



wwPDB X-ray Structure Validation Summary Report ⓘ

Oct 2, 2023 – 02:21 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

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity : **FAILED**
Xtrriage (Phenix) : 1.13
EDS : **FAILED**
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) : 2.35.1

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.

There are no overall percentile quality scores available for this entry.

MolProbity and EDS failed to run properly - the sequence quality summary graphics cannot be shown.

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

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

3 Data and refinement statistics i

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

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α , β , γ	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
$\langle I/\sigma(I) \rangle$ ¹	1.97 (at 2.20Å)	Xtrriage
Refinement program	PHENIX (1.13_2998)	Depositor
R, R_{free}	0.214 , 0.245	Depositor
Wilson B-factor (Å ²)	31.8	Xtrriage
Anisotropy	0.555	Xtrriage
L-test for twinning ²	$\langle L \rangle = 0.47$, $\langle L^2 \rangle = 0.30$	Xtrriage
Estimated twinning fraction	0.469 for h,-k,-l 0.469 for -h,k,-l 0.470 for -h,-k,l	Xtrriage
Total number of atoms	39500	wwPDB-VP
Average B, all atoms (Å ²)	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.*

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.

4 Model quality [i](#)

4.1 Standard geometry [i](#)

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

4.2 Too-close contacts [i](#)

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

4.3 Torsion angles [i](#)

4.3.1 Protein backbone [i](#)

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

4.3.2 Protein sidechains [i](#)

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

4.3.3 RNA [i](#)

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

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

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

4.5 Carbohydrates [i](#)

There are no monosaccharides in this entry.

4.6 Ligand geometry [i](#)

There are no ligands in this entry.

4.7 Other polymers [i](#)

There are no such residues in this entry.

4.8 Polymer linkage issues

There are no chain breaks in this entry.

5 Fit of model and data [i](#)

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

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

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

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

5.3 Carbohydrates [i](#)

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

5.4 Ligands [i](#)

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

5.5 Other polymers [i](#)

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