



wwPDB X-ray Structure Validation Summary Report ⓘ

Aug 26, 2025 – 02:12 PM EDT

PDB ID : 9MK5 / pdb_00009mk5
Title : Crystal structure of Neisseria meningitidis ClpP protease complex with small molecule activator, Diocatin
Authors : Mabanglo, M.F.; Houry, W.A.
Deposited on : 2024-12-16
Resolution : 1.90 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	:	4-5-2 with Phenix2.0rc1
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0rc1
EDS	:	3.0
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20231227.v01 (using entries in the PDB archive December 27th 2023)
CCP4	:	9.0.006 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.45.1

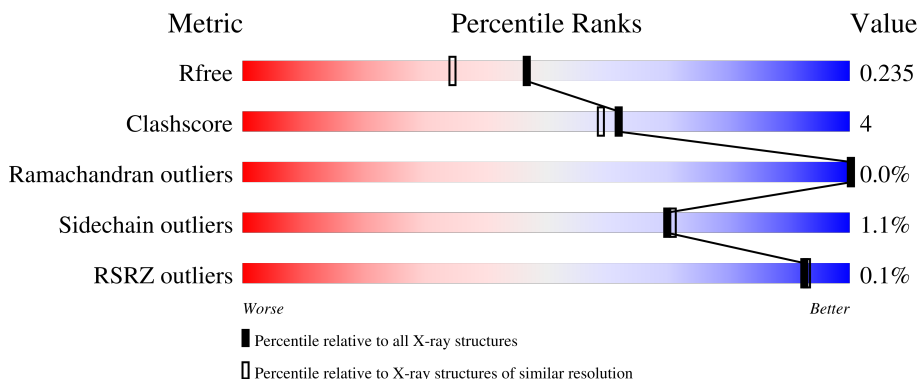
1 Overall quality at a glance ⓘ

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.90 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.











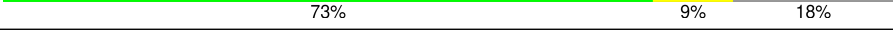
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	164625	7293 (1.90-1.90)
Clashscore	180529	8090 (1.90-1.90)
Ramachandran outliers	177936	8022 (1.90-1.90)
Sidechain outliers	177891	8022 (1.90-1.90)
RSRZ outliers	164620	7292 (1.90-1.90)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	218	<div> <div>75%</div> <div>9%</div> <div>16%</div> </div>
1	B	218	<div> <div>76%</div> <div>9%</div> <div>15%</div> </div>
1	C	218	<div> <div>73%</div> <div>10%</div> <div>17%</div> </div>
1	D	218	<div> <div>76%</div> <div>7%</div> <div>17%</div> </div>
1	E	218	<div> <div>75%</div> <div>8%</div> <div>17%</div> </div>

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Mol	Chain	Length	Quality of chain
1	F	218	 73%12%14%
1	G	218	 74%11%16%
1	H	218	 76%6%17%
1	I	218	 78%7%15%
1	J	218	 78%6%16%
1	K	218	 76%7%16%
1	L	218	 72%10%18%
1	M	218	 75%9%17%
1	N	218	 73%9%18%

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 20870 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	183	Total	C	N	O	S	0	0	0
			1426	903	242	273	8			
1	B	185	Total	C	N	O	S	0	0	0
			1440	912	244	276	8			
1	C	181	Total	C	N	O	S	0	0	0
			1408	889	240	271	8			
1	D	182	Total	C	N	O	S	0	0	0
			1415	894	241	272	8			
1	E	182	Total	C	N	O	S	0	0	0
			1420	898	241	273	8			
1	F	187	Total	C	N	O	S	0	0	0
			1459	924	249	278	8			
1	G	184	Total	C	N	O	S	0	0	0
			1432	906	243	275	8			
1	H	181	Total	C	N	O	S	0	0	0
			1409	889	240	272	8			
1	I	185	Total	C	N	O	S	0	0	0
			1441	913	244	276	8			
1	J	183	Total	C	N	O	S	0	0	0
			1428	904	242	274	8			
1	K	184	Total	C	N	O	S	0	0	0
			1439	910	246	275	8			
1	L	179	Total	C	N	O	S	0	0	0
			1400	882	241	269	8			
1	M	182	Total	C	N	O	S	0	0	0
			1418	897	241	272	8			
1	N	178	Total	C	N	O	S	0	0	0
			1385	872	237	268	8			

There are 196 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-13	HIS	-	expression tag	UNP Q9JZ38

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Chain	Residue	Modelled	Actual	Comment	Reference
A	-12	HIS	-	expression tag	UNP Q9JZ38
A	-11	HIS	-	expression tag	UNP Q9JZ38
A	-10	HIS	-	expression tag	UNP Q9JZ38
A	-9	HIS	-	expression tag	UNP Q9JZ38
A	-8	HIS	-	expression tag	UNP Q9JZ38
A	-7	GLU	-	expression tag	UNP Q9JZ38
A	-6	ASN	-	expression tag	UNP Q9JZ38
A	-5	LEU	-	expression tag	UNP Q9JZ38
A	-4	TYR	-	expression tag	UNP Q9JZ38
A	-3	PHE	-	expression tag	UNP Q9JZ38
A	-2	GLN	-	expression tag	UNP Q9JZ38
A	-1	SER	-	expression tag	UNP Q9JZ38
A	0	ASN	-	expression tag	UNP Q9JZ38
B	-13	HIS	-	expression tag	UNP Q9JZ38
B	-12	HIS	-	expression tag	UNP Q9JZ38
B	-11	HIS	-	expression tag	UNP Q9JZ38
B	-10	HIS	-	expression tag	UNP Q9JZ38
B	-9	HIS	-	expression tag	UNP Q9JZ38
B	-8	HIS	-	expression tag	UNP Q9JZ38
B	-7	GLU	-	expression tag	UNP Q9JZ38
B	-6	ASN	-	expression tag	UNP Q9JZ38
B	-5	LEU	-	expression tag	UNP Q9JZ38
B	-4	TYR	-	expression tag	UNP Q9JZ38
B	-3	PHE	-	expression tag	UNP Q9JZ38
B	-2	GLN	-	expression tag	UNP Q9JZ38
B	-1	SER	-	expression tag	UNP Q9JZ38
B	0	ASN	-	expression tag	UNP Q9JZ38
C	-13	HIS	-	expression tag	UNP Q9JZ38
C	-12	HIS	-	expression tag	UNP Q9JZ38
C	-11	HIS	-	expression tag	UNP Q9JZ38
C	-10	HIS	-	expression tag	UNP Q9JZ38
C	-9	HIS	-	expression tag	UNP Q9JZ38
C	-8	HIS	-	expression tag	UNP Q9JZ38
C	-7	GLU	-	expression tag	UNP Q9JZ38
C	-6	ASN	-	expression tag	UNP Q9JZ38
C	-5	LEU	-	expression tag	UNP Q9JZ38
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C	-3	PHE	-	expression tag	UNP Q9JZ38
C	-2	GLN	-	expression tag	UNP Q9JZ38
C	-1	SER	-	expression tag	UNP Q9JZ38
C	0	ASN	-	expression tag	UNP Q9JZ38
D	-13	HIS	-	expression tag	UNP Q9JZ38

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Chain	Residue	Modelled	Actual	Comment	Reference
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D	-11	HIS	-	expression tag	UNP Q9JZ38
D	-10	HIS	-	expression tag	UNP Q9JZ38
D	-9	HIS	-	expression tag	UNP Q9JZ38
D	-8	HIS	-	expression tag	UNP Q9JZ38
D	-7	GLU	-	expression tag	UNP Q9JZ38
D	-6	ASN	-	expression tag	UNP Q9JZ38
D	-5	LEU	-	expression tag	UNP Q9JZ38
D	-4	TYR	-	expression tag	UNP Q9JZ38
D	-3	PHE	-	expression tag	UNP Q9JZ38
D	-2	GLN	-	expression tag	UNP Q9JZ38
D	-1	SER	-	expression tag	UNP Q9JZ38
D	0	ASN	-	expression tag	UNP Q9JZ38
E	-13	HIS	-	expression tag	UNP Q9JZ38
E	-12	HIS	-	expression tag	UNP Q9JZ38
E	-11	HIS	-	expression tag	UNP Q9JZ38
E	-10	HIS	-	expression tag	UNP Q9JZ38
E	-9	HIS	-	expression tag	UNP Q9JZ38
E	-8	HIS	-	expression tag	UNP Q9JZ38
E	-7	GLU	-	expression tag	UNP Q9JZ38
E	-6	ASN	-	expression tag	UNP Q9JZ38
E	-5	LEU	-	expression tag	UNP Q9JZ38
E	-4	TYR	-	expression tag	UNP Q9JZ38
E	-3	PHE	-	expression tag	UNP Q9JZ38
E	-2	GLN	-	expression tag	UNP Q9JZ38
E	-1	SER	-	expression tag	UNP Q9JZ38
E	0	ASN	-	expression tag	UNP Q9JZ38
F	-13	HIS	-	expression tag	UNP Q9JZ38
F	-12	HIS	-	expression tag	UNP Q9JZ38
F	-11	HIS	-	expression tag	UNP Q9JZ38
F	-10	HIS	-	expression tag	UNP Q9JZ38
F	-9	HIS	-	expression tag	UNP Q9JZ38
F	-8	HIS	-	expression tag	UNP Q9JZ38
F	-7	GLU	-	expression tag	UNP Q9JZ38
F	-6	ASN	-	expression tag	UNP Q9JZ38
F	-5	LEU	-	expression tag	UNP Q9JZ38
F	-4	TYR	-	expression tag	UNP Q9JZ38
F	-3	PHE	-	expression tag	UNP Q9JZ38
F	-2	GLN	-	expression tag	UNP Q9JZ38
F	-1	SER	-	expression tag	UNP Q9JZ38
F	0	ASN	-	expression tag	UNP Q9JZ38
G	-13	HIS	-	expression tag	UNP Q9JZ38

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Chain	Residue	Modelled	Actual	Comment	Reference
G	-12	HIS	-	expression tag	UNP Q9JZ38
G	-11	HIS	-	expression tag	UNP Q9JZ38
G	-10	HIS	-	expression tag	UNP Q9JZ38
G	-9	HIS	-	expression tag	UNP Q9JZ38
G	-8	HIS	-	expression tag	UNP Q9JZ38
G	-7	GLU	-	expression tag	UNP Q9JZ38
G	-6	ASN	-	expression tag	UNP Q9JZ38
G	-5	LEU	-	expression tag	UNP Q9JZ38
G	-4	TYR	-	expression tag	UNP Q9JZ38
G	-3	PHE	-	expression tag	UNP Q9JZ38
G	-2	GLN	-	expression tag	UNP Q9JZ38
G	-1	SER	-	expression tag	UNP Q9JZ38
G	0	ASN	-	expression tag	UNP Q9JZ38
H	-13	HIS	-	expression tag	UNP Q9JZ38
H	-12	HIS	-	expression tag	UNP Q9JZ38
H	-11	HIS	-	expression tag	UNP Q9JZ38
H	-10	HIS	-	expression tag	UNP Q9JZ38
H	-9	HIS	-	expression tag	UNP Q9JZ38
H	-8	HIS	-	expression tag	UNP Q9JZ38
H	-7	GLU	-	expression tag	UNP Q9JZ38
H	-6	ASN	-	expression tag	UNP Q9JZ38
H	-5	LEU	-	expression tag	UNP Q9JZ38
H	-4	TYR	-	expression tag	UNP Q9JZ38
H	-3	PHE	-	expression tag	UNP Q9JZ38
H	-2	GLN	-	expression tag	UNP Q9JZ38
H	-1	SER	-	expression tag	UNP Q9JZ38
H	0	ASN	-	expression tag	UNP Q9JZ38
I	-13	HIS	-	expression tag	UNP Q9JZ38
I	-12	HIS	-	expression tag	UNP Q9JZ38
I	-11	HIS	-	expression tag	UNP Q9JZ38
I	-10	HIS	-	expression tag	UNP Q9JZ38
I	-9	HIS	-	expression tag	UNP Q9JZ38
I	-8	HIS	-	expression tag	UNP Q9JZ38
I	-7	GLU	-	expression tag	UNP Q9JZ38
I	-6	ASN	-	expression tag	UNP Q9JZ38
I	-5	LEU	-	expression tag	UNP Q9JZ38
I	-4	TYR	-	expression tag	UNP Q9JZ38
I	-3	PHE	-	expression tag	UNP Q9JZ38
I	-2	GLN	-	expression tag	UNP Q9JZ38
I	-1	SER	-	expression tag	UNP Q9JZ38
I	0	ASN	-	expression tag	UNP Q9JZ38
J	-13	HIS	-	expression tag	UNP Q9JZ38

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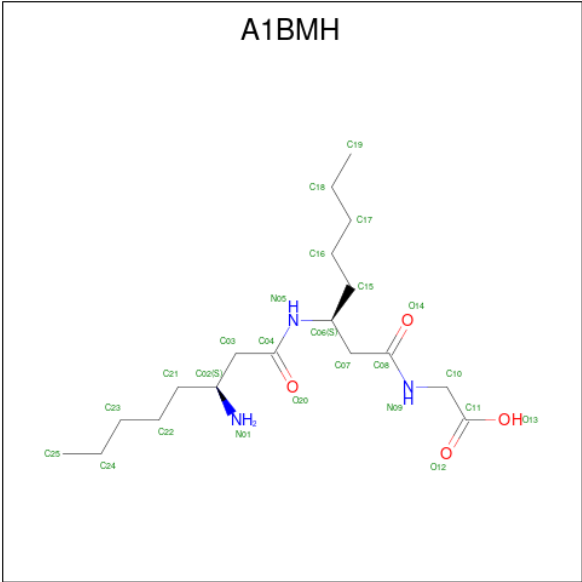
Chain	Residue	Modelled	Actual	Comment	Reference
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J	-11	HIS	-	expression tag	UNP Q9JZ38
J	-10	HIS	-	expression tag	UNP Q9JZ38
J	-9	HIS	-	expression tag	UNP Q9JZ38
J	-8	HIS	-	expression tag	UNP Q9JZ38
J	-7	GLU	-	expression tag	UNP Q9JZ38
J	-6	ASN	-	expression tag	UNP Q9JZ38
J	-5	LEU	-	expression tag	UNP Q9JZ38
J	-4	TYR	-	expression tag	UNP Q9JZ38
J	-3	PHE	-	expression tag	UNP Q9JZ38
J	-2	GLN	-	expression tag	UNP Q9JZ38
J	-1	SER	-	expression tag	UNP Q9JZ38
J	0	ASN	-	expression tag	UNP Q9JZ38
K	-13	HIS	-	expression tag	UNP Q9JZ38
K	-12	HIS	-	expression tag	UNP Q9JZ38
K	-11	HIS	-	expression tag	UNP Q9JZ38
K	-10	HIS	-	expression tag	UNP Q9JZ38
K	-9	HIS	-	expression tag	UNP Q9JZ38
K	-8	HIS	-	expression tag	UNP Q9JZ38
K	-7	GLU	-	expression tag	UNP Q9JZ38
K	-6	ASN	-	expression tag	UNP Q9JZ38
K	-5	LEU	-	expression tag	UNP Q9JZ38
K	-4	TYR	-	expression tag	UNP Q9JZ38
K	-3	PHE	-	expression tag	UNP Q9JZ38
K	-2	GLN	-	expression tag	UNP Q9JZ38
K	-1	SER	-	expression tag	UNP Q9JZ38
K	0	ASN	-	expression tag	UNP Q9JZ38
L	-13	HIS	-	expression tag	UNP Q9JZ38
L	-12	HIS	-	expression tag	UNP Q9JZ38
L	-11	HIS	-	expression tag	UNP Q9JZ38
L	-10	HIS	-	expression tag	UNP Q9JZ38
L	-9	HIS	-	expression tag	UNP Q9JZ38
L	-8	HIS	-	expression tag	UNP Q9JZ38
L	-7	GLU	-	expression tag	UNP Q9JZ38
L	-6	ASN	-	expression tag	UNP Q9JZ38
L	-5	LEU	-	expression tag	UNP Q9JZ38
L	-4	TYR	-	expression tag	UNP Q9JZ38
L	-3	PHE	-	expression tag	UNP Q9JZ38
L	-2	GLN	-	expression tag	UNP Q9JZ38
L	-1	SER	-	expression tag	UNP Q9JZ38
L	0	ASN	-	expression tag	UNP Q9JZ38
M	-13	HIS	-	expression tag	UNP Q9JZ38

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Chain	Residue	Modelled	Actual	Comment	Reference
M	-12	HIS	-	expression tag	UNP Q9JZ38
M	-11	HIS	-	expression tag	UNP Q9JZ38
M	-10	HIS	-	expression tag	UNP Q9JZ38
M	-9	HIS	-	expression tag	UNP Q9JZ38
M	-8	HIS	-	expression tag	UNP Q9JZ38
M	-7	GLU	-	expression tag	UNP Q9JZ38
M	-6	ASN	-	expression tag	UNP Q9JZ38
M	-5	LEU	-	expression tag	UNP Q9JZ38
M	-4	TYR	-	expression tag	UNP Q9JZ38
M	-3	PHE	-	expression tag	UNP Q9JZ38
M	-2	GLN	-	expression tag	UNP Q9JZ38
M	-1	SER	-	expression tag	UNP Q9JZ38
M	0	ASN	-	expression tag	UNP Q9JZ38
N	-13	HIS	-	expression tag	UNP Q9JZ38
N	-12	HIS	-	expression tag	UNP Q9JZ38
N	-11	HIS	-	expression tag	UNP Q9JZ38
N	-10	HIS	-	expression tag	UNP Q9JZ38
N	-9	HIS	-	expression tag	UNP Q9JZ38
N	-8	HIS	-	expression tag	UNP Q9JZ38
N	-7	GLU	-	expression tag	UNP Q9JZ38
N	-6	ASN	-	expression tag	UNP Q9JZ38
N	-5	LEU	-	expression tag	UNP Q9JZ38
N	-4	TYR	-	expression tag	UNP Q9JZ38
N	-3	PHE	-	expression tag	UNP Q9JZ38
N	-2	GLN	-	expression tag	UNP Q9JZ38
N	-1	SER	-	expression tag	UNP Q9JZ38
N	0	ASN	-	expression tag	UNP Q9JZ38

- Molecule 2 is N-{(3S)-3-[(3S)-3-aminooctanamido]octanoyl}glycine (CCD ID: A1BMH) (formula: C₁₈H₃₅N₃O₄).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	1	Total	C	N	O	0	0
			25	18	3	4		
2	B	1	Total	C	N	O	0	0
			25	18	3	4		
2	C	1	Total	C	N	O	0	0
			25	18	3	4		
2	F	1	Total	C	N	O	0	0
			25	18	3	4		
2	K	1	Total	C	N	O	0	0
			25	18	3	4		

- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	49	Total	O	0	0
			49	49		
3	B	68	Total	O	0	0
			68	68		
3	C	63	Total	O	0	0
			63	63		
3	D	57	Total	O	0	0
			57	57		
3	E	52	Total	O	0	0
			52	52		
3	F	74	Total	O	0	0
			74	74		
3	G	52	Total	O	0	0
			52	52		

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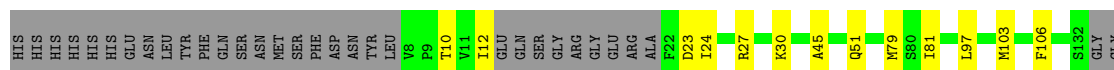
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	H	60	Total 60	O 60	0	0
3	I	60	Total 60	O 60	0	0
3	J	50	Total 50	O 50	0	0
3	K	59	Total 59	O 59	0	0
3	L	59	Total 59	O 59	0	0
3	M	60	Total 60	O 60	0	0
3	N	62	Total 62	O 62	0	0



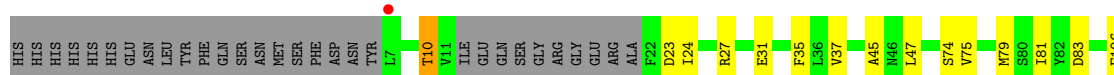
- Molecule 1: ATP-dependent Clp protease proteolytic subunit

Chain E: 75% 8% 17%



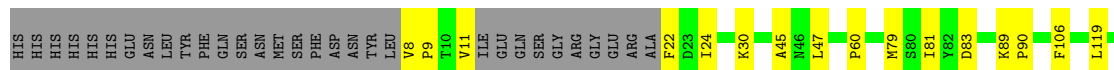
- Molecule 1: ATP-dependent Clp protease proteolytic subunit

Chain F: 73% 12% 14%



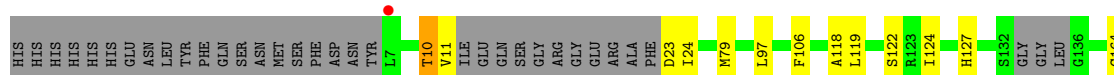
- Molecule 1: ATP-dependent Clp protease proteolytic subunit

Chain G: 74% 11% 16%



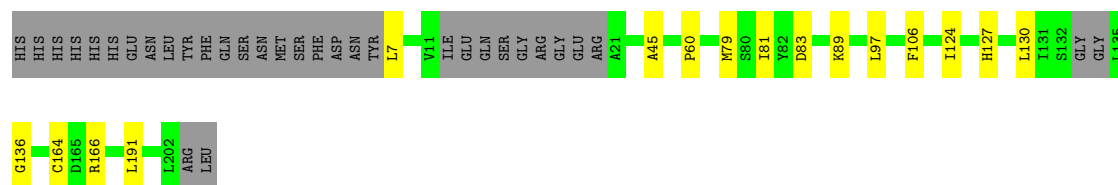
- Molecule 1: ATP-dependent Clp protease proteolytic subunit

Chain H: 76% 6% 17%



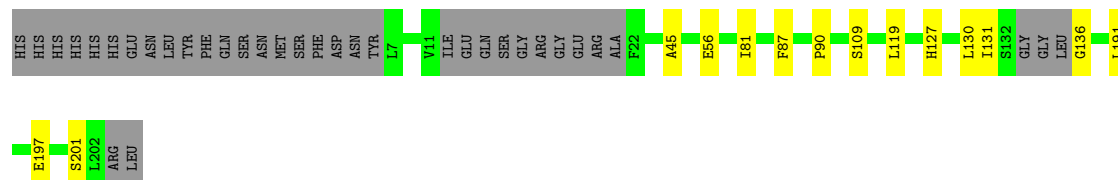
- Molecule 1: ATP-dependent Clp protease proteolytic subunit

Chain I: 78% 7% 15%



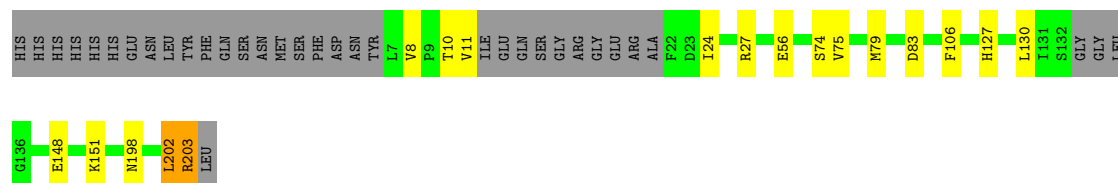
- Molecule 1: ATP-dependent Clp protease proteolytic subunit

Chain J: 78% 6% 16%



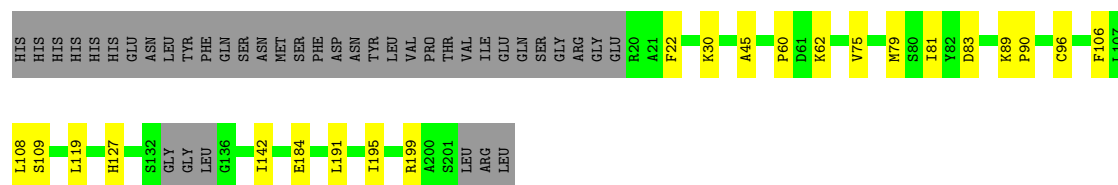
- Molecule 1: ATP-dependent Clp protease proteolytic subunit

Chain K: 76% 7% 16%



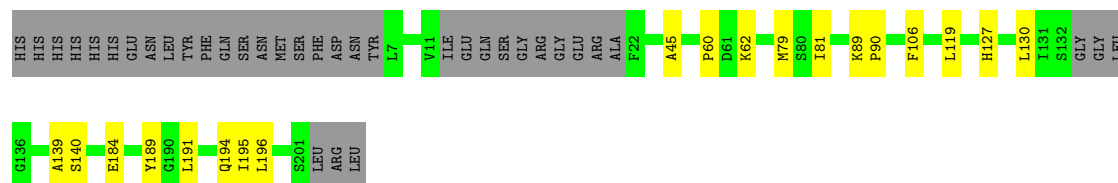
- Molecule 1: ATP-dependent Clp protease proteolytic subunit

Chain L: 72% 10% 18%



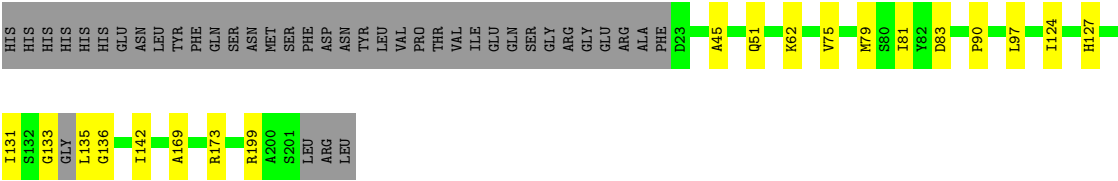
- Molecule 1: ATP-dependent Clp protease proteolytic subunit

Chain M: 75% 9% 17%



- Molecule 1: ATP-dependent Clp protease proteolytic subunit

Chain N: 73% 9% 18%



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	97.44Å 127.30Å 119.09Å 90.00° 90.26° 90.00°	Depositor
Resolution (Å)	97.43 – 1.90 97.43 – 1.90	Depositor EDS
% Data completeness (in resolution range)	99.0 (97.43-1.90) 97.7 (97.43-1.90)	Depositor EDS
R_{merge}	0.13	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.50 (at 1.90Å)	Xtriage
Refinement program	PHENIX 1.21.2_5419	Depositor
R, R_{free}	0.202 , 0.236 0.203 , 0.235	Depositor DCC
R_{free} test set	11334 reflections (4.99%)	wwPDB-VP
Wilson B-factor (Å ²)	28.6	Xtriage
Anisotropy	0.350	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 29.3	EDS
L-test for twinning ²	$\langle L \rangle = 0.46$, $\langle L^2 \rangle = 0.28$	Xtriage
Estimated twinning fraction	0.215 for h,-k,-l	Xtriage
F_o, F_c correlation	0.97	EDS
Total number of atoms	20870	wwPDB-VP
Average B, all atoms (Å ²)	31.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.10% 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.

5 Model quality [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: A1BMH

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	0.35	0/1446	0.54	0/1946
1	B	0.42	0/1460	0.57	0/1965
1	C	0.36	0/1429	0.55	0/1923
1	D	0.33	0/1435	0.54	0/1931
1	E	0.34	0/1440	0.55	0/1938
1	F	0.37	0/1479	0.56	0/1990
1	G	0.36	0/1452	0.58	0/1954
1	H	0.36	0/1428	0.55	0/1922
1	I	0.42	0/1461	0.60	1/1967 (0.1%)
1	J	0.35	0/1448	0.56	0/1949
1	K	0.36	0/1459	0.58	0/1963
1	L	0.37	0/1420	0.58	0/1909
1	M	0.38	0/1438	0.58	0/1935
1	N	0.38	0/1404	0.57	0/1888
All	All	0.37	0/20199	0.57	1/27180 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	I	136	GLY	N-CA-C	5.01	125.06	113.18

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen

atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	1426	0	1436	18	0
1	B	1440	0	1452	12	0
1	C	1408	0	1414	13	0
1	D	1415	0	1419	9	0
1	E	1420	0	1427	12	0
1	F	1459	0	1476	22	0
1	G	1432	0	1441	22	0
1	H	1409	0	1418	9	0
1	I	1441	0	1454	8	0
1	J	1428	0	1438	9	0
1	K	1439	0	1451	17	0
1	L	1400	0	1403	14	0
1	M	1418	0	1423	15	0
1	N	1385	0	1390	13	0
2	A	25	0	0	3	0
2	B	25	0	0	2	0
2	C	25	0	0	1	0
2	F	25	0	0	4	0
2	K	25	0	0	2	0
3	A	49	0	0	0	0
3	B	68	0	0	1	0
3	C	63	0	0	0	0
3	D	57	0	0	0	0
3	E	52	0	0	0	0
3	F	74	0	0	1	0
3	G	52	0	0	0	0
3	H	60	0	0	0	0
3	I	60	0	0	0	0
3	J	50	0	0	0	0
3	K	59	0	0	0	0
3	L	59	0	0	0	0
3	M	60	0	0	1	0
3	N	62	0	0	0	0
All	All	20870	0	20042	162	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 4.

The worst 5 of 162 close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:203:ARG:HH21	1:K:203:ARG:HG3	1.16	1.08
1:A:75:VAL:HG23	2:A:301:A1BMH:C03	2.05	0.85
1:K:203:ARG:HG3	1:K:203:ARG:NH2	1.89	0.80
1:J:197:GLU:HG2	1:J:201:SER:OG	1.86	0.75
1:A:199:ARG:HD2	1:G:89:LYS:HE3	1.69	0.75

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	177/218 (81%)	173 (98%)	4 (2%)	0	100	100
1	B	179/218 (82%)	174 (97%)	5 (3%)	0	100	100
1	C	179/218 (82%)	172 (96%)	6 (3%)	1 (1%)	22	13
1	D	176/218 (81%)	173 (98%)	3 (2%)	0	100	100
1	E	176/218 (81%)	172 (98%)	4 (2%)	0	100	100
1	F	181/218 (83%)	178 (98%)	3 (2%)	0	100	100
1	G	178/218 (82%)	175 (98%)	3 (2%)	0	100	100
1	H	175/218 (80%)	171 (98%)	4 (2%)	0	100	100
1	I	179/218 (82%)	176 (98%)	3 (2%)	0	100	100
1	J	177/218 (81%)	174 (98%)	3 (2%)	0	100	100
1	K	178/218 (82%)	175 (98%)	3 (2%)	0	100	100
1	L	175/218 (80%)	172 (98%)	3 (2%)	0	100	100
1	M	176/218 (81%)	173 (98%)	3 (2%)	0	100	100
1	N	174/218 (80%)	170 (98%)	4 (2%)	0	100	100
All	All	2480/3052 (81%)	2428 (98%)	51 (2%)	1 (0%)	100	100

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	135	LEU

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	156/187 (83%)	154 (99%)	2 (1%)	65	65
1	B	158/187 (84%)	156 (99%)	2 (1%)	65	65
1	C	153/187 (82%)	151 (99%)	2 (1%)	65	65
1	D	154/187 (82%)	151 (98%)	3 (2%)	52	49
1	E	156/187 (83%)	154 (99%)	2 (1%)	65	65
1	F	160/187 (86%)	158 (99%)	2 (1%)	65	65
1	G	157/187 (84%)	156 (99%)	1 (1%)	84	86
1	H	155/187 (83%)	153 (99%)	2 (1%)	65	65
1	I	158/187 (84%)	156 (99%)	2 (1%)	65	65
1	J	157/187 (84%)	157 (100%)	0	100	100
1	K	158/187 (84%)	154 (98%)	4 (2%)	42	37
1	L	152/187 (81%)	151 (99%)	1 (1%)	81	83
1	M	155/187 (83%)	155 (100%)	0	100	100
1	N	151/187 (81%)	150 (99%)	1 (1%)	81	83
All	All	2180/2618 (83%)	2156 (99%)	24 (1%)	70	71

5 of 24 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	H	10	THR
1	I	130	LEU
1	I	7	LEU
1	K	10	THR
1	D	8	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 8 such sidechains are listed below:

Mol	Chain	Res	Type
1	M	194	GLN
1	J	194	GLN
1	I	194	GLN
1	H	46	ASN
1	J	46	ASN

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 oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

5 ligands are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. 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 $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
2	A1BMH	C	301	-	24,24,24	2.31	4 (16%)	26,28,28	2.30	5 (19%)
2	A1BMH	A	301	-	24,24,24	2.15	6 (25%)	26,28,28	2.20	6 (23%)
2	A1BMH	B	301	-	24,24,24	2.40	5 (20%)	26,28,28	2.18	4 (15%)
2	A1BMH	K	301	-	24,24,24	2.27	4 (16%)	26,28,28	1.84	4 (15%)
2	A1BMH	F	301	-	24,24,24	2.10	5 (20%)	26,28,28	2.37	8 (30%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the

Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns.
'-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	A1BMH	C	301	-	-	11/27/27/27	-
2	A1BMH	A	301	-	-	11/27/27/27	-
2	A1BMH	B	301	-	-	13/27/27/27	-
2	A1BMH	K	301	-	-	12/27/27/27	-
2	A1BMH	F	301	-	-	10/27/27/27	-

The worst 5 of 24 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	301	A1BMH	C04-N05	7.45	1.49	1.34
2	B	301	A1BMH	C04-N05	7.43	1.49	1.34
2	K	301	A1BMH	C04-N05	7.01	1.48	1.34
2	C	301	A1BMH	C08-N09	6.39	1.48	1.33
2	K	301	A1BMH	C08-N09	6.33	1.48	1.33

The worst 5 of 27 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	301	A1BMH	C06-C07-C08	9.94	126.51	112.41
2	B	301	A1BMH	C06-C07-C08	8.88	125.02	112.41
2	A	301	A1BMH	C06-C07-C08	7.86	123.56	112.41
2	K	301	A1BMH	C06-C07-C08	7.16	122.57	112.41
2	F	301	A1BMH	C06-C07-C08	7.03	122.39	112.41

There are no chirality outliers.

5 of 57 torsion outliers are listed below:

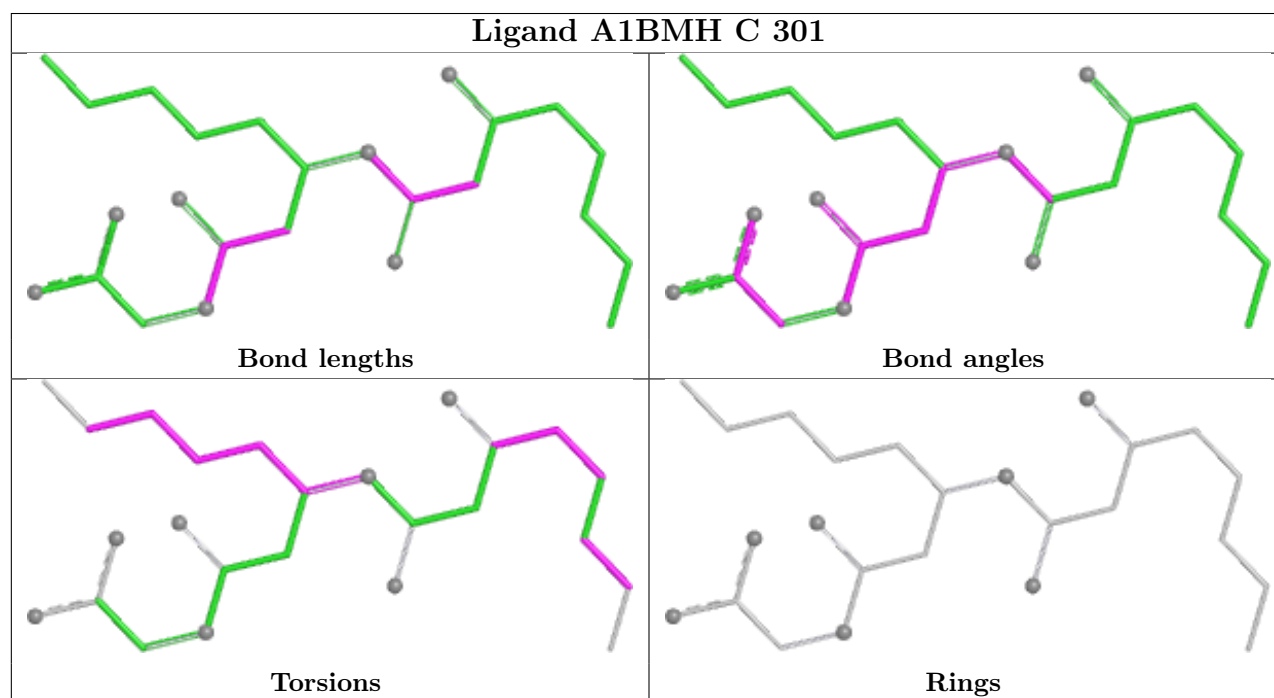
Mol	Chain	Res	Type	Atoms
2	A	301	A1BMH	N01-C02-C03-C04
2	A	301	A1BMH	C07-C06-C15-C16
2	B	301	A1BMH	C21-C02-C03-C04
2	B	301	A1BMH	N01-C02-C03-C04
2	B	301	A1BMH	C15-C06-C07-C08

There are no ring outliers.

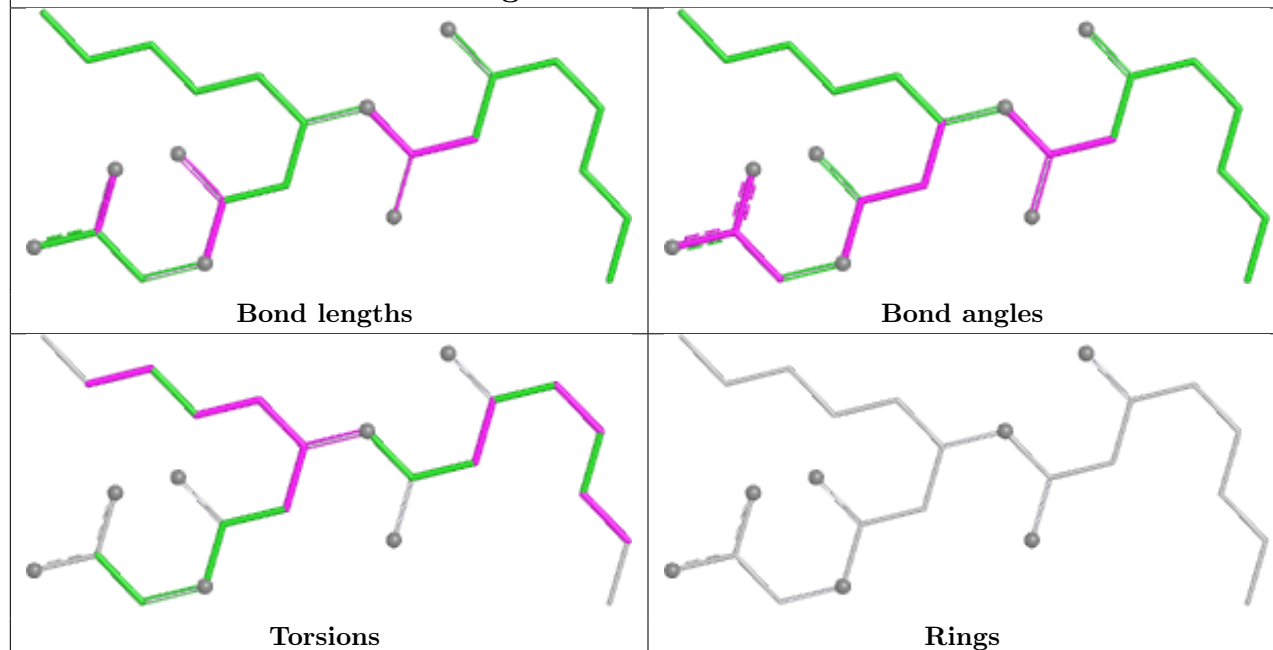
5 monomers are involved in 12 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	C	301	A1BMH	1	0
2	A	301	A1BMH	3	0
2	B	301	A1BMH	2	0
2	K	301	A1BMH	2	0
2	F	301	A1BMH	4	0

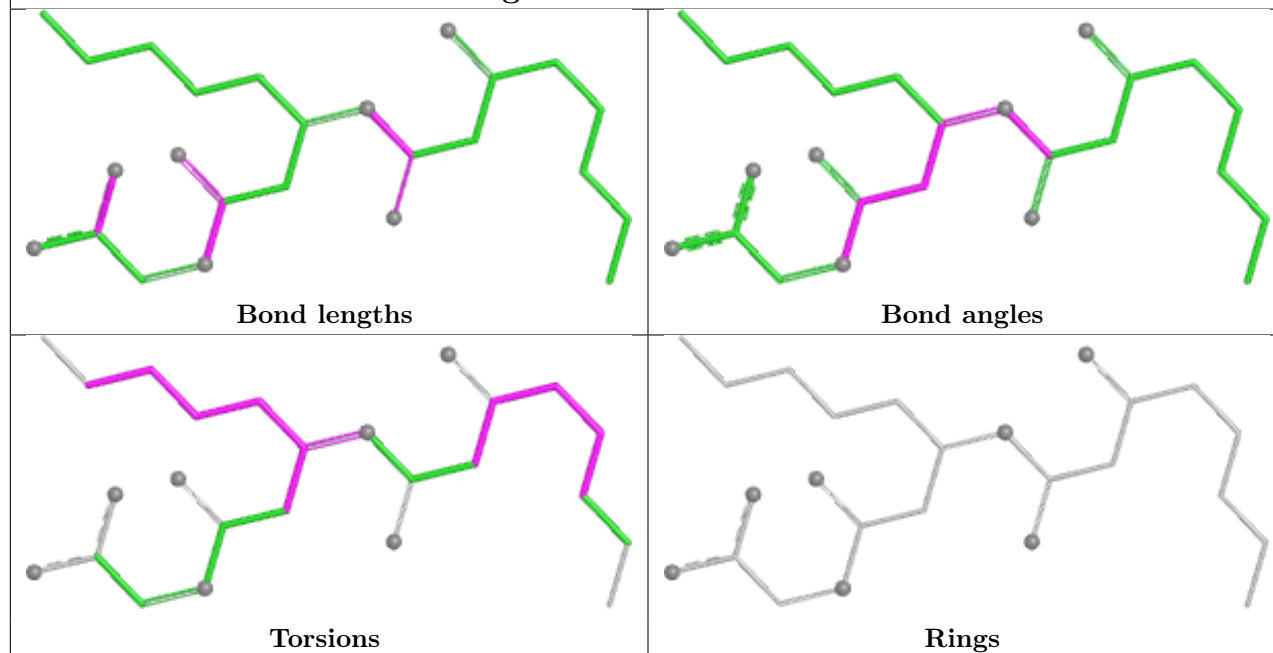
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

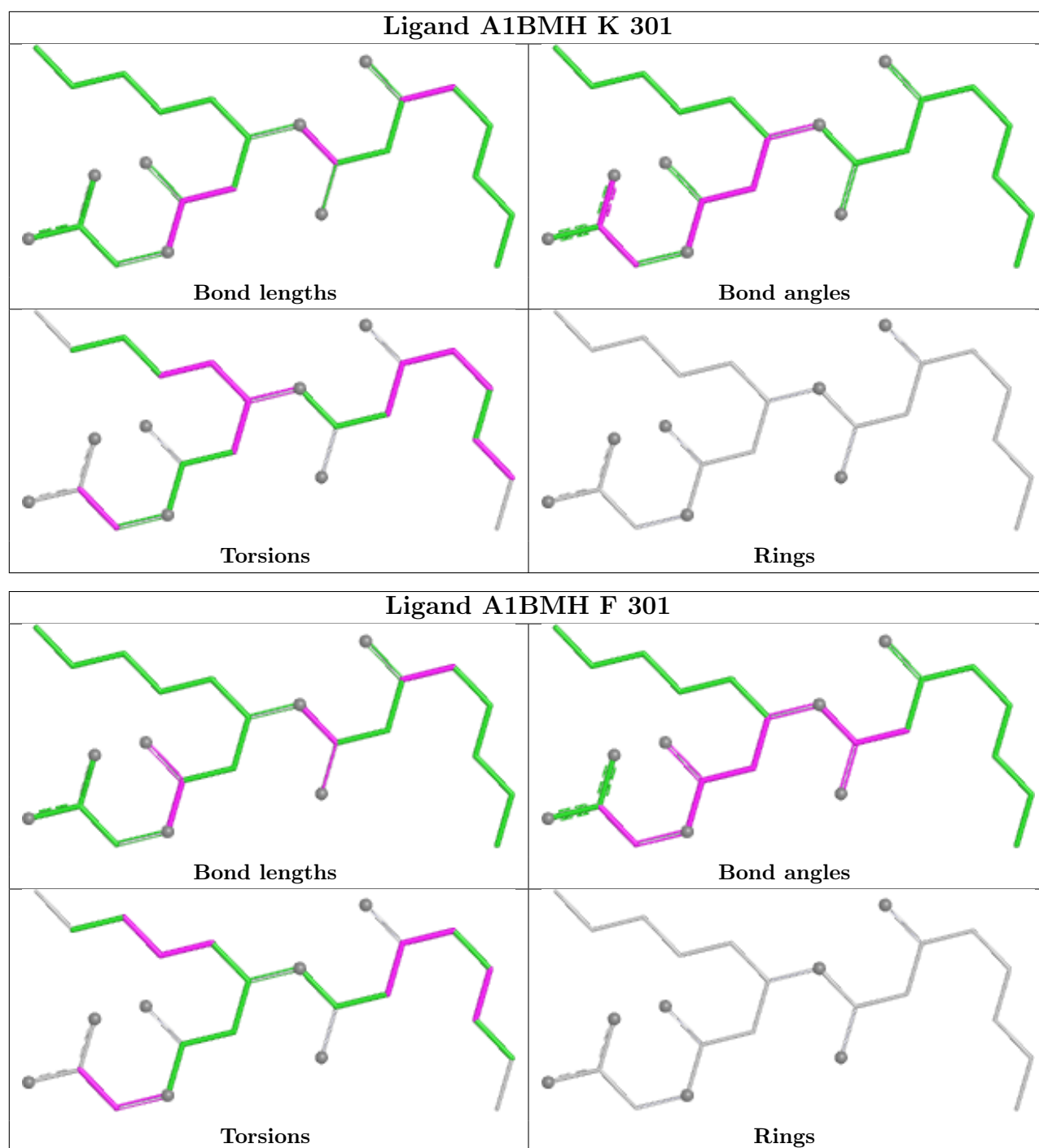


Ligand A1BMH A 301



Ligand A1BMH B 301





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 [i](#)

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

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	183/218 (83%)	-1.17	0 100 100	23, 29, 50, 63	0
1	B	185/218 (84%)	-1.21	0 100 100	22, 27, 48, 73	0
1	C	181/218 (83%)	-1.25	0 100 100	23, 29, 43, 66	0
1	D	182/218 (83%)	-1.21	0 100 100	24, 30, 48, 64	0
1	E	182/218 (83%)	-1.19	0 100 100	24, 31, 47, 67	0
1	F	187/218 (85%)	-1.23	1 (0%) 87 88	21, 28, 50, 67	0
1	G	184/218 (84%)	-1.22	0 100 100	23, 28, 49, 61	0
1	H	181/218 (83%)	-1.25	1 (0%) 85 87	21, 27, 44, 71	0
1	I	185/218 (84%)	-1.25	0 100 100	22, 28, 44, 58	0
1	J	183/218 (83%)	-1.20	0 100 100	22, 29, 46, 59	0
1	K	184/218 (84%)	-1.22	0 100 100	22, 29, 50, 67	0
1	L	179/218 (82%)	-1.28	0 100 100	23, 28, 45, 87	0
1	M	182/218 (83%)	-1.20	0 100 100	22, 28, 44, 59	0
1	N	178/218 (81%)	-1.29	0 100 100	21, 27, 40, 63	0
All	All	2556/3052 (83%)	-1.23	2 (0%) 92 93	21, 28, 48, 87	0

All (2) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	H	7	LEU	2.4
1	F	7	LEU	2.1

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

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

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

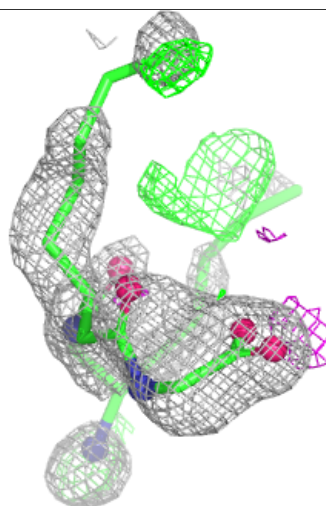
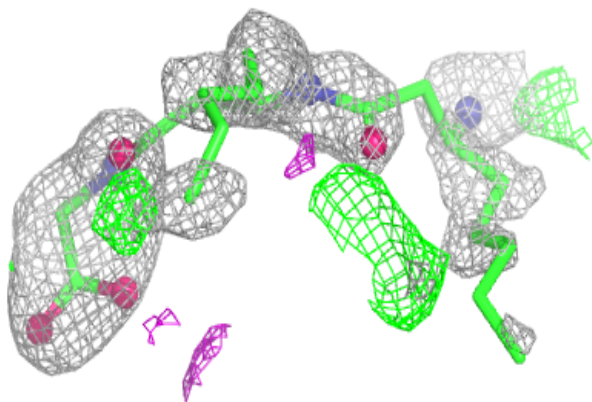
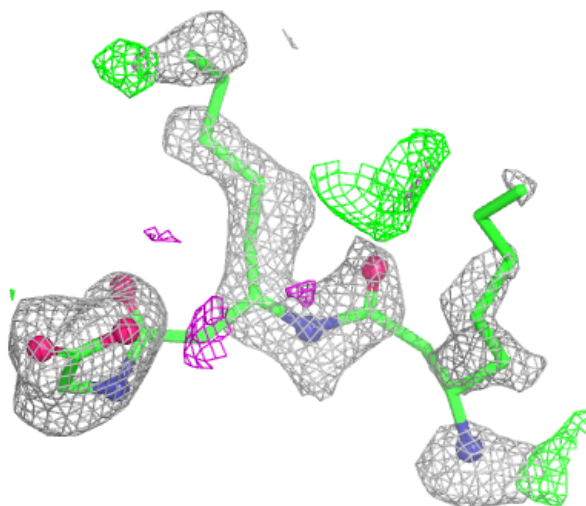
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
2	A1BMH	A	301	25/25	0.94	0.11	27,38,44,48	25
2	A1BMH	F	301	25/25	0.95	0.10	33,39,43,49	25
2	A1BMH	C	301	25/25	0.97	0.10	36,43,48,50	25
2	A1BMH	B	301	25/25	0.97	0.09	33,39,43,47	25
2	A1BMH	K	301	25/25	0.97	0.08	31,40,47,54	25

The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation to approximate a three-dimensional view.

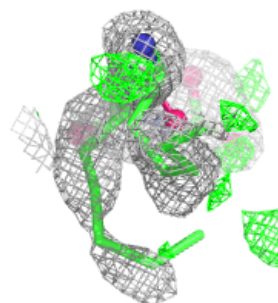
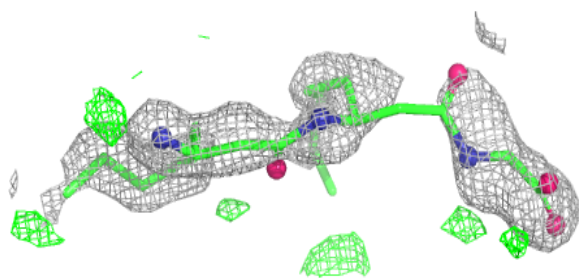
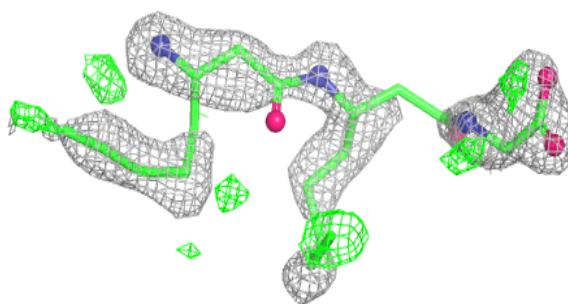
Electron density around A1BMH A 301:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

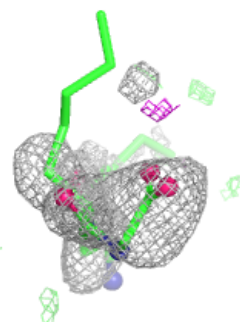
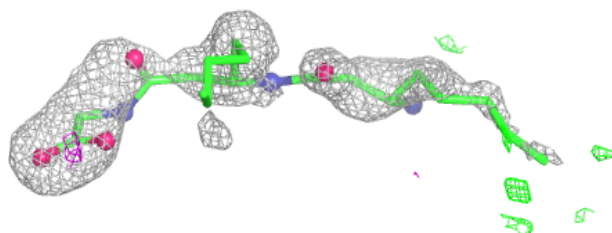
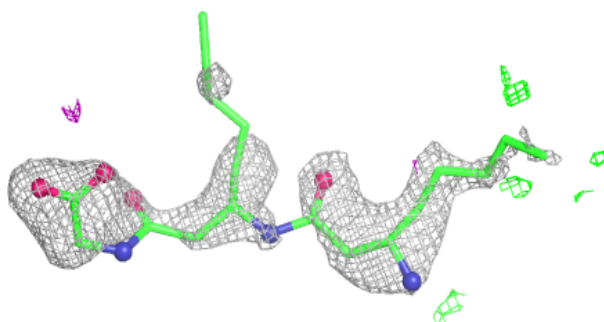


Electron density around A1BMH F 301:

$2mF_o - DF_c$ (at 0.7 rmsd) in gray
 $mF_o - DF_c$ (at 3 rmsd) in purple (negative)
and green (positive)

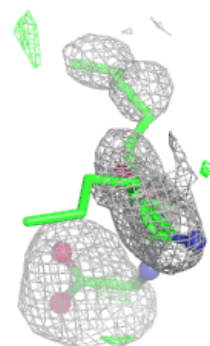
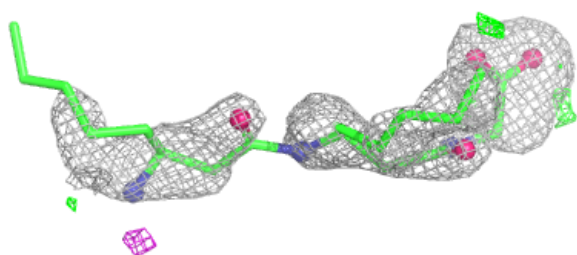
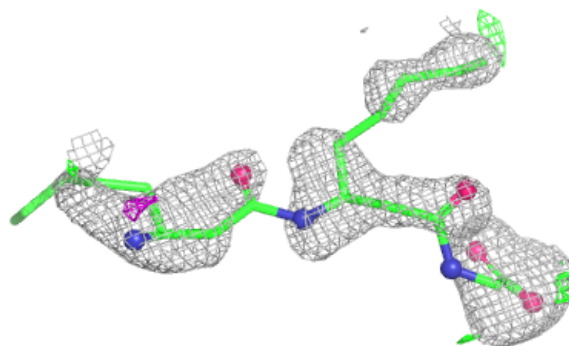
**Electron density around A1BMH C 301:**

$2mF_o - DF_c$ (at 0.7 rmsd) in gray
 $mF_o - DF_c$ (at 3 rmsd) in purple (negative)
and green (positive)

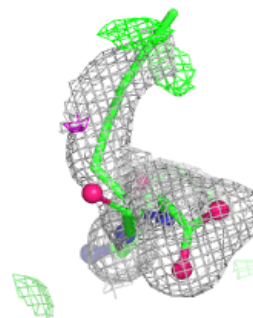
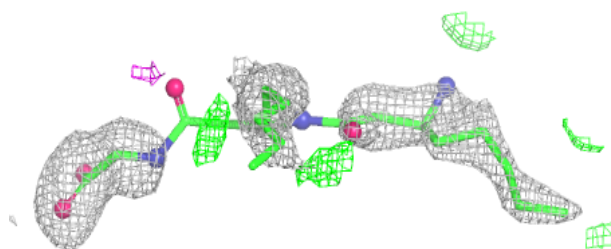
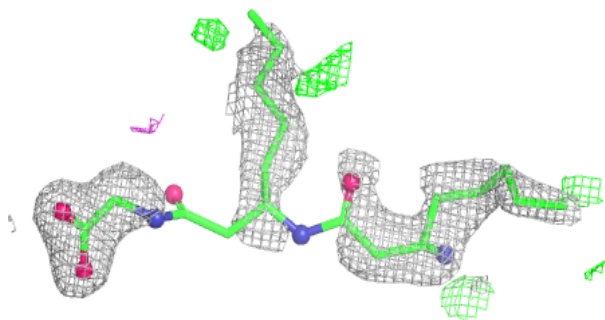


Electron density around A1BMH B 301:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

**Electron density around A1BMH K 301:**

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



6.5 Other polymers [i](#)

There are no such residues in this entry.