wwPDB X-ray Structure Validation Summary Report (i)

Oct 2, 2023 – 08:05 AM EDT

PDB ID	:	6NAQ
Title	:	Crystal structure of Neisseria meningitidis ClpP protease in Apo form
Authors	:	Houry, W.A.; Mabanglo, M.F.; Pai, E.F.; Eger, B.T.; Bryson, S.
Deposited on	:	2018-12-06
Resolution	:	2.02 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 (i) 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 (i)) were used in the production of this report:

MolProbity	:	FAILED
Xtriage (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 2.02 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 3 unique types of molecules in this entry. The entry contains 20681 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	184	Total	C	N	O	S	0	0	0
			1428	902	243	275	8			
1	B	183	Total	C	N	O	S	0	0	0
			1422	899	242	273	8			
1	C	182	Total	C	N	O	S	0	0	0
			1415	894	241	272	8			
1	D	183	Total	C	N	O	S	0	0	0
			1422	899	242	273	8			
1	E	184	Total	C	N	O	S	0	0	0
			1430	905	243	274	8			
1	F	183	Total	C	N	O	S	0	0	0
			1422	899	242	273	8			
1	G	187	Total	C	N	O	S	0	0	0
			1456	920	249	279	8			
1	H	187	Total	C	N	O	S	0	0	0
			1455	920	249	278	8			
1	I	185	Total	C	N	O	S	0	0	0
			1436	908	244	276	8			
1	J	186	Total	C	N	O	S	0	0	0
			1448	915	248	277	8			
1	K	184	Total	C	N	O	S	0	0	0
			1428	902	243	275	8			
1	L	183	Total	C	N	O	S	0	0	0
			1423	900	242	273	8			
1	M	183	Total	C	N	O	S	0	0	0
			1421	897	242	274	8			
1	N	184	Total	C	N	O	S	0	0	0
			1428	902	243	275	8			

There are 196 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-13	HIS	-	expression tag	UNP I4E574

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Chain	Residue	Modelled	Actual	Comment	Reference
A	-12	HIS	-	expression tag	UNP I4E574
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	GLU	-	expression tag	UNP I4E574
A	-6	ASN	-	expression tag	UNP I4E574
A	-5	LEU	-	expression tag	UNP I4E574
A	-4	TYR	-	expression tag	UNP I4E574
A	-3	PHE	-	expression tag	UNP I4E574
A	-2	GLN	-	expression tag	UNP I4E574
A	-1	SER	-	expression tag	UNP I4E574
A	0	ASN	-	expression tag	UNP I4E574
B	-13	HIS	-	expression tag	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	GLU	-	expression tag	UNP I4E574
B	-6	ASN	-	expression tag	UNP I4E574
B	-5	LEU	-	expression tag	UNP I4E574
B	-4	TYR	-	expression tag	UNP I4E574
B	-3	PHE	-	expression tag	UNP I4E574
B	-2	GLN	-	expression tag	UNP I4E574
B	-1	SER	-	expression tag	UNP I4E574
B	0	ASN	-	expression tag	UNP I4E574
C	-13	HIS	-	expression tag	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	GLU	-	expression tag	UNP I4E574
C	-6	ASN	-	expression tag	UNP I4E574
C	-5	LEU	-	expression tag	UNP I4E574
C	-4	TYR	-	expression tag	UNP I4E574
C	-3	PHE	-	expression tag	UNP I4E574
C	-2	GLN	-	expression tag	UNP I4E574
C	-1	SER	-	expression tag	UNP I4E574
C	0	ASN	-	expression tag	UNP I4E574
D	-13	HIS	-	expression tag	UNP I4E574

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Chain	Residue	Modelled	Actual	Comment	Reference
D	-12	HIS	-	expression tag	UNP I4E574
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	GLU	-	expression tag	UNP I4E574
D	-6	ASN	-	expression tag	UNP I4E574
D	-5	LEU	-	expression tag	UNP I4E574
D	-4	TYR	-	expression tag	UNP I4E574
D	-3	PHE	-	expression tag	UNP I4E574
D	-2	GLN	-	expression tag	UNP I4E574
D	-1	SER	-	expression tag	UNP I4E574
D	0	ASN	-	expression tag	UNP I4E574
E	-13	HIS	-	expression tag	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	GLU	-	expression tag	UNP I4E574
E	-6	ASN	-	expression tag	UNP I4E574
E	-5	LEU	-	expression tag	UNP I4E574
E	-4	TYR	-	expression tag	UNP I4E574
E	-3	PHE	-	expression tag	UNP I4E574
E	-2	GLN	-	expression tag	UNP I4E574
E	-1	SER	-	expression tag	UNP I4E574
E	0	ASN	-	expression tag	UNP I4E574
F	-13	HIS	-	expression tag	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	GLU	-	expression tag	UNP I4E574
F	-6	ASN	-	expression tag	UNP I4E574
F	-5	LEU	-	expression tag	UNP I4E574
F	-4	TYR	-	expression tag	UNP I4E574
F	-3	PHE	-	expression tag	UNP I4E574
F	-2	GLN	-	expression tag	UNP I4E574
F	-1	SER	-	expression tag	UNP I4E574
F	0	ASN	-	expression tag	UNP I4E574
G	-13	HIS	-	expression tag	UNP I4E574

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Chain	Residue	Modelled	Actual	Comment	Reference
G	-12	HIS	-	expression tag	UNP I4E574
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	GLU	-	expression tag	UNP I4E574
G	-6	ASN	-	expression tag	UNP I4E574
G	-5	LEU	-	expression tag	UNP I4E574
G	-4	TYR	-	expression tag	UNP I4E574
G	-3	PHE	-	expression tag	UNP I4E574
G	-2	GLN	-	expression tag	UNP I4E574
G	-1	SER	-	expression tag	UNP I4E574
G	0	ASN	-	expression tag	UNP I4E574
H	-13	HIS	-	expression tag	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	GLU	-	expression tag	UNP I4E574
H	-6	ASN	-	expression tag	UNP I4E574
H	-5	LEU	-	expression tag	UNP I4E574
H	-4	TYR	-	expression tag	UNP I4E574
H	-3	PHE	-	expression tag	UNP I4E574
H	-2	GLN	-	expression tag	UNP I4E574
H	-1	SER	-	expression tag	UNP I4E574
H	0	ASN	-	expression tag	UNP I4E574
I	-13	HIS	-	expression tag	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	GLU	-	expression tag	UNP I4E574
I	-6	ASN	-	expression tag	UNP I4E574
I	-5	LEU	-	expression tag	UNP I4E574
I	-4	TYR	-	expression tag	UNP I4E574
I	-3	PHE	-	expression tag	UNP I4E574
I	-2	GLN	-	expression tag	UNP I4E574
I	-1	SER	-	expression tag	UNP I4E574
I	0	ASN	-	expression tag	UNP I4E574
J	-13	HIS	-	expression tag	UNP I4E574

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Chain	Residue	Modelled	Actual	Comment	Reference
J	-12	HIS	-	expression tag	UNP I4E574
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	GLU	-	expression tag	UNP I4E574
J	-6	ASN	-	expression tag	UNP I4E574
J	-5	LEU	-	expression tag	UNP I4E574
J	-4	TYR	-	expression tag	UNP I4E574
J	-3	PHE	-	expression tag	UNP I4E574
J	-2	GLN	-	expression tag	UNP I4E574
J	-1	SER	-	expression tag	UNP I4E574
J	0	ASN	-	expression tag	UNP I4E574
K	-13	HIS	-	expression tag	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	GLU	-	expression tag	UNP I4E574
K	-6	ASN	-	expression tag	UNP I4E574
K	-5	LEU	-	expression tag	UNP I4E574
K	-4	TYR	-	expression tag	UNP I4E574
K	-3	PHE	-	expression tag	UNP I4E574
K	-2	GLN	-	expression tag	UNP I4E574
K	-1	SER	-	expression tag	UNP I4E574
K	0	ASN	-	expression tag	UNP I4E574
L	-13	HIS	-	expression tag	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	GLU	-	expression tag	UNP I4E574
L	-6	ASN	-	expression tag	UNP I4E574
L	-5	LEU	-	expression tag	UNP I4E574
L	-4	TYR	-	expression tag	UNP I4E574
L	-3	PHE	-	expression tag	UNP I4E574
L	-2	GLN	-	expression tag	UNP I4E574
L	-1	SER	-	expression tag	UNP I4E574
L	0	ASN	-	expression tag	UNP I4E574
M	-13	HIS	-	expression tag	UNP I4E574

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Chain	Residue	Modelled	Actual	Comment	Reference
M	-12	HIS	-	expression tag	UNP I4E574
M	-11	HIS	-	expression tag	UNP I4E574
M	-10	HIS	-	expression tag	UNP I4E574
M	-9	HIS	-	expression tag	UNP I4E574
M	-8	HIS	-	expression tag	UNP I4E574
M	-7	GLU	-	expression tag	UNP I4E574
M	-6	ASN	-	expression tag	UNP I4E574
M	-5	LEU	-	expression tag	UNP I4E574
M	-4	TYR	-	expression tag	UNP I4E574
M	-3	PHE	-	expression tag	UNP I4E574
M	-2	GLN	-	expression tag	UNP I4E574
M	-1	SER	-	expression tag	UNP I4E574
M	0	ASN	-	expression tag	UNP I4E574
N	-13	HIS	-	expression tag	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	GLU	-	expression tag	UNP I4E574
N	-6	ASN	-	expression tag	UNP I4E574
N	-5	LEU	-	expression tag	UNP I4E574
N	-4	TYR	-	expression tag	UNP I4E574
N	-3	PHE	-	expression tag	UNP I4E574
N	-2	GLN	-	expression tag	UNP I4E574
N	-1	SER	-	expression tag	UNP I4E574
N	0	ASN	-	expression tag	UNP I4E574

- Molecule 2 is POTASSIUM ION (three-letter code: K) (formula: K).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	1	Total 1	K 1	0	0
2	B	1	Total 1	K 1	0	0
2	C	1	Total 1	K 1	0	0
2	D	1	Total 1	K 1	0	0
2	E	1	Total 1	K 1	0	0
2	F	1	Total 1	K 1	0	0

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	G	1	Total 1	K 1	0	0
2	H	1	Total 1	K 1	0	0
2	I	1	Total 1	K 1	0	0
2	J	1	Total 1	K 1	0	0
2	K	1	Total 1	K 1	0	0
2	L	1	Total 1	K 1	0	0
2	M	1	Total 1	K 1	0	0
2	N	1	Total 1	K 1	0	0

- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	55	Total 55	O 55	0	0
3	B	54	Total 54	O 54	0	0
3	C	45	Total 45	O 45	0	0
3	D	43	Total 43	O 43	0	0
3	E	31	Total 31	O 31	0	0
3	F	37	Total 37	O 37	0	0
3	G	51	Total 51	O 51	0	0
3	H	32	Total 32	O 32	0	0
3	I	29	Total 29	O 29	0	0
3	J	44	Total 44	O 44	0	0
3	K	48	Total 48	O 48	0	0

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	L	54	Total 54	O 54	0	0
3	M	58	Total 58	O 58	0	0
3	N	52	Total 52	O 52	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	98.58Å 127.94Å 120.19Å 90.00° 90.19° 90.00°	Depositor
Resolution (Å)	51.39 – 2.02	Depositor
% Data completeness (in resolution range)	97.7 (51.39-2.02)	Depositor
R_{merge}	0.10	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.76 (at 2.01Å)	Xtriage
Refinement program	PHENIX 1.8.4_1496	Depositor
R, R_{free}	0.207 , 0.246	Depositor
Wilson B-factor (Å^2)	19.3	Xtriage
Anisotropy	0.936	Xtriage
L-test for twinning[2]	$< |L| > = 0.44, < L^2 > = 0.26$	Xtriage
Estimated twinning fraction	0.370 for h,-k,-l	Xtriage
Total number of atoms	20681	wwPDB-VP
Average B, all atoms (Å^2)	25.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.74% of the height of the origin peak. No significant pseudotranslation is detected.*

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[1]Intensities estimated from amplitudes.

[2]Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

4 Model quality ⓘ

4.1 Standard geometry ⓘ

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

4.2 Too-close contacts ⓘ

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

4.3 Torsion angles ⓘ

4.3.1 Protein backbone ⓘ

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

4.3.2 Protein sidechains ⓘ

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

4.3.3 RNA ⓘ

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

4.4 Non-standard residues in protein, DNA, RNA chains ⓘ

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

4.5 Carbohydrates ⓘ

There are no monosaccharides in this entry.

4.6 Ligand geometry ⓘ

Of 14 ligands modelled in this entry, 14 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

4.7 Other polymers ⓘ

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 ⓘ

5.1 Protein, DNA and RNA chains ⓘ

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

5.2 Non-standard residues in protein, DNA, RNA chains ⓘ

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

5.3 Carbohydrates ⓘ

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

5.4 Ligands ⓘ

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

5.5 Other polymers ⓘ

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