



wwPDB X-ray Structure Validation Summary Report ⓘ

Mar 1, 2026 – 05:10 PM UTC

PDB ID : 9MJP / pdb_00009mjp
Title : Crystal structure of Neisseria meningitidis ClpP protease complex with boronate compound BC8a
Authors : Mabanglo, M.F.; Houry, W.A.
Deposited on : 2024-12-16
Resolution : 1.99 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 Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

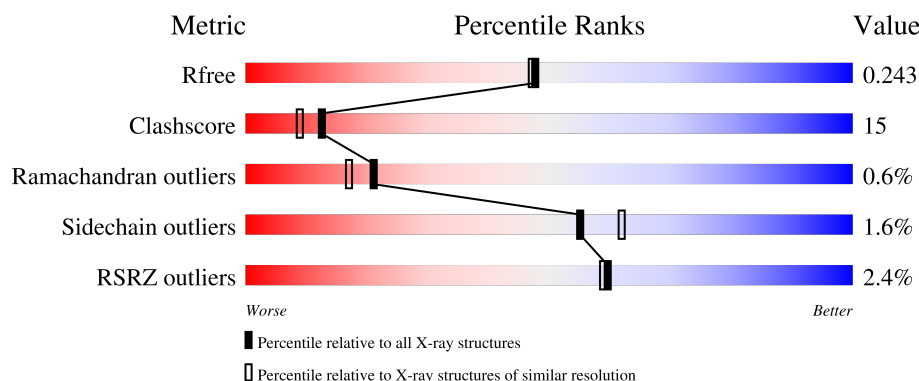
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.99 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}	180053	10052 (2.00-2.00)
Clashscore	190562	11152 (2.00-2.00)
Ramachandran outliers	187476	11031 (2.00-2.00)
Sidechain outliers	187428	11029 (2.00-2.00)
RSRZ outliers	180081	10067 (2.00-2.00)

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	2% 52% 28% 20%
1	B	218	3% 49% 31% 18%
1	C	218	4% 52% 27% 20%
1	D	218	0% 51% 28% 20%
1	E	218	0% 51% 27% 21%

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Mol	Chain	Length	Quality of chain
1	F	218	
1	G	218	
1	H	218	
1	I	218	
1	J	218	
1	K	218	
1	L	218	
1	M	218	
1	N	218	

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 19946 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	175	Total	C	N	O	S	0	0	0
			1374	868	234	264	8			
1	B	178	Total	C	N	O	S	0	0	0
			1391	878	237	268	8			
1	C	174	Total	C	N	O	S	0	0	0
			1362	859	233	262	8			
1	D	174	Total	C	N	O	S	0	0	0
			1368	865	233	262	8			
1	E	172	Total	C	N	O	S	0	0	0
			1352	856	228	260	8			
1	F	174	Total	C	N	O	S	0	0	0
			1368	865	233	262	8			
1	G	181	Total	C	N	O	S	0	0	0
			1416	896	240	272	8			
1	H	180	Total	C	N	O	S	0	0	0
			1405	887	239	271	8			
1	I	178	Total	C	N	O	S	0	0	0
			1394	881	237	268	8			
1	J	175	Total	C	N	O	S	0	0	0
			1369	862	234	265	8			
1	K	175	Total	C	N	O	S	0	0	0
			1374	868	234	264	8			
1	L	174	Total	C	N	O	S	0	0	0
			1363	859	233	263	8			
1	M	177	Total	C	N	O	S	0	0	0
			1390	879	236	267	8			
1	N	172	Total	C	N	O	S	0	0	0
			1347	847	231	261	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
C	-4	TYR	-	expression tag	UNP Q9JZ38
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	6	HIS	-	expression tag	UNP Q9JZ38

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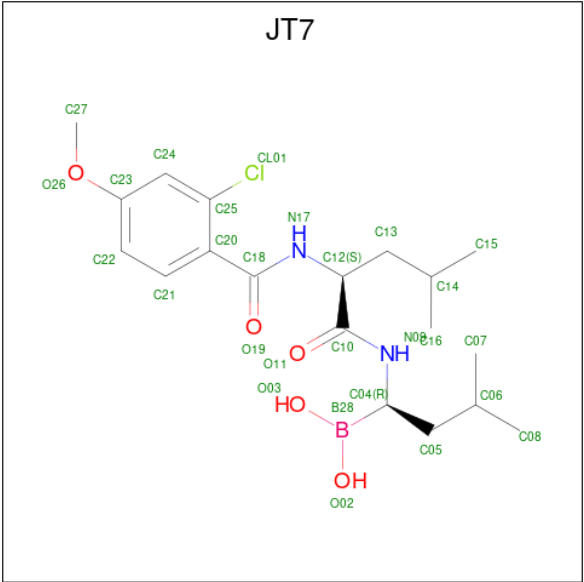
Chain	Residue	Modelled	Actual	Comment	Reference
J	7	HIS	-	expression tag	UNP Q9JZ38
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J	9	HIS	-	expression tag	UNP Q9JZ38
J	10	HIS	-	expression tag	UNP Q9JZ38
J	11	HIS	-	expression tag	UNP Q9JZ38
J	12	GLU	-	expression tag	UNP Q9JZ38
J	13	ASN	-	expression tag	UNP Q9JZ38
J	14	LEU	-	expression tag	UNP Q9JZ38
J	15	TYR	-	expression tag	UNP Q9JZ38
J	16	PHE	-	expression tag	UNP Q9JZ38
J	17	GLN	-	expression tag	UNP Q9JZ38
J	18	SER	-	expression tag	UNP Q9JZ38
J	19	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-[(1R)-1-borono-3-methylbutyl]-N 2 -(2-chloro-4-methoxybenzene-1-carbonyl)-L-leucinamide (CCD ID: JT7) (formula: $C_{19}H_{30}BClN_2O_5$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
2	A	1	Total 28	B 1	C 19	Cl 1	N 2	O 5	0	0
2	B	1	Total 28	B 1	C 19	Cl 1	N 2	O 5	0	0
2	C	1	Total 28	B 1	C 19	Cl 1	N 2	O 5	0	0
2	D	1	Total 28	B 1	C 19	Cl 1	N 2	O 5	0	0
2	E	1	Total 28	B 1	C 19	Cl 1	N 2	O 5	0	0
2	F	1	Total 28	B 1	C 19	Cl 1	N 2	O 5	0	0
2	G	1	Total 28	B 1	C 19	Cl 1	N 2	O 5	0	0
2	H	1	Total 28	B 1	C 19	Cl 1	N 2	O 5	0	0
2	I	1	Total 28	B 1	C 19	Cl 1	N 2	O 5	0	0
2	J	1	Total 28	B 1	C 19	Cl 1	N 2	O 5	0	0
2	K	1	Total 28	B 1	C 19	Cl 1	N 2	O 5	0	0
2	L	1	Total 28	B 1	C 19	Cl 1	N 2	O 5	0	0
2	M	1	Total 28	B 1	C 19	Cl 1	N 2	O 5	0	0
2	N	1	Total 28	B 1	C 19	Cl 1	N 2	O 5	0	0

- Molecule 3 is water.

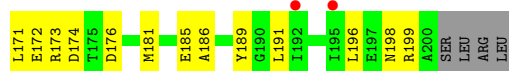
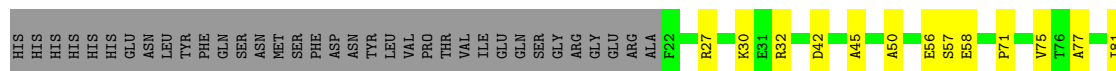
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
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3	B	20	Total O 20 20	0	0
3	C	28	Total O 28 28	0	0
3	D	23	Total O 23 23	0	0
3	E	14	Total O 14 14	0	0
3	F	18	Total O 18 18	0	0
3	G	20	Total O 20 20	0	0
3	H	25	Total O 25 25	0	0
3	I	27	Total O 27 27	0	0
3	J	19	Total O 19 19	0	0
3	K	22	Total O 22 22	0	0
3	L	23	Total O 23 23	0	0
3	M	8	Total O 8 8	0	0
3	N	20	Total O 20 20	0	0

- Molecule 1: ATP-dependent Clp protease proteolytic subunit

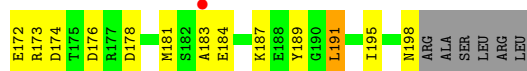
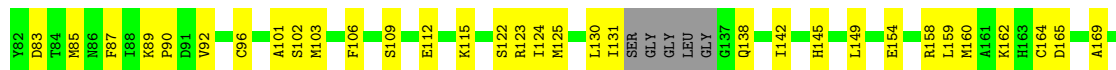
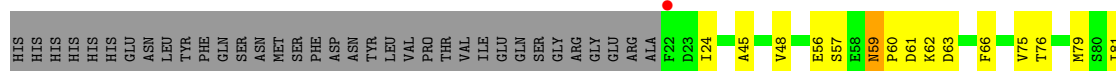




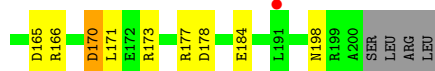
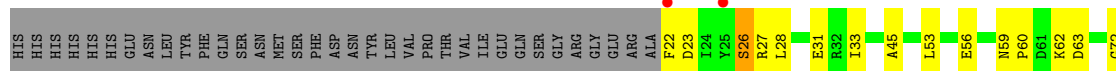
- Molecule 1: ATP-dependent Clp protease proteolytic subunit



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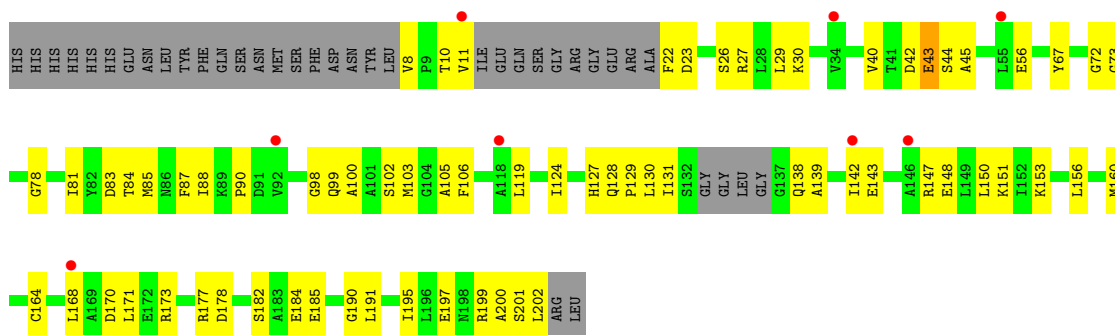


- Molecule 1: ATP-dependent Clp protease proteolytic subunit

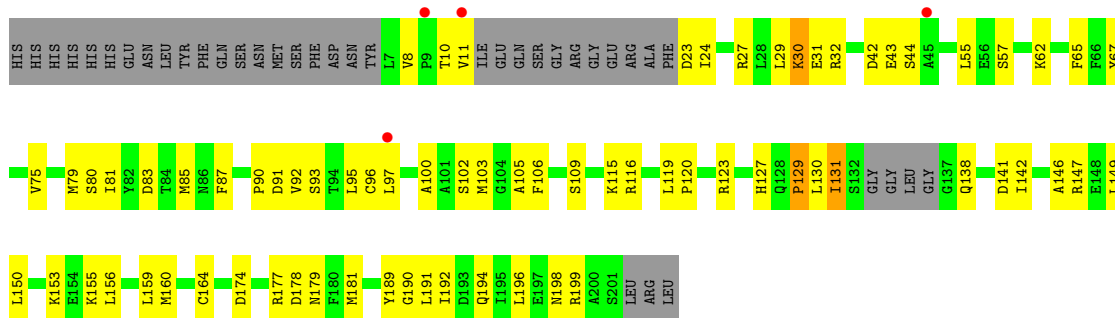


- Molecule 1: ATP-dependent Clp protease proteolytic subunit

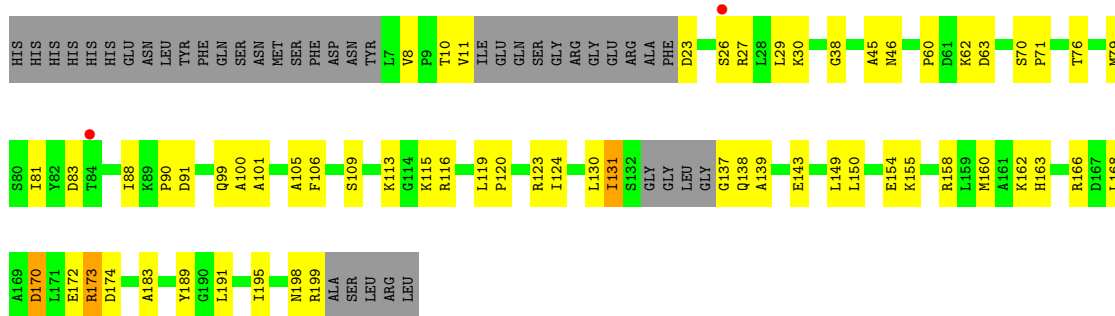




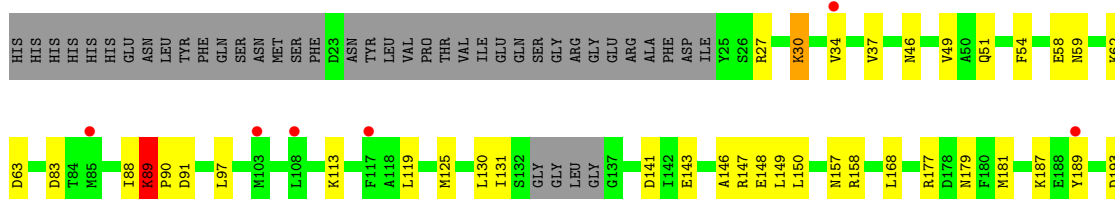
- Molecule 1: ATP-dependent Clp protease proteolytic subunit



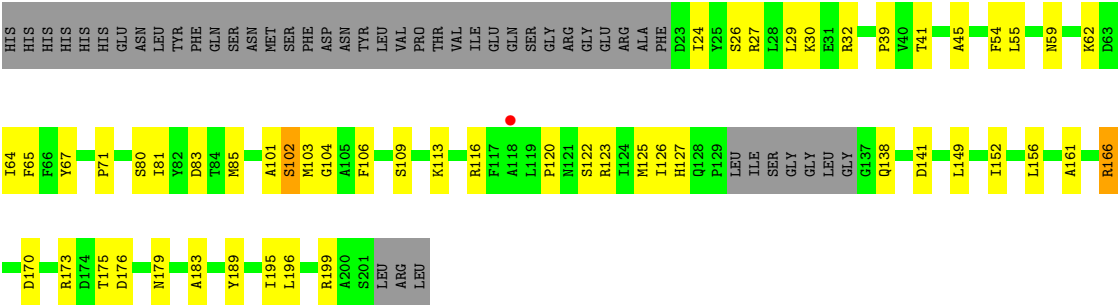
- Molecule 1: ATP-dependent Clp protease proteolytic subunit



- Molecule 1: ATP-dependent Clp protease proteolytic subunit







4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	97.12Å 127.55Å 119.39Å 90.00° 89.98° 90.00°	Depositor
Resolution (Å)	48.68 – 1.99 48.68 – 1.99	Depositor EDS
% Data completeness (in resolution range)	92.5 (48.68-1.99) 90.3 (48.68-1.99)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.31 (at 1.98Å)	Xtriage
Refinement program	PHENIX 1.21.2_5419	Depositor
R, R_{free}	0.195 , 0.234 0.196 , 0.243	Depositor DCC
R_{free} test set	2007 reflections (1.09%)	wwPDB-VP
Wilson B-factor (Å ²)	32.8	Xtriage
Anisotropy	0.655	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 34.2	EDS
L-test for twinning ²	$\langle L \rangle = 0.40$, $\langle L^2 \rangle = 0.22$	Xtriage
Estimated twinning fraction	0.458 for h,-k,-l	Xtriage
Reported twinning fraction	0.490 for h,-k,-l	Depositor
Outliers	0 of 183680 reflections	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	19946	wwPDB-VP
Average B, all atoms (Å ²)	40.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.22% 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

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: JT7

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	0.19	0/1394	0.47	0/1875
1	B	0.20	0/1410	0.52	1/1898 (0.1%)
1	C	0.31	0/1381	0.55	0/1858
1	D	0.22	0/1388	0.49	0/1867
1	E	0.24	0/1372	0.59	3/1846 (0.2%)
1	F	0.29	0/1388	0.53	2/1867 (0.1%)
1	G	0.20	0/1436	0.44	0/1933
1	H	0.25	0/1424	0.50	0/1917
1	I	0.22	0/1413	0.49	0/1902
1	J	0.19	0/1387	0.46	0/1864
1	K	0.20	0/1394	0.44	0/1875
1	L	0.20	0/1382	0.48	0/1859
1	M	0.20	0/1410	0.47	0/1896
1	N	0.29	1/1366 (0.1%)	0.47	0/1837
All	All	0.23	1/19545 (0.0%)	0.49	6/26294 (0.0%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	C	0	1
1	H	0	1
1	J	0	1
All	All	0	3

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	N	102	SER	C-O	-5.22	1.17	1.24

The worst 5 of 6 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	197	GLU	N-CA-C	-7.26	96.48	110.56
1	E	60	PRO	N-CD-CG	-6.91	92.84	103.20
1	E	60	PRO	CA-N-CD	-6.02	103.58	112.00
1	E	60	PRO	CA-CB-CG	-5.62	93.83	104.50
1	F	170	ASP	CA-C-N	5.24	128.07	120.79

There are no chirality outliers.

All (3) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	C	30	LYS	Peptide
1	H	30	LYS	Peptide
1	J	89	LYS	Peptide

5.2 Too-close contacts

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	1374	0	1376	51	0
1	B	1391	0	1398	62	0
1	C	1362	0	1364	55	0
1	D	1368	0	1371	53	0
1	E	1352	0	1353	51	0
1	F	1368	0	1371	49	0
1	G	1416	0	1423	60	0
1	H	1405	0	1414	56	0
1	I	1394	0	1404	47	0
1	J	1369	0	1371	33	0
1	K	1374	0	1376	41	0
1	L	1363	0	1367	51	0
1	M	1390	0	1394	55	0
1	N	1347	0	1345	44	0
2	A	28	0	0	0	0
2	B	28	0	0	4	0
2	C	28	0	0	2	0
2	D	28	0	0	4	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	E	28	0	0	3	0
2	F	28	0	0	2	0
2	G	28	0	0	4	0
2	H	28	0	0	3	0
2	I	28	0	0	1	0
2	J	28	0	0	0	0
2	K	28	0	0	4	0
2	L	28	0	0	3	0
2	M	28	0	0	2	0
2	N	28	0	0	2	0
3	A	14	0	0	5	0
3	B	20	0	0	1	0
3	C	28	0	0	3	0
3	D	23	0	0	3	0
3	E	14	0	0	1	0
3	F	18	0	0	0	0
3	G	20	0	0	2	0
3	H	25	0	0	3	0
3	I	27	0	0	1	0
3	J	19	0	0	2	0
3	K	22	0	0	1	0
3	L	23	0	0	6	0
3	M	8	0	0	0	0
3	N	20	0	0	2	0
All	All	19946	0	19327	598	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 15.

The worst 5 of 598 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:M:166:ARG:HH21	1:M:189:TYR:HA	1.29	0.98
1:L:74:SER:O	3:L:401:HOH:O	1.83	0.96
1:F:56:GLU:OE1	1:G:199:ARG:NH2	2.00	0.94
1:E:63:ASP:OD2	1:E:115:LYS:NZ	2.05	0.89
1:B:54:PHE:HE1	1:C:27:ARG:HG3	1.38	0.88

There are no symmetry-related clashes.

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	171/218 (78%)	155 (91%)	13 (8%)	3 (2%)	6	3
1	B	172/218 (79%)	152 (88%)	19 (11%)	1 (1%)	21	17
1	C	170/218 (78%)	153 (90%)	14 (8%)	3 (2%)	6	3
1	D	170/218 (78%)	154 (91%)	15 (9%)	1 (1%)	21	17
1	E	168/218 (77%)	157 (94%)	10 (6%)	1 (1%)	21	17
1	F	170/218 (78%)	158 (93%)	12 (7%)	0	100	100
1	G	175/218 (80%)	162 (93%)	11 (6%)	2 (1%)	11	7
1	H	174/218 (80%)	163 (94%)	10 (6%)	1 (1%)	21	17
1	I	172/218 (79%)	162 (94%)	10 (6%)	0	100	100
1	J	170/218 (78%)	158 (93%)	11 (6%)	1 (1%)	21	17
1	K	171/218 (78%)	160 (94%)	11 (6%)	0	100	100
1	L	170/218 (78%)	161 (95%)	8 (5%)	1 (1%)	21	17
1	M	171/218 (78%)	162 (95%)	8 (5%)	1 (1%)	21	17
1	N	168/218 (77%)	159 (95%)	9 (5%)	0	100	100
All	All	2392/3052 (78%)	2216 (93%)	161 (7%)	15 (1%)	21	17

5 of 15 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	197	GLU
1	A	131	ILE
1	D	165	ASP
1	G	201	SER
1	A	178	ASP

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	150/187 (80%)	149 (99%)	1 (1%)	76	82
1	B	153/187 (82%)	149 (97%)	4 (3%)	40	44
1	C	148/187 (79%)	144 (97%)	4 (3%)	39	42
1	D	149/187 (80%)	145 (97%)	4 (3%)	39	42
1	E	148/187 (79%)	146 (99%)	2 (1%)	59	66
1	F	149/187 (80%)	148 (99%)	1 (1%)	76	82
1	G	156/187 (83%)	156 (100%)	0	100	100
1	H	155/187 (83%)	153 (99%)	2 (1%)	61	68
1	I	154/187 (82%)	150 (97%)	4 (3%)	40	44
1	J	150/187 (80%)	147 (98%)	3 (2%)	48	54
1	K	150/187 (80%)	148 (99%)	2 (1%)	61	68
1	L	149/187 (80%)	146 (98%)	3 (2%)	48	54
1	M	153/187 (82%)	152 (99%)	1 (1%)	76	82
1	N	147/187 (79%)	145 (99%)	2 (1%)	59	66
All	All	2111/2618 (81%)	2078 (98%)	33 (2%)	55	62

5 of 33 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	L	142	ILE
1	L	184	GLU
1	N	166	ARG
1	D	171	LEU
1	D	152	ILE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 22 such sidechains are listed below:

Mol	Chain	Res	Type
1	J	51	GLN

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Mol	Chain	Res	Type
1	K	51	GLN
1	J	138	GLN
1	L	138	GLN
1	D	157	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](#)

14 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	JT7	B	301	1	24,28,28	1.81	4 (16%)	33,38,38	1.11	4 (12%)
2	JT7	E	301	1	24,28,28	1.90	4 (16%)	33,38,38	1.61	7 (21%)
2	JT7	L	301	1	24,28,28	1.87	4 (16%)	33,38,38	1.11	3 (9%)
2	JT7	M	301	1	24,28,28	1.83	4 (16%)	33,38,38	1.29	2 (6%)
2	JT7	A	301	1	24,28,28	1.86	5 (20%)	33,38,38	1.22	3 (9%)
2	JT7	G	301	1	24,28,28	1.87	5 (20%)	33,38,38	1.22	3 (9%)
2	JT7	C	301	1	24,28,28	1.87	5 (20%)	33,38,38	1.22	3 (9%)
2	JT7	F	301	1	24,28,28	1.79	5 (20%)	33,38,38	1.75	8 (24%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	JT7	N	301	-	24,28,28	1.90	4 (16%)	33,38,38	1.61	7 (21%)
2	JT7	H	401	1	24,28,28	1.78	4 (16%)	33,38,38	1.12	1 (3%)
2	JT7	J	301	1	24,28,28	1.92	5 (20%)	33,38,38	1.12	3 (9%)
2	JT7	D	301	1	24,28,28	1.90	4 (16%)	33,38,38	1.61	7 (21%)
2	JT7	K	301	1	24,28,28	1.82	4 (16%)	33,38,38	1.08	2 (6%)
2	JT7	I	301	1	24,28,28	1.82	4 (16%)	33,38,38	1.15	2 (6%)

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	JT7	B	301	1	-	7/25/30/30	0/1/1/1
2	JT7	E	301	1	-	12/25/30/30	0/1/1/1
2	JT7	L	301	1	-	9/25/30/30	0/1/1/1
2	JT7	M	301	1	-	8/25/30/30	0/1/1/1
2	JT7	A	301	1	-	10/25/30/30	0/1/1/1
2	JT7	G	301	1	-	10/25/30/30	0/1/1/1
2	JT7	C	301	1	-	10/25/30/30	0/1/1/1
2	JT7	F	301	1	-	10/25/30/30	0/1/1/1
2	JT7	N	301	-	-	12/25/30/30	0/1/1/1
2	JT7	H	401	1	-	6/25/30/30	0/1/1/1
2	JT7	J	301	1	-	10/25/30/30	0/1/1/1
2	JT7	D	301	1	-	12/25/30/30	0/1/1/1
2	JT7	K	301	1	-	12/25/30/30	0/1/1/1
2	JT7	I	301	1	-	9/25/30/30	0/1/1/1

The worst 5 of 61 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	J	301	JT7	C10-N09	5.86	1.46	1.34
2	N	301	JT7	C10-N09	5.75	1.46	1.34
2	D	301	JT7	C10-N09	5.74	1.46	1.34
2	E	301	JT7	C10-N09	5.74	1.46	1.34
2	G	301	JT7	C10-N09	5.70	1.46	1.34

The worst 5 of 55 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	F	301	JT7	C24-C25-C20	-5.28	117.27	121.59
2	D	301	JT7	C13-C12-N17	-4.19	101.13	110.58
2	E	301	JT7	C13-C12-N17	-4.18	101.14	110.58
2	N	301	JT7	C13-C12-N17	-4.18	101.14	110.58
2	M	301	JT7	C13-C12-N17	-3.58	102.51	110.58

There are no chirality outliers.

5 of 137 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	B	301	JT7	B28-C04-C05-C06
2	D	301	JT7	B28-C04-C05-C06
2	D	301	JT7	C04-C05-C06-C08
2	E	301	JT7	B28-C04-C05-C06
2	E	301	JT7	C04-C05-C06-C08

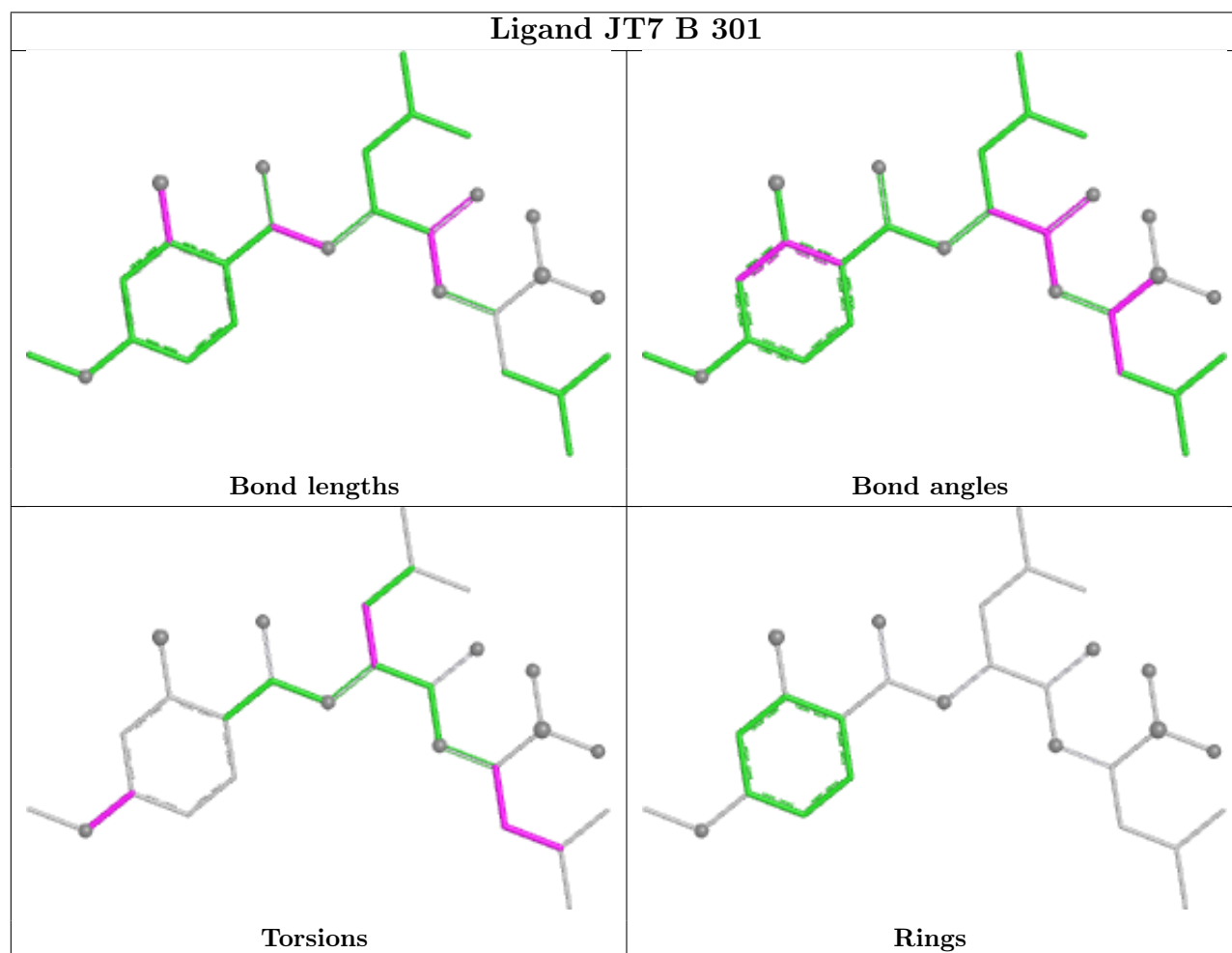
There are no ring outliers.

12 monomers are involved in 34 short contacts:

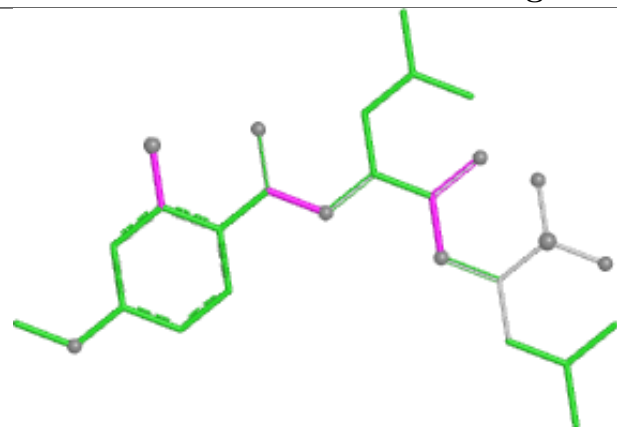
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	301	JT7	4	0
2	E	301	JT7	3	0
2	L	301	JT7	3	0
2	M	301	JT7	2	0
2	G	301	JT7	4	0
2	C	301	JT7	2	0
2	F	301	JT7	2	0
2	N	301	JT7	2	0
2	H	401	JT7	3	0
2	D	301	JT7	4	0
2	K	301	JT7	4	0
2	I	301	JT7	1	0

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.

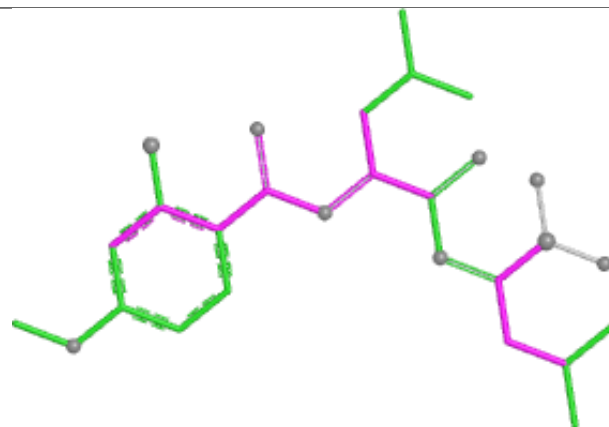
The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.



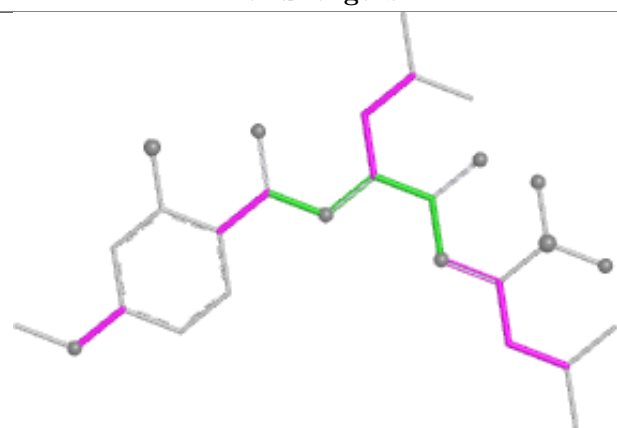
Ligand JT7 E 301



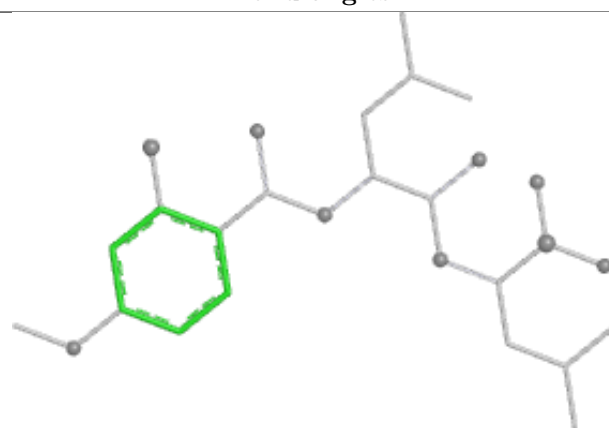
Bond lengths



Bond angles

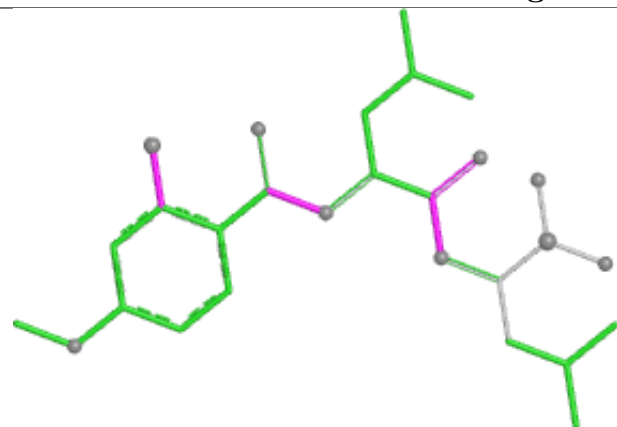


Torsions

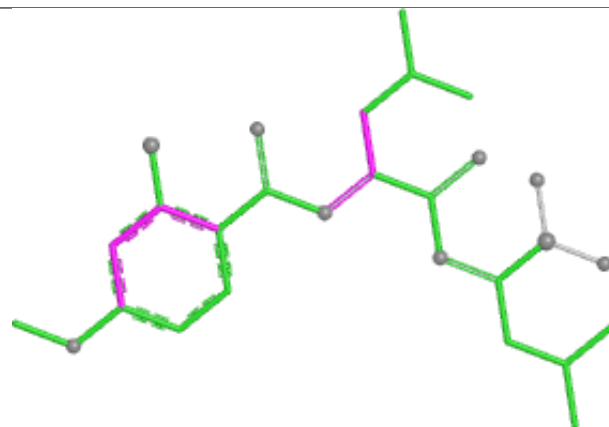


Rings

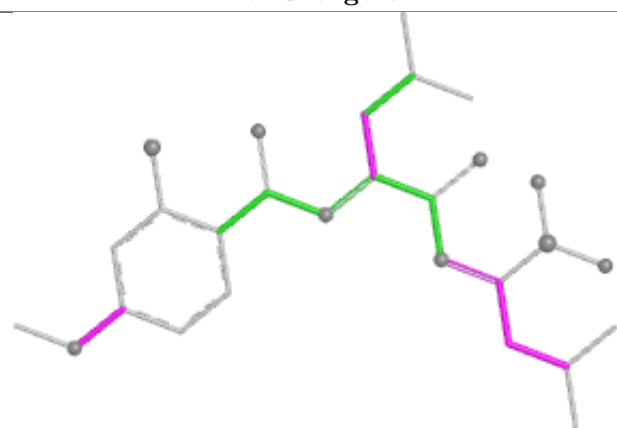
Ligand JT7 L 301



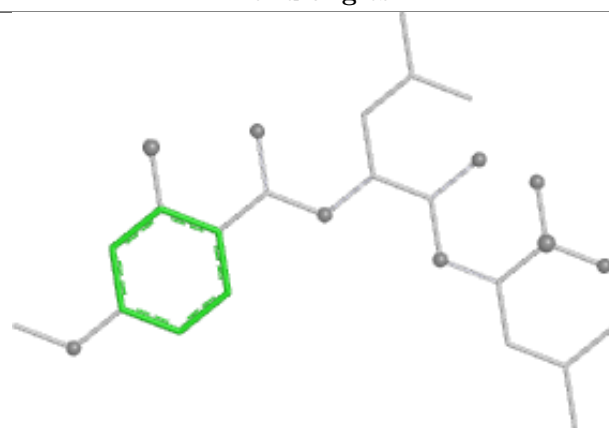
Bond lengths



Bond angles

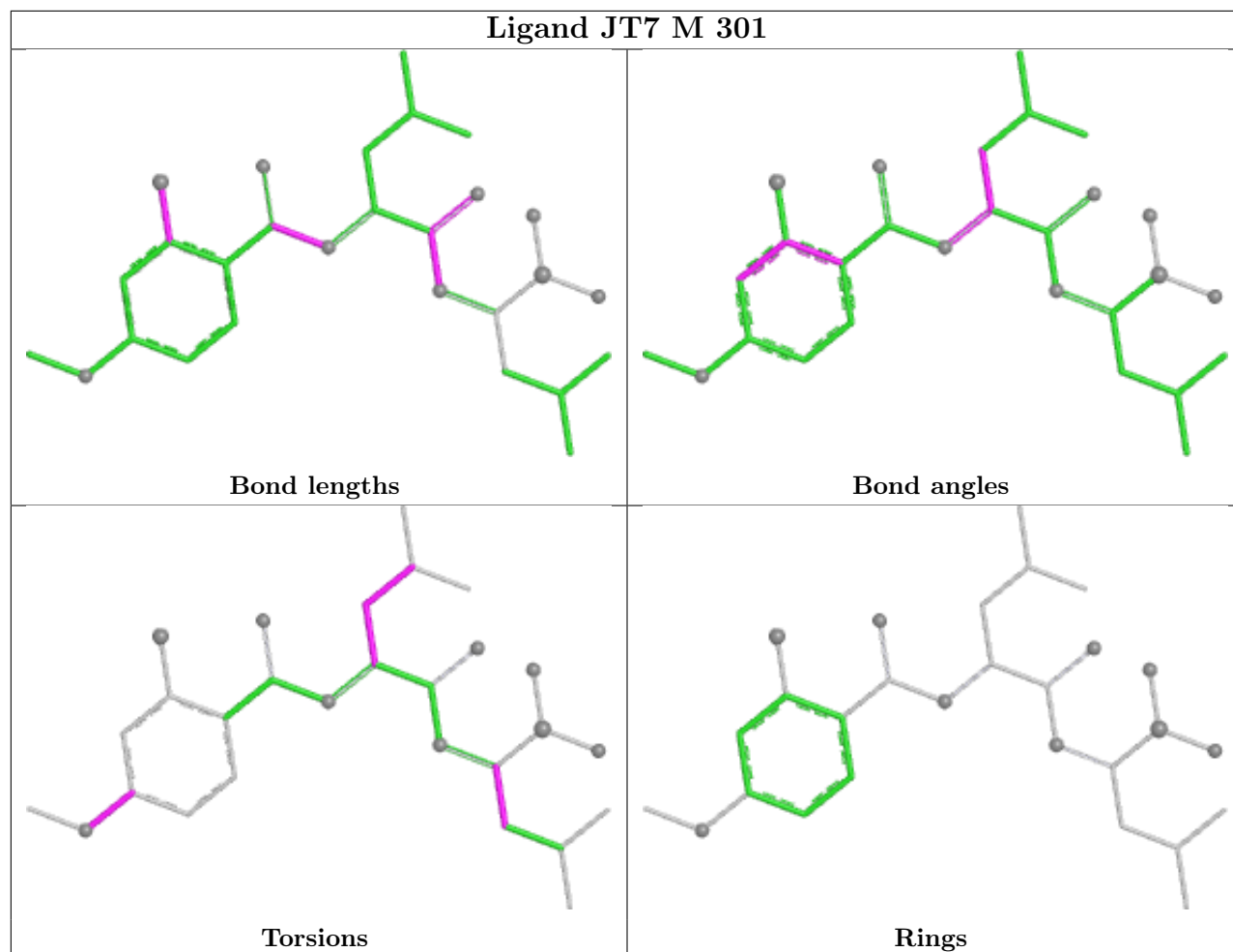


Torsions

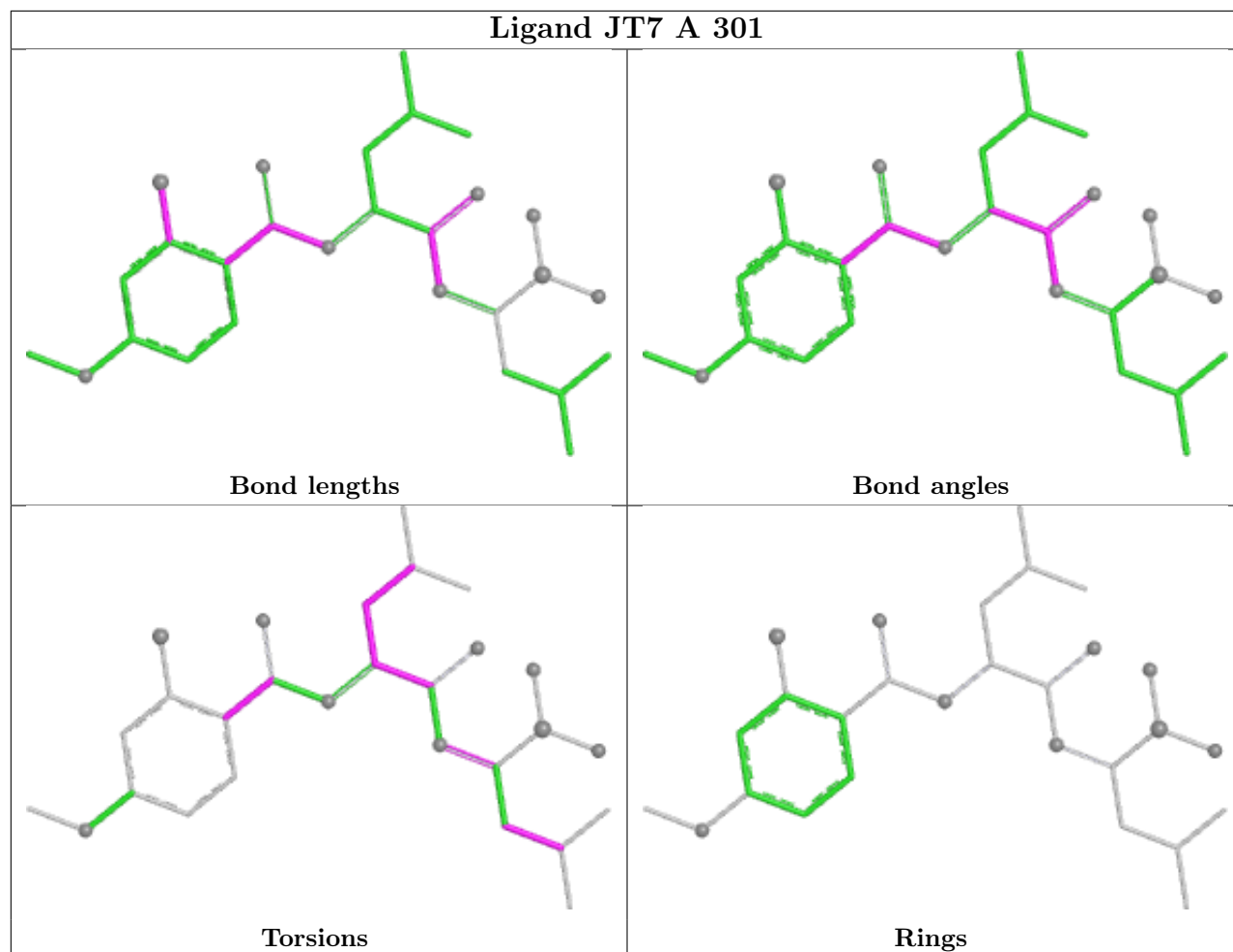


Rings

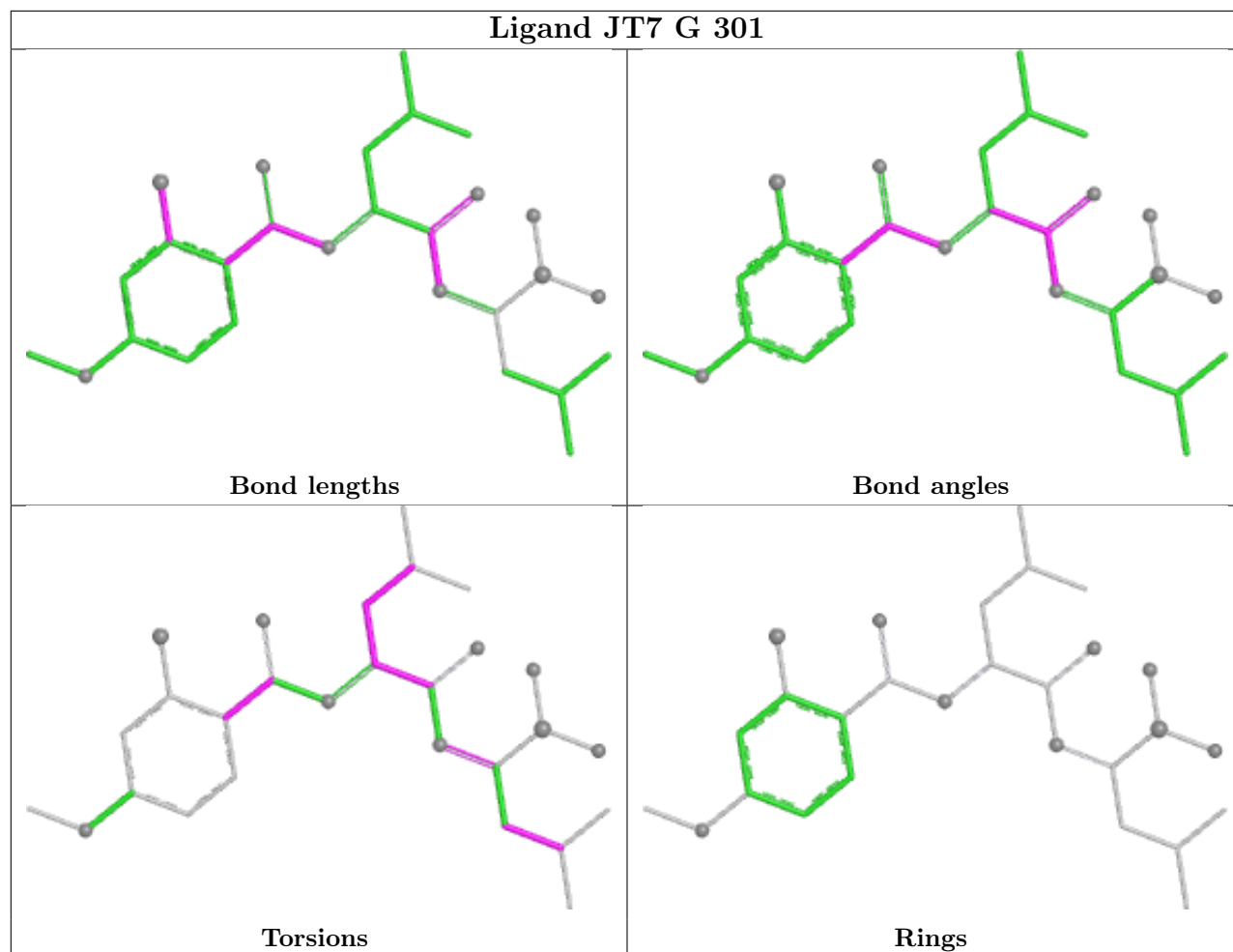
Ligand JT7 M 301



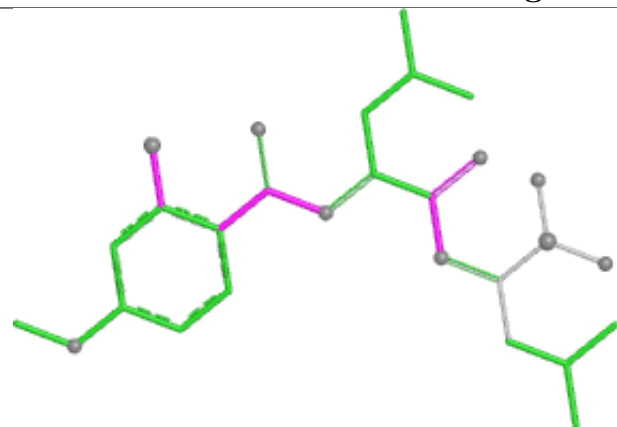
Ligand JT7 A 301



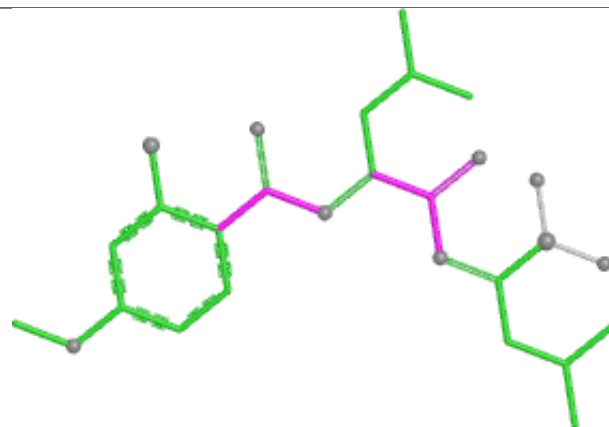
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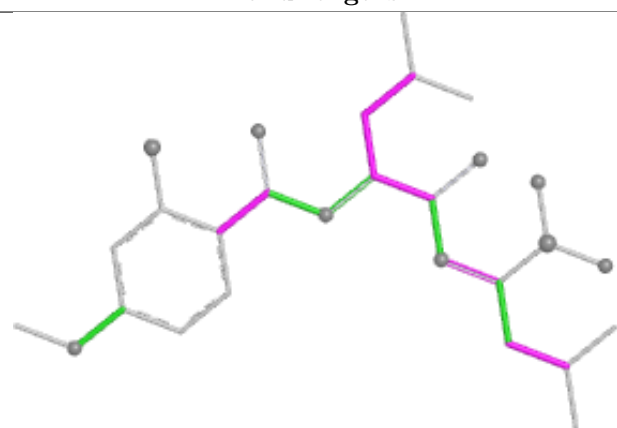
Ligand JT7 C 301



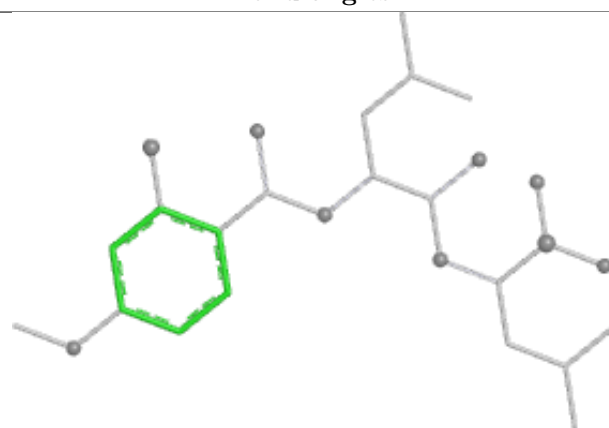
Bond lengths



Bond angles

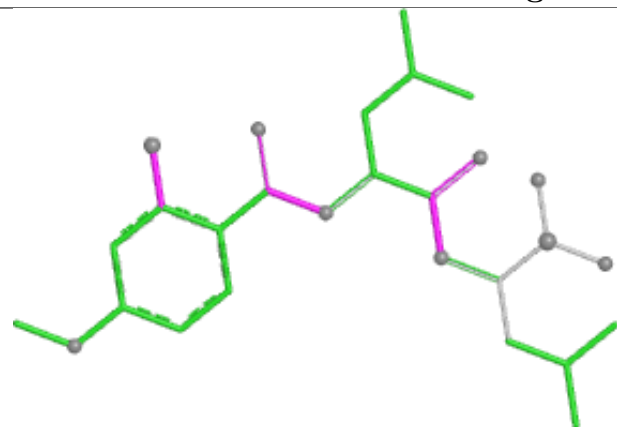


Torsions

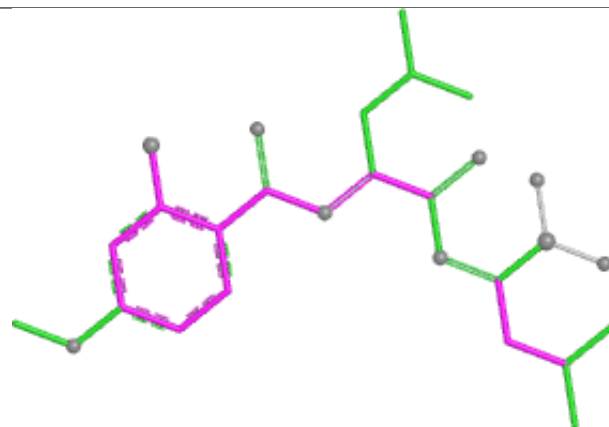


Rings

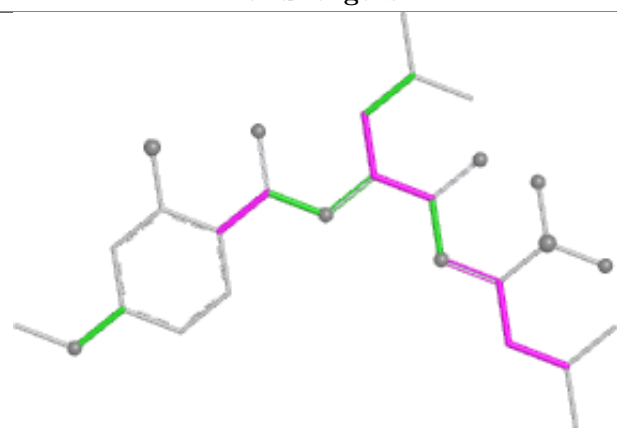
Ligand JT7 F 301



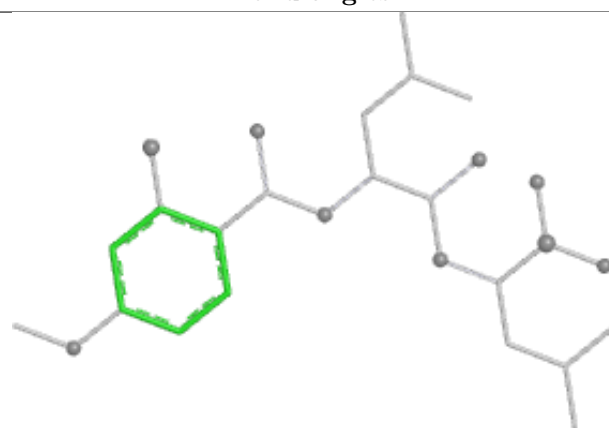
Bond lengths



Bond angles

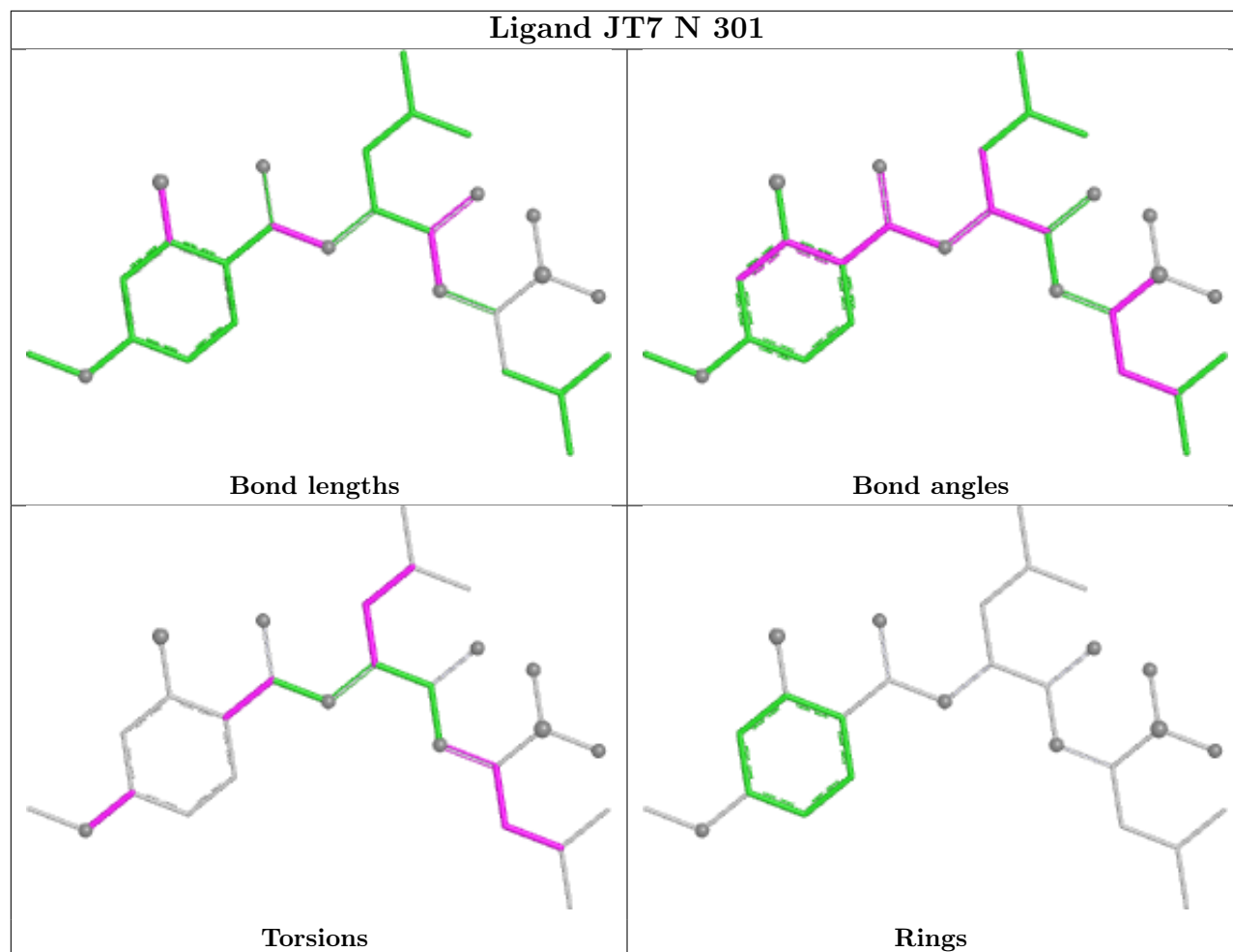


Torsions

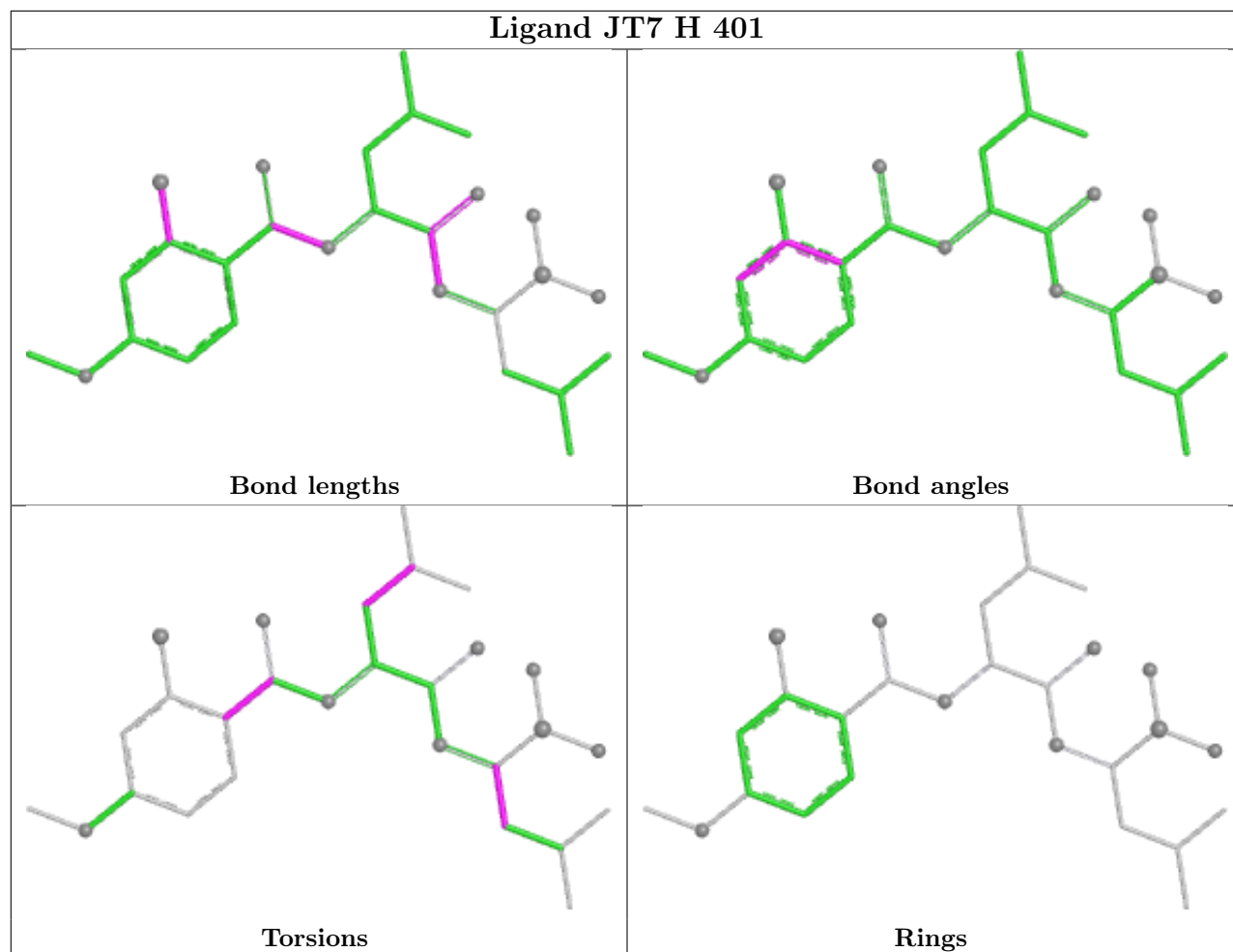


Rings

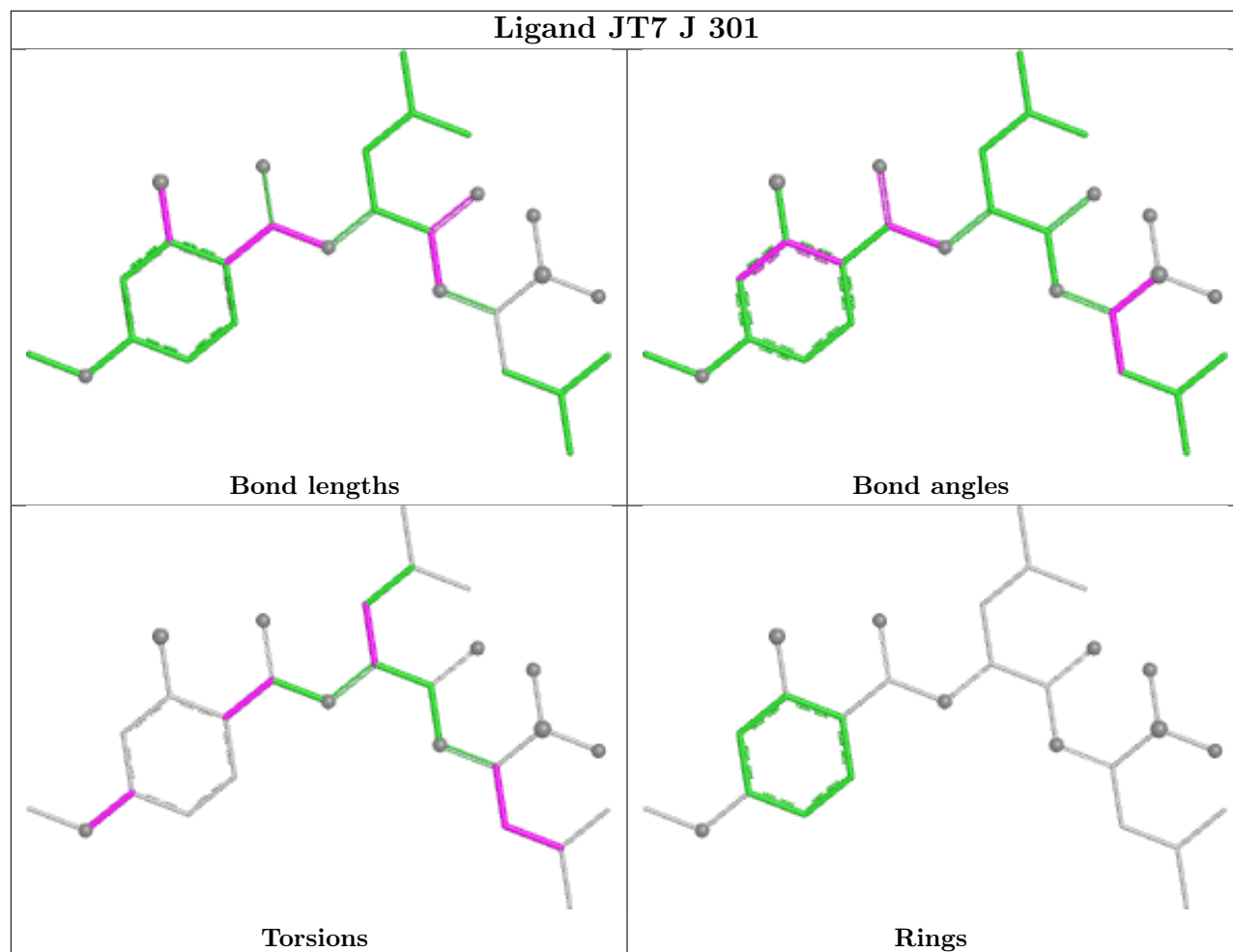
Ligand JT7 N 301



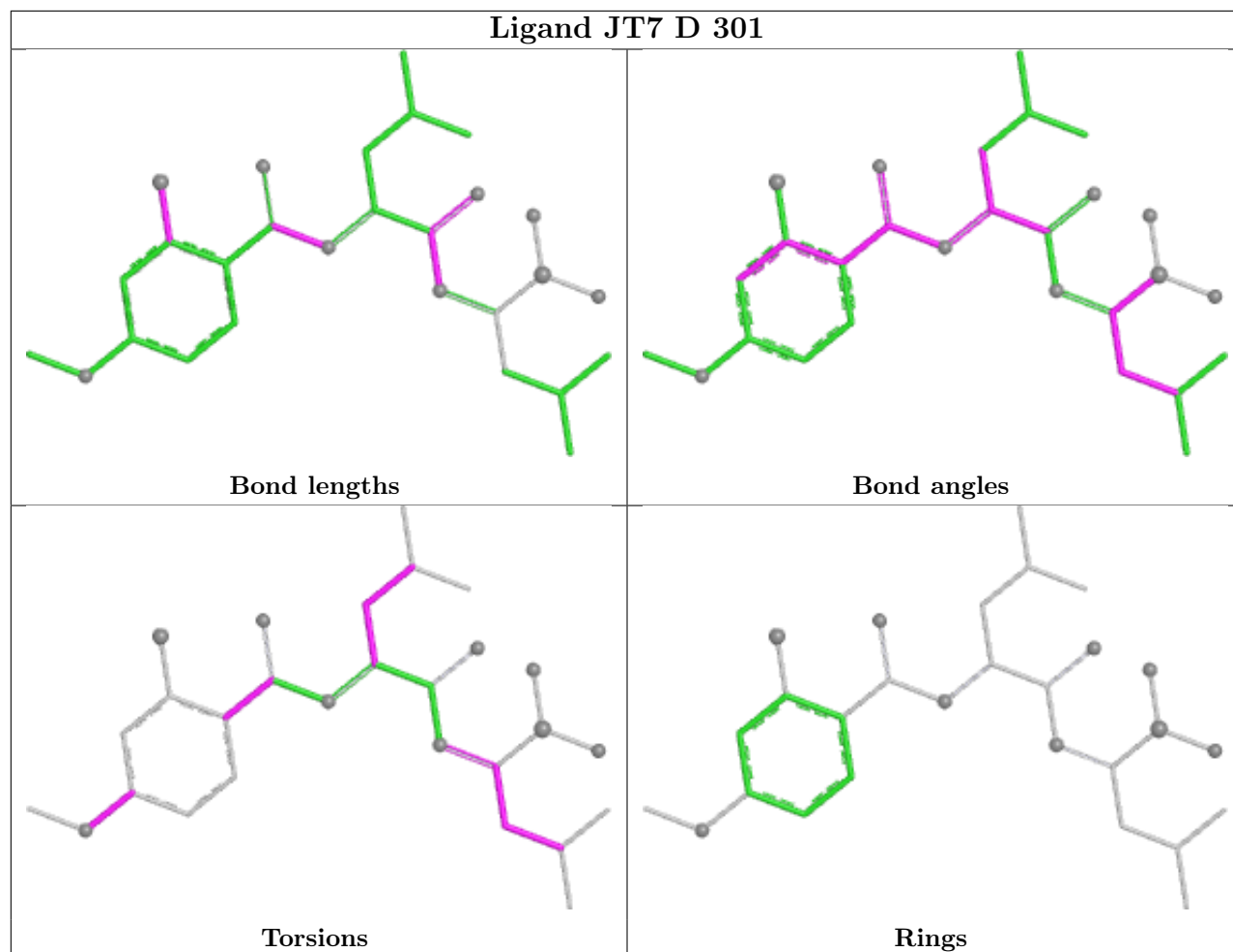
Ligand JT7 H 401



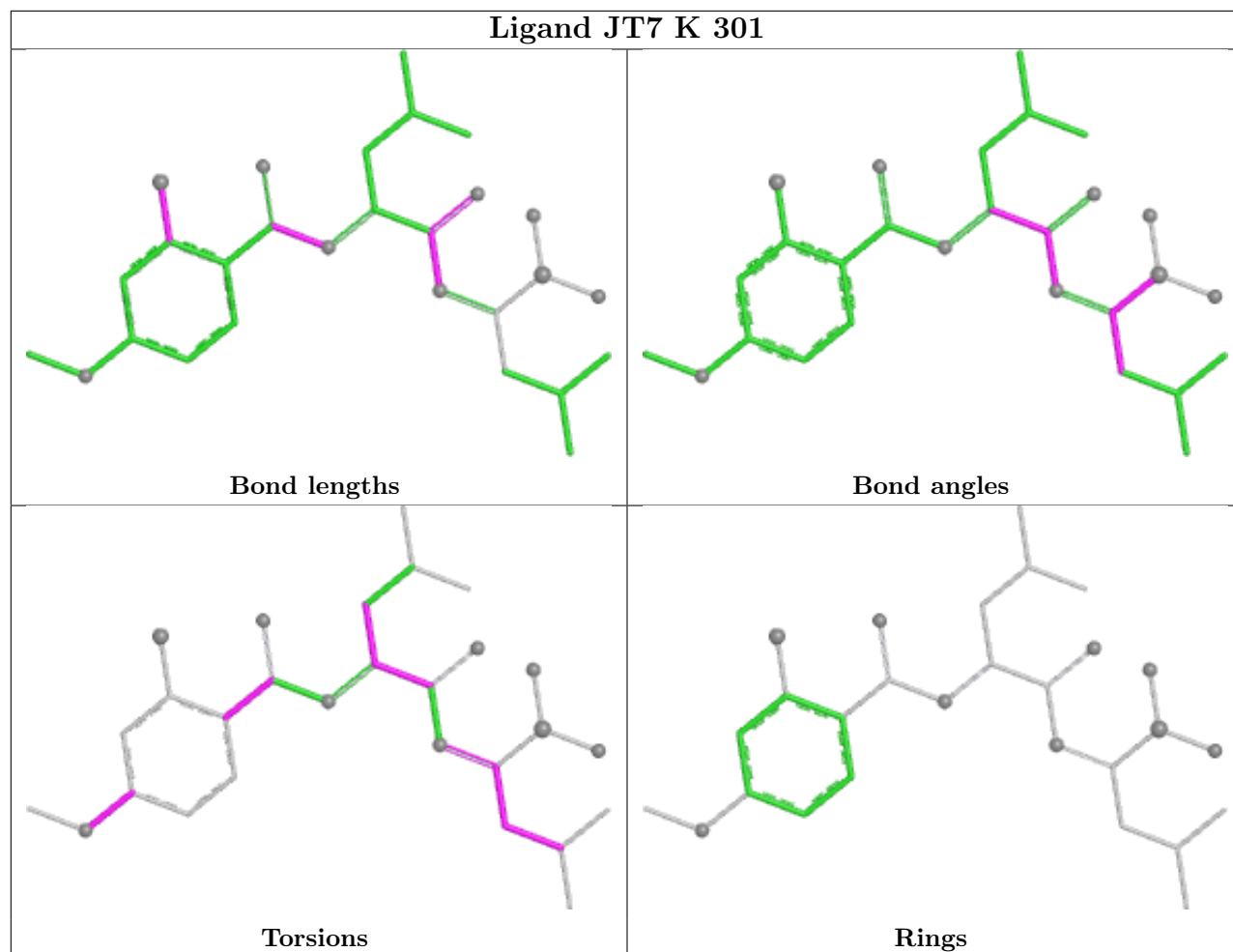
Ligand JT7 J 301

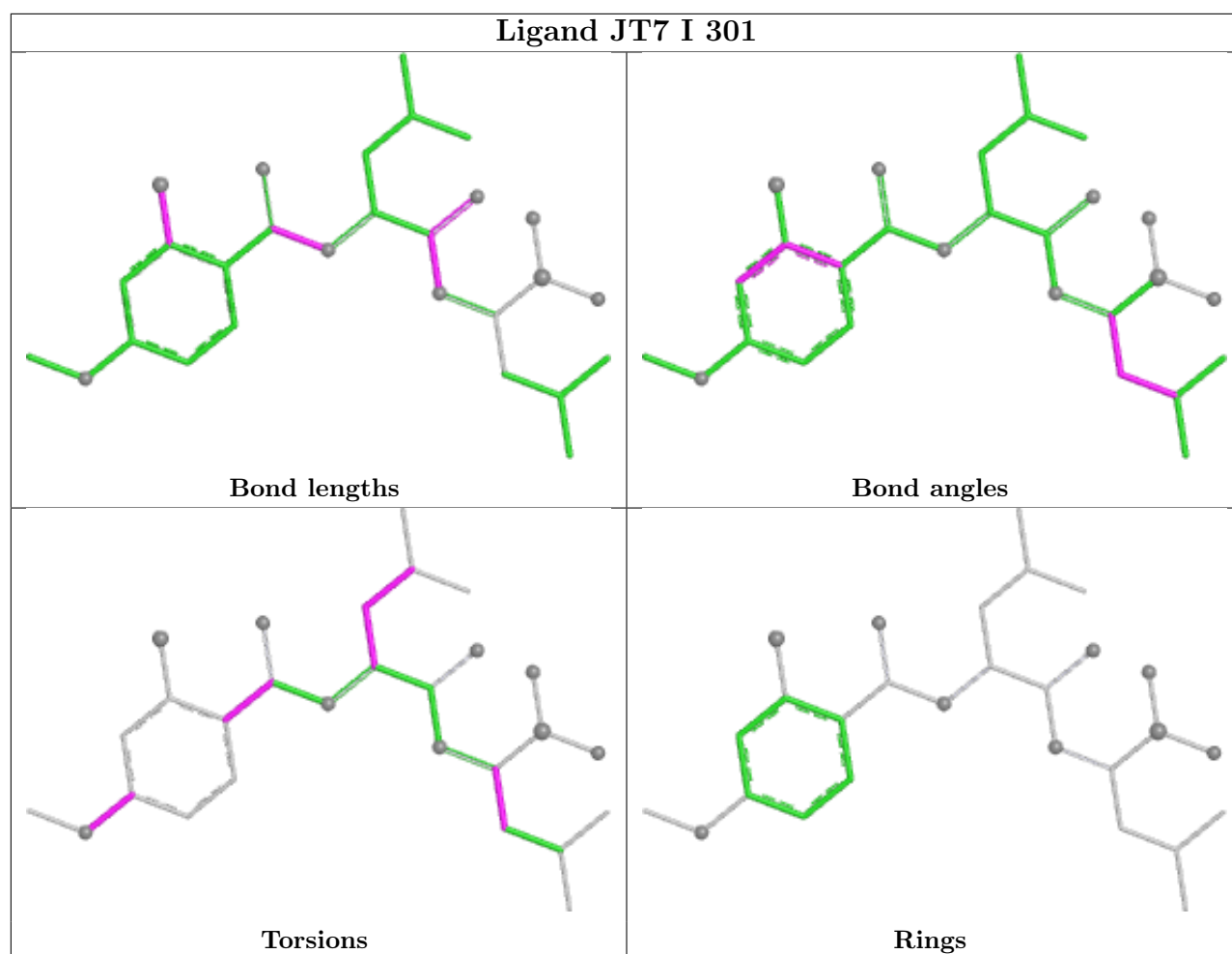


Ligand JT7 D 301



Ligand JT7 K 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	175/218 (80%)	0.48	5 (2%) 53 52	31, 47, 58, 65	0
1	B	178/218 (81%)	0.40	7 (3%) 43 42	32, 42, 55, 67	0
1	C	174/218 (79%)	0.36	9 (5%) 33 31	32, 42, 56, 67	0
1	D	174/218 (79%)	0.26	3 (1%) 69 68	33, 43, 57, 65	0
1	E	172/218 (78%)	0.23	2 (1%) 76 76	30, 41, 55, 84	0
1	F	174/218 (79%)	0.22	3 (1%) 69 68	23, 37, 48, 66	0
1	G	181/218 (83%)	0.33	8 (4%) 39 38	31, 42, 54, 67	0
1	H	180/218 (82%)	0.08	4 (2%) 62 61	24, 32, 45, 62	0
1	I	178/218 (81%)	0.22	2 (1%) 78 77	21, 35, 49, 61	0
1	J	175/218 (80%)	0.28	6 (3%) 48 47	28, 39, 49, 58	0
1	K	175/218 (80%)	0.17	3 (1%) 69 68	23, 35, 45, 54	0
1	L	174/218 (79%)	0.24	2 (1%) 78 77	27, 37, 48, 53	0
1	M	177/218 (81%)	0.29	4 (2%) 61 60	26, 36, 53, 67	0
1	N	172/218 (78%)	0.10	1 (0%) 85 85	20, 35, 45, 55	0
All	All	2459/3052 (80%)	0.26	59 (2%) 59 59	20, 39, 53, 84	0

The worst 5 of 59 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	K	67	TYR	4.4
1	L	183	ALA	4.1
1	G	146	ALA	3.7
1	C	191	LEU	3.6
1	B	66	PHE	3.6

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

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

6.3 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

6.4 Ligands ⓘ

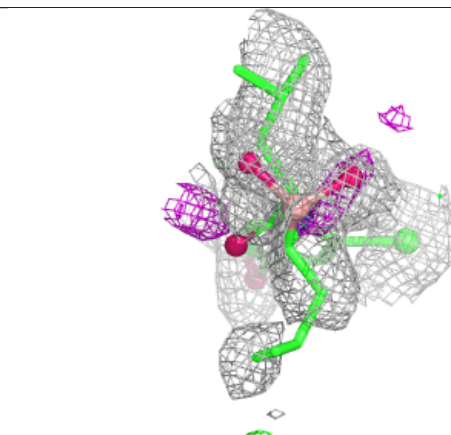
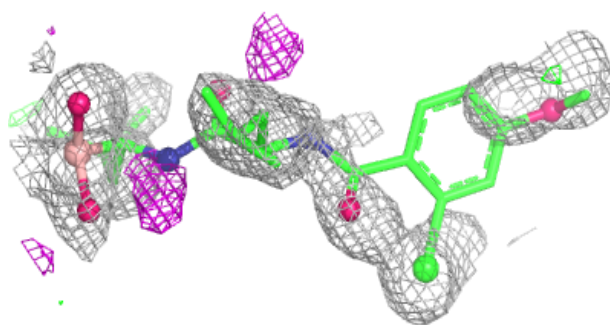
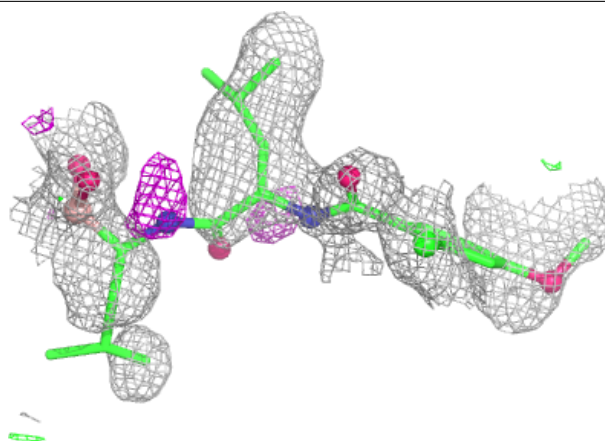
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
2	JT7	M	301	28/28	0.92	0.13	39,51,75,78	0
2	JT7	G	301	28/28	0.94	0.10	40,49,62,64	0
2	JT7	J	301	28/28	0.94	0.12	39,49,70,88	0
2	JT7	L	301	28/28	0.94	0.12	40,45,63,67	0
2	JT7	C	301	28/28	0.94	0.12	42,51,59,63	0
2	JT7	F	301	28/28	0.95	0.09	39,48,64,70	0
2	JT7	K	301	28/28	0.95	0.10	34,40,49,53	0
2	JT7	D	301	28/28	0.95	0.13	54,64,82,85	0
2	JT7	I	301	28/28	0.95	0.09	41,45,58,59	0
2	JT7	N	301	28/28	0.95	0.13	40,54,63,65	0
2	JT7	E	301	28/28	0.96	0.09	43,51,70,76	0
2	JT7	H	401	28/28	0.96	0.08	34,41,52,54	0
2	JT7	A	301	28/28	0.97	0.11	48,62,80,81	0
2	JT7	B	301	28/28	0.97	0.09	37,50,64,72	0

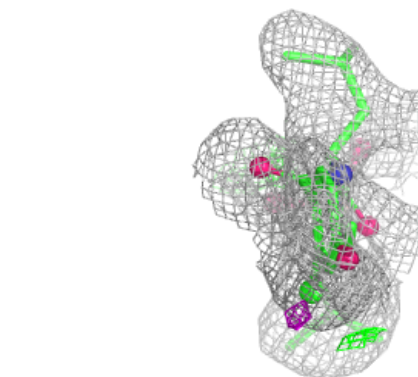
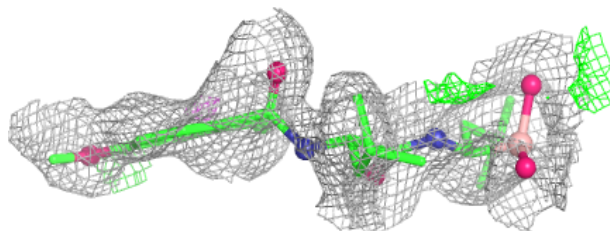
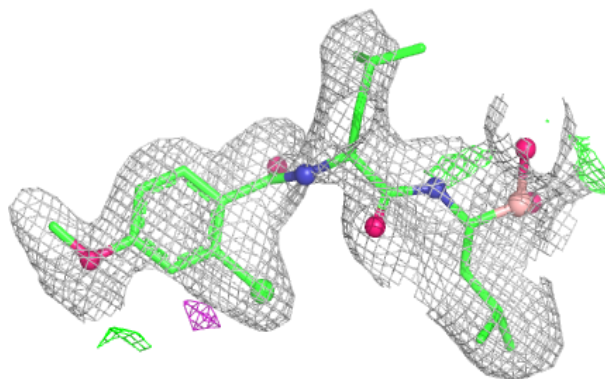
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around JT7 M 301:

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

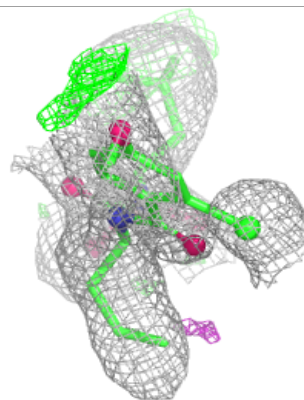
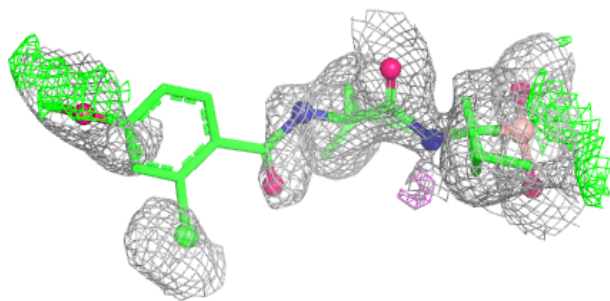
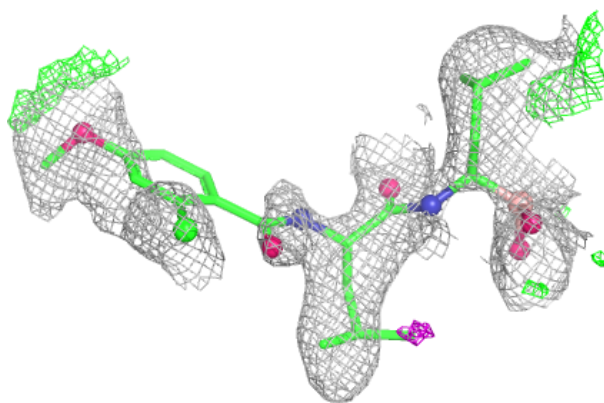
**Electron density around JT7 G 301:**

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 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

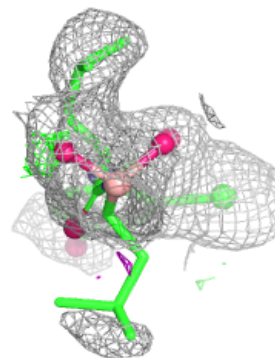
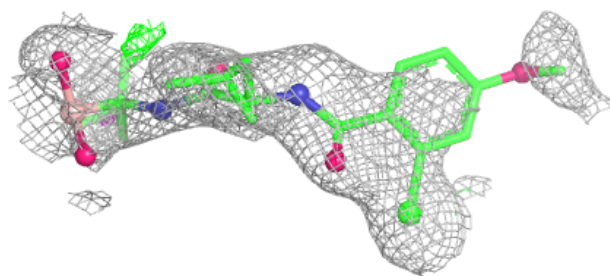
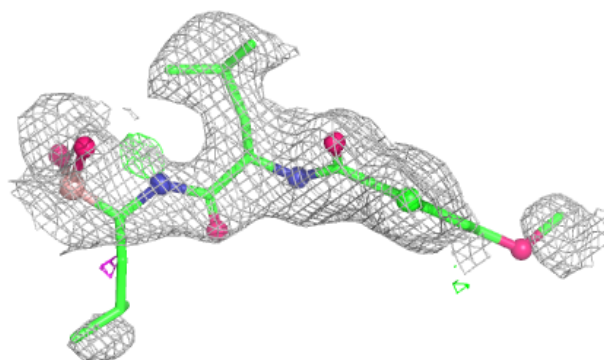


Electron density around JT7 J 301:

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 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

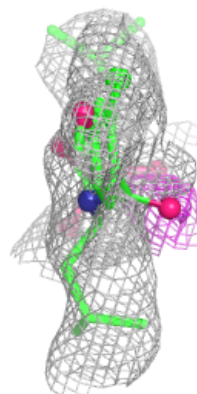
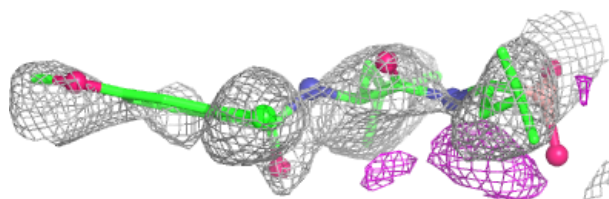
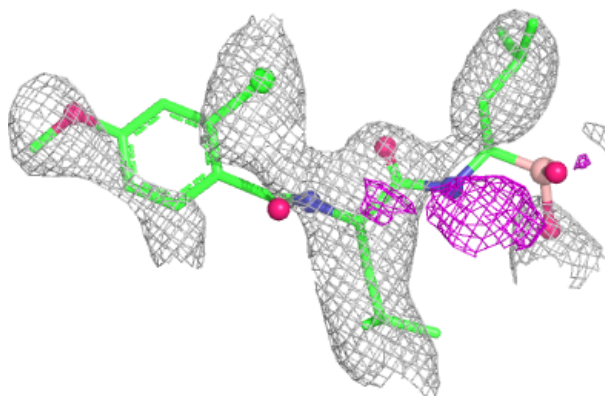
**Electron density around JT7 L 301:**

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 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

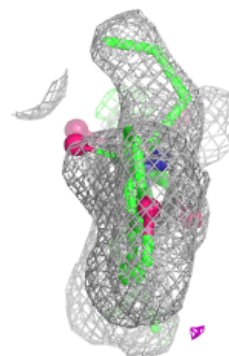
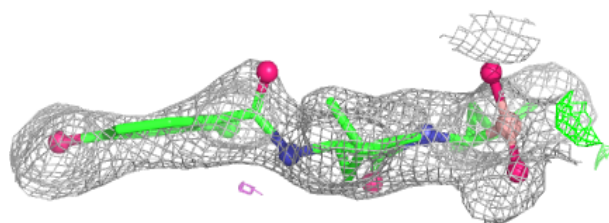
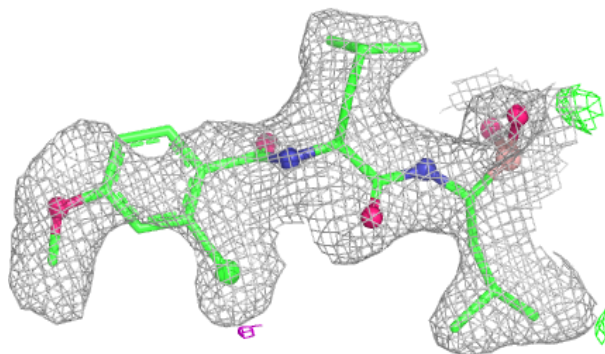


Electron density around JT7 C 301:

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 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

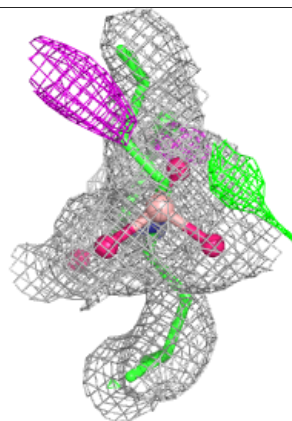
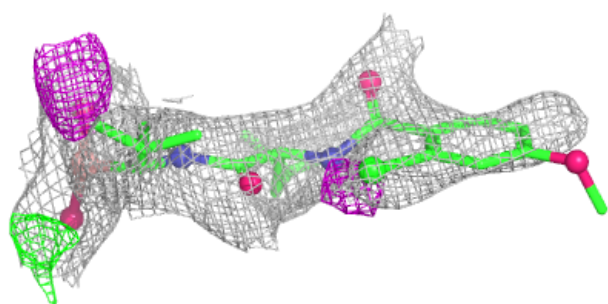
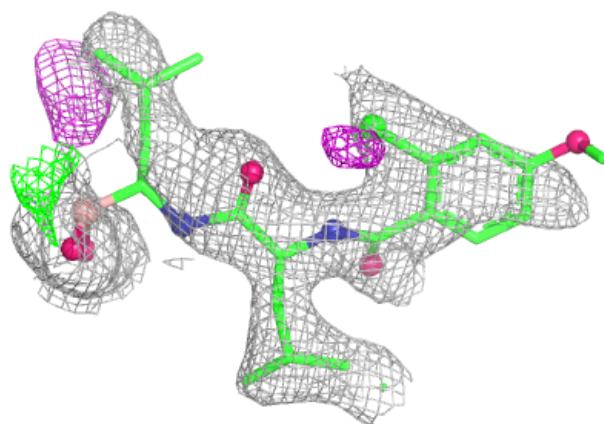
**Electron density around JT7 F 301:**

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 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

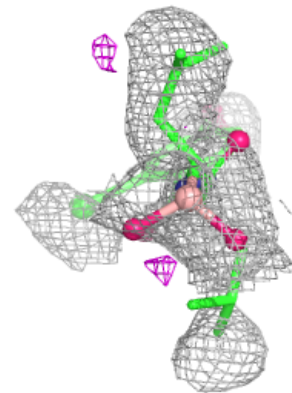
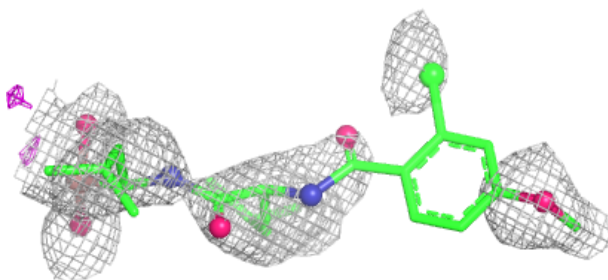
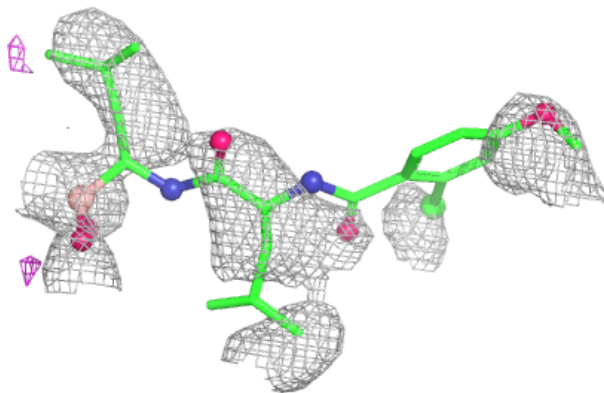


Electron density around JT7 K 301:

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 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

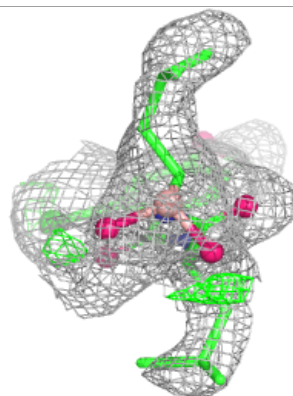
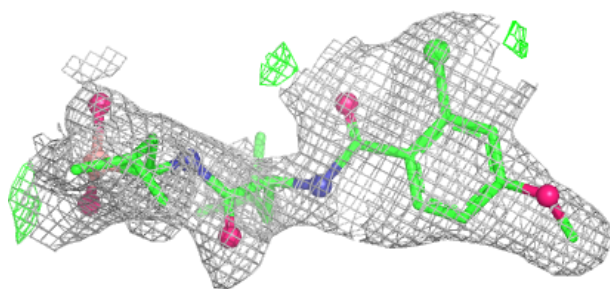
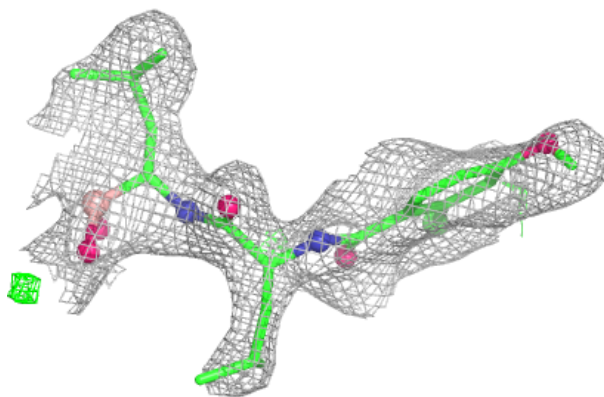
**Electron density around JT7 D 301:**

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 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

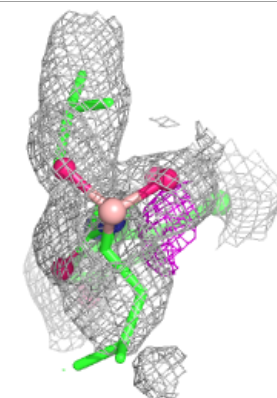
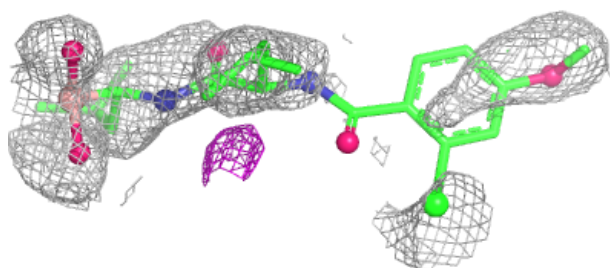
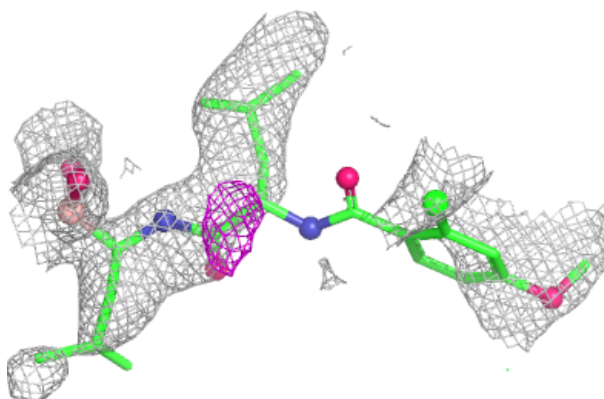


Electron density around JT7 I 301:

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

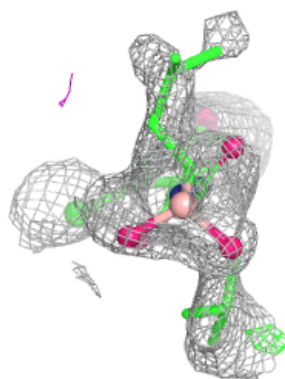
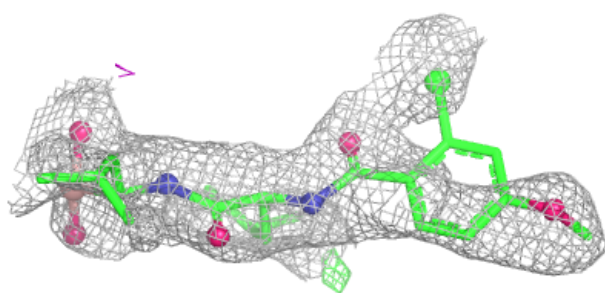
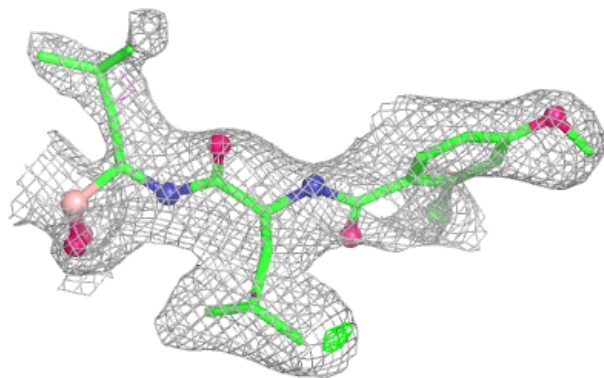
**Electron density around JT7 N 301:**

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 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

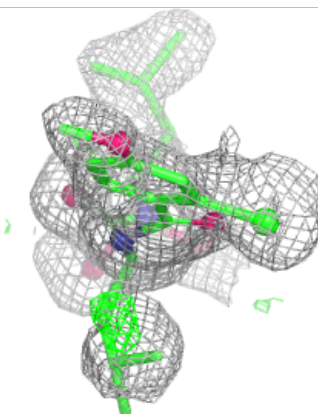
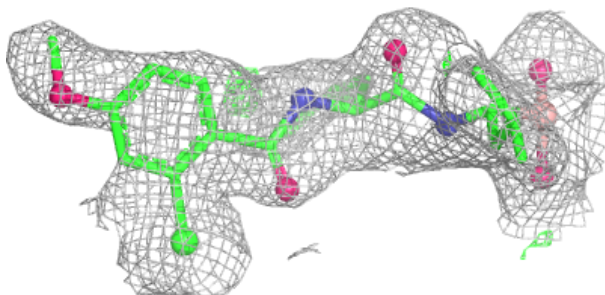
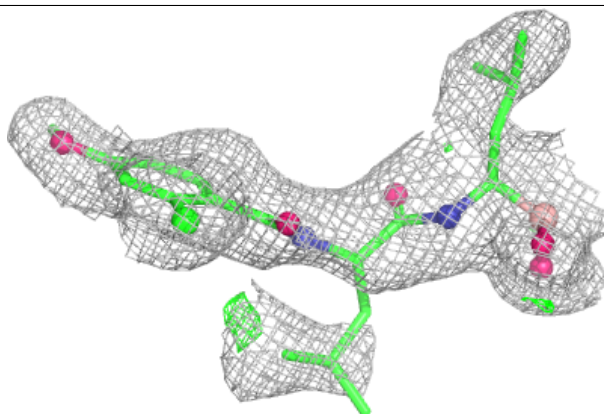


Electron density around JT7 E 301:

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

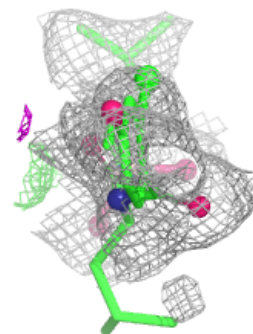
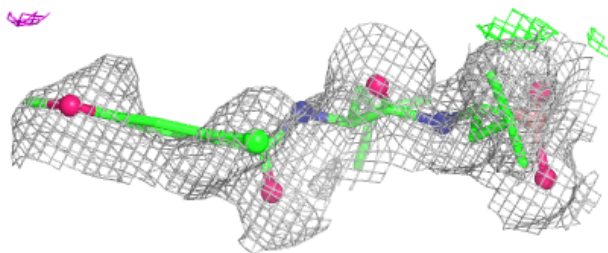
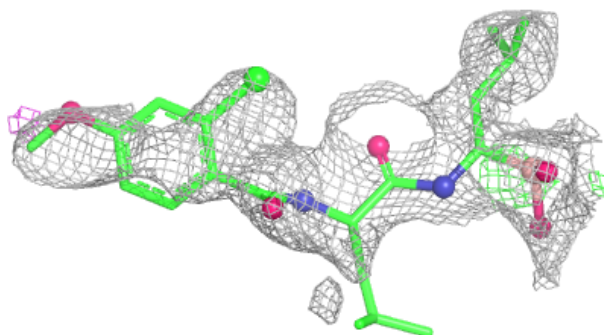
**Electron density around JT7 H 401:**

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 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

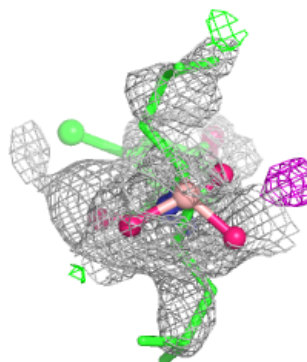
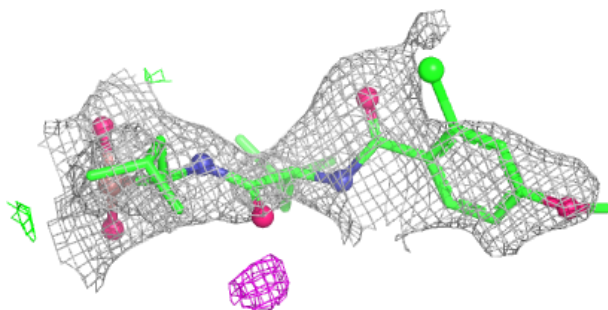
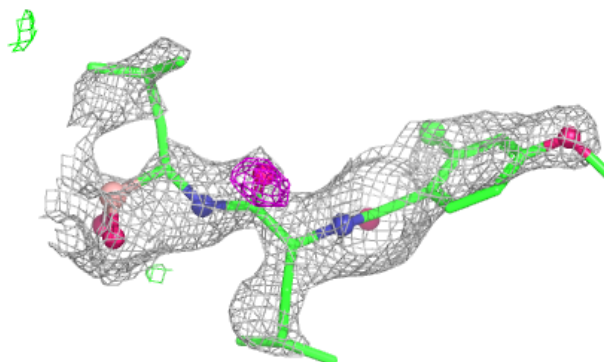


Electron density around JT7 A 301:

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

**Electron density around JT7 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)



6.5 Other polymers [i](#)

There are no such residues in this entry.