



wwPDB X-ray Structure Validation Summary Report ⓘ

Sep 14, 2026 – 10:21 AM EDT

PDB ID : 11OP / pdb_000011op
Title : Crystal Structure of M. tuberculosis ClpP1P2 bound to ONC201
Authors : Burnside, C.M.; Fei, F.; Schmitz, K.R.; Sello, J.K.
Deposited on : 2026-03-06
Resolution : 3.11 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	:	9.0.015 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.50

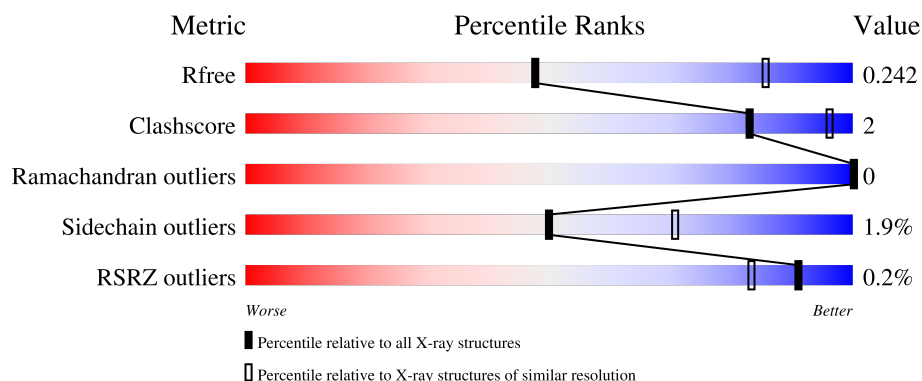
1 Overall quality at a glance ⓘ

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.11 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	1816 (3.14-3.10)
Clashscore	190562	1906 (3.14-3.10)
Ramachandran outliers	187476	1802 (3.14-3.10)
Sidechain outliers	187428	1802 (3.14-3.10)
RSRZ outliers	180081	1816 (3.14-3.10)

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	214	 86% 6% 8%
1	B	214	 87% 6% 7%
1	C	214	 87% 7% 6%
1	D	214	 87% 5% 7%
1	E	214	 85% 8% 7%

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Mol	Chain	Length	Quality of chain
1	F	214	 87% 5% 8%
1	G	214	 88% 5% 7%
2	H	194	 87% 9%
2	I	194	 83% 8% 9%
2	J	194	 84% 8% 8%
2	K	194	 85% 8% 7%
2	L	194	 83% 8% 9%
2	M	194	 80% 12% 7%
2	N	194	 86% 5% 9%

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
3	BEZ	C	801	-	X	-	-
3	BEZ	G	801	-	X	-	-
4	LEU	B	803	-	X	-	-

2 Entry composition

There are 12 unique types of molecules in this entry. The entry contains 41180 atoms, of which 20461 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 2.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	197	Total	C	H	N	O	S	0	0	0
			3023	951	1511	257	296	8			
1	B	199	Total	C	H	N	O	S	0	0	0
			3035	957	1515	256	299	8			
1	C	202	Total	C	H	N	O	S	0	0	0
			3101	973	1552	265	303	8			
1	D	198	Total	C	H	N	O	S	0	0	0
			3030	954	1513	258	297	8			
1	E	200	Total	C	H	N	O	S	0	0	0
			3039	957	1514	260	300	8			
1	F	197	Total	C	H	N	O	S	0	0	0
			2998	946	1496	254	294	8			
1	G	200	Total	C	H	N	O	S	0	0	0
			3063	963	1532	260	300	8			

There are 84 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	12	MET	-	initiating methionine	UNP P9WPC3
A	215	ALA	-	expression tag	UNP P9WPC3
A	216	ALA	-	expression tag	UNP P9WPC3
A	217	ALA	-	expression tag	UNP P9WPC3
A	218	LEU	-	expression tag	UNP P9WPC3
A	219	GLU	-	expression tag	UNP P9WPC3
A	220	HIS	-	expression tag	UNP P9WPC3
A	221	HIS	-	expression tag	UNP P9WPC3
A	222	HIS	-	expression tag	UNP P9WPC3
A	223	HIS	-	expression tag	UNP P9WPC3
A	224	HIS	-	expression tag	UNP P9WPC3
A	225	HIS	-	expression tag	UNP P9WPC3
B	12	MET	-	initiating methionine	UNP P9WPC3
B	215	ALA	-	expression tag	UNP P9WPC3
B	216	ALA	-	expression tag	UNP P9WPC3

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Chain	Residue	Modelled	Actual	Comment	Reference
B	217	ALA	-	expression tag	UNP P9WPC3
B	218	LEU	-	expression tag	UNP P9WPC3
B	219	GLU	-	expression tag	UNP P9WPC3
B	220	HIS	-	expression tag	UNP P9WPC3
B	221	HIS	-	expression tag	UNP P9WPC3
B	222	HIS	-	expression tag	UNP P9WPC3
B	223	HIS	-	expression tag	UNP P9WPC3
B	224	HIS	-	expression tag	UNP P9WPC3
B	225	HIS	-	expression tag	UNP P9WPC3
C	12	MET	-	initiating methionine	UNP P9WPC3
C	215	ALA	-	expression tag	UNP P9WPC3
C	216	ALA	-	expression tag	UNP P9WPC3
C	217	ALA	-	expression tag	UNP P9WPC3
C	218	LEU	-	expression tag	UNP P9WPC3
C	219	GLU	-	expression tag	UNP P9WPC3
C	220	HIS	-	expression tag	UNP P9WPC3
C	221	HIS	-	expression tag	UNP P9WPC3
C	222	HIS	-	expression tag	UNP P9WPC3
C	223	HIS	-	expression tag	UNP P9WPC3
C	224	HIS	-	expression tag	UNP P9WPC3
C	225	HIS	-	expression tag	UNP P9WPC3
D	12	MET	-	initiating methionine	UNP P9WPC3
D	215	ALA	-	expression tag	UNP P9WPC3
D	216	ALA	-	expression tag	UNP P9WPC3
D	217	ALA	-	expression tag	UNP P9WPC3
D	218	LEU	-	expression tag	UNP P9WPC3
D	219	GLU	-	expression tag	UNP P9WPC3
D	220	HIS	-	expression tag	UNP P9WPC3
D	221	HIS	-	expression tag	UNP P9WPC3
D	222	HIS	-	expression tag	UNP P9WPC3
D	223	HIS	-	expression tag	UNP P9WPC3
D	224	HIS	-	expression tag	UNP P9WPC3
D	225	HIS	-	expression tag	UNP P9WPC3
E	12	MET	-	initiating methionine	UNP P9WPC3
E	215	ALA	-	expression tag	UNP P9WPC3
E	216	ALA	-	expression tag	UNP P9WPC3
E	217	ALA	-	expression tag	UNP P9WPC3
E	218	LEU	-	expression tag	UNP P9WPC3
E	219	GLU	-	expression tag	UNP P9WPC3
E	220	HIS	-	expression tag	UNP P9WPC3
E	221	HIS	-	expression tag	UNP P9WPC3
E	222	HIS	-	expression tag	UNP P9WPC3

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Chain	Residue	Modelled	Actual	Comment	Reference
E	223	HIS	-	expression tag	UNP P9WPC3
E	224	HIS	-	expression tag	UNP P9WPC3
E	225	HIS	-	expression tag	UNP P9WPC3
F	12	MET	-	initiating methionine	UNP P9WPC3
F	215	ALA	-	expression tag	UNP P9WPC3
F	216	ALA	-	expression tag	UNP P9WPC3
F	217	ALA	-	expression tag	UNP P9WPC3
F	218	LEU	-	expression tag	UNP P9WPC3
F	219	GLU	-	expression tag	UNP P9WPC3
F	220	HIS	-	expression tag	UNP P9WPC3
F	221	HIS	-	expression tag	UNP P9WPC3
F	222	HIS	-	expression tag	UNP P9WPC3
F	223	HIS	-	expression tag	UNP P9WPC3
F	224	HIS	-	expression tag	UNP P9WPC3
F	225	HIS	-	expression tag	UNP P9WPC3
G	12	MET	-	initiating methionine	UNP P9WPC3
G	215	ALA	-	expression tag	UNP P9WPC3
G	216	ALA	-	expression tag	UNP P9WPC3
G	217	ALA	-	expression tag	UNP P9WPC3
G	218	LEU	-	expression tag	UNP P9WPC3
G	219	GLU	-	expression tag	UNP P9WPC3
G	220	HIS	-	expression tag	UNP P9WPC3
G	221	HIS	-	expression tag	UNP P9WPC3
G	222	HIS	-	expression tag	UNP P9WPC3
G	223	HIS	-	expression tag	UNP P9WPC3
G	224	HIS	-	expression tag	UNP P9WPC3
G	225	HIS	-	expression tag	UNP P9WPC3

- Molecule 2 is a protein called ATP-dependent Clp protease proteolytic subunit 1.

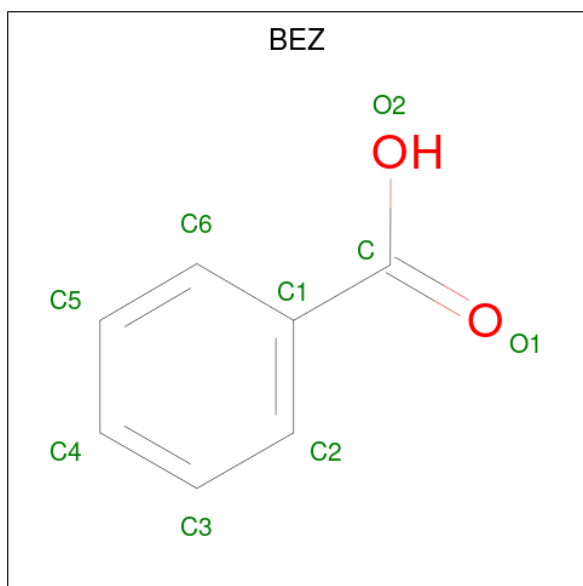
Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
2	H	176	Total	C	H	N	O	S	0	0	0
			2626	840	1303	221	253	9			
2	I	176	Total	C	H	N	O	S	0	0	0
			2626	840	1303	221	253	9			
2	J	178	Total	C	H	N	O	S	0	0	0
			2661	849	1321	226	256	9			
2	K	180	Total	C	H	N	O	S	0	0	0
			2661	853	1317	222	260	9			
2	L	177	Total	C	H	N	O	S	0	0	0
			2636	843	1306	222	256	9			
2	M	180	Total	C	H	N	O	S	0	0	0
			2616	844	1285	222	256	9			

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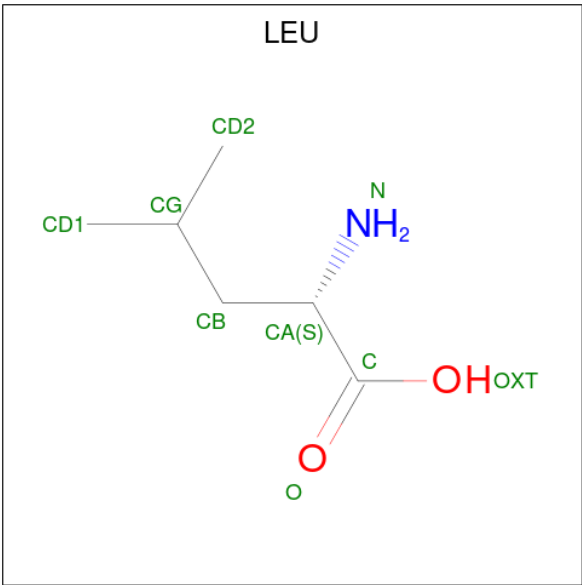
Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
2	N	176	Total	C	H	N	O	S	0	0	0
			2629	840	1304	221	255	9			

- Molecule 3 is BENZOIC ACID (CCD ID: BEZ) (formula: $C_7H_6O_2$).



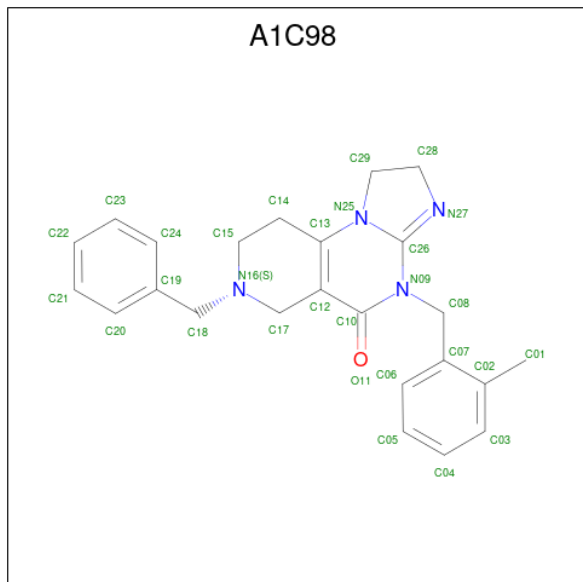
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	A	1	Total	C	H	O	0	0
			13	7	5	1		
3	B	1	Total	C	H	O	0	0
			13	7	5	1		
3	C	1	Total	C	H	O	0	0
			13	7	5	1		
3	D	1	Total	C	H	O	0	0
			13	7	5	1		
3	E	1	Total	C	H	O	0	0
			13	7	5	1		
3	F	1	Total	C	H	O	0	0
			13	7	5	1		
3	G	1	Total	C	H	O	0	0
			13	7	5	1		

- Molecule 4 is LEUCINE (CCD ID: LEU) (formula: $C_6H_{13}NO_2$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
4	A	1	Total	C	H	N	O	0	0
			19	6	11	1	1		
4	A	1	Total	C	H	N	O	0	0
			20	6	11	1	2		
4	B	1	Total	C	H	N	O	0	0
			19	6	11	1	1		
4	B	1	Total	C	H	N	O	0	0
			20	6	11	1	2		
4	C	1	Total	C	H	N	O	0	0
			19	6	11	1	1		
4	C	1	Total	C	H	N	O	0	0
			20	6	11	1	2		
4	D	1	Total	C	H	N	O	0	0
			19	6	11	1	1		
4	D	1	Total	C	H	N	O	0	0
			20	6	11	1	2		
4	E	1	Total	C	H	N	O	0	0
			19	6	11	1	1		
4	E	1	Total	C	H	N	O	0	0
			20	6	11	1	2		
4	F	1	Total	C	H	N	O	0	0
			19	6	11	1	1		
4	F	1	Total	C	H	N	O	0	0
			20	6	11	1	2		
4	G	1	Total	C	H	N	O	0	0
			19	6	11	1	1		
4	G	1	Total	C	H	N	O	0	0
			20	6	11	1	2		

- Molecule 5 is Dordaviprone (CCD ID: A1C98) (formula: $C_{24}H_{26}N_4O$) (labeled as "Ligand of Interest" by depositor).



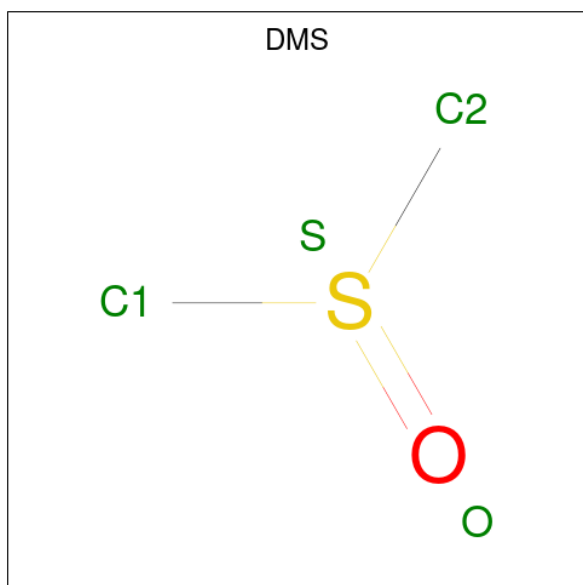
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
5	A	1	Total	C	H	N	O	0	0
			55	24	26	4	1		
5	B	1	Total	C	H	N	O	0	0
			55	24	26	4	1		
5	C	1	Total	C	H	N	O	0	0
			55	24	26	4	1		
5	D	1	Total	C	H	N	O	0	0
			55	24	26	4	1		
5	E	1	Total	C	H	N	O	0	0
			55	24	26	4	1		
5	E	1	Total	C	H	N	O	0	0
			55	24	26	4	1		
5	G	1	Total	C	H	N	O	0	0
			55	24	26	4	1		
5	H	1	Total	C	H	N	O	0	0
			55	24	26	4	1		
5	I	1	Total	C	H	N	O	0	0
			55	24	26	4	1		
5	J	1	Total	C	H	N	O	0	0
			55	24	26	4	1		
5	K	1	Total	C	H	N	O	0	0
			55	24	26	4	1		
5	L	1	Total	C	H	N	O	0	0
			55	24	26	4	1		

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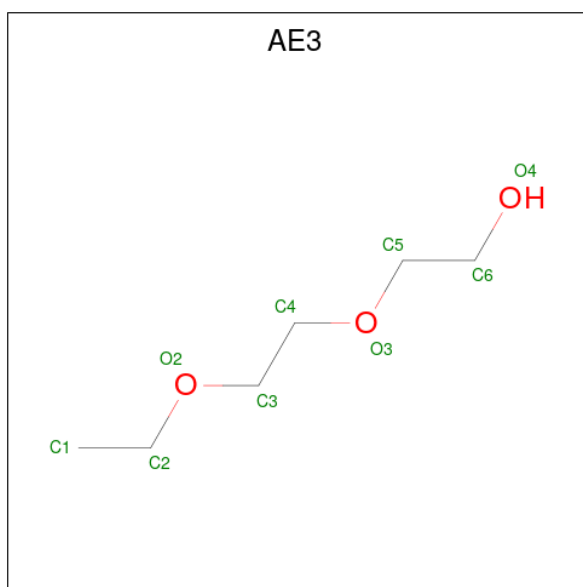
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
5	M	1	Total	C	H	N	O	0	0
			55	24	26	4	1		
5	N	1	Total	C	H	N	O	0	0
			55	24	26	4	1		

- Molecule 6 is DIMETHYL SULFOXIDE (CCD ID: DMS) (formula: C_2H_6OS).



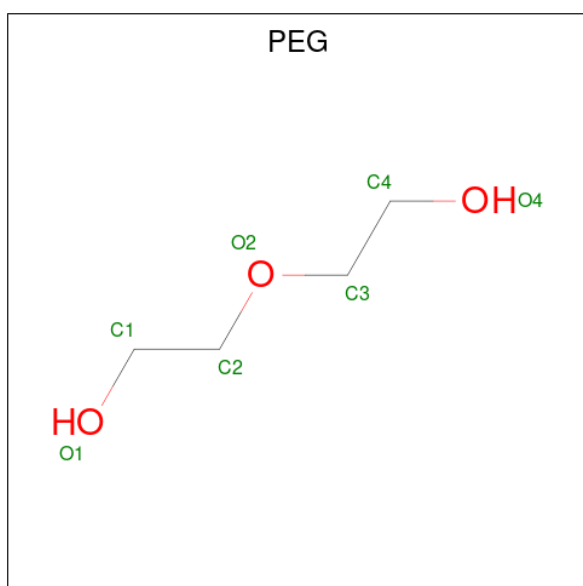
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
6	A	1	Total	C	H	O	S	0	0
			10	2	6	1	1		
6	B	1	Total	C	H	O	S	0	0
			10	2	6	1	1		
6	C	1	Total	C	H	O	S	0	0
			10	2	6	1	1		
6	D	1	Total	C	H	O	S	0	0
			10	2	6	1	1		
6	E	1	Total	C	H	O	S	0	0
			10	2	6	1	1		
6	F	1	Total	C	H	O	S	0	0
			10	2	6	1	1		
6	G	1	Total	C	H	O	S	0	0
			10	2	6	1	1		

- Molecule 7 is 2-(2-ETHOXYETHOXY)ETHANOL (CCD ID: AE3) (formula: $C_6H_{14}O_3$).



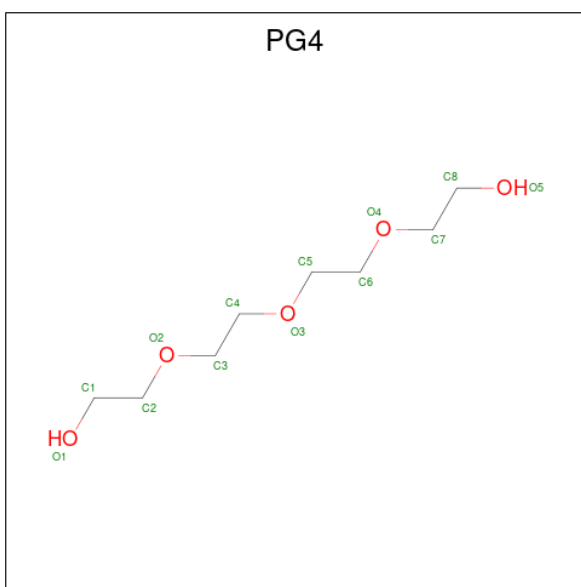
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
7	A	1	Total	C	H	O	0	0
			23	6	14	3		
7	D	1	Total	C	H	O	0	0
			23	6	14	3		

- Molecule 8 is DI(HYDROXYETHYL)ETHER (CCD ID: PEG) (formula: $C_4H_{10}O_3$).



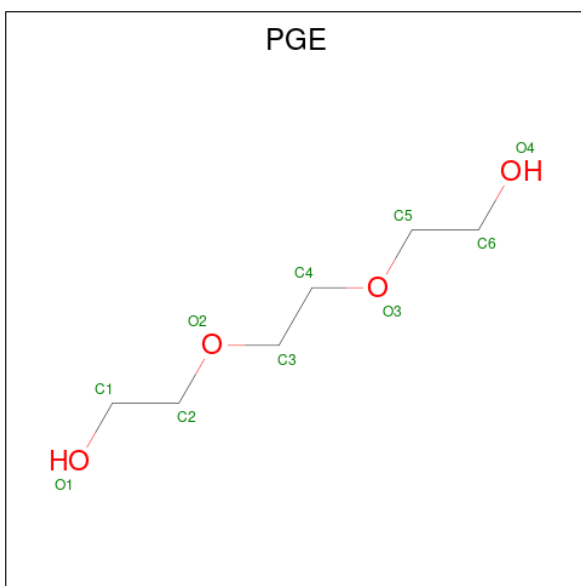
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
8	C	1	Total	C	H	O	0	0
			17	4	10	3		

- Molecule 9 is TETRAETHYLENE GLYCOL (CCD ID: PG4) (formula: $C_8H_{18}O_5$).



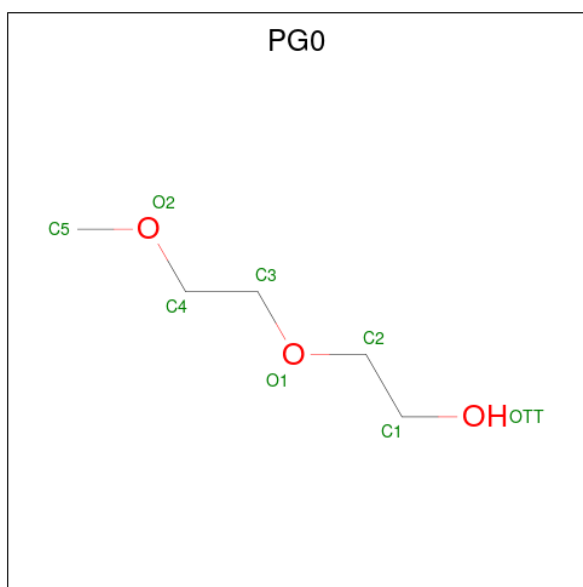
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
9	C	1	Total	C	H	O	0	0
			31	8	18	5		

- Molecule 10 is TRIETHYLENE GLYCOL (CCD ID: PGE) (formula: $C_6H_{14}O_4$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
10	E	1	Total	C	H	O	0	0
			24	6	14	4		

- Molecule 11 is 2-(2-METHOXYETHOXY)ETHANOL (CCD ID: PG0) (formula: $C_5H_{12}O_3$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
11	F	1	Total	C	H	O	0	0
			20	5	12	3		
11	G	1	Total	C	H	O	0	0
			20	5	12	3		

- Molecule 12 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
12	A	8	Total	O	0	0
			8	8		
12	B	9	Total	O	0	0
			9	9		
12	C	9	Total	O	0	0
			9	9		
12	D	7	Total	O	0	0
			7	7		
12	E	6	Total	O	0	0
			6	6		
12	F	9	Total	O	0	0
			9	9		
12	G	8	Total	O	0	0
			8	8		
12	H	1	Total	O	0	0
			1	1		
12	I	6	Total	O	0	0
			6	6		
12	J	3	Total	O	0	0
			3	3		

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
12	K	2	Total 2	O 2	0	0
12	L	2	Total 2	O 2	0	0
12	M	2	Total 2	O 2	0	0
12	N	2	Total 2	O 2	0	0

3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ($RSRZ > 2$). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

- Molecule 1: ATP-dependent Clp protease proteolytic subunit 2

Chain A: 



- Molecule 1: ATP-dependent Clp protease proteolytic subunit 2

Chain B: 



- Molecule 1: ATP-dependent Clp protease proteolytic subunit 2

Chain C: 



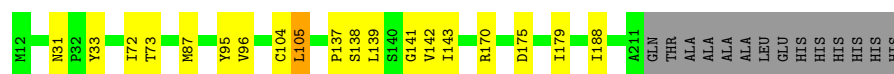
- Molecule 1: ATP-dependent Clp protease proteolytic subunit 2

Chain D: 



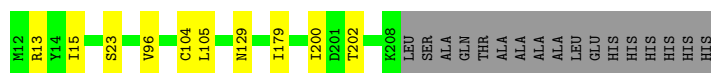
- Molecule 1: ATP-dependent Clp protease proteolytic subunit 2

Chain E: 



- Molecule 1: ATP-dependent Clp protease proteolytic subunit 2

Chain F: 



- Molecule 1: ATP-dependent Clp protease proteolytic subunit 2

Chain G: 88% 5% 7%



- Molecule 2: ATP-dependent Clp protease proteolytic subunit 1

Chain H: 87% 9%



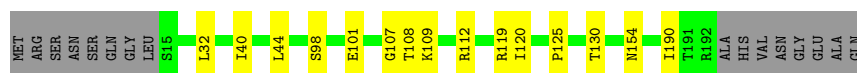
- Molecule 2: ATP-dependent Clp protease proteolytic subunit 1

Chain I: 83% 8% 9%



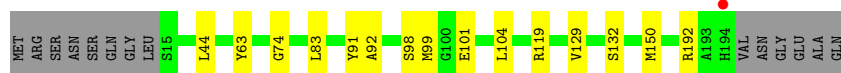
- Molecule 2: ATP-dependent Clp protease proteolytic subunit 1

Chain J: 84% 8% 8%



- Molecule 2: ATP-dependent Clp protease proteolytic subunit 1

Chain K: 85% 8% 7%



- Molecule 2: ATP-dependent Clp protease proteolytic subunit 1

Chain L: 83% 8% 9%

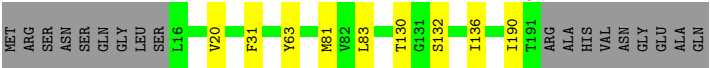
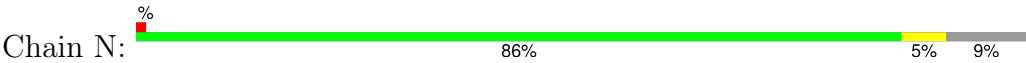


- Molecule 2: ATP-dependent Clp protease proteolytic subunit 1

Chain M: 80% 12% 7%



● Molecule 2: ATP-dependent Clp protease proteolytic subunit 1



4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	210.27Å 181.83Å 95.13Å 90.00° 94.72° 90.00°	Depositor
Resolution (Å)	31.59 – 3.11 31.59 – 3.11	Depositor EDS
% Data completeness (in resolution range)	86.7 (31.59-3.11) 79.4 (31.59-3.11)	Depositor EDS
R_{merge}	0.15	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.57 (at 3.12Å)	Xtriage
Refinement program	PHENIX 1.21.2_5419	Depositor
R, R_{free}	0.187 , 0.242 0.187 , 0.242	Depositor DCC
R_{free} test set	2861 reflections (5.01%)	wwPDB-VP
Wilson B-factor (Å ²)	68.0	Xtriage
Anisotropy	0.093	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.36 , 46.1	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	41180	wwPDB-VP
Average B, all atoms (Å ²)	79.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.07% 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: DMS, BEZ, PGE, AE3, PG0, PG4, PEG, A1C98

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	0.29	0/1534	0.52	3/2077 (0.1%)
1	B	0.36	0/1542	0.53	0/2089
1	C	0.28	0/1571	0.45	0/2127
1	D	0.40	1/1539 (0.1%)	0.50	0/2084
1	E	0.41	1/1547 (0.1%)	0.57	2/2095 (0.1%)
1	F	0.31	0/1524	0.50	0/2065
1	G	0.27	0/1553	0.41	0/2103
2	H	0.30	0/1345	0.54	1/1821 (0.1%)
2	I	0.39	0/1345	0.57	1/1821 (0.1%)
2	J	0.34	0/1362	0.50	0/1843
2	K	0.42	0/1366	0.65	1/1851 (0.1%)
2	L	0.33	0/1352	0.47	0/1830
2	M	0.45	0/1354	0.70	4/1838 (0.2%)
2	N	0.35	0/1347	0.50	0/1823
All	All	0.35	2/20281 (0.0%)	0.53	12/27467 (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
2	M	0	2

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	E	105	LEU	C-N	7.03	1.43	1.33
1	D	104	CYS	C-N	6.00	1.41	1.33

The worst 5 of 12 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	M	191	THR	N-CA-C	8.07	120.63	107.32
1	A	128	PRO	N-CA-C	7.39	123.25	113.57
1	A	128	PRO	CB-CA-C	-6.81	102.17	112.11
2	K	192	ARG	N-CA-C	5.99	119.36	111.28
2	M	191	THR	CB-CA-C	-5.84	104.05	111.70

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	M	112	ARG	Sidechain
2	M	173	ARG	Sidechain

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	1512	1511	1506	7	0
1	B	1520	1515	1514	9	0
1	C	1549	1552	1547	12	0
1	D	1517	1513	1508	10	0
1	E	1525	1514	1509	9	0
1	F	1502	1496	1491	8	0
1	G	1531	1532	1527	7	0
2	H	1323	1303	1302	4	0
2	I	1323	1303	1302	7	0
2	J	1340	1321	1320	7	0
2	K	1344	1317	1316	8	0
2	L	1330	1306	1304	10	0
2	M	1331	1285	1284	13	0
2	N	1325	1304	1302	5	0
3	A	8	5	5	0	0
3	B	8	5	5	0	0
3	C	8	5	5	0	0
3	D	8	5	5	0	0
3	E	8	5	5	1	0
3	F	8	5	5	0	0
3	G	8	5	5	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	A	17	22	22	1	0
4	B	17	22	22	0	0
4	C	17	22	22	1	0
4	D	17	22	22	0	0
4	E	17	22	22	1	0
4	F	17	22	22	0	0
4	G	17	22	22	0	0
5	A	29	26	0	0	0
5	B	29	26	0	0	0
5	C	29	26	0	0	0
5	D	29	26	0	0	0
5	E	58	52	0	0	0
5	G	29	26	0	0	0
5	H	29	26	0	0	0
5	I	29	26	0	0	0
5	J	29	26	0	0	0
5	K	29	26	0	0	0
5	L	29	26	0	0	0
5	M	29	26	0	0	0
5	N	29	26	0	0	0
6	A	4	6	6	0	0
6	B	4	6	6	0	0
6	C	4	6	6	0	0
6	D	4	6	6	0	0
6	E	4	6	6	0	0
6	F	4	6	6	1	0
6	G	4	6	6	0	0
7	A	9	14	14	1	0
7	D	9	14	14	0	0
8	C	7	10	10	1	0
9	C	13	18	18	1	0
10	E	10	14	14	1	0
11	F	8	12	12	0	0
11	G	8	12	12	0	0
12	A	8	0	0	0	0
12	B	9	0	0	0	0
12	C	9	0	0	0	0
12	D	7	0	0	0	0
12	E	6	0	0	0	0
12	F	9	0	0	0	0
12	G	8	0	0	0	0
12	H	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
12	I	6	0	0	0	0
12	J	3	0	0	0	0
12	K	2	0	0	0	0
12	L	2	0	0	0	0
12	M	2	0	0	0	0
12	N	2	0	0	0	0
All	All	20719	20461	20057	96	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 2.

The worst 5 of 96 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:A:105:LEU:HD23	1:G:57:MET:SD	2.24	0.77
2:M:121:LEU:HD22	2:M:174:TRP:CZ2	2.21	0.75
10:E:807:PGE:H3	1:F:15:ILE:HG23	1.69	0.74
2:K:74:GLY:HA3	2:K:99:MET:HE2	1.74	0.69
1:E:139:LEU:HD21	1:E:143:ILE:HG12	1.76	0.67

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	195/214 (91%)	184 (94%)	11 (6%)	0	100	100
1	B	197/214 (92%)	183 (93%)	14 (7%)	0	100	100
1	C	200/214 (94%)	190 (95%)	10 (5%)	0	100	100
1	D	196/214 (92%)	184 (94%)	12 (6%)	0	100	100
1	E	198/214 (92%)	180 (91%)	18 (9%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	F	195/214 (91%)	184 (94%)	11 (6%)	0	100	100
1	G	198/214 (92%)	190 (96%)	8 (4%)	0	100	100
2	H	174/194 (90%)	165 (95%)	9 (5%)	0	100	100
2	I	174/194 (90%)	165 (95%)	9 (5%)	0	100	100
2	J	176/194 (91%)	161 (92%)	15 (8%)	0	100	100
2	K	178/194 (92%)	166 (93%)	12 (7%)	0	100	100
2	L	175/194 (90%)	170 (97%)	5 (3%)	0	100	100
2	M	178/194 (92%)	165 (93%)	13 (7%)	0	100	100
2	N	174/194 (90%)	164 (94%)	10 (6%)	0	100	100
All	All	2608/2856 (91%)	2451 (94%)	157 (6%)	0	100	100

There are no Ramachandran outliers to report.

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	161/176 (92%)	158 (98%)	3 (2%)	50	71
1	B	162/176 (92%)	160 (99%)	2 (1%)	63	76
1	C	165/176 (94%)	163 (99%)	2 (1%)	63	76
1	D	161/176 (92%)	158 (98%)	3 (2%)	50	71
1	E	161/176 (92%)	157 (98%)	4 (2%)	42	66
1	F	159/176 (90%)	157 (99%)	2 (1%)	61	75
1	G	163/176 (93%)	159 (98%)	4 (2%)	42	66
2	H	132/151 (87%)	132 (100%)	0	100	100
2	I	132/151 (87%)	130 (98%)	2 (2%)	57	73
2	J	134/151 (89%)	130 (97%)	4 (3%)	36	63
2	K	134/151 (89%)	132 (98%)	2 (2%)	57	73
2	L	133/151 (88%)	131 (98%)	2 (2%)	57	73

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	M	130/151 (86%)	126 (97%)	4 (3%)	35	62
2	N	133/151 (88%)	130 (98%)	3 (2%)	44	68
All	All	2060/2289 (90%)	2023 (98%)	37 (2%)	50	71

5 of 37 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	L	72	SER
2	N	81	MET
2	L	122	MET
2	M	181	LEU
1	E	175	ASP

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (1) such sidechains are listed below:

Mol	Chain	Res	Type
1	G	47	GLN

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](#)

49 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
5	A1C98	A	804	-	33,33,33	5.25	15 (45%)	40,47,47	2.91	9 (22%)
4	LEU	B	803	4	6,8,8	2.24	3 (50%)	5,10,10	2.04	3 (60%)
4	LEU	G	802	3,4	5,7,8	1.06	0	6,8,10	0.50	0
6	DMS	C	807	-	3,3,3	0.65	0	3,3,3	0.61	0
5	A1C98	G	804	-	33,33,33	5.30	16 (48%)	40,47,47	3.07	10 (25%)
8	PEG	C	805	-	6,6,6	0.25	0	5,5,5	0.31	0
6	DMS	B	805	-	3,3,3	0.58	0	3,3,3	0.28	0
4	LEU	F	802	3,4	5,7,8	0.94	0	6,8,10	1.46	1 (16%)
10	PGE	E	807	-	9,9,9	0.32	0	8,8,8	0.60	0
5	A1C98	L	901	-	33,33,33	5.27	17 (51%)	40,47,47	3.21	11 (27%)
4	LEU	E	802	3,4	5,7,8	0.58	0	6,8,10	0.86	0
3	BEZ	E	801	4	8,8,9	1.25	1 (12%)	9,9,11	1.57	1 (11%)
7	AE3	D	806	-	8,8,8	0.36	0	7,7,7	0.20	0
4	LEU	B	802	3,4	5,7,8	1.95	2 (40%)	6,8,10	0.42	0
3	BEZ	F	801	4	8,8,9	1.03	1 (12%)	9,9,11	2.79	4 (44%)
4	LEU	D	803	4	6,8,8	1.06	1 (16%)	5,10,10	0.32	0
4	LEU	C	803	4	6,8,8	2.36	1 (16%)	5,10,10	1.72	1 (20%)
5	A1C98	E	806	-	33,33,33	5.26	15 (45%)	40,47,47	2.89	10 (25%)
4	LEU	A	802	3,4	5,7,8	0.50	0	6,8,10	0.22	0
5	A1C98	B	804	-	33,33,33	5.32	15 (45%)	40,47,47	2.84	5 (12%)
5	A1C98	E	804	-	33,33,33	5.30	15 (45%)	40,47,47	2.96	9 (22%)
5	A1C98	I	901	-	33,33,33	5.30	14 (42%)	40,47,47	3.15	10 (25%)
7	AE3	A	806	-	8,8,8	0.36	0	7,7,7	0.36	0
6	DMS	A	805	-	3,3,3	0.63	0	3,3,3	0.19	0
6	DMS	E	805	-	3,3,3	0.70	0	3,3,3	0.29	0
3	BEZ	G	801	4	8,8,9	2.07	3 (37%)	9,9,11	2.03	4 (44%)
6	DMS	F	805	-	3,3,3	0.62	0	3,3,3	0.49	0
4	LEU	E	803	4	6,8,8	0.94	0	5,10,10	2.17	3 (60%)
4	LEU	D	802	3,4	5,7,8	0.39	0	6,8,10	0.30	0
4	LEU	C	802	3,4	5,7,8	0.42	0	6,8,10	0.25	0
4	LEU	G	803	4	6,8,8	2.42	3 (50%)	5,10,10	2.32	3 (60%)
5	A1C98	D	804	-	33,33,33	5.29	15 (45%)	40,47,47	2.92	10 (25%)
3	BEZ	A	801	4	8,8,9	1.72	2 (25%)	9,9,11	2.34	4 (44%)
11	PG0	G	805	-	7,7,7	0.39	0	6,6,6	0.35	0
5	A1C98	C	804	-	33,33,33	5.32	16 (48%)	40,47,47	2.91	9 (22%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
5	A1C98	J	901	-	33,33,33	5.28	16 (48%)	40,47,47	3.25	10 (25%)
3	BEZ	C	801	4	8,8,9	1.93	3 (37%)	9,9,11	3.64	6 (66%)
3	BEZ	B	801	4	8,8,9	1.70	2 (25%)	9,9,11	2.43	4 (44%)
5	A1C98	K	901	-	33,33,33	5.32	15 (45%)	40,47,47	3.08	11 (27%)
6	DMS	G	806	-	3,3,3	0.64	0	3,3,3	0.16	0
9	PG4	C	806	-	12,12,12	0.31	0	11,11,11	0.23	0
5	A1C98	N	901	-	33,33,33	5.29	16 (48%)	40,47,47	3.18	10 (25%)
11	PG0	F	804	-	7,7,7	0.30	0	6,6,6	0.11	0
5	A1C98	H	901	-	33,33,33	5.26	16 (48%)	40,47,47	3.16	11 (27%)
5	A1C98	M	901	-	33,33,33	5.45	15 (45%)	40,47,47	3.12	9 (22%)
6	DMS	D	805	-	3,3,3	0.63	0	3,3,3	0.33	0
4	LEU	F	803	4	6,8,8	1.54	1 (16%)	5,10,10	0.48	0
3	BEZ	D	801	4	8,8,9	2.31	2 (25%)	9,9,11	3.58	4 (44%)
4	LEU	A	803	4	6,8,8	1.74	1 (16%)	5,10,10	0.96	0

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
5	A1C98	A	804	-	-	0/8/23/23	0/5/5/5
4	LEU	B	803	4	-	5/8/8/8	-
4	LEU	G	802	3,4	-	2/5/6/8	-
5	A1C98	G	804	-	-	0/8/23/23	0/5/5/5
8	PEG	C	805	-	-	2/4/4/4	-
4	LEU	F	802	3,4	-	1/5/6/8	-
10	PGE	E	807	-	-	3/7/7/7	-
5	A1C98	L	901	-	-	0/8/23/23	0/5/5/5
4	LEU	E	802	3,4	-	0/5/6/8	-
3	BEZ	E	801	4	-	2/2/2/4	0/1/1/1
7	AE3	D	806	-	-	0/6/6/6	-
4	LEU	B	802	3,4	-	0/5/6/8	-
3	BEZ	F	801	4	-	2/2/2/4	0/1/1/1
4	LEU	D	803	4	-	0/8/8/8	-
4	LEU	C	803	4	-	1/8/8/8	-
5	A1C98	E	806	-	-	0/8/23/23	0/5/5/5
4	LEU	A	802	3,4	-	0/5/6/8	-
5	A1C98	B	804	-	-	0/8/23/23	0/5/5/5

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	A1C98	E	804	-	-	0/8/23/23	0/5/5/5
5	A1C98	I	901	-	-	2/8/23/23	0/5/5/5
7	AE3	A	806	-	-	4/6/6/6	-
3	BEZ	G	801	4	-	1/2/2/4	0/1/1/1
4	LEU	E	803	4	-	1/8/8/8	-
4	LEU	D	802	3,4	-	0/5/6/8	-
4	LEU	C	802	3,4	-	0/5/6/8	-
4	LEU	G	803	4	-	2/8/8/8	-
5	A1C98	D	804	-	-	0/8/23/23	0/5/5/5
3	BEZ	A	801	4	-	1/2/2/4	0/1/1/1
11	PG0	G	805	-	-	2/5/5/5	-
5	A1C98	C	804	-	-	0/8/23/23	0/5/5/5
5	A1C98	J	901	-	-	0/8/23/23	0/5/5/5
3	BEZ	C	801	4	-	2/2/2/4	0/1/1/1
3	BEZ	B	801	4	-	0/2/2/4	0/1/1/1
5	A1C98	K	901	-	-	2/8/23/23	0/5/5/5
11	PG0	F	804	-	-	3/5/5/5	-
9	PG4	C	806	-	-	5/10/10/10	-
5	A1C98	N	901	-	-	0/8/23/23	0/5/5/5
5	A1C98	H	901	-	-	0/8/23/23	0/5/5/5
5	A1C98	M	901	-	-	2/8/23/23	0/5/5/5
4	LEU	F	803	4	-	2/8/8/8	-
3	BEZ	D	801	4	-	1/2/2/4	0/1/1/1
4	LEU	A	803	4	-	2/8/8/8	-

The worst 5 of 242 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	D	804	A1C98	C26-N27	17.14	1.41	1.28
5	B	804	A1C98	C26-N27	17.12	1.41	1.28
5	E	804	A1C98	C26-N27	17.10	1.41	1.28
5	K	901	A1C98	C26-N27	17.08	1.41	1.28
5	I	901	A1C98	C26-N27	16.96	1.41	1.28

The worst 5 of 172 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	J	901	A1C98	C28-C29-N25	15.58	112.56	101.30
5	L	901	A1C98	C28-C29-N25	15.45	112.47	101.30
5	N	901	A1C98	C28-C29-N25	15.42	112.44	101.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	H	901	A1C98	C28-C29-N25	15.38	112.42	101.30
5	I	901	A1C98	C28-C29-N25	15.15	112.25	101.30

There are no chirality outliers.

5 of 50 torsion outliers are listed below:

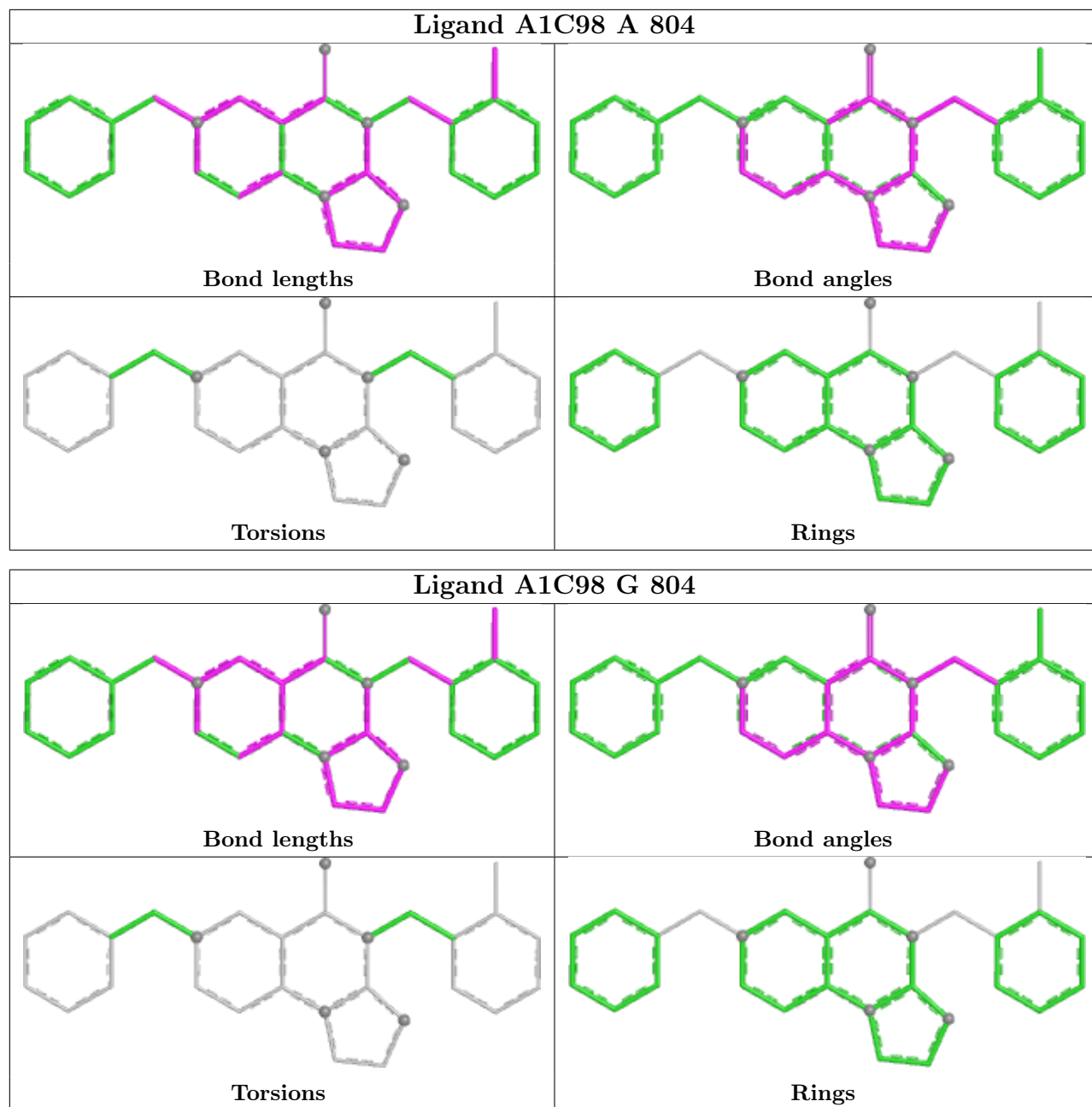
Mol	Chain	Res	Type	Atoms
4	B	803	LEU	N-CA-CB-CG
4	E	803	LEU	N-CA-CB-CG
4	F	802	LEU	O-C-CA-CB
4	G	803	LEU	N-CA-CB-CG
3	F	801	BEZ	O1-C-C1-C2

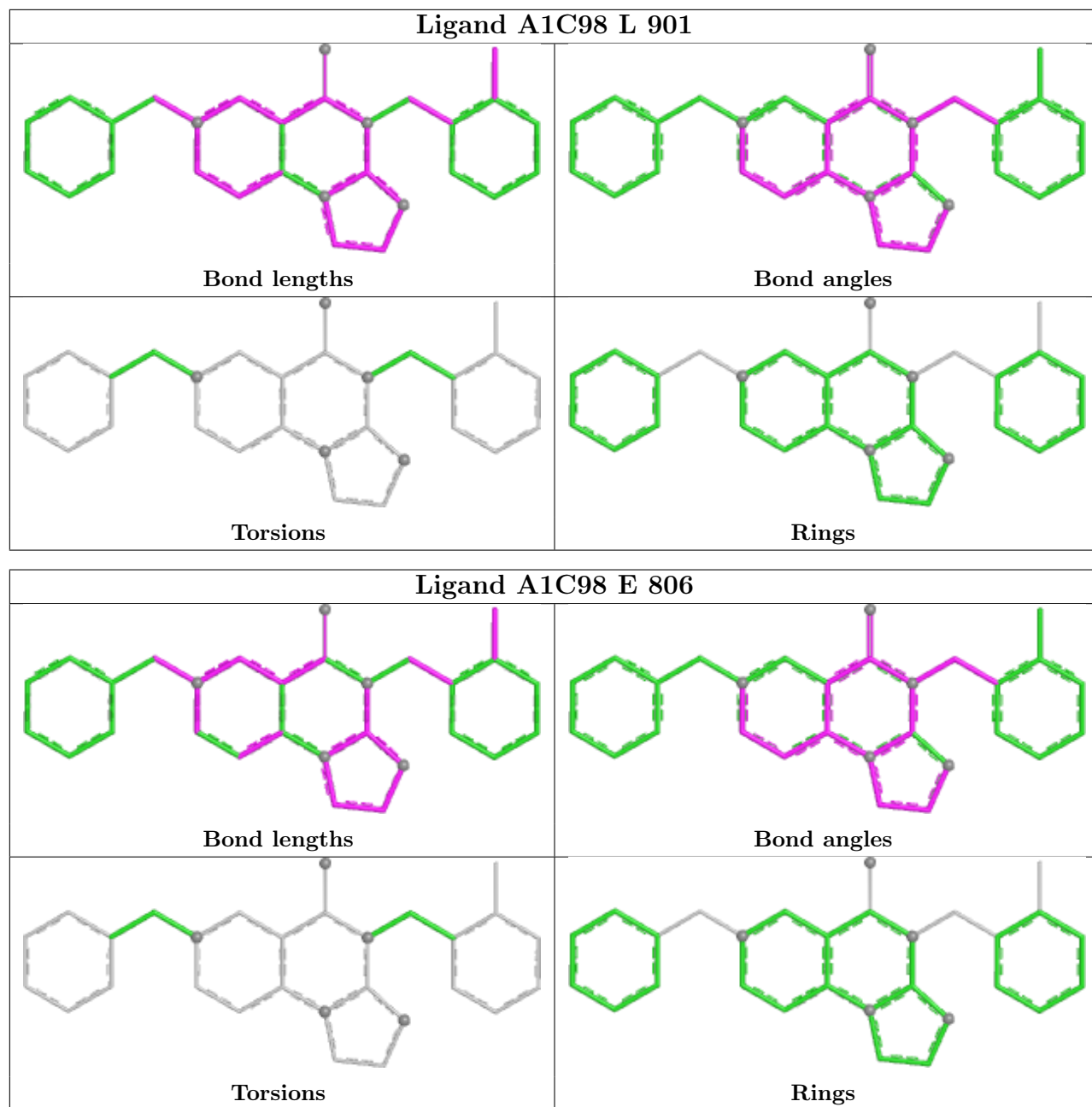
There are no ring outliers.

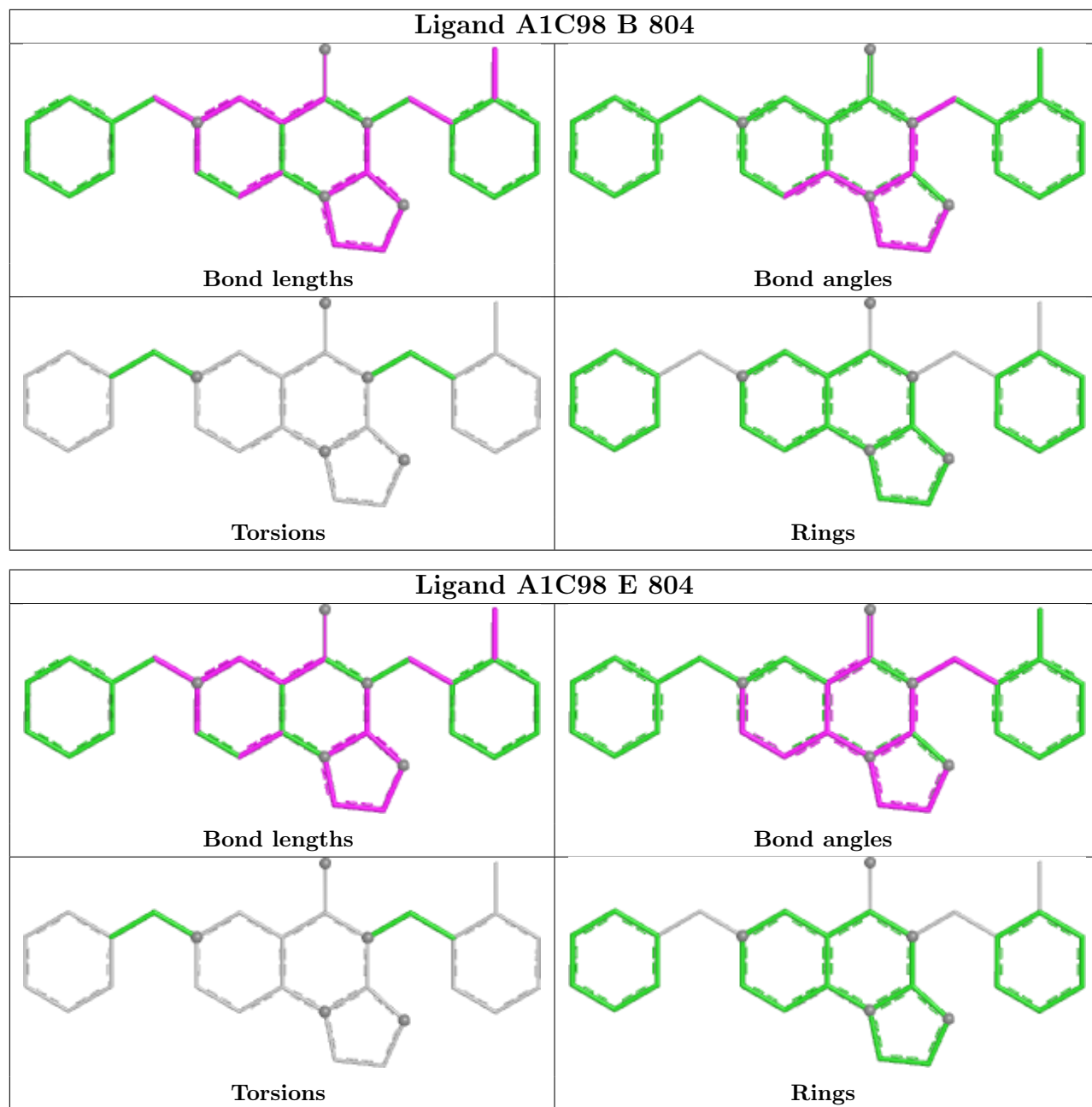
10 monomers are involved in 9 short contacts:

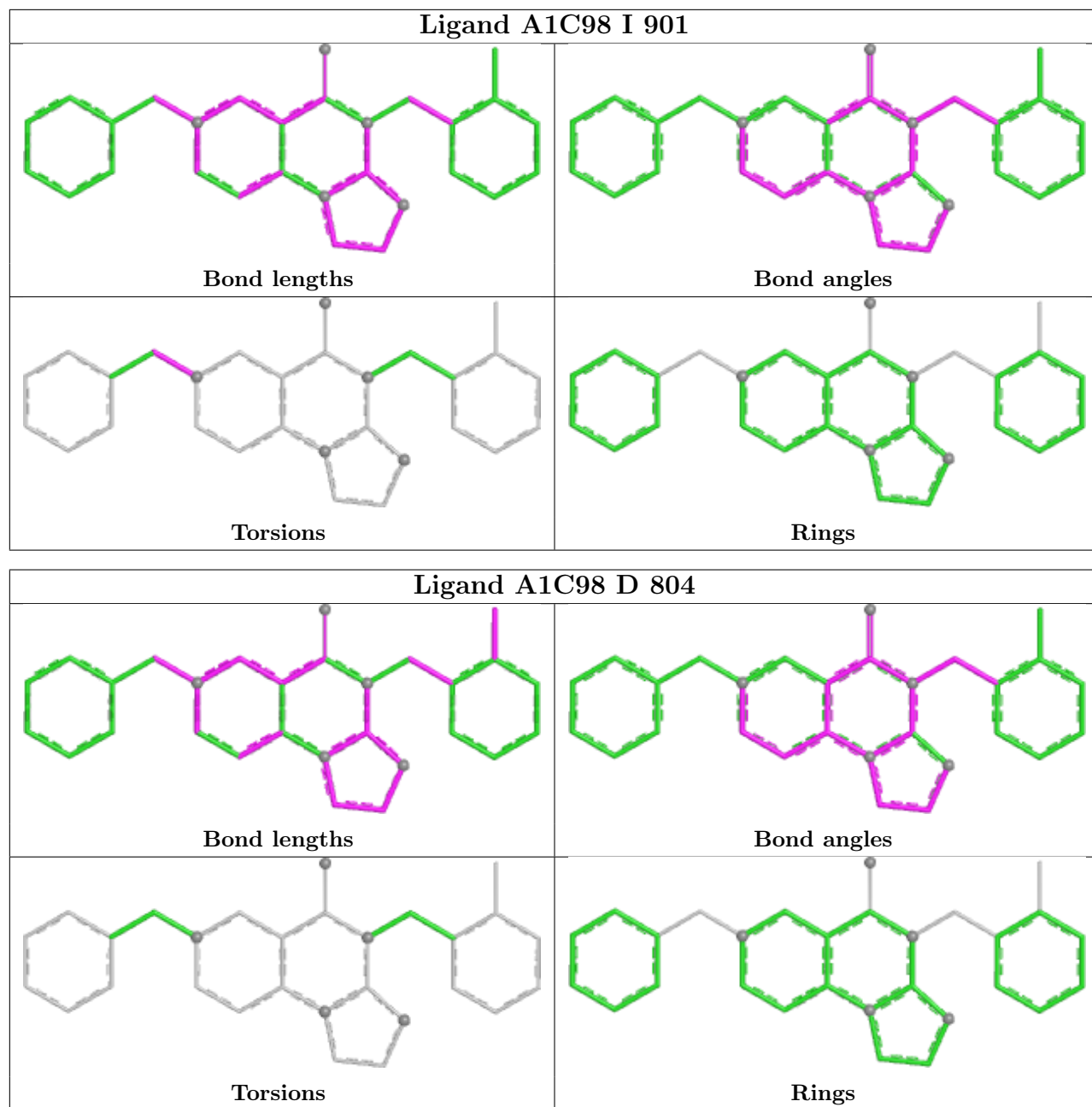
Mol	Chain	Res	Type	Clashes	Symm-Clashes
8	C	805	PEG	1	0
10	E	807	PGE	1	0
4	E	802	LEU	1	0
3	E	801	BEZ	1	0
4	C	803	LEU	1	0
7	A	806	AE3	1	0
6	F	805	DMS	1	0
4	E	803	LEU	1	0
9	C	806	PG4	1	0
4	A	803	LEU	1	0

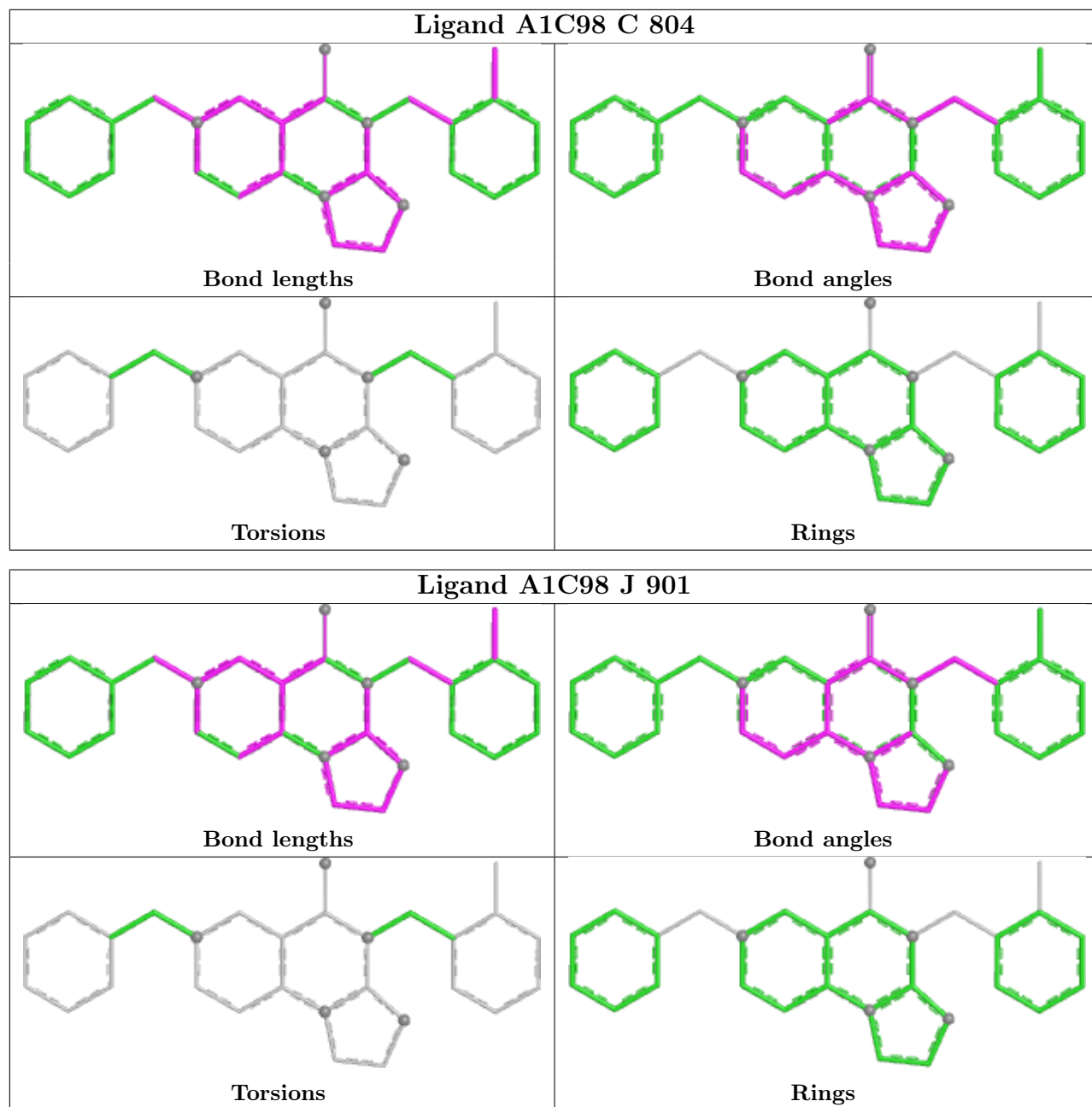
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. 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.

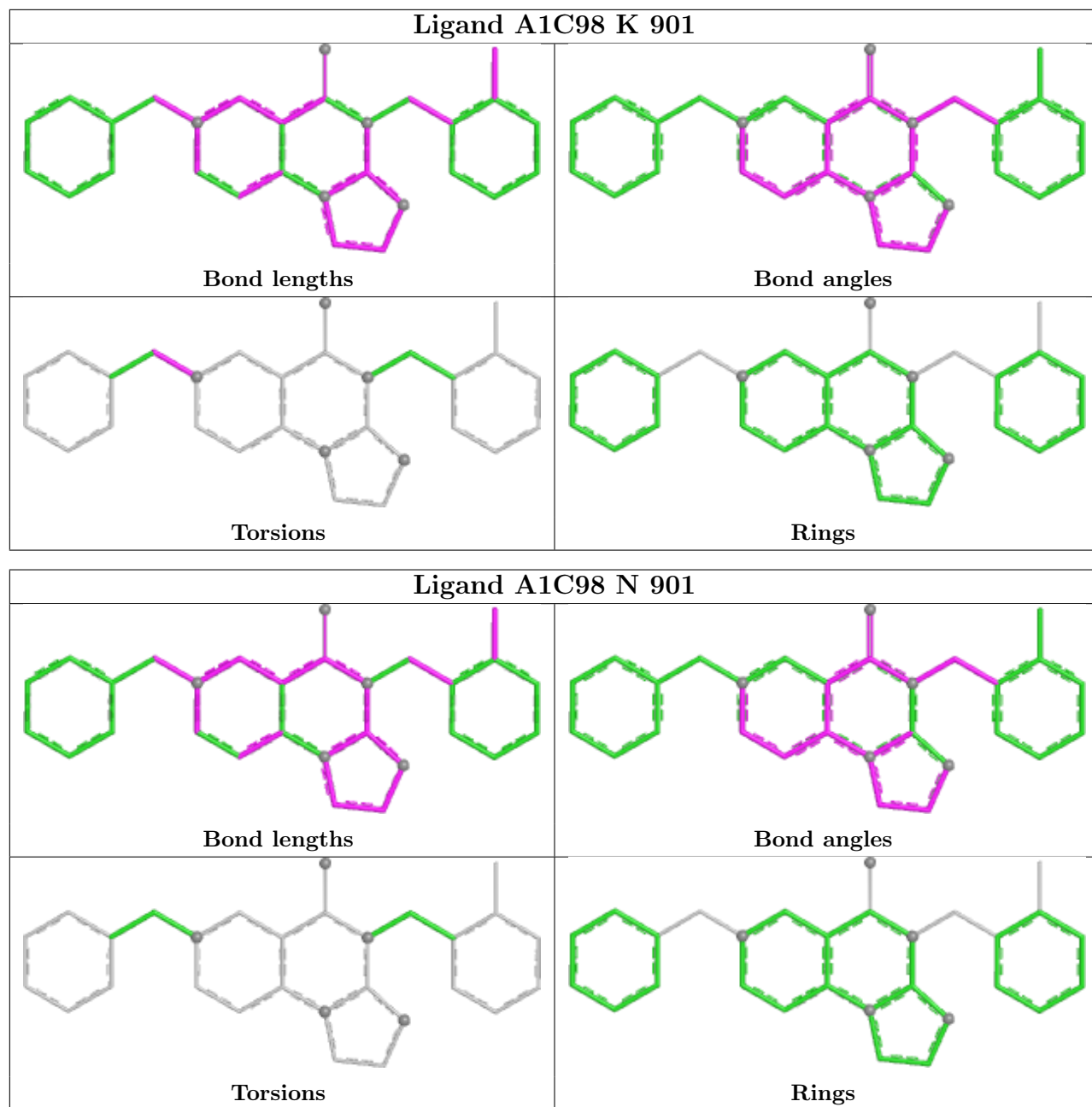


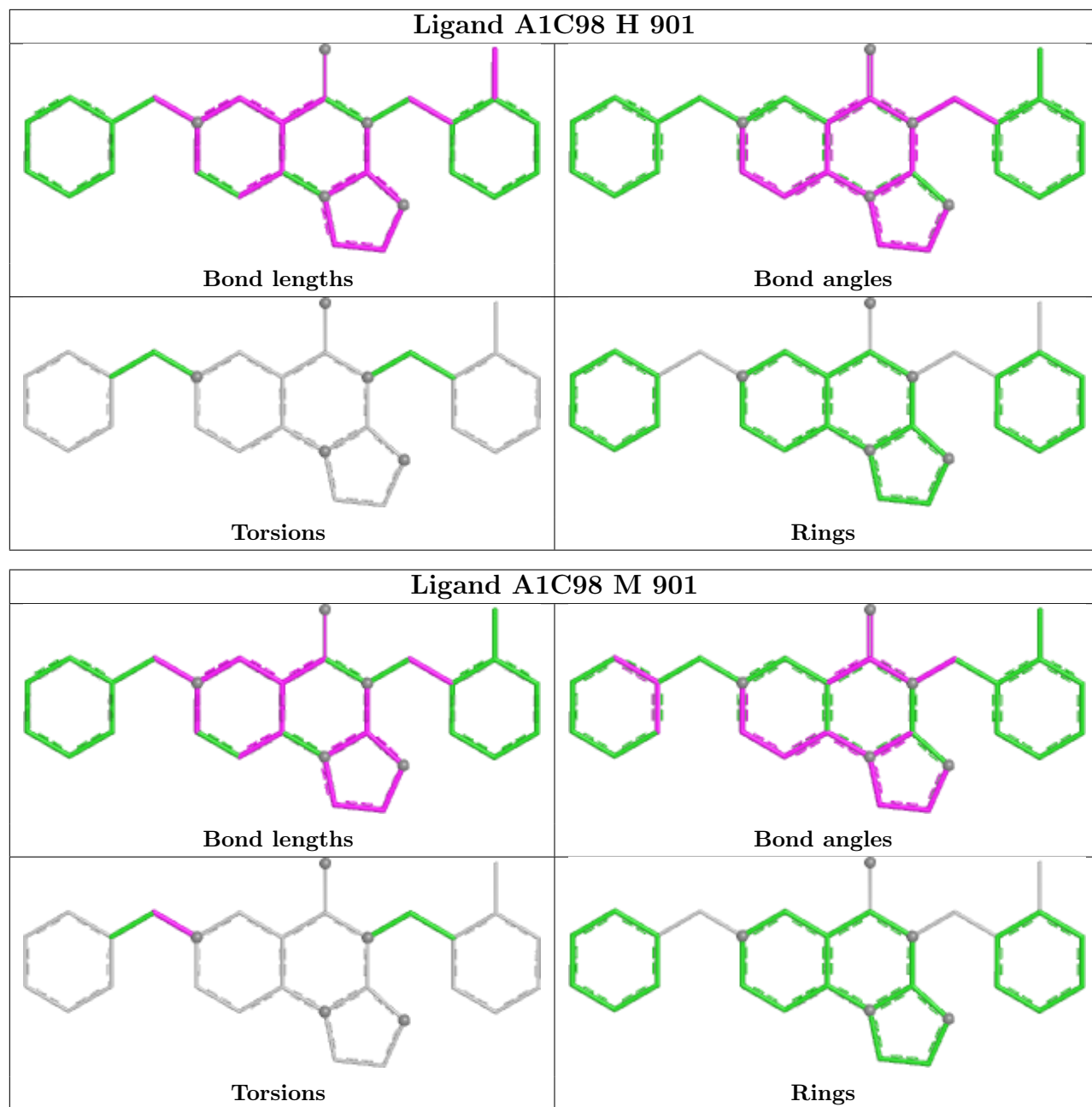












5.7 Other polymers [i](#)

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

6.1 Protein, DNA and RNA chains

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	197/214 (92%)	-0.66	0	100	100	49, 65, 82, 101	0
1	B	199/214 (92%)	-0.63	0	100	100	50, 65, 84, 130	0
1	C	202/214 (94%)	-0.61	0	100	100	47, 66, 87, 130	0
1	D	198/214 (92%)	-0.53	0	100	100	50, 69, 90, 110	0
1	E	200/214 (93%)	-0.56	0	100	100	50, 73, 89, 123	0
1	F	197/214 (92%)	-0.54	0	100	100	54, 72, 90, 111	0
1	G	200/214 (93%)	-0.57	0	100	100	53, 69, 87, 124	0
2	H	176/194 (90%)	-0.46	1 (0%)	85	70	62, 82, 109, 123	0
2	I	176/194 (90%)	-0.44	0	100	100	62, 82, 105, 135	0
2	J	178/194 (91%)	-0.33	0	100	100	60, 85, 117, 135	0
2	K	180/194 (92%)	-0.24	1 (0%)	85	70	69, 92, 119, 141	0
2	L	177/194 (91%)	-0.26	1 (0%)	85	70	72, 94, 116, 165	0
2	M	180/194 (92%)	-0.29	0	100	100	71, 91, 116, 133	0
2	N	176/194 (90%)	-0.36	1 (0%)	85	70	62, 85, 115, 140	0
All	All	2636/2856 (92%)	-0.47	4 (0%)	91	83	47, 77, 107, 165	0

All (4) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	K	194	HIS	3.8
2	N	191	THR	2.9
2	L	191	THR	2.6
2	H	18	ASP	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(Å ²)	Q<0.9
6	DMS	G	806	4/4	0.58	0.16	65,82,98,121	0
4	LEU	D	803	9/9	0.61	0.19	30,30,91,93	0
6	DMS	D	805	4/4	0.64	0.18	65,78,112,117	0
11	PG0	G	805	8/8	0.65	0.17	58,73,97,97	0
6	DMS	E	805	4/4	0.67	0.13	55,66,72,107	0
4	LEU	C	803	9/9	0.70	0.17	30,30,73,73	0
4	LEU	E	802	8/9	0.70	0.18	30,30,82,84	0
4	LEU	G	802	8/9	0.72	0.17	30,30,74,88	0
6	DMS	A	805	4/4	0.72	0.17	59,89,110,113	0
4	LEU	A	802	8/9	0.72	0.17	30,30,67,74	0
4	LEU	F	803	9/9	0.73	0.18	30,30,93,93	0
4	LEU	C	802	8/9	0.74	0.15	30,30,71,81	0
4	LEU	B	802	8/9	0.75	0.16	30,30,77,81	0
6	DMS	F	805	4/4	0.75	0.15	61,73,103,107	0
6	DMS	B	805	4/4	0.76	0.18	73,88,96,113	0
7	AE3	D	806	9/9	0.79	0.12	53,69,82,82	0
7	AE3	A	806	9/9	0.79	0.12	62,76,86,88	0
6	DMS	C	807	4/4	0.80	0.15	59,71,72,121	0
4	LEU	D	802	8/9	0.80	0.16	30,30,77,86	0
11	PG0	F	804	8/8	0.85	0.11	56,78,94,94	0
4	LEU	F	802	8/9	0.85	0.13	76,86,103,103	0
9	PG4	C	806	13/13	0.86	0.08	51,81,98,106	0
5	A1C98	M	901	29/29	0.87	0.14	91,111,137,149	0
5	A1C98	N	901	29/29	0.87	0.14	94,116,140,142	0
5	A1C98	J	901	29/29	0.89	0.15	100,124,149,156	0
5	A1C98	I	901	29/29	0.90	0.13	86,105,129,133	0
10	PGE	E	807	10/10	0.90	0.10	58,79,95,100	0

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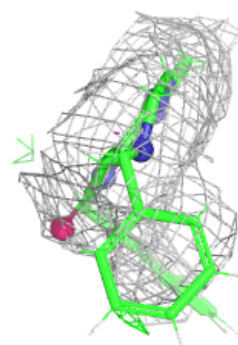
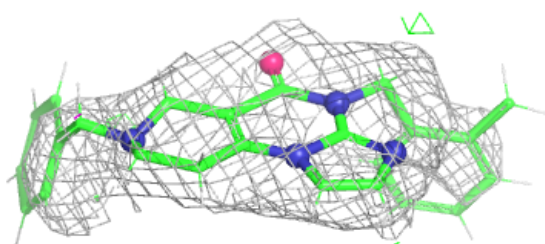
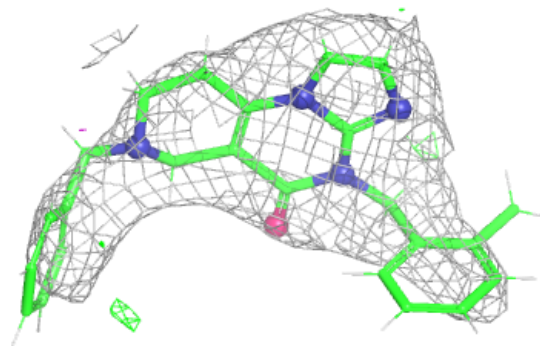
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
3	BEZ	F	801	8/9	0.91	0.13	83,85,103,105	0
5	A1C98	K	901	29/29	0.91	0.12	100,116,139,144	0
5	A1C98	L	901	29/29	0.91	0.11	88,105,126,132	0
4	LEU	G	803	9/9	0.92	0.12	70,85,97,99	0
5	A1C98	H	901	29/29	0.92	0.12	82,103,122,140	0
3	BEZ	C	801	8/9	0.92	0.12	57,68,80,85	0
3	BEZ	D	801	8/9	0.93	0.13	58,70,97,97	0
8	PEG	C	805	7/7	0.93	0.06	39,61,74,74	0
4	LEU	B	803	9/9	0.93	0.10	65,84,95,95	0
4	LEU	E	803	9/9	0.94	0.11	76,91,101,101	0
4	LEU	A	803	9/9	0.94	0.12	66,82,94,94	0
3	BEZ	G	801	8/9	0.95	0.10	65,76,90,91	0
5	A1C98	B	804	29/29	0.95	0.09	55,67,80,88	0
5	A1C98	D	804	29/29	0.95	0.11	52,72,98,112	0
5	A1C98	G	804	29/29	0.95	0.09	60,76,103,112	0
3	BEZ	B	801	8/9	0.95	0.12	65,73,87,95	0
5	A1C98	E	804	29/29	0.96	0.09	61,78,94,110	0
5	A1C98	E	806	29/29	0.96	0.08	59,76,92,96	0
5	A1C98	A	804	29/29	0.96	0.08	50,66,82,83	0
3	BEZ	A	801	8/9	0.96	0.10	57,67,81,83	0
5	A1C98	C	804	29/29	0.96	0.10	54,72,98,103	0
3	BEZ	E	801	8/9	0.96	0.09	66,73,88,90	0

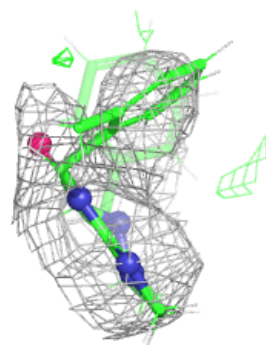
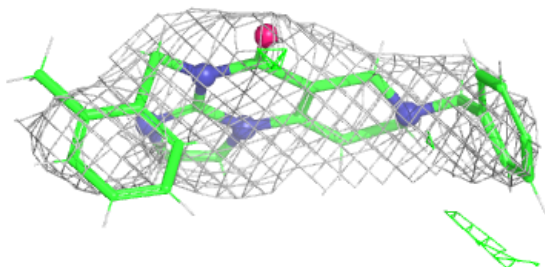
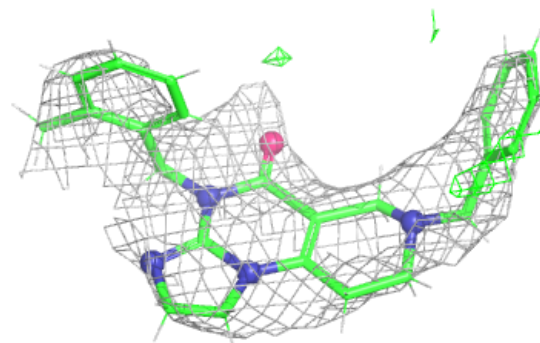
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around A1C98 M 901:

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

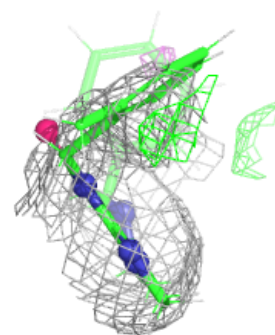
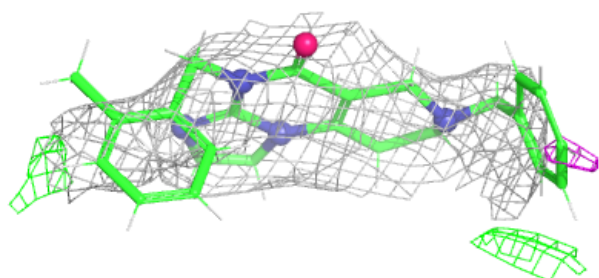
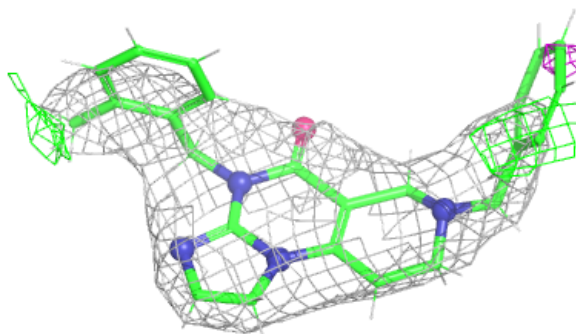
**Electron density around A1C98 N 901:**

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

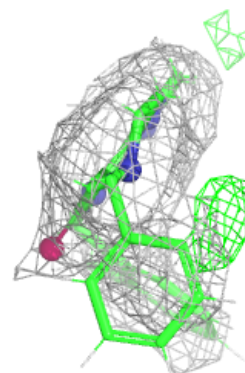
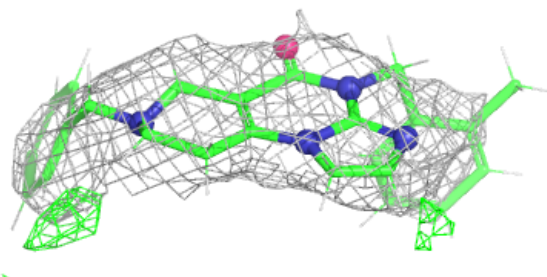
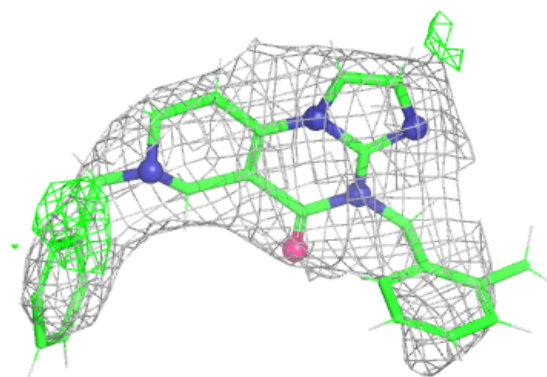


Electron density around A1C98 J 901:

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

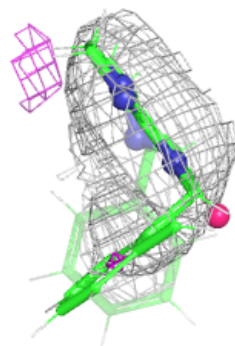
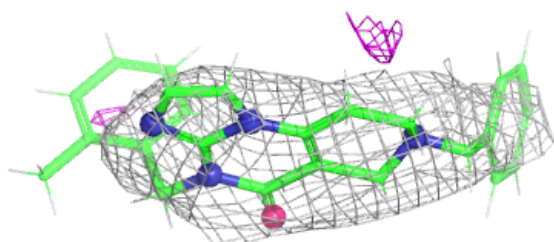
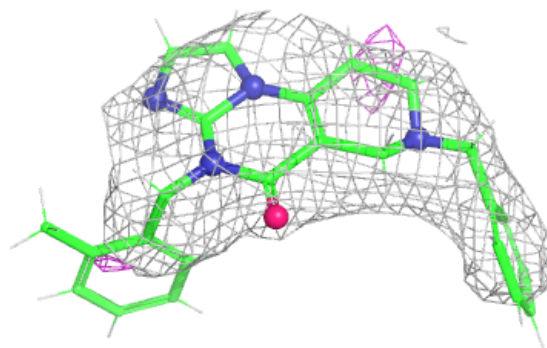
**Electron density around A1C98 I 901:**

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and green (positive)

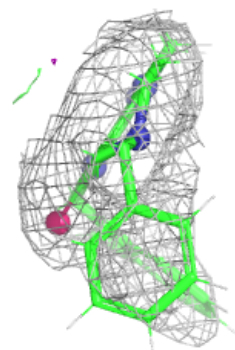
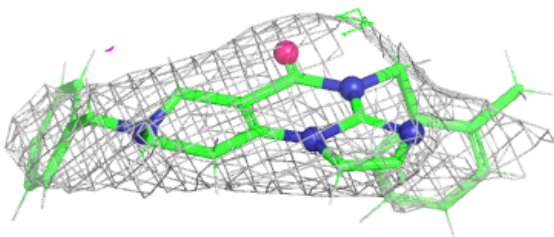
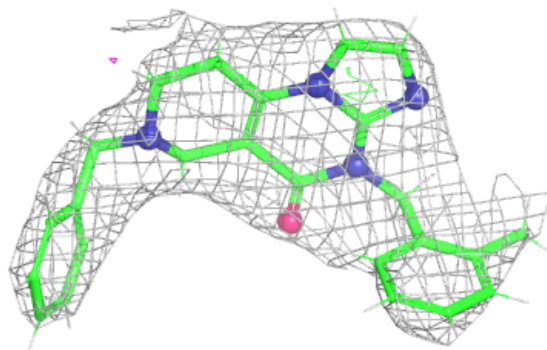


Electron density around A1C98 K 901:

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

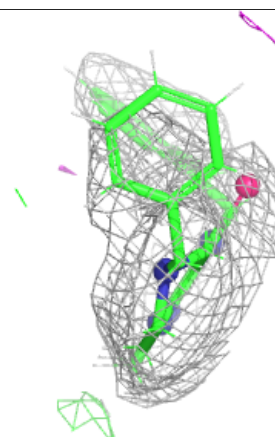
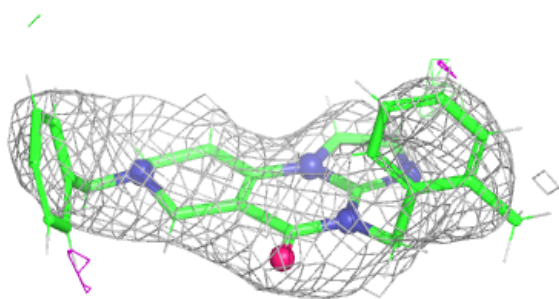
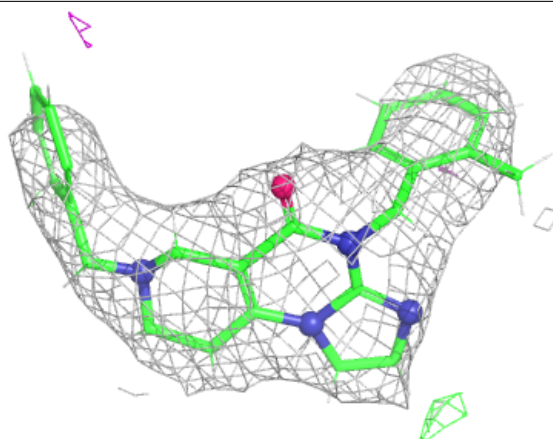
**Electron density around A1C98 L 901:**

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and green (positive)



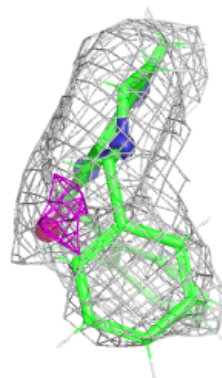
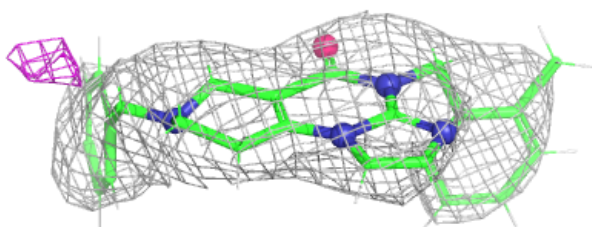
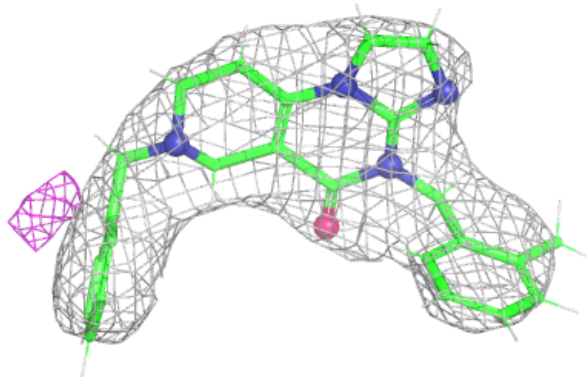
Electron density around A1C98 H 901:

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and green (positive)

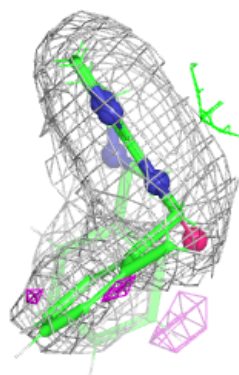
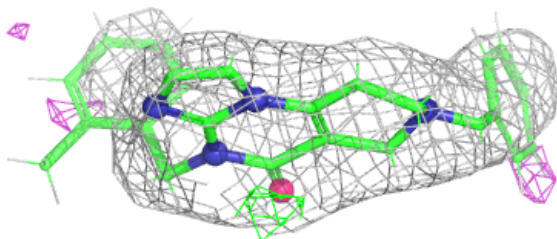
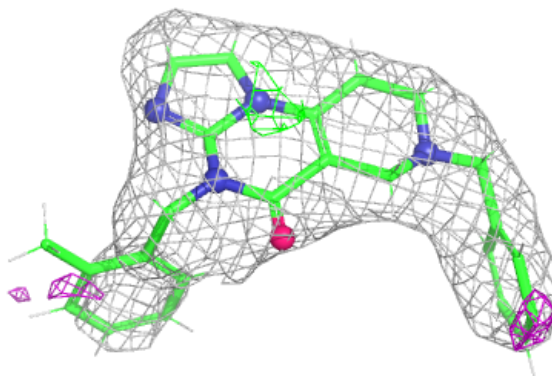


Electron density around A1C98 B 804:

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

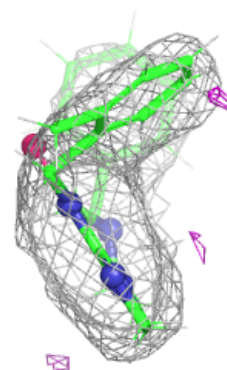
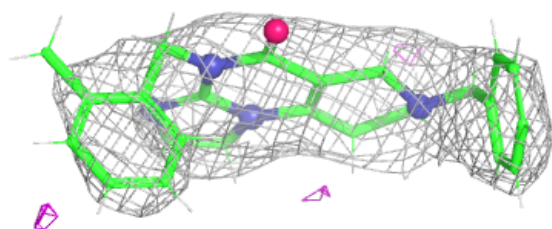
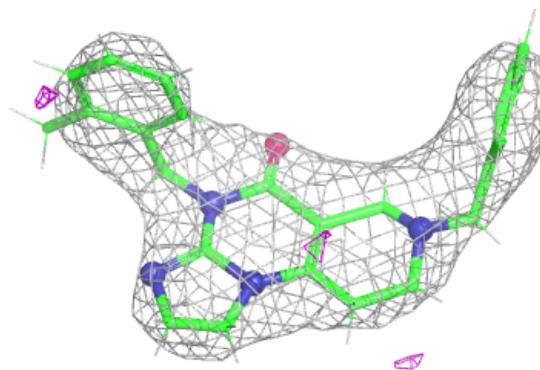
**Electron density around A1C98 D 804:**

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

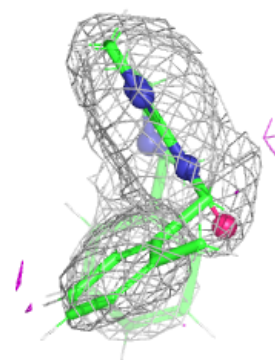
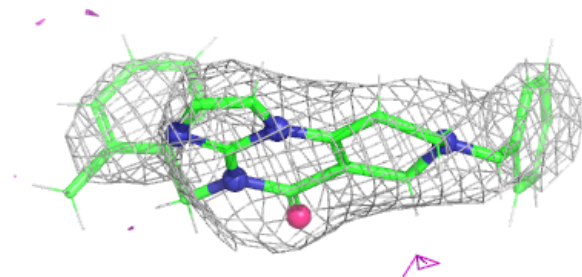
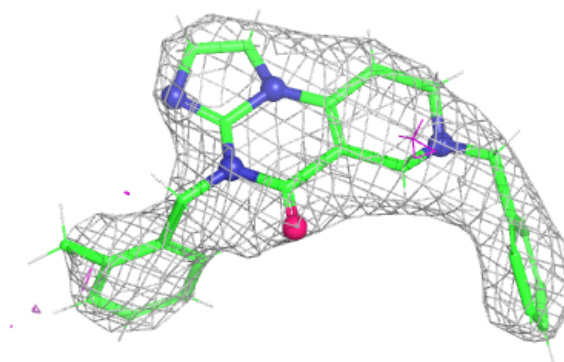


Electron density around A1C98 G 804:

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and green (positive)

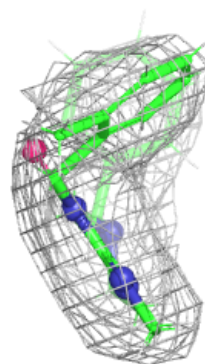
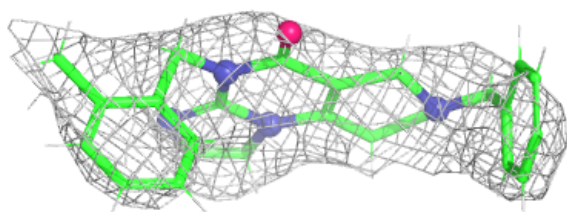
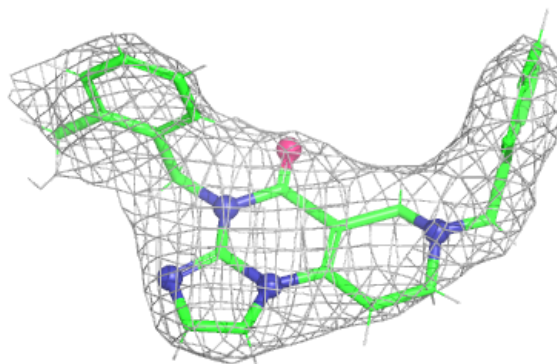
**Electron density around A1C98 E 804:**

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

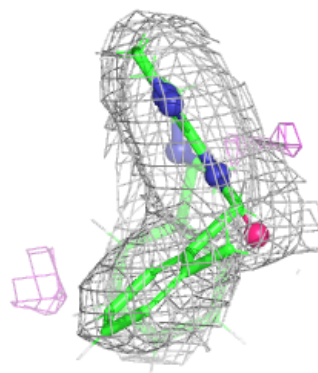
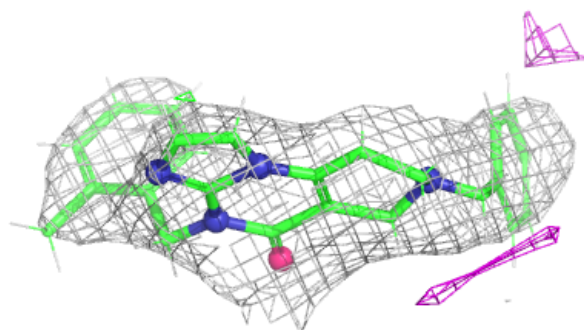
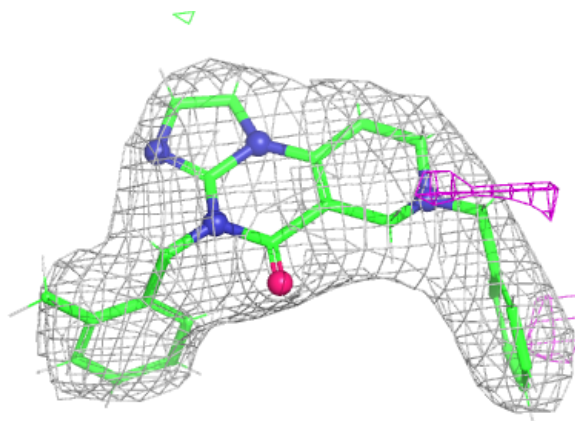


Electron density around A1C98 E 806:

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

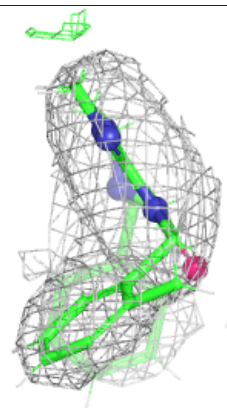
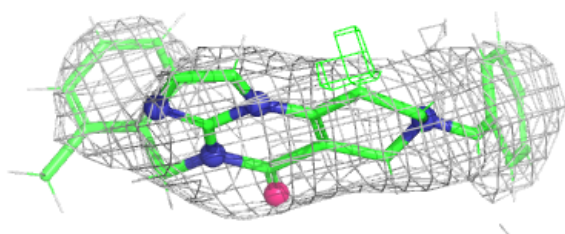
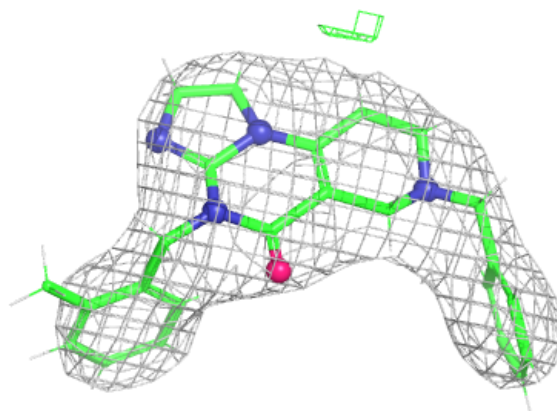
**Electron density around A1C98 A 804:**

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



Electron density around A1C98 C 804:

$2mF_o-DF_c$ (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.