engineered mutation	UNP A0A0H5Q9L9
T	-12	HIS	-	expression tag	UNP A0A0H5Q9L9
T	-11	HIS	-	expression tag	UNP A0A0H5Q9L9
T	-10	HIS	-	expression tag	UNP A0A0H5Q9L9
T	-9	HIS	-	expression tag	UNP A0A0H5Q9L9
T	-8	HIS	-	expression tag	UNP A0A0H5Q9L9
T	-7	HIS	-	expression tag	UNP A0A0H5Q9L9
T	-6	GLU	-	expression tag	UNP A0A0H5Q9L9
T	-5	ASN	-	expression tag	UNP A0A0H5Q9L9
T	-4	LEU	-	expression tag	UNP A0A0H5Q9L9
T	-3	TYR	-	expression tag	UNP A0A0H5Q9L9
T	-2	PHE	-	expression tag	UNP A0A0H5Q9L9
T	-1	GLN	-	expression tag	UNP A0A0H5Q9L9
T	0	GLY	-	expression tag	UNP A0A0H5Q9L9
T	31	ALA	GLU	engineered mutation	UNP A0A0H5Q9L9
T	58	ALA	GLU	engineered mutation	UNP A0A0H5Q9L9
U	-12	HIS	-	expression tag	UNP A0A0H5Q9L9
U	-11	HIS	-	expression tag	UNP A0A0H5Q9L9
U	-10	HIS	-	expression tag	UNP A0A0H5Q9L9
U	-9	HIS	-	expression tag	UNP A0A0H5Q9L9
U	-8	HIS	-	expression tag	UNP A0A0H5Q9L9
U	-7	HIS	-	expression tag	UNP A0A0H5Q9L9
U	-6	GLU	-	expression tag	UNP A0A0H5Q9L9
U	-5	ASN	-	expression tag	UNP A0A0H5Q9L9
U	-4	LEU	-	expression tag	UNP A0A0H5Q9L9

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Chain	Residue	Modelled	Actual	Comment	Reference
U	-3	TYR	-	expression tag	UNP A0A0H5Q9L9
U	-2	PHE	-	expression tag	UNP A0A0H5Q9L9
U	-1	GLN	-	expression tag	UNP A0A0H5Q9L9
U	0	GLY	-	expression tag	UNP A0A0H5Q9L9
U	31	ALA	GLU	engineered mutation	UNP A0A0H5Q9L9
U	58	ALA	GLU	engineered mutation	UNP A0A0H5Q9L9
V	-12	HIS	-	expression tag	UNP A0A0H5Q9L9
V	-11	HIS	-	expression tag	UNP A0A0H5Q9L9
V	-10	HIS	-	expression tag	UNP A0A0H5Q9L9
V	-9	HIS	-	expression tag	UNP A0A0H5Q9L9
V	-8	HIS	-	expression tag	UNP A0A0H5Q9L9
V	-7	HIS	-	expression tag	UNP A0A0H5Q9L9
V	-6	GLU	-	expression tag	UNP A0A0H5Q9L9
V	-5	ASN	-	expression tag	UNP A0A0H5Q9L9
V	-4	LEU	-	expression tag	UNP A0A0H5Q9L9
V	-3	TYR	-	expression tag	UNP A0A0H5Q9L9
V	-2	PHE	-	expression tag	UNP A0A0H5Q9L9
V	-1	GLN	-	expression tag	UNP A0A0H5Q9L9
V	0	GLY	-	expression tag	UNP A0A0H5Q9L9
V	31	ALA	GLU	engineered mutation	UNP A0A0H5Q9L9
V	58	ALA	GLU	engineered mutation	UNP A0A0H5Q9L9
W	-12	HIS	-	expression tag	UNP A0A0H5Q9L9
W	-11	HIS	-	expression tag	UNP A0A0H5Q9L9
W	-10	HIS	-	expression tag	UNP A0A0H5Q9L9
W	-9	HIS	-	expression tag	UNP A0A0H5Q9L9
W	-8	HIS	-	expression tag	UNP A0A0H5Q9L9
W	-7	HIS	-	expression tag	UNP A0A0H5Q9L9
W	-6	GLU	-	expression tag	UNP A0A0H5Q9L9
W	-5	ASN	-	expression tag	UNP A0A0H5Q9L9
W	-4	LEU	-	expression tag	UNP A0A0H5Q9L9
W	-3	TYR	-	expression tag	UNP A0A0H5Q9L9
W	-2	PHE	-	expression tag	UNP A0A0H5Q9L9
W	-1	GLN	-	expression tag	UNP A0A0H5Q9L9
W	0	GLY	-	expression tag	UNP A0A0H5Q9L9
W	31	ALA	GLU	engineered mutation	UNP A0A0H5Q9L9
W	58	ALA	GLU	engineered mutation	UNP A0A0H5Q9L9
X	-12	HIS	-	expression tag	UNP A0A0H5Q9L9
X	-11	HIS	-	expression tag	UNP A0A0H5Q9L9
X	-10	HIS	-	expression tag	UNP A0A0H5Q9L9
X	-9	HIS	-	expression tag	UNP A0A0H5Q9L9
X	-8	HIS	-	expression tag	UNP A0A0H5Q9L9
X	-7	HIS	-	expression tag	UNP A0A0H5Q9L9

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Chain	Residue	Modelled	Actual	Comment	Reference
X	-6	GLU	-	expression tag	UNP A0A0H5Q9L9
X	-5	ASN	-	expression tag	UNP A0A0H5Q9L9
X	-4	LEU	-	expression tag	UNP A0A0H5Q9L9
X	-3	TYR	-	expression tag	UNP A0A0H5Q9L9
X	-2	PHE	-	expression tag	UNP A0A0H5Q9L9
X	-1	GLN	-	expression tag	UNP A0A0H5Q9L9
X	0	GLY	-	expression tag	UNP A0A0H5Q9L9
X	31	ALA	GLU	engineered mutation	UNP A0A0H5Q9L9
X	58	ALA	GLU	engineered mutation	UNP A0A0H5Q9L9
Y	-12	HIS	-	expression tag	UNP A0A0H5Q9L9
Y	-11	HIS	-	expression tag	UNP A0A0H5Q9L9
Y	-10	HIS	-	expression tag	UNP A0A0H5Q9L9
Y	-9	HIS	-	expression tag	UNP A0A0H5Q9L9
Y	-8	HIS	-	expression tag	UNP A0A0H5Q9L9
Y	-7	HIS	-	expression tag	UNP A0A0H5Q9L9
Y	-6	GLU	-	expression tag	UNP A0A0H5Q9L9
Y	-5	ASN	-	expression tag	UNP A0A0H5Q9L9
Y	-4	LEU	-	expression tag	UNP A0A0H5Q9L9
Y	-3	TYR	-	expression tag	UNP A0A0H5Q9L9
Y	-2	PHE	-	expression tag	UNP A0A0H5Q9L9
Y	-1	GLN	-	expression tag	UNP A0A0H5Q9L9
Y	0	GLY	-	expression tag	UNP A0A0H5Q9L9
Y	31	ALA	GLU	engineered mutation	UNP A0A0H5Q9L9
Y	58	ALA	GLU	engineered mutation	UNP A0A0H5Q9L9
Z	-12	HIS	-	expression tag	UNP A0A0H5Q9L9
Z	-11	HIS	-	expression tag	UNP A0A0H5Q9L9
Z	-10	HIS	-	expression tag	UNP A0A0H5Q9L9
Z	-9	HIS	-	expression tag	UNP A0A0H5Q9L9
Z	-8	HIS	-	expression tag	UNP A0A0H5Q9L9
Z	-7	HIS	-	expression tag	UNP A0A0H5Q9L9
Z	-6	GLU	-	expression tag	UNP A0A0H5Q9L9
Z	-5	ASN	-	expression tag	UNP A0A0H5Q9L9
Z	-4	LEU	-	expression tag	UNP A0A0H5Q9L9
Z	-3	TYR	-	expression tag	UNP A0A0H5Q9L9
Z	-2	PHE	-	expression tag	UNP A0A0H5Q9L9
Z	-1	GLN	-	expression tag	UNP A0A0H5Q9L9
Z	0	GLY	-	expression tag	UNP A0A0H5Q9L9
Z	31	ALA	GLU	engineered mutation	UNP A0A0H5Q9L9
Z	58	ALA	GLU	engineered mutation	UNP A0A0H5Q9L9
a	-12	HIS	-	expression tag	UNP A0A0H5Q9L9
a	-11	HIS	-	expression tag	UNP A0A0H5Q9L9
a	-10	HIS	-	expression tag	UNP A0A0H5Q9L9

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Chain	Residue	Modelled	Actual	Comment	Reference
a	-9	HIS	-	expression tag	UNP A0A0H5Q9L9
a	-8	HIS	-	expression tag	UNP A0A0H5Q9L9
a	-7	HIS	-	expression tag	UNP A0A0H5Q9L9
a	-6	GLU	-	expression tag	UNP A0A0H5Q9L9
a	-5	ASN	-	expression tag	UNP A0A0H5Q9L9
a	-4	LEU	-	expression tag	UNP A0A0H5Q9L9
a	-3	TYR	-	expression tag	UNP A0A0H5Q9L9
a	-2	PHE	-	expression tag	UNP A0A0H5Q9L9
a	-1	GLN	-	expression tag	UNP A0A0H5Q9L9
a	0	GLY	-	expression tag	UNP A0A0H5Q9L9
a	31	ALA	GLU	engineered mutation	UNP A0A0H5Q9L9
a	58	ALA	GLU	engineered mutation	UNP A0A0H5Q9L9
b	-12	HIS	-	expression tag	UNP A0A0H5Q9L9
b	-11	HIS	-	expression tag	UNP A0A0H5Q9L9
b	-10	HIS	-	expression tag	UNP A0A0H5Q9L9
b	-9	HIS	-	expression tag	UNP A0A0H5Q9L9
b	-8	HIS	-	expression tag	UNP A0A0H5Q9L9
b	-7	HIS	-	expression tag	UNP A0A0H5Q9L9
b	-6	GLU	-	expression tag	UNP A0A0H5Q9L9
b	-5	ASN	-	expression tag	UNP A0A0H5Q9L9
b	-4	LEU	-	expression tag	UNP A0A0H5Q9L9
b	-3	TYR	-	expression tag	UNP A0A0H5Q9L9
b	-2	PHE	-	expression tag	UNP A0A0H5Q9L9
b	-1	GLN	-	expression tag	UNP A0A0H5Q9L9
b	0	GLY	-	expression tag	UNP A0A0H5Q9L9
b	31	ALA	GLU	engineered mutation	UNP A0A0H5Q9L9
b	58	ALA	GLU	engineered mutation	UNP A0A0H5Q9L9

- Molecule 2 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	50	Total O 50 50	0	0
2	B	50	Total O 50 50	0	0
2	C	57	Total O 57 57	0	0
2	D	45	Total O 45 45	0	0
2	E	44	Total O 44 44	0	0
2	F	57	Total O 57 57	0	0

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	G	54	Total O 54 54	0	0
2	H	56	Total O 56 56	0	0
2	I	55	Total O 55 55	0	0
2	J	32	Total O 32 32	0	0
2	K	44	Total O 44 44	0	0
2	L	47	Total O 47 47	0	0
2	M	49	Total O 49 49	0	0
2	N	53	Total O 53 53	0	0
2	O	60	Total O 60 60	0	0
2	P	46	Total O 46 46	0	0
2	Q	57	Total O 57 57	0	0
2	R	42	Total O 42 42	0	0
2	S	32	Total O 32 32	0	0
2	T	50	Total O 50 50	0	0
2	U	50	Total O 50 50	0	0
2	V	64	Total O 64 64	0	0
2	W	44	Total O 44 44	0	0
2	X	42	Total O 42 42	0	0
2	Y	54	Total O 54 54	0	0
2	Z	51	Total O 51 51	0	0
2	a	52	Total O 52 52	0	0

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<b>Mol</b>	<b>Chain</b>	<b>Residues</b>	<b>Atoms</b>		<b>ZeroOcc</b>	<b>AltConf</b>
2	b	49	Total	O	0	0
			49	49		

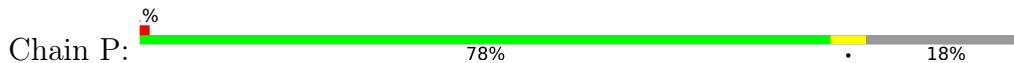






LEU

- Molecule 1: ATP-dependent Clp protease proteolytic subunit

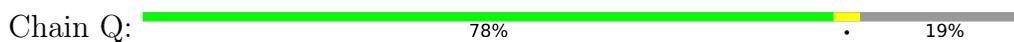


LEU

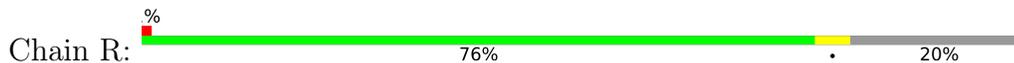
ARG

LEU

- Molecule 1: ATP-dependent Clp protease proteolytic subunit

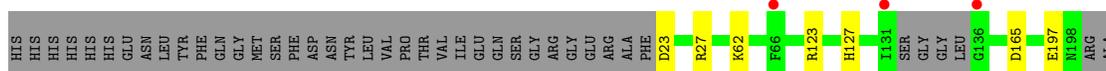
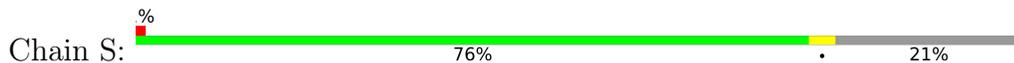


- Molecule 1: ATP-dependent Clp protease proteolytic subunit



LEU

- Molecule 1: ATP-dependent Clp protease proteolytic subunit



SER

LEU

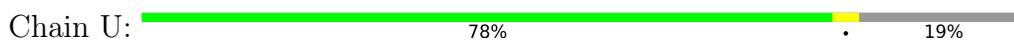
ARG

LEU

- Molecule 1: ATP-dependent Clp protease proteolytic subunit

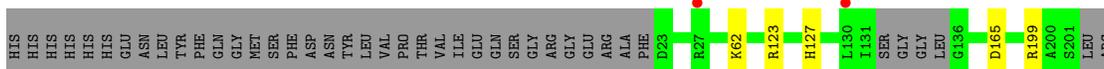
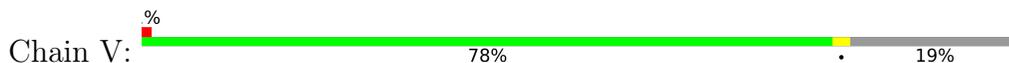


- Molecule 1: ATP-dependent Clp protease proteolytic subunit





- Molecule 1: ATP-dependent Clp protease proteolytic subunit



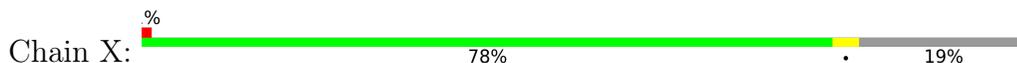
LEU

- Molecule 1: ATP-dependent Clp protease proteolytic subunit

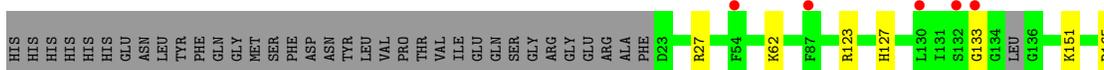


LEU  
ARG  
LEU

- Molecule 1: ATP-dependent Clp protease proteolytic subunit



- Molecule 1: ATP-dependent Clp protease proteolytic subunit



L202  
ARG  
LEU

- Molecule 1: ATP-dependent Clp protease proteolytic subunit



- Molecule 1: ATP-dependent Clp protease proteolytic subunit



## 4 Data and refinement statistics i

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	98.71Å 119.84Å 127.86Å 90.02° 89.99° 90.02°	Depositor
Resolution (Å)	46.05 – 2.20 46.05 – 2.20	Depositor EDS
% Data completeness (in resolution range)	95.2 (46.05-2.20) 95.1 (46.05-2.20)	Depositor EDS
$R_{merge}$	0.05	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.97 (at 2.20Å)	Xtrriage
Refinement program	PHENIX (1.13_2998)	Depositor
R, $R_{free}$	0.214 , 0.245 0.214 , 0.246	Depositor DCC
$R_{free}$ test set	1991 reflections (0.70%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	31.8	Xtrriage
Anisotropy	0.555	Xtrriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.34 , 31.5	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.47$ , $\langle L^2 \rangle = 0.30$	Xtrriage
Estimated twinning fraction	0.469 for h,-k,-l 0.469 for -h,k,-l 0.470 for -h,-k,l	Xtrriage
$F_o, F_c$ correlation	0.94	EDS
Total number of atoms	39500	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	39.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.47% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical 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	0.45	0/1374	0.66	0/1849
1	B	0.45	0/1374	0.63	0/1849
1	C	0.45	0/1378	0.62	0/1854
1	D	0.46	0/1384	0.63	0/1862
1	E	0.46	0/1367	0.61	0/1839
1	F	0.46	0/1405	0.64	0/1890
1	G	0.49	0/1396	0.63	0/1878
1	H	1.10	3/1378 (0.2%)	0.68	1/1854 (0.1%)
1	I	0.53	1/1372 (0.1%)	0.69	1/1846 (0.1%)
1	J	0.49	1/1386 (0.1%)	0.65	1/1865 (0.1%)
1	K	0.47	0/1386	0.67	2/1865 (0.1%)
1	L	0.46	0/1378	0.65	0/1854
1	M	0.54	1/1363 (0.1%)	0.67	2/1834 (0.1%)
1	N	0.49	0/1392	0.67	2/1873 (0.1%)
1	O	0.48	1/1374 (0.1%)	0.63	0/1849
1	P	0.46	0/1390	0.65	1/1870 (0.1%)
1	Q	0.43	0/1378	0.60	0/1854
1	R	0.49	0/1372	0.70	4/1846 (0.2%)
1	S	0.50	1/1356 (0.1%)	0.63	0/1825
1	T	0.47	0/1386	0.63	0/1865
1	U	0.43	0/1384	0.62	0/1862
1	V	0.46	0/1378	0.61	0/1854
1	W	0.46	0/1372	0.65	2/1846 (0.1%)
1	X	0.46	0/1386	0.61	0/1865
1	Y	0.49	0/1400	0.73	3/1883 (0.2%)
1	Z	0.47	0/1378	0.64	1/1854 (0.1%)
1	a	0.47	0/1374	0.62	0/1849
1	b	0.55	2/1386 (0.1%)	0.69	2/1865 (0.1%)
All	All	0.51	10/38647 (0.0%)	0.65	22/51999 (0.0%)

The worst 5 of 10 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	H	43	GLU	CD-OE1	36.16	1.65	1.25
1	M	194	GLN	CD-OE1	-8.39	1.05	1.24
1	I	43	GLU	CG-CD	-7.73	1.40	1.51
1	H	43	GLU	CG-CD	-6.29	1.42	1.51
1	H	43	GLU	CB-CG	-6.12	1.40	1.52

The worst 5 of 22 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	Y	27	ARG	NE-CZ-NH2	-12.59	114.00	120.30
1	Y	27	ARG	NE-CZ-NH1	9.05	124.83	120.30
1	I	198	ASN	C-N-CA	8.32	142.51	121.70
1	N	198	ASN	O-C-N	-8.06	109.81	122.70
1	P	198	ASN	C-N-CA	-7.46	103.06	121.70

There are no chirality outliers.

There are no planarity outliers.

## 5.2 Too-close contacts [i](#)

Due to software issues we are unable to calculate clashes - this section is therefore empty.

## 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	170/217 (78%)	165 (97%)	5 (3%)	0	100	100
1	B	170/217 (78%)	164 (96%)	6 (4%)	0	100	100
1	C	171/217 (79%)	165 (96%)	5 (3%)	1 (1%)	25	26
1	D	171/217 (79%)	166 (97%)	4 (2%)	1 (1%)	25	26
1	E	169/217 (78%)	164 (97%)	5 (3%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	F	174/217 (80%)	168 (97%)	5 (3%)	1 (1%)	25	26
1	G	174/217 (80%)	169 (97%)	5 (3%)	0	100	100
1	H	171/217 (79%)	166 (97%)	5 (3%)	0	100	100
1	I	170/217 (78%)	165 (97%)	5 (3%)	0	100	100
1	J	172/217 (79%)	168 (98%)	4 (2%)	0	100	100
1	K	172/217 (79%)	168 (98%)	4 (2%)	0	100	100
1	L	171/217 (79%)	165 (96%)	6 (4%)	0	100	100
1	M	168/217 (77%)	164 (98%)	4 (2%)	0	100	100
1	N	173/217 (80%)	168 (97%)	4 (2%)	1 (1%)	25	26
1	O	170/217 (78%)	165 (97%)	5 (3%)	0	100	100
1	P	173/217 (80%)	166 (96%)	6 (4%)	1 (1%)	25	26
1	Q	171/217 (79%)	165 (96%)	6 (4%)	0	100	100
1	R	170/217 (78%)	166 (98%)	4 (2%)	0	100	100
1	S	168/217 (77%)	164 (98%)	4 (2%)	0	100	100
1	T	172/217 (79%)	167 (97%)	5 (3%)	0	100	100
1	U	172/217 (79%)	167 (97%)	5 (3%)	0	100	100
1	V	171/217 (79%)	166 (97%)	5 (3%)	0	100	100
1	W	170/217 (78%)	165 (97%)	5 (3%)	0	100	100
1	X	172/217 (79%)	167 (97%)	5 (3%)	0	100	100
1	Y	175/217 (81%)	169 (97%)	5 (3%)	1 (1%)	25	26
1	Z	171/217 (79%)	166 (97%)	5 (3%)	0	100	100
1	a	170/217 (78%)	165 (97%)	5 (3%)	0	100	100
1	b	172/217 (79%)	166 (96%)	5 (3%)	1 (1%)	25	26
All	All	4793/6076 (79%)	4649 (97%)	137 (3%)	7 (0%)	51	60

5 of 7 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	F	200	ALA
1	N	200	ALA
1	C	199	ARG
1	b	200	ALA
1	D	24	ILE

### 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	147/183 (80%)	141 (96%)	6 (4%)	30	39
1	B	147/183 (80%)	140 (95%)	7 (5%)	25	32
1	C	147/183 (80%)	141 (96%)	6 (4%)	30	39
1	D	147/183 (80%)	143 (97%)	4 (3%)	44	57
1	E	146/183 (80%)	140 (96%)	6 (4%)	30	39
1	F	150/183 (82%)	145 (97%)	5 (3%)	38	49
1	G	149/183 (81%)	144 (97%)	5 (3%)	37	47
1	H	147/183 (80%)	141 (96%)	6 (4%)	30	39
1	I	146/183 (80%)	140 (96%)	6 (4%)	30	39
1	J	148/183 (81%)	142 (96%)	6 (4%)	30	39
1	K	148/183 (81%)	143 (97%)	5 (3%)	37	47
1	L	147/183 (80%)	142 (97%)	5 (3%)	37	47
1	M	146/183 (80%)	141 (97%)	5 (3%)	37	47
1	N	149/183 (81%)	142 (95%)	7 (5%)	26	33
1	O	147/183 (80%)	142 (97%)	5 (3%)	37	47
1	P	148/183 (81%)	142 (96%)	6 (4%)	30	39
1	Q	147/183 (80%)	141 (96%)	6 (4%)	30	39
1	R	146/183 (80%)	140 (96%)	6 (4%)	30	39
1	S	145/183 (79%)	139 (96%)	6 (4%)	30	39
1	T	148/183 (81%)	144 (97%)	4 (3%)	44	57
1	U	148/183 (81%)	142 (96%)	6 (4%)	30	39
1	V	147/183 (80%)	142 (97%)	5 (3%)	37	47
1	W	146/183 (80%)	140 (96%)	6 (4%)	30	39
1	X	148/183 (81%)	142 (96%)	6 (4%)	30	39
1	Y	149/183 (81%)	145 (97%)	4 (3%)	44	57
1	Z	147/183 (80%)	143 (97%)	4 (3%)	44	57

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	a	147/183 (80%)	143 (97%)	4 (3%)	44 57
1	b	148/183 (81%)	144 (97%)	4 (3%)	44 57
All	All	4125/5124 (80%)	3974 (96%)	151 (4%)	34 43

5 of 151 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	U	123	ARG
1	a	62	LYS
1	V	123	ARG
1	X	43	GLU
1	b	165	ASP

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (1) such sidechains are listed below:

Mol	Chain	Res	Type
1	H	194	GLN

### 5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

## 5.5 Carbohydrates [i](#)

There are no monosaccharides in this entry.

## 5.6 Ligand geometry [i](#)

There are no ligands in this entry.

## 5.7 Other polymers [i](#)

There are no such residues in this entry.

## 5.8 Polymer linkage issues

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, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	A	174/217 (80%)	-0.03	0 <b>100</b> <b>100</b>	27, 34, 65, 102	0
1	B	174/217 (80%)	-0.03	1 (0%) 89 88	26, 33, 57, 74	0
1	C	175/217 (80%)	-0.01	0 <b>100</b> <b>100</b>	27, 34, 63, 76	0
1	D	175/217 (80%)	0.06	2 (1%) 80 79	30, 37, 69, 82	0
1	E	173/217 (79%)	0.17	5 (2%) 51 49	30, 39, 65, 81	0
1	F	178/217 (82%)	0.11	1 (0%) 89 88	28, 36, 64, 107	0
1	G	178/217 (82%)	0.08	0 <b>100</b> <b>100</b>	27, 34, 69, 96	0
1	H	175/217 (80%)	0.00	1 (0%) 89 88	28, 34, 62, 83	0
1	I	174/217 (80%)	0.13	2 (1%) 80 79	30, 37, 67, 82	0
1	J	176/217 (81%)	0.17	4 (2%) 60 58	30, 39, 71, 91	0
1	K	176/217 (81%)	0.01	5 (2%) 53 51	28, 35, 63, 84	0
1	L	175/217 (80%)	0.10	3 (1%) 70 68	28, 34, 67, 88	0
1	M	172/217 (79%)	-0.02	0 <b>100</b> <b>100</b>	28, 34, 60, 80	0
1	N	177/217 (81%)	-0.06	0 <b>100</b> <b>100</b>	26, 32, 62, 74	0
1	O	174/217 (80%)	0.10	1 (0%) 89 88	27, 34, 60, 79	0
1	P	177/217 (81%)	-0.01	3 (1%) 70 68	26, 33, 62, 108	0
1	Q	175/217 (80%)	-0.02	1 (0%) 89 88	28, 34, 63, 101	0
1	R	174/217 (80%)	0.10	2 (1%) 80 79	29, 37, 65, 82	0
1	S	172/217 (79%)	0.12	3 (1%) 70 68	30, 39, 65, 82	0
1	T	176/217 (81%)	0.01	1 (0%) 89 88	28, 35, 62, 74	0
1	U	176/217 (81%)	0.02	1 (0%) 89 88	28, 33, 64, 87	0
1	V	175/217 (80%)	-0.05	2 (1%) 80 79	28, 34, 64, 79	0
1	W	174/217 (80%)	0.14	2 (1%) 80 79	29, 37, 64, 81	0
1	X	176/217 (81%)	0.18	2 (1%) 80 79	31, 39, 67, 94	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å <sup>2</sup> )	Q<0.9
1	Y	179/217 (82%)	0.16	5 (2%) 53 51	28, 35, 66, 141	0
1	Z	175/217 (80%)	0.09	1 (0%) 89 88	28, 34, 64, 105	0
1	a	174/217 (80%)	0.05	1 (0%) 89 88	27, 34, 68, 80	0
1	b	176/217 (81%)	-0.01	0 100 100	25, 33, 62, 77	0
All	All	4905/6076 (80%)	0.06	49 (0%) 82 81	25, 35, 66, 141	0

The worst 5 of 49 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	L	199	ARG	3.6
1	P	54	PHE	3.5
1	Q	24	ILE	2.9
1	S	131	ILE	2.9
1	E	58	ALA	2.8

## 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.