



# Full wwPDB X-ray Structure Validation Report ⓘ

Aug 19, 2020 – 11:01 AM BST

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 Full wwPDB X-ray Structure Validation 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 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	:	<b>FAILED</b>
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.13.1

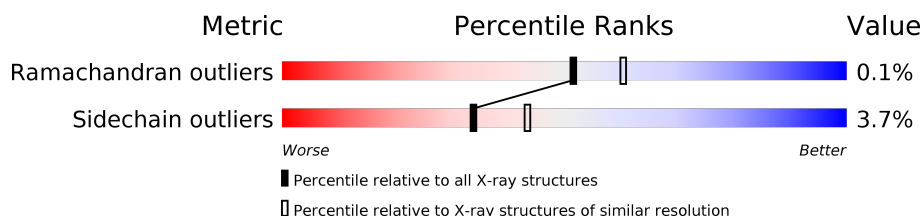
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 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))
Ramachandran outliers	138981	5503 (2.20-2.20)
Sidechain outliers	138945	5504 (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 on 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  $\leq 5\%$ .

Note EDS failed to run properly.

Mol	Chain	Length	Quality of chain
1	A	217	77% 20%
1	B	217	77% 20%
1	C	217	77% 19%
1	D	217	78% 19%
1	E	217	77% 20%
1	F	217	79% 18%
1	G	217	80% 18%
1	H	217	77% 19%
1	I	217	76% 20%

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Length	Quality of chain
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

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

*Continued on next page...*

*Continued from previous page...*

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

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

*Continued on next page...*

*Continued from previous page...*

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

*Continued on next page...*

*Continued from previous page...*

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

*Continued on next page...*

*Continued from previous page...*

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

*Continued on next page...*



*Continued from previous page...*

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

*Continued on next page...*

*Continued from previous page...*

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

*Continued on next page...*

*Continued from previous page...*

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

*Continued on next page...*

*Continued from previous page...*

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

*Continued on next page...*

*Continued from previous page...*

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

*Continued on next page...*

*Continued from previous page...*

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

*Continued on next page...*

*Continued from previous page...*

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

*Continued on next page...*

*Continued from previous page...*

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

*Continued on next page...*

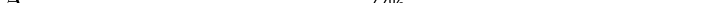


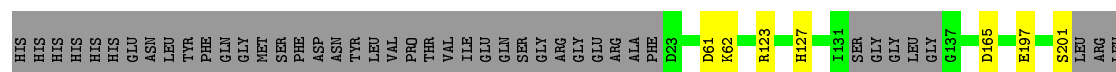
*Continued from previous page...*

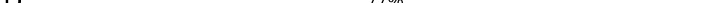
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	b	49	Total	O	0	0
			49	49		

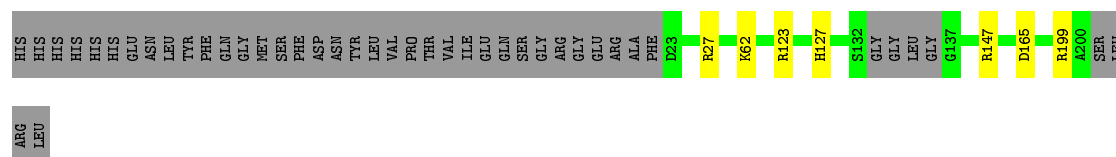


Note EDS failed to run properly.

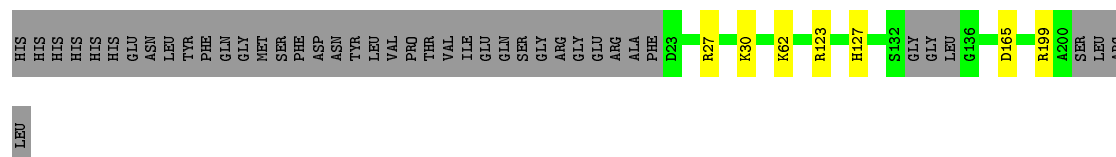
- Chain A:  77% 20%

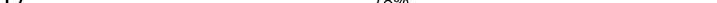


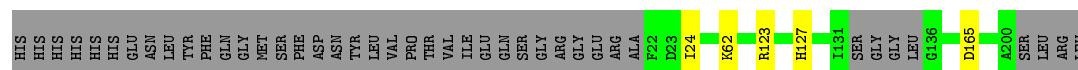
- Chain B:  77% 20%

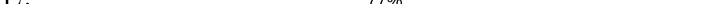


- Chain C:  77% 1% 19%

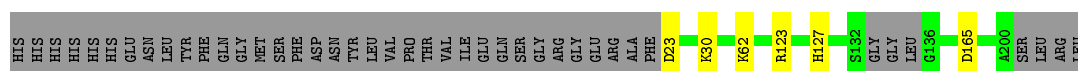


- Chain D:  78% • 19%

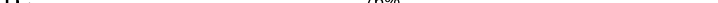


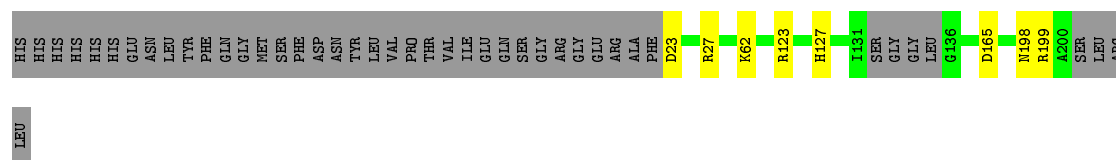
- Chain E:  77% 20%





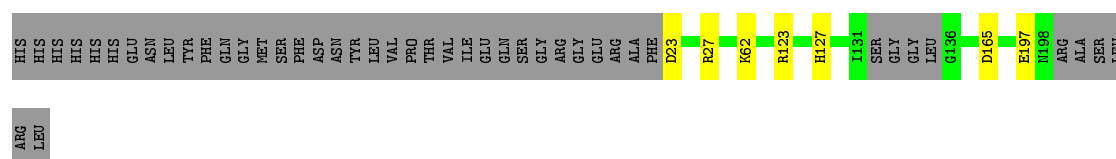
- Molecule 1: ATP-dependent Clp protease proteolytic subunit

Chain R:  76% . 20%



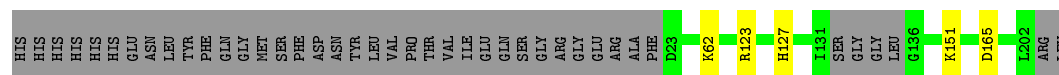
- Molecule 1: ATP-dependent Clp protease proteolytic subunit

Chain S:  76% 21%




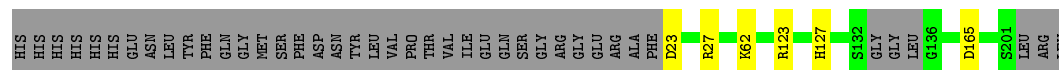
- Molecule 1: ATP-dependent Clp protease proteolytic subunit

Chain T:  79% • 19%



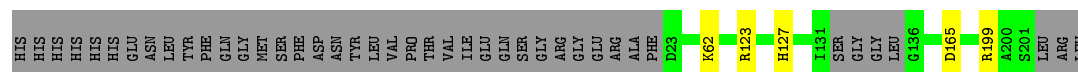
- Molecule 1: ATP-dependent Clp protease proteolytic subunit

Chain U:  78% . 19%



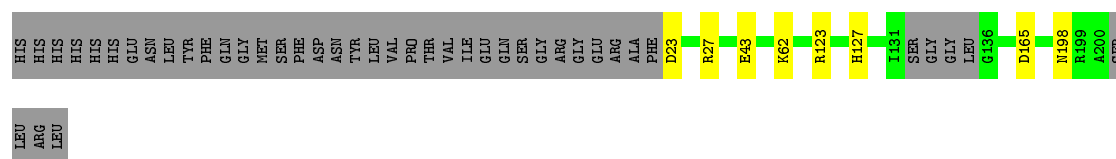
- Molecule 1: ATP-dependent Clp protease proteolytic subunit

Chain V:  78% 19%




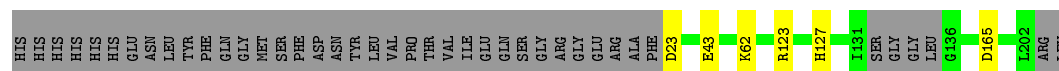
- Molecule 1: ATP-dependent Clp protease proteolytic subunit

Chain W:  76% . 20%




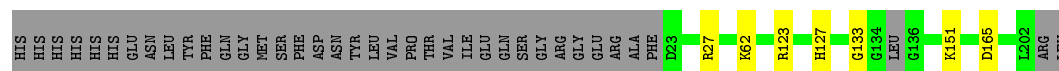
- Molecule 1: ATP-dependent Clp protease proteolytic subunit

Chain X:  78% 19%




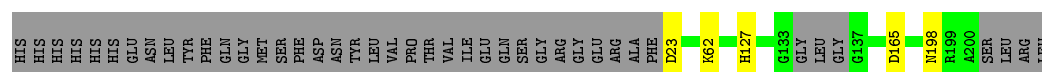
- Molecule 1: ATP-dependent Clp protease proteolytic subunit

Chain Y:  79% 18%



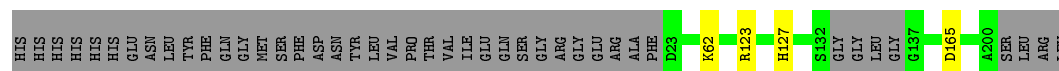
- Molecule 1: ATP-dependent Clp protease proteolytic subunit

Chain Z:  78% 19%




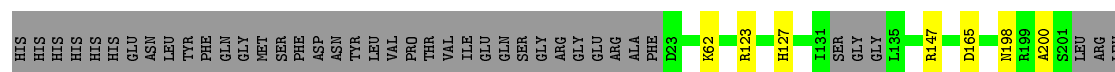
- Molecule 1: ATP-dependent Clp protease proteolytic subunit

Chain a:  78% 20%



- Molecule 1: ATP-dependent Clp protease proteolytic subunit

Chain b:  78% 19%



## 4 Data and refinement statistics

EDS failed to run properly - this section is therefore incomplete.

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	Depositor
% Data completeness (in resolution range)	95.2 (46.05-2.20)	Depositor
$R_{merge}$	0.05	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.97 (at 2.20Å)	Xtriage
Refinement program	PHENIX (1.13_2998)	Depositor
R, $R_{free}$	0.214 , 0.245	Depositor
Wilson B-factor (Å <sup>2</sup> )	31.8	Xtriage
Anisotropy	0.555	Xtriage
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.47$ , $\langle L^2 \rangle = 0.30$	Xtriage
Estimated twinning fraction	0.469 for h,-k,-l 0.469 for -h,k,-l 0.470 for -h,-k,l	Xtriage
Total number of atoms	39500	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	39.0	wwPDB-VP

Xtriage'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 ⓘ

### 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	0.45	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%)

All (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
1	S	197	GLU	CB-CG	-5.99	1.40	1.52
1	O	43	GLU	CB-CG	5.19	1.62	1.52
1	b	147	ARG	CZ-NH2	5.10	1.39	1.33
1	J	197	GLU	CB-CG	-5.01	1.42	1.52
1	b	147	ARG	NE-CZ	5.01	1.39	1.33

All (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
1	b	147	ARG	NE-CZ-NH1	-7.24	116.68	120.30
1	K	30	LYS	CD-CE-NZ	-6.50	96.75	111.70
1	M	147	ARG	NE-CZ-NH2	-6.48	117.06	120.30
1	K	198	ASN	O-C-N	-6.10	112.94	122.70
1	W	43	GLU	CA-CB-CG	5.97	126.55	113.40
1	H	43	GLU	OE1-CD-OE2	-5.90	116.22	123.30
1	R	198	ASN	C-N-CA	5.75	136.09	121.70
1	W	198	ASN	C-N-CA	5.69	135.93	121.70
1	M	147	ARG	NE-CZ-NH1	5.61	123.11	120.30
1	R	198	ASN	O-C-N	5.59	131.65	122.70
1	Z	198	ASN	O-C-N	5.59	131.64	122.70
1	R	198	ASN	CA-C-N	-5.53	105.03	117.20
1	Y	27	ARG	CG-CD-NE	-5.36	100.54	111.80
1	J	184	GLU	CA-CB-CG	5.34	125.16	113.40
1	b	198	ASN	O-C-N	-5.23	114.33	122.70
1	R	199	ARG	CA-CB-CG	5.21	124.86	113.40
1	N	198	ASN	CA-C-N	5.17	128.57	117.20

There are no chirality outliers.

There are no planarity outliers.

## 5.2 Too-close contacts

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

## 5.3 Torsion angles

### 5.3.1 Protein backbone

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	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
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

*Continued on next page...*

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
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

All (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
1	P	135	LEU
1	Y	133	GLY

### 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	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

Continued on next page...

*Continued from previous page...*

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
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
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

All (151) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	62	LYS
1	A	123	ARG
1	A	127	HIS
1	A	165	ASP
1	A	197	GLU
1	A	201	SER
1	B	27	ARG
1	B	62	LYS
1	B	123	ARG

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
1	B	127	HIS
1	B	147	ARG
1	B	165	ASP
1	B	199	ARG
1	C	27	ARG
1	C	30	LYS
1	C	62	LYS
1	C	123	ARG
1	C	127	HIS
1	C	165	ASP
1	D	62	LYS
1	D	123	ARG
1	D	127	HIS
1	D	165	ASP
1	E	23	ASP
1	E	27	ARG
1	E	62	LYS
1	E	123	ARG
1	E	127	HIS
1	E	165	ASP
1	F	62	LYS
1	F	123	ARG
1	F	127	HIS
1	F	151	LYS
1	F	165	ASP
1	G	23	ASP
1	G	62	LYS
1	G	127	HIS
1	G	132	SER
1	G	165	ASP
1	H	27	ARG
1	H	30	LYS
1	H	62	LYS
1	H	123	ARG
1	H	127	HIS
1	H	165	ASP
1	I	23	ASP
1	I	27	ARG
1	I	62	LYS
1	I	123	ARG
1	I	127	HIS
1	I	165	ASP

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
1	J	23	ASP
1	J	62	LYS
1	J	123	ARG
1	J	127	HIS
1	J	162	LYS
1	J	165	ASP
1	K	62	LYS
1	K	123	ARG
1	K	127	HIS
1	K	165	ASP
1	K	201	SER
1	L	23	ASP
1	L	62	LYS
1	L	123	ARG
1	L	127	HIS
1	L	165	ASP
1	M	23	ASP
1	M	62	LYS
1	M	123	ARG
1	M	127	HIS
1	M	165	ASP
1	N	23	ASP
1	N	27	ARG
1	N	62	LYS
1	N	123	ARG
1	N	127	HIS
1	N	147	ARG
1	N	165	ASP
1	O	23	ASP
1	O	62	LYS
1	O	123	ARG
1	O	127	HIS
1	O	165	ASP
1	P	27	ARG
1	P	62	LYS
1	P	123	ARG
1	P	127	HIS
1	P	165	ASP
1	P	197	GLU
1	Q	23	ASP
1	Q	30	LYS
1	Q	62	LYS

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
1	Q	123	ARG
1	Q	127	HIS
1	Q	165	ASP
1	R	23	ASP
1	R	27	ARG
1	R	62	LYS
1	R	123	ARG
1	R	127	HIS
1	R	165	ASP
1	S	23	ASP
1	S	27	ARG
1	S	62	LYS
1	S	123	ARG
1	S	127	HIS
1	S	165	ASP
1	T	62	LYS
1	T	123	ARG
1	T	127	HIS
1	T	165	ASP
1	U	23	ASP
1	U	27	ARG
1	U	62	LYS
1	U	123	ARG
1	U	127	HIS
1	U	165	ASP
1	V	62	LYS
1	V	123	ARG
1	V	127	HIS
1	V	165	ASP
1	V	199	ARG
1	W	23	ASP
1	W	27	ARG
1	W	62	LYS
1	W	123	ARG
1	W	127	HIS
1	W	165	ASP
1	X	23	ASP
1	X	43	GLU
1	X	62	LYS
1	X	123	ARG
1	X	127	HIS
1	X	165	ASP

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
1	Y	62	LYS
1	Y	123	ARG
1	Y	127	HIS
1	Y	165	ASP
1	Z	23	ASP
1	Z	62	LYS
1	Z	127	HIS
1	Z	165	ASP
1	a	62	LYS
1	a	123	ARG
1	a	127	HIS
1	a	165	ASP
1	b	62	LYS
1	b	123	ARG
1	b	127	HIS
1	b	165	ASP

Some 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 [i](#)

There are no chain breaks in this entry.

## 6 Fit of model and data

### 6.1 Protein, DNA and RNA chains

EDS failed to run properly - this section is therefore empty.

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

EDS failed to run properly - this section is therefore empty.

### 6.3 Carbohydrates

EDS failed to run properly - this section is therefore empty.

### 6.4 Ligands

EDS failed to run properly - this section is therefore empty.

### 6.5 Other polymers

EDS failed to run properly - this section is therefore empty.