



wwPDB X-ray Structure Validation Summary Report ⓘ

Oct 2, 2023 – 01:55 AM EDT

PDB ID : 6NAW
Title : Crystal structure of Neisseria meningitidis ClpP E58A activated mutant
Authors : Mabanglo, M.F.; Houry, W.A.
Deposited on : 2018-12-06
Resolution : 2.40 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 2.40 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 20353 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	177	1384	876	236	264	8	0	0	0
1	B	178	1392	882	237	265	8	0	0	0
1	C	175	1363	859	234	262	8	0	0	0
1	D	179	1396	884	238	266	8	0	0	0
1	E	177	1380	875	233	264	8	0	0	0
1	F	179	1396	884	238	266	8	0	0	0
1	G	183	1420	898	242	272	8	0	0	0
1	H	180	1399	884	239	268	8	0	0	0
1	I	178	1388	878	237	265	8	0	0	0
1	J	180	1399	884	239	268	8	0	0	0
1	K	183	1416	894	242	272	8	0	0	0
1	L	175	1363	859	234	262	8	0	0	0
1	M	178	1391	881	237	265	8	0	0	0
1	N	176	1371	865	235	263	8	0	0	0

There are 196 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-12	HIS	-	expression tag	UNP I4E574

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Chain	Residue	Modelled	Actual	Comment	Reference
A	-11	HIS	-	expression tag	UNP I4E574
A	-10	HIS	-	expression tag	UNP I4E574
A	-9	HIS	-	expression tag	UNP I4E574
A	-8	HIS	-	expression tag	UNP I4E574
A	-7	HIS	-	expression tag	UNP I4E574
A	-6	GLU	-	expression tag	UNP I4E574
A	-5	ASN	-	expression tag	UNP I4E574
A	-4	LEU	-	expression tag	UNP I4E574
A	-3	TYR	-	expression tag	UNP I4E574
A	-2	PHE	-	expression tag	UNP I4E574
A	-1	GLN	-	expression tag	UNP I4E574
A	0	GLY	-	expression tag	UNP I4E574
A	58	ALA	GLU	engineered mutation	UNP I4E574
B	-12	HIS	-	expression tag	UNP I4E574
B	-11	HIS	-	expression tag	UNP I4E574
B	-10	HIS	-	expression tag	UNP I4E574
B	-9	HIS	-	expression tag	UNP I4E574
B	-8	HIS	-	expression tag	UNP I4E574
B	-7	HIS	-	expression tag	UNP I4E574
B	-6	GLU	-	expression tag	UNP I4E574
B	-5	ASN	-	expression tag	UNP I4E574
B	-4	LEU	-	expression tag	UNP I4E574
B	-3	TYR	-	expression tag	UNP I4E574
B	-2	PHE	-	expression tag	UNP I4E574
B	-1	GLN	-	expression tag	UNP I4E574
B	0	GLY	-	expression tag	UNP I4E574
B	58	ALA	GLU	engineered mutation	UNP I4E574
C	-12	HIS	-	expression tag	UNP I4E574
C	-11	HIS	-	expression tag	UNP I4E574
C	-10	HIS	-	expression tag	UNP I4E574
C	-9	HIS	-	expression tag	UNP I4E574
C	-8	HIS	-	expression tag	UNP I4E574
C	-7	HIS	-	expression tag	UNP I4E574
C	-6	GLU	-	expression tag	UNP I4E574
C	-5	ASN	-	expression tag	UNP I4E574
C	-4	LEU	-	expression tag	UNP I4E574
C	-3	TYR	-	expression tag	UNP I4E574
C	-2	PHE	-	expression tag	UNP I4E574
C	-1	GLN	-	expression tag	UNP I4E574
C	0	GLY	-	expression tag	UNP I4E574
C	58	ALA	GLU	engineered mutation	UNP I4E574
D	-12	HIS	-	expression tag	UNP I4E574

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Chain	Residue	Modelled	Actual	Comment	Reference
D	-11	HIS	-	expression tag	UNP I4E574
D	-10	HIS	-	expression tag	UNP I4E574
D	-9	HIS	-	expression tag	UNP I4E574
D	-8	HIS	-	expression tag	UNP I4E574
D	-7	HIS	-	expression tag	UNP I4E574
D	-6	GLU	-	expression tag	UNP I4E574
D	-5	ASN	-	expression tag	UNP I4E574
D	-4	LEU	-	expression tag	UNP I4E574
D	-3	TYR	-	expression tag	UNP I4E574
D	-2	PHE	-	expression tag	UNP I4E574
D	-1	GLN	-	expression tag	UNP I4E574
D	0	GLY	-	expression tag	UNP I4E574
D	58	ALA	GLU	engineered mutation	UNP I4E574
E	-12	HIS	-	expression tag	UNP I4E574
E	-11	HIS	-	expression tag	UNP I4E574
E	-10	HIS	-	expression tag	UNP I4E574
E	-9	HIS	-	expression tag	UNP I4E574
E	-8	HIS	-	expression tag	UNP I4E574
E	-7	HIS	-	expression tag	UNP I4E574
E	-6	GLU	-	expression tag	UNP I4E574
E	-5	ASN	-	expression tag	UNP I4E574
E	-4	LEU	-	expression tag	UNP I4E574
E	-3	TYR	-	expression tag	UNP I4E574
E	-2	PHE	-	expression tag	UNP I4E574
E	-1	GLN	-	expression tag	UNP I4E574
E	0	GLY	-	expression tag	UNP I4E574
E	58	ALA	GLU	engineered mutation	UNP I4E574
F	-12	HIS	-	expression tag	UNP I4E574
F	-11	HIS	-	expression tag	UNP I4E574
F	-10	HIS	-	expression tag	UNP I4E574
F	-9	HIS	-	expression tag	UNP I4E574
F	-8	HIS	-	expression tag	UNP I4E574
F	-7	HIS	-	expression tag	UNP I4E574
F	-6	GLU	-	expression tag	UNP I4E574
F	-5	ASN	-	expression tag	UNP I4E574
F	-4	LEU	-	expression tag	UNP I4E574
F	-3	TYR	-	expression tag	UNP I4E574
F	-2	PHE	-	expression tag	UNP I4E574
F	-1	GLN	-	expression tag	UNP I4E574
F	0	GLY	-	expression tag	UNP I4E574
F	58	ALA	GLU	engineered mutation	UNP I4E574
G	-12	HIS	-	expression tag	UNP I4E574

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Chain	Residue	Modelled	Actual	Comment	Reference
G	-11	HIS	-	expression tag	UNP I4E574
G	-10	HIS	-	expression tag	UNP I4E574
G	-9	HIS	-	expression tag	UNP I4E574
G	-8	HIS	-	expression tag	UNP I4E574
G	-7	HIS	-	expression tag	UNP I4E574
G	-6	GLU	-	expression tag	UNP I4E574
G	-5	ASN	-	expression tag	UNP I4E574
G	-4	LEU	-	expression tag	UNP I4E574
G	-3	TYR	-	expression tag	UNP I4E574
G	-2	PHE	-	expression tag	UNP I4E574
G	-1	GLN	-	expression tag	UNP I4E574
G	0	GLY	-	expression tag	UNP I4E574
G	58	ALA	GLU	engineered mutation	UNP I4E574
H	-12	HIS	-	expression tag	UNP I4E574
H	-11	HIS	-	expression tag	UNP I4E574
H	-10	HIS	-	expression tag	UNP I4E574
H	-9	HIS	-	expression tag	UNP I4E574
H	-8	HIS	-	expression tag	UNP I4E574
H	-7	HIS	-	expression tag	UNP I4E574
H	-6	GLU	-	expression tag	UNP I4E574
H	-5	ASN	-	expression tag	UNP I4E574
H	-4	LEU	-	expression tag	UNP I4E574
H	-3	TYR	-	expression tag	UNP I4E574
H	-2	PHE	-	expression tag	UNP I4E574
H	-1	GLN	-	expression tag	UNP I4E574
H	0	GLY	-	expression tag	UNP I4E574
H	58	ALA	GLU	engineered mutation	UNP I4E574
I	-12	HIS	-	expression tag	UNP I4E574
I	-11	HIS	-	expression tag	UNP I4E574
I	-10	HIS	-	expression tag	UNP I4E574
I	-9	HIS	-	expression tag	UNP I4E574
I	-8	HIS	-	expression tag	UNP I4E574
I	-7	HIS	-	expression tag	UNP I4E574
I	-6	GLU	-	expression tag	UNP I4E574
I	-5	ASN	-	expression tag	UNP I4E574
I	-4	LEU	-	expression tag	UNP I4E574
I	-3	TYR	-	expression tag	UNP I4E574
I	-2	PHE	-	expression tag	UNP I4E574
I	-1	GLN	-	expression tag	UNP I4E574
I	0	GLY	-	expression tag	UNP I4E574
I	58	ALA	GLU	engineered mutation	UNP I4E574
J	-12	HIS	-	expression tag	UNP I4E574

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Chain	Residue	Modelled	Actual	Comment	Reference
J	-11	HIS	-	expression tag	UNP I4E574
J	-10	HIS	-	expression tag	UNP I4E574
J	-9	HIS	-	expression tag	UNP I4E574
J	-8	HIS	-	expression tag	UNP I4E574
J	-7	HIS	-	expression tag	UNP I4E574
J	-6	GLU	-	expression tag	UNP I4E574
J	-5	ASN	-	expression tag	UNP I4E574
J	-4	LEU	-	expression tag	UNP I4E574
J	-3	TYR	-	expression tag	UNP I4E574
J	-2	PHE	-	expression tag	UNP I4E574
J	-1	GLN	-	expression tag	UNP I4E574
J	0	GLY	-	expression tag	UNP I4E574
J	58	ALA	GLU	engineered mutation	UNP I4E574
K	-12	HIS	-	expression tag	UNP I4E574
K	-11	HIS	-	expression tag	UNP I4E574
K	-10	HIS	-	expression tag	UNP I4E574
K	-9	HIS	-	expression tag	UNP I4E574
K	-8	HIS	-	expression tag	UNP I4E574
K	-7	HIS	-	expression tag	UNP I4E574
K	-6	GLU	-	expression tag	UNP I4E574
K	-5	ASN	-	expression tag	UNP I4E574
K	-4	LEU	-	expression tag	UNP I4E574
K	-3	TYR	-	expression tag	UNP I4E574
K	-2	PHE	-	expression tag	UNP I4E574
K	-1	GLN	-	expression tag	UNP I4E574
K	0	GLY	-	expression tag	UNP I4E574
K	58	ALA	GLU	engineered mutation	UNP I4E574
L	-12	HIS	-	expression tag	UNP I4E574
L	-11	HIS	-	expression tag	UNP I4E574
L	-10	HIS	-	expression tag	UNP I4E574
L	-9	HIS	-	expression tag	UNP I4E574
L	-8	HIS	-	expression tag	UNP I4E574
L	-7	HIS	-	expression tag	UNP I4E574
L	-6	GLU	-	expression tag	UNP I4E574
L	-5	ASN	-	expression tag	UNP I4E574
L	-4	LEU	-	expression tag	UNP I4E574
L	-3	TYR	-	expression tag	UNP I4E574
L	-2	PHE	-	expression tag	UNP I4E574
L	-1	GLN	-	expression tag	UNP I4E574
L	0	GLY	-	expression tag	UNP I4E574
L	58	ALA	GLU	engineered mutation	UNP I4E574
M	-12	HIS	-	expression tag	UNP I4E574

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Chain	Residue	Modelled	Actual	Comment	Reference
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M	-10	HIS	-	expression tag	UNP I4E574
M	-9	HIS	-	expression tag	UNP I4E574
M	-8	HIS	-	expression tag	UNP I4E574
M	-7	HIS	-	expression tag	UNP I4E574
M	-6	GLU	-	expression tag	UNP I4E574
M	-5	ASN	-	expression tag	UNP I4E574
M	-4	LEU	-	expression tag	UNP I4E574
M	-3	TYR	-	expression tag	UNP I4E574
M	-2	PHE	-	expression tag	UNP I4E574
M	-1	GLN	-	expression tag	UNP I4E574
M	0	GLY	-	expression tag	UNP I4E574
M	58	ALA	GLU	engineered mutation	UNP I4E574
N	-12	HIS	-	expression tag	UNP I4E574
N	-11	HIS	-	expression tag	UNP I4E574
N	-10	HIS	-	expression tag	UNP I4E574
N	-9	HIS	-	expression tag	UNP I4E574
N	-8	HIS	-	expression tag	UNP I4E574
N	-7	HIS	-	expression tag	UNP I4E574
N	-6	GLU	-	expression tag	UNP I4E574
N	-5	ASN	-	expression tag	UNP I4E574
N	-4	LEU	-	expression tag	UNP I4E574
N	-3	TYR	-	expression tag	UNP I4E574
N	-2	PHE	-	expression tag	UNP I4E574
N	-1	GLN	-	expression tag	UNP I4E574
N	0	GLY	-	expression tag	UNP I4E574
N	58	ALA	GLU	engineered mutation	UNP I4E574

- Molecule 2 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	64	Total O 64 64	0	0
2	B	74	Total O 74 74	0	0
2	C	65	Total O 65 65	0	0
2	D	56	Total O 56 56	0	0
2	E	53	Total O 53 53	0	0
2	F	75	Total O 75 75	0	0

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	G	61	Total O 61 61	0	0
2	H	64	Total O 64 64	0	0
2	I	58	Total O 58 58	0	0
2	J	58	Total O 58 58	0	0
2	K	75	Total O 75 75	0	0
2	L	65	Total O 65 65	0	0
2	M	55	Total O 55 55	0	0
2	N	72	Total O 72 72	0	0

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 21 1	Depositor
Cell constants a, b, c, α , β , γ	98.12Å 119.36Å 127.64Å 90.00° 89.99° 90.00°	Depositor
Resolution (Å)	42.76 – 2.40	Depositor
% Data completeness (in resolution range)	99.8 (42.76-2.40)	Depositor
R_{merge}	0.17	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.79 (at 2.39Å)	Xtrriage
Refinement program	PHENIX (1.13_2998)	Depositor
R, R_{free}	0.193 , 0.252	Depositor
Wilson B-factor (Å ²)	29.9	Xtrriage
Anisotropy	0.580	Xtrriage
L-test for twinning ²	$\langle L \rangle = 0.51$, $\langle L^2 \rangle = 0.35$	Xtrriage
Estimated twinning fraction	0.469 for h,-k,-l	Xtrriage
Total number of atoms	20353	wwPDB-VP
Average B, all atoms (Å ²)	36.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.54% of the height of the origin peak. No significant pseudotranslation is detected.*

¹ Intensities estimated from amplitudes.

² 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.

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.