



wwPDB X-ray Structure Validation Summary Report ⓘ

May 8, 2024 – 06:12 PM JST

PDB ID : 8YLB
Title : Cocrystal structures of agonists compound 1 with HsClpP
Authors : Zhao, N.; Zhu, Y.; Bao, R.
Deposited on : 2024-03-06
Resolution : 2.15 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 : 4.02b-467
Mogul : 1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix) : 1.13
EDS : 2.36.2
buster-report : 1.1.7 (2018)
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac : 5.8.0158
CCP4 : 7.0.044 (Gargrove)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.36.2

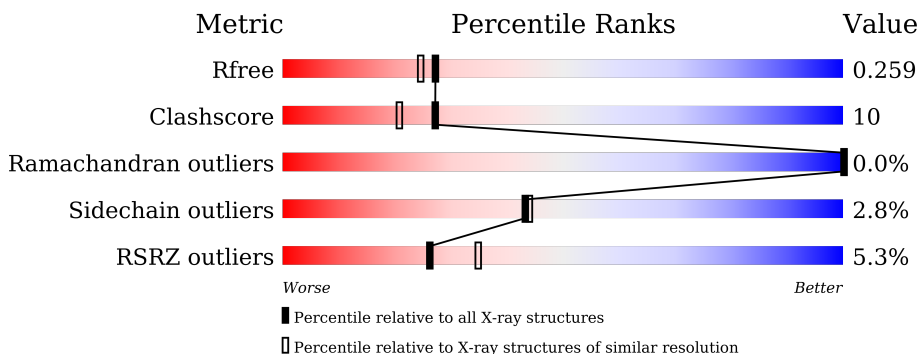
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.15 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}	130704	1479 (2.16-2.16)
Clashscore	141614	1585 (2.16-2.16)
Ramachandran outliers	138981	1560 (2.16-2.16)
Sidechain outliers	138945	1559 (2.16-2.16)
RSRZ outliers	127900	1456 (2.16-2.16)

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	220	
1	B	220	
1	C	220	
1	D	220	
1	E	220	
1	F	220	

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Mol	Chain	Length	Quality of chain
1	G	220	<p>3% 65% 11% 23%</p>
1	H	220	<p>7% 51% 23% 25%</p>
1	I	220	<p>4% 59% 19% 22%</p>
1	J	220	<p>6% 59% 18% 23%</p>
1	K	220	<p>3% 60% 18% 22%</p>
1	L	220	<p>3% 69% 9% 23%</p>
1	M	220	<p>5% 65% 13% 22%</p>
1	N	220	<p>5% 55% 21% 22%</p>

2 Entry composition i

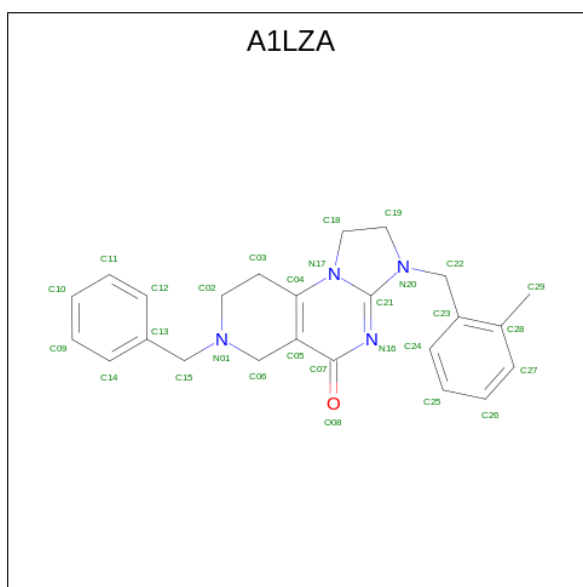
There are 3 unique types of molecules in this entry. The entry contains 19734 atoms, of which 294 are hydrogens and 0 are deuteriums.

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, mitochondrial.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	176	Total 1383	C 882	N 236	O 252	S 13	0	1	0
1	B	173	Total 1346	C 862	N 228	O 243	S 13	0	0	0
1	C	171	Total 1335	C 856	N 226	O 240	S 13	0	0	0
1	D	171	Total 1333	C 854	N 226	O 240	S 13	0	0	0
1	E	171	Total 1333	C 854	N 226	O 240	S 13	0	0	0
1	F	166	Total 1298	C 831	N 219	O 235	S 13	0	0	0
1	G	170	Total 1334	C 854	N 226	O 241	S 13	0	1	0
1	H	166	Total 1307	C 834	N 221	O 238	S 14	0	2	0
1	I	172	Total 1349	C 864	N 228	O 244	S 13	0	1	0
1	J	169	Total 1327	C 850	N 224	O 240	S 13	0	1	0
1	K	171	Total 1338	C 855	N 227	O 243	S 13	0	0	0
1	L	170	Total 1327	C 850	N 225	O 239	S 13	0	0	0
1	M	171	Total 1340	C 858	N 227	O 242	S 13	0	1	0
1	N	172	Total 1347	C 861	N 228	O 245	S 13	0	1	0

- Molecule 2 is 5-[(2-methylphenyl)methyl]-11-(phenylmethyl)-2,5,7,11-tetrazatricyclo[7.4.0.0[^]{2,6}]trideca-1(9),6-dien-8-one (three-letter code: A1LZA) (formula: C₂₄H₂₆N₄O) (labeled as "Ligand of Interest" by depositor).



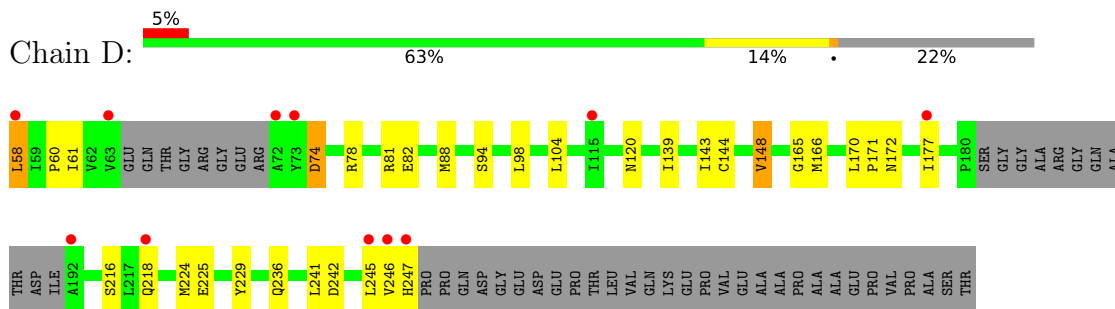
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	
			Total	C	H	N			O
2	A	1	Total	C	H	N	O	0	0
			50	24	21	4	1		
2	B	1	Total	C	H	N	O	0	0
			50	24	21	4	1		
2	C	1	Total	C	H	N	O	0	0
			50	24	21	4	1		
2	D	1	Total	C	H	N	O	0	0
			50	24	21	4	1		
2	E	1	Total	C	H	N	O	0	0
			50	24	21	4	1		
2	F	1	Total	C	H	N	O	0	0
			50	24	21	4	1		
2	G	1	Total	C	H	N	O	0	0
			50	24	21	4	1		
2	H	1	Total	C	H	N	O	0	0
			50	24	21	4	1		
2	I	1	Total	C	H	N	O	0	0
			50	24	21	4	1		
2	J	1	Total	C	H	N	O	0	0
			50	24	21	4	1		
2	K	1	Total	C	H	N	O	0	0
			50	24	21	4	1		
2	L	1	Total	C	H	N	O	0	0
			50	24	21	4	1		
2	M	1	Total	C	H	N	O	0	0
			50	24	21	4	1		
2	N	1	Total	C	H	N	O	0	0
			50	24	21	4	1		

- Molecule 3 is water.

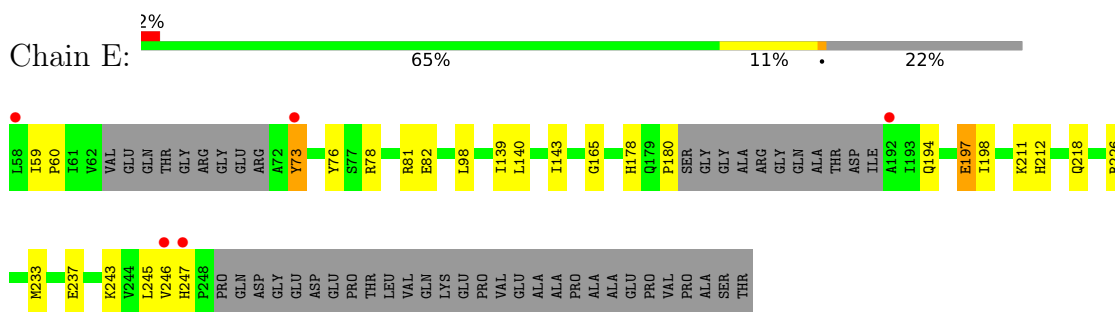
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	30	Total O 30 30	0	0
3	B	25	Total O 25 25	0	0
3	C	12	Total O 12 12	0	0
3	D	16	Total O 16 16	0	0
3	E	33	Total O 33 33	0	0
3	F	31	Total O 31 31	0	0
3	G	28	Total O 28 28	0	0
3	H	9	Total O 9 9	0	0
3	I	17	Total O 17 17	0	0
3	J	20	Total O 20 20	0	0
3	K	30	Total O 30 30	0	0
3	L	37	Total O 37 37	0	0
3	M	39	Total O 39 39	0	0
3	N	10	Total O 10 10	0	0

VAL
PRO
ALA
SER
THR

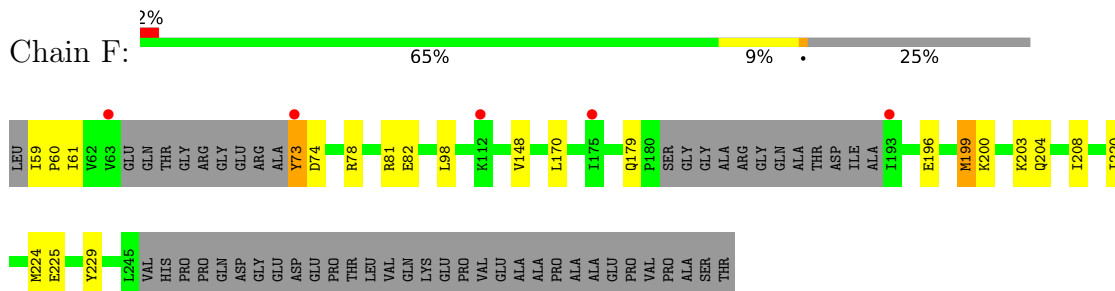
- Molecule 1: ATP-dependent Clp protease proteolytic subunit, mitochondrial



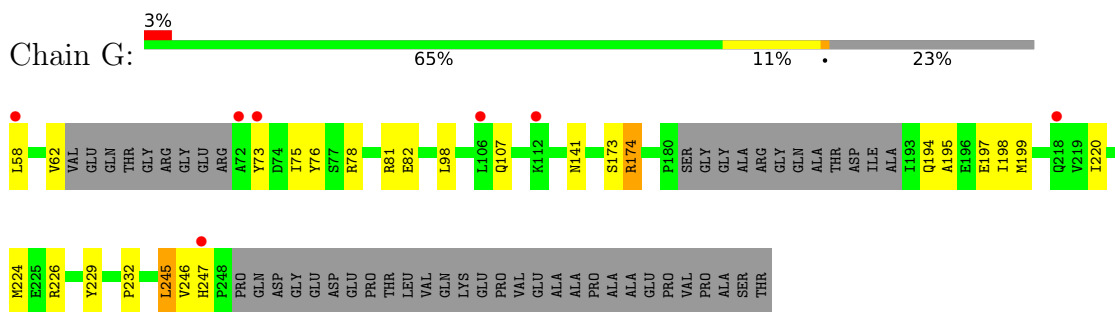
- Molecule 1: ATP-dependent Clp protease proteolytic subunit, mitochondrial



- Molecule 1: ATP-dependent Clp protease proteolytic subunit, mitochondrial



- Molecule 1: ATP-dependent Clp protease proteolytic subunit, mitochondrial



- Molecule 1: ATP-dependent Clp protease proteolytic subunit, mitochondrial



4 Data and refinement statistics i

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	120.24Å 96.74Å 124.54Å 90.00° 94.44° 90.00°	Depositor
Resolution (Å)	19.88 – 2.15 19.88 – 2.15	Depositor EDS
% Data completeness (in resolution range)	99.6 (19.88-2.15) 99.6 (19.88-2.15)	Depositor EDS
R_{merge}	0.25	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.10 (at 2.15Å)	Xtrriage
Refinement program	PHENIX (1.19.2_4158: ???)	Depositor
R, R_{free}	0.207 , 0.260 0.208 , 0.259	Depositor DCC
R_{free} test set	2016 reflections (1.31%)	wwPDB-VP
Wilson B-factor (Å ²)	34.6	Xtrriage
Anisotropy	0.240	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.36 , 45.6	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtrriage
Estimated twinning fraction	0.013 for l,-k,h	Xtrriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	19734	wwPDB-VP
Average B, all atoms (Å ²)	37.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 6.33% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: A1LZA

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	0.42	0/1407	0.61	0/1902
1	B	0.40	0/1370	0.61	0/1853
1	C	0.37	0/1359	0.59	0/1838
1	D	0.43	0/1356	0.62	0/1833
1	E	0.41	0/1357	0.61	0/1835
1	F	0.43	0/1320	0.62	0/1783
1	G	0.39	0/1358	0.62	0/1836
1	H	0.37	0/1328	0.59	0/1792
1	I	0.35	0/1372	0.57	0/1855
1	J	0.39	0/1349	0.59	0/1823
1	K	0.41	0/1361	0.61	0/1839
1	L	0.40	0/1351	0.62	0/1827
1	M	0.45	0/1365	0.64	0/1847
1	N	0.37	0/1371	0.60	0/1854
All	All	0.40	0/19024	0.61	0/25717

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	1383	0	1423	35	0
1	B	1346	0	1390	33	0
1	C	1335	0	1380	43	0
1	D	1333	0	1378	33	0
1	E	1333	0	1376	26	0
1	F	1298	0	1341	18	0
1	G	1334	0	1375	21	0
1	H	1307	0	1351	70	0
1	I	1349	0	1392	34	0
1	J	1327	0	1373	32	0
1	K	1338	0	1376	28	0
1	L	1327	0	1369	14	0
1	M	1340	0	1380	34	0
1	N	1347	0	1384	47	0
2	A	29	21	0	1	0
2	B	29	21	0	2	0
2	C	29	21	0	1	0
2	D	29	21	0	1	0
2	E	29	21	0	1	0
2	F	29	21	0	0	0
2	G	29	21	0	1	0
2	H	29	21	0	1	0
2	I	29	21	0	1	0
2	J	29	21	0	0	0
2	K	29	21	0	0	0
2	L	29	21	0	1	0
2	M	29	21	0	0	0
2	N	29	21	0	0	0
3	A	30	0	0	4	0
3	B	25	0	0	0	0
3	C	12	0	0	1	0
3	D	16	0	0	0	0
3	E	33	0	0	1	0
3	F	31	0	0	1	0
3	G	28	0	0	2	0
3	H	9	0	0	0	0
3	I	17	0	0	2	0
3	J	20	0	0	3	0
3	K	30	0	0	1	0
3	L	37	0	0	0	0
3	M	39	0	0	1	0
3	N	10	0	0	1	0
All	All	19440	294	19288	386	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 10.

The worst 5 of 386 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:J:73:TYR:OH	1:J:81:ARG:NH1	1.76	1.16
1:B:192:ALA:HB1	1:H:181:SER:HB3	1.40	1.01
1:H:193:ILE:HD11	1:H:198:ILE:HD13	1.42	0.99
1:B:196:GLU:HA	1:H:199:MET:HE1	1.45	0.94
1:H:148:VAL:HG12	1:H:170:LEU:HD12	1.49	0.94

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	171/220 (78%)	168 (98%)	3 (2%)	0	100	100
1	B	167/220 (76%)	162 (97%)	5 (3%)	0	100	100
1	C	165/220 (75%)	159 (96%)	6 (4%)	0	100	100
1	D	165/220 (75%)	162 (98%)	3 (2%)	0	100	100
1	E	165/220 (75%)	161 (98%)	4 (2%)	0	100	100
1	F	160/220 (73%)	155 (97%)	5 (3%)	0	100	100
1	G	165/220 (75%)	161 (98%)	4 (2%)	0	100	100
1	H	162/220 (74%)	155 (96%)	7 (4%)	0	100	100
1	I	167/220 (76%)	162 (97%)	5 (3%)	0	100	100
1	J	164/220 (74%)	159 (97%)	4 (2%)	1 (1%)	25	18
1	K	165/220 (75%)	161 (98%)	4 (2%)	0	100	100
1	L	164/220 (74%)	161 (98%)	3 (2%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	M	166/220 (76%)	159 (96%)	7 (4%)	0	100	100
1	N	167/220 (76%)	161 (96%)	6 (4%)	0	100	100
All	All	2313/3080 (75%)	2246 (97%)	66 (3%)	1 (0%)	100	100

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	J	110	SER

5.3.2 Protein sidechains [i](#)

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	155/184 (84%)	150 (97%)	5 (3%)	39	38
1	B	150/184 (82%)	147 (98%)	3 (2%)	55	59
1	C	149/184 (81%)	144 (97%)	5 (3%)	37	35
1	D	148/184 (80%)	144 (97%)	4 (3%)	44	46
1	E	148/184 (80%)	144 (97%)	4 (3%)	44	46
1	F	145/184 (79%)	141 (97%)	4 (3%)	43	44
1	G	149/184 (81%)	145 (97%)	4 (3%)	44	46
1	H	147/184 (80%)	142 (97%)	5 (3%)	37	35
1	I	150/184 (82%)	145 (97%)	5 (3%)	38	37
1	J	148/184 (80%)	145 (98%)	3 (2%)	55	59
1	K	149/184 (81%)	145 (97%)	4 (3%)	44	46
1	L	148/184 (80%)	145 (98%)	3 (2%)	55	59
1	M	150/184 (82%)	148 (99%)	2 (1%)	69	74
1	N	150/184 (82%)	142 (95%)	8 (5%)	22	19
All	All	2086/2576 (81%)	2027 (97%)	59 (3%)	43	44

5 of 59 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	G	245	LEU
1	N	168	HIS
1	I	174	ARG
1	N	108	SER
1	M	74	ASP

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 7 such sidechains are listed below:

Mol	Chain	Res	Type
1	G	107	GLN
1	H	137	GLN
1	M	247	HIS
1	L	204	GLN
1	E	179	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 monosaccharides 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	A1LZA	C	301	-	33,33,33	3.78	13 (39%)	39,47,47	3.19	14 (35%)
2	A1LZA	D	301	-	33,33,33	3.66	13 (39%)	39,47,47	3.08	11 (28%)
2	A1LZA	N	301	-	33,33,33	3.73	13 (39%)	39,47,47	3.25	13 (33%)
2	A1LZA	G	301	-	33,33,33	3.91	14 (42%)	39,47,47	3.16	12 (30%)
2	A1LZA	K	301	-	33,33,33	3.68	12 (36%)	39,47,47	3.30	11 (28%)
2	A1LZA	M	301	-	33,33,33	3.90	14 (42%)	39,47,47	3.19	11 (28%)
2	A1LZA	J	301	-	33,33,33	3.63	13 (39%)	39,47,47	3.15	10 (25%)
2	A1LZA	H	301	-	33,33,33	3.83	13 (39%)	39,47,47	3.19	11 (28%)
2	A1LZA	I	301	-	33,33,33	3.75	13 (39%)	39,47,47	3.22	13 (33%)
2	A1LZA	B	301	-	33,33,33	3.97	14 (42%)	39,47,47	3.19	10 (25%)
2	A1LZA	A	301	-	33,33,33	3.86	15 (45%)	39,47,47	3.23	12 (30%)
2	A1LZA	E	301	-	33,33,33	3.66	13 (39%)	39,47,47	3.25	12 (30%)
2	A1LZA	L	301	-	33,33,33	3.95	15 (45%)	39,47,47	3.22	12 (30%)
2	A1LZA	F	301	-	33,33,33	3.81	13 (39%)	39,47,47	3.15	12 (30%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '2' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	A1LZA	C	301	-	-	3/8/26/26	0/5/5/5
2	A1LZA	D	301	-	-	2/8/26/26	0/5/5/5
2	A1LZA	N	301	-	-	2/8/26/26	0/5/5/5
2	A1LZA	G	301	-	-	2/8/26/26	0/5/5/5
2	A1LZA	K	301	-	-	2/8/26/26	0/5/5/5
2	A1LZA	M	301	-	-	2/8/26/26	0/5/5/5
2	A1LZA	J	301	-	-	2/8/26/26	0/5/5/5
2	A1LZA	H	301	-	-	1/8/26/26	0/5/5/5
2	A1LZA	I	301	-	-	2/8/26/26	0/5/5/5
2	A1LZA	B	301	-	-	2/8/26/26	0/5/5/5
2	A1LZA	A	301	-	-	2/8/26/26	0/5/5/5
2	A1LZA	E	301	-	-	2/8/26/26	0/5/5/5
2	A1LZA	L	301	-	-	2/8/26/26	0/5/5/5
2	A1LZA	F	301	-	-	2/8/26/26	0/5/5/5

The worst 5 of 188 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	L	301	A1LZA	C06-N01	-15.69	1.32	1.46
2	M	301	A1LZA	C06-N01	-15.55	1.32	1.46
2	B	301	A1LZA	C06-N01	-15.50	1.32	1.46
2	G	301	A1LZA	C06-N01	-15.48	1.32	1.46
2	A	301	A1LZA	C06-N01	-15.24	1.32	1.46

The worst 5 of 164 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	301	A1LZA	C03-C02-N01	11.28	121.48	111.23
2	N	301	A1LZA	C03-C02-N01	10.97	121.19	111.23
2	E	301	A1LZA	C03-C02-N01	10.88	121.12	111.23
2	J	301	A1LZA	C03-C02-N01	10.83	121.07	111.23
2	K	301	A1LZA	C03-C02-N01	10.71	120.96	111.23

There are no chirality outliers.

5 of 28 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	301	A1LZA	C13-C15-N01-C02
2	H	301	A1LZA	C13-C15-N01-C02
2	M	301	A1LZA	C13-C15-N01-C02
2	D	301	A1LZA	C13-C15-N01-C02
2	F	301	A1LZA	C13-C15-N01-C02

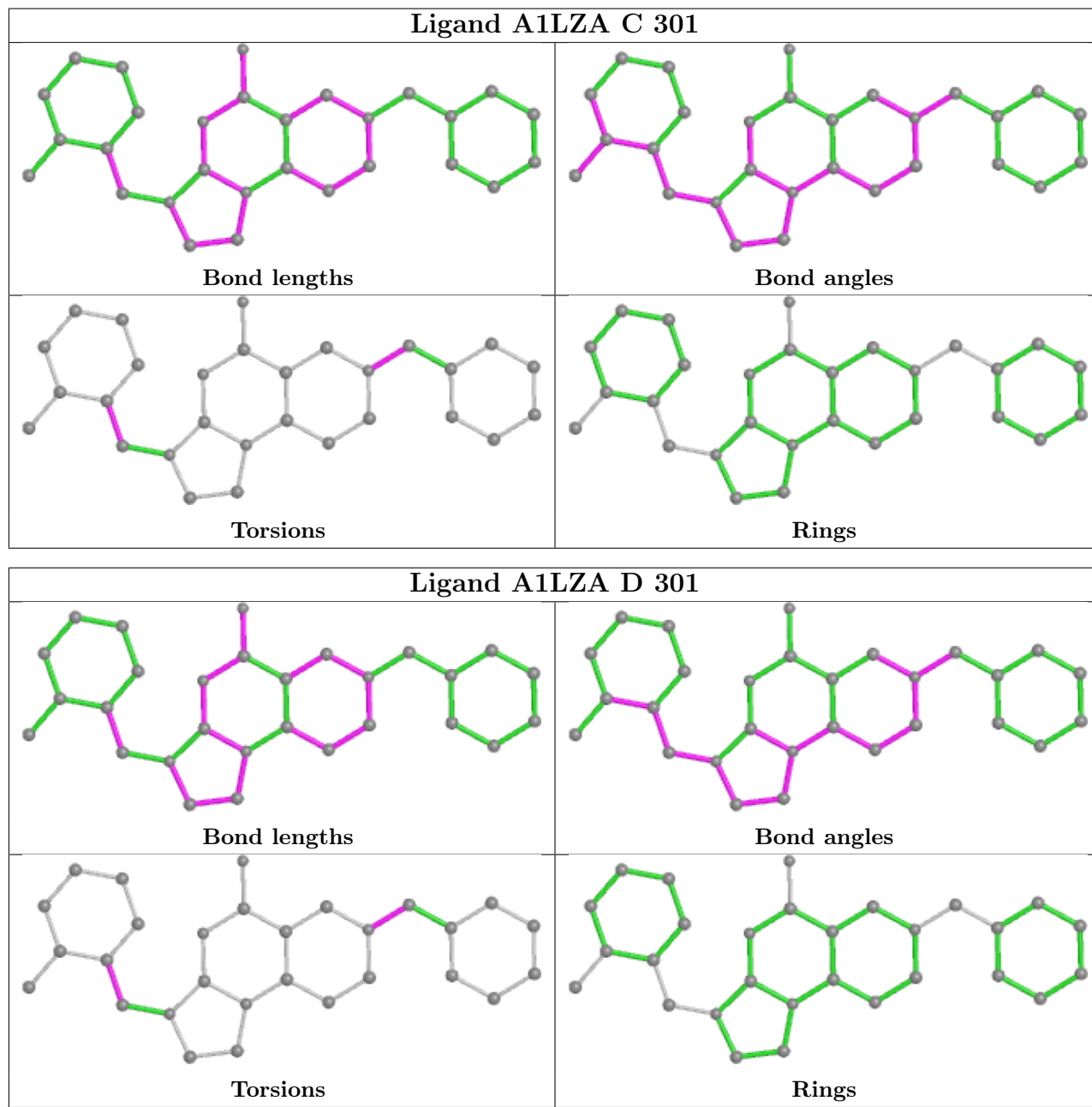
There are no ring outliers.

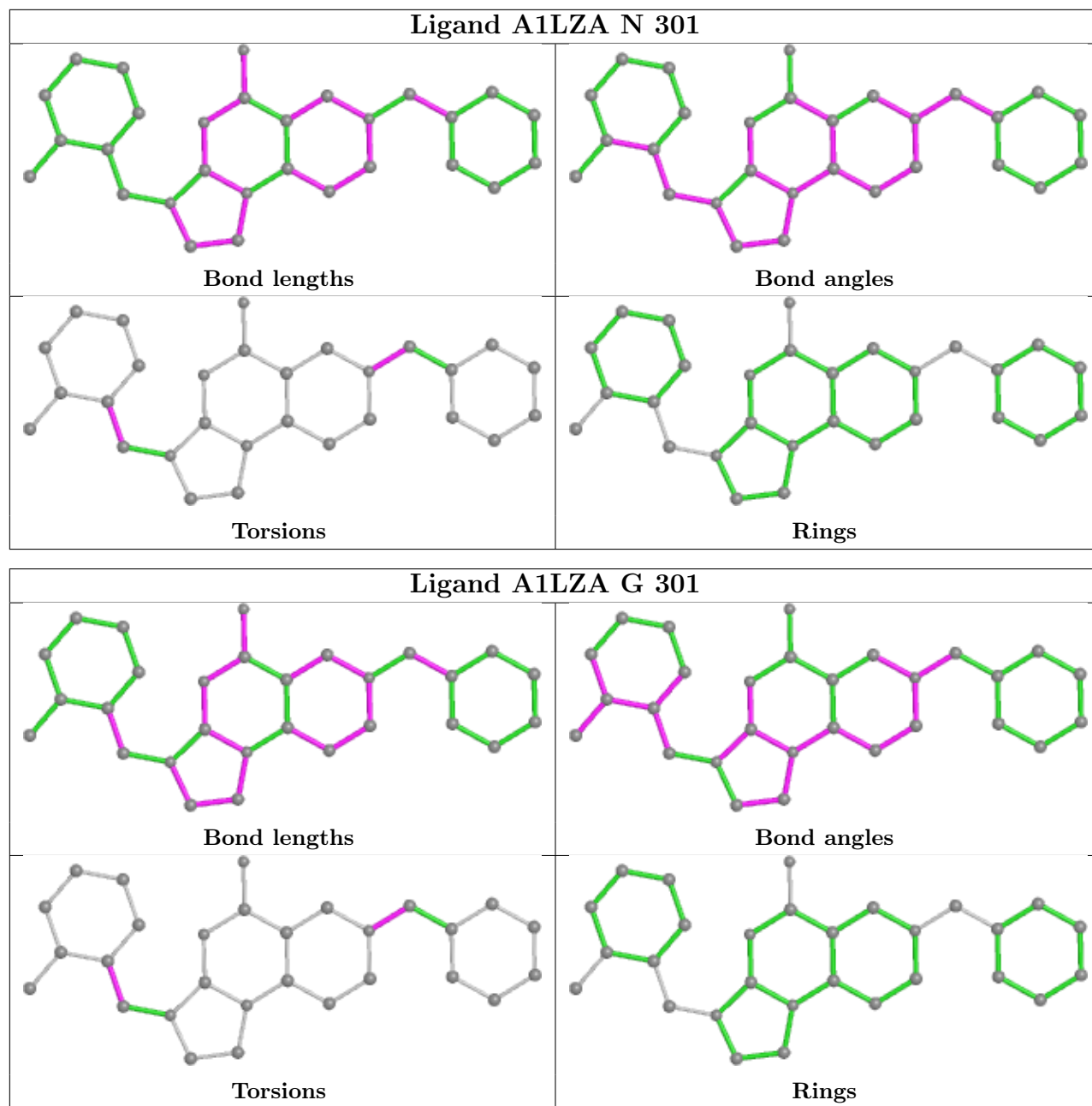
9 monomers are involved in 10 short contacts:

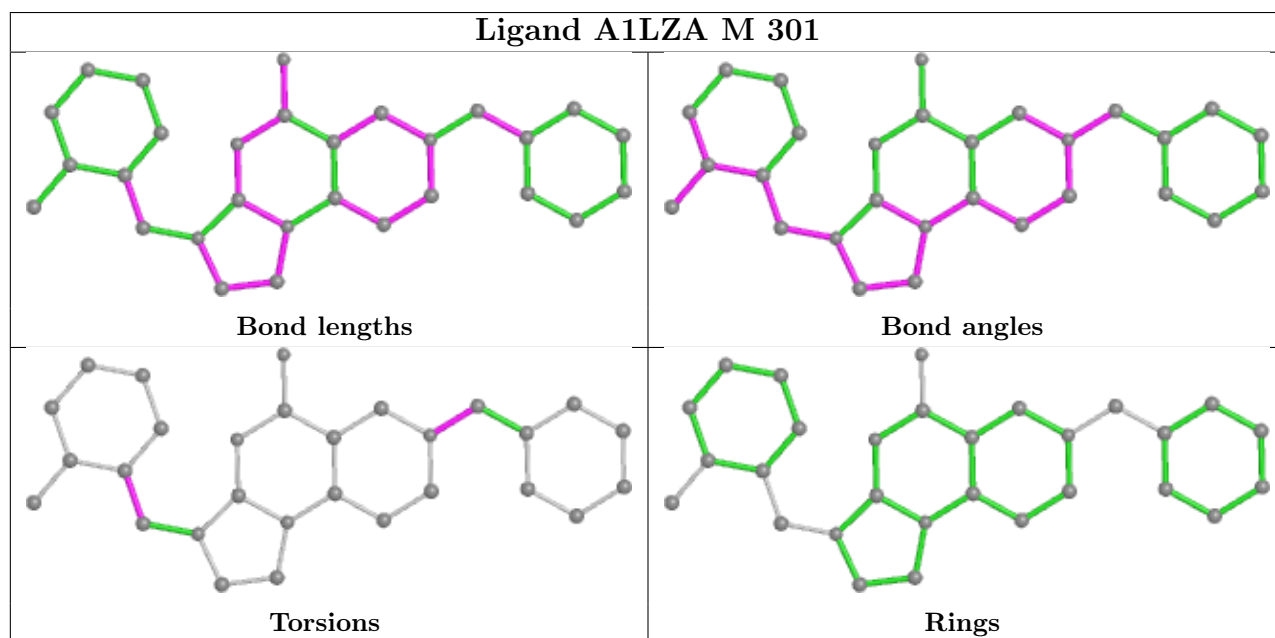
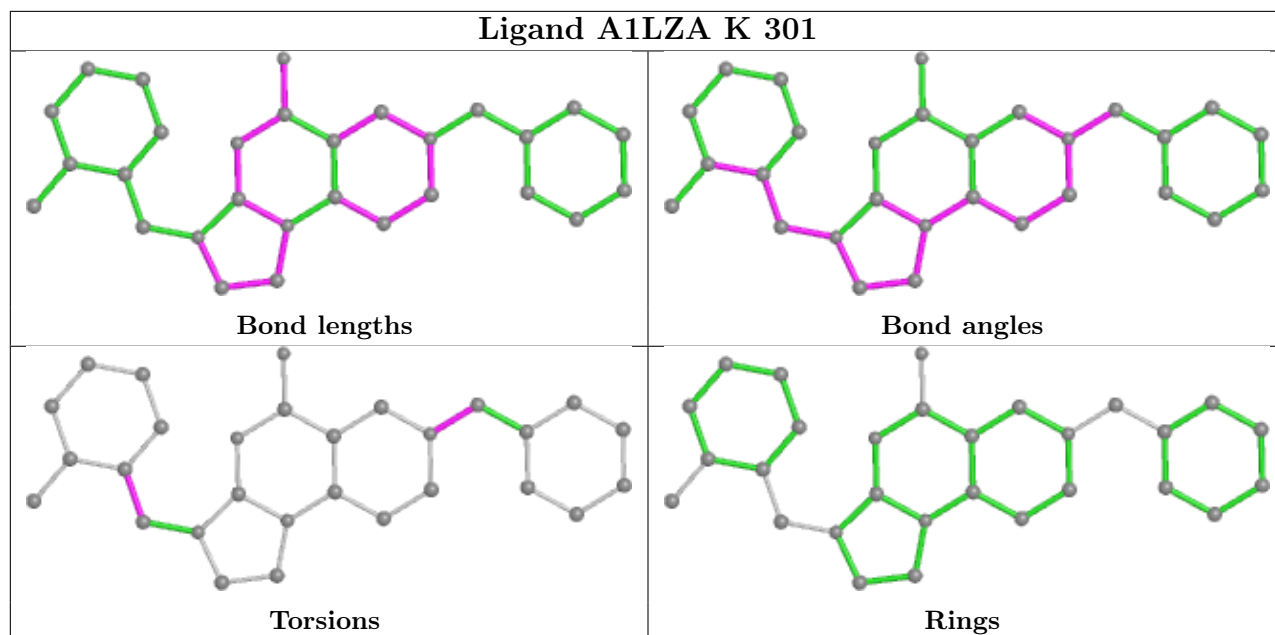
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	C	301	A1LZA	1	0
2	D	301	A1LZA	1	0
2	G	301	A1LZA	1	0
2	H	301	A1LZA	1	0
2	I	301	A1LZA	1	0
2	B	301	A1LZA	2	0
2	A	301	A1LZA	1	0
2	E	301	A1LZA	1	0
2	L	301	A1LZA	1	0

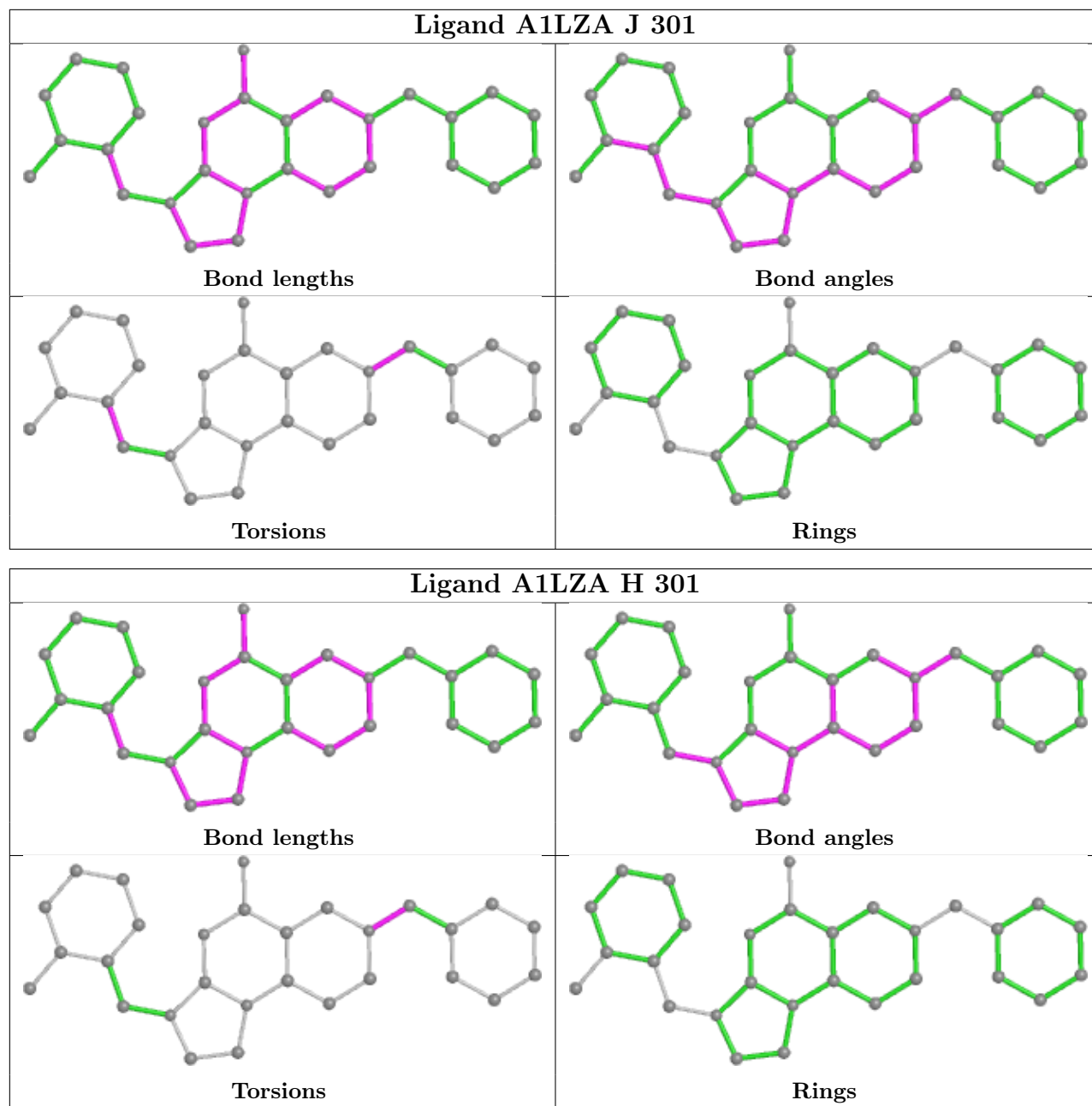
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In

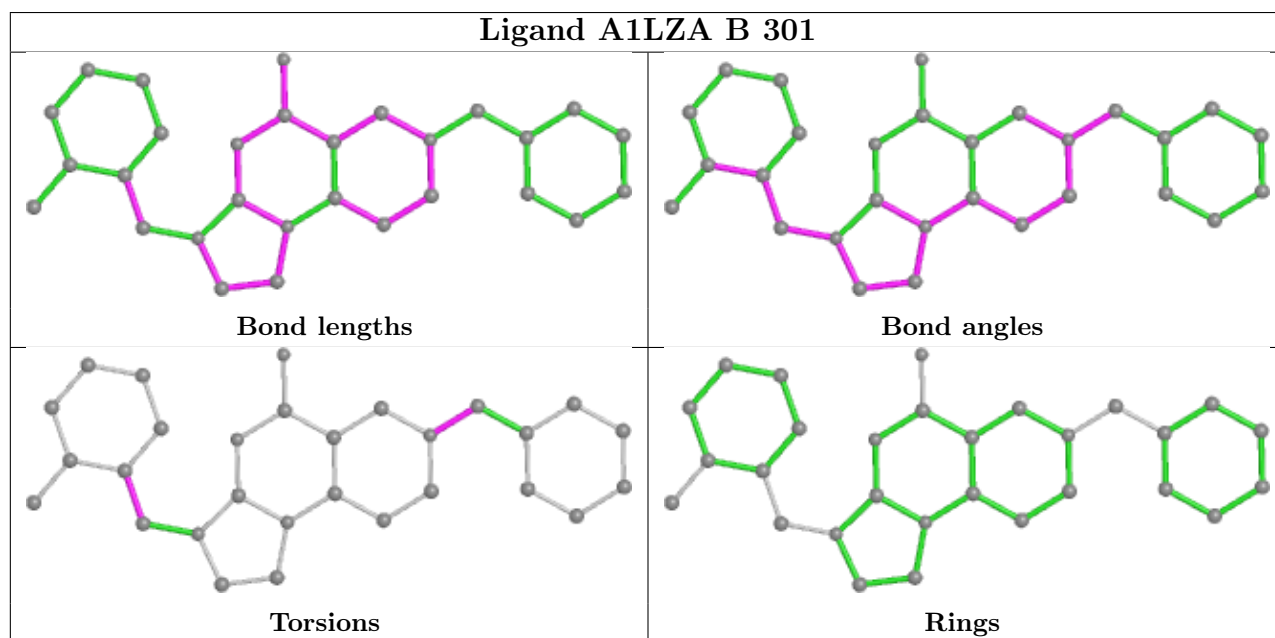
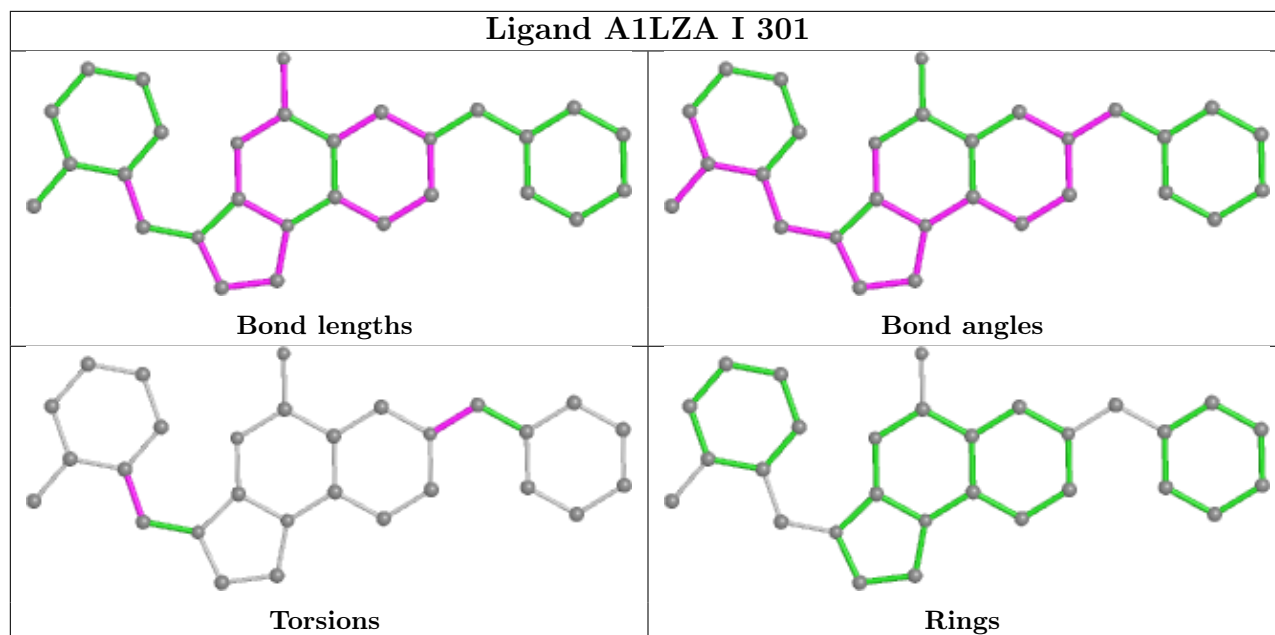
addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. 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.

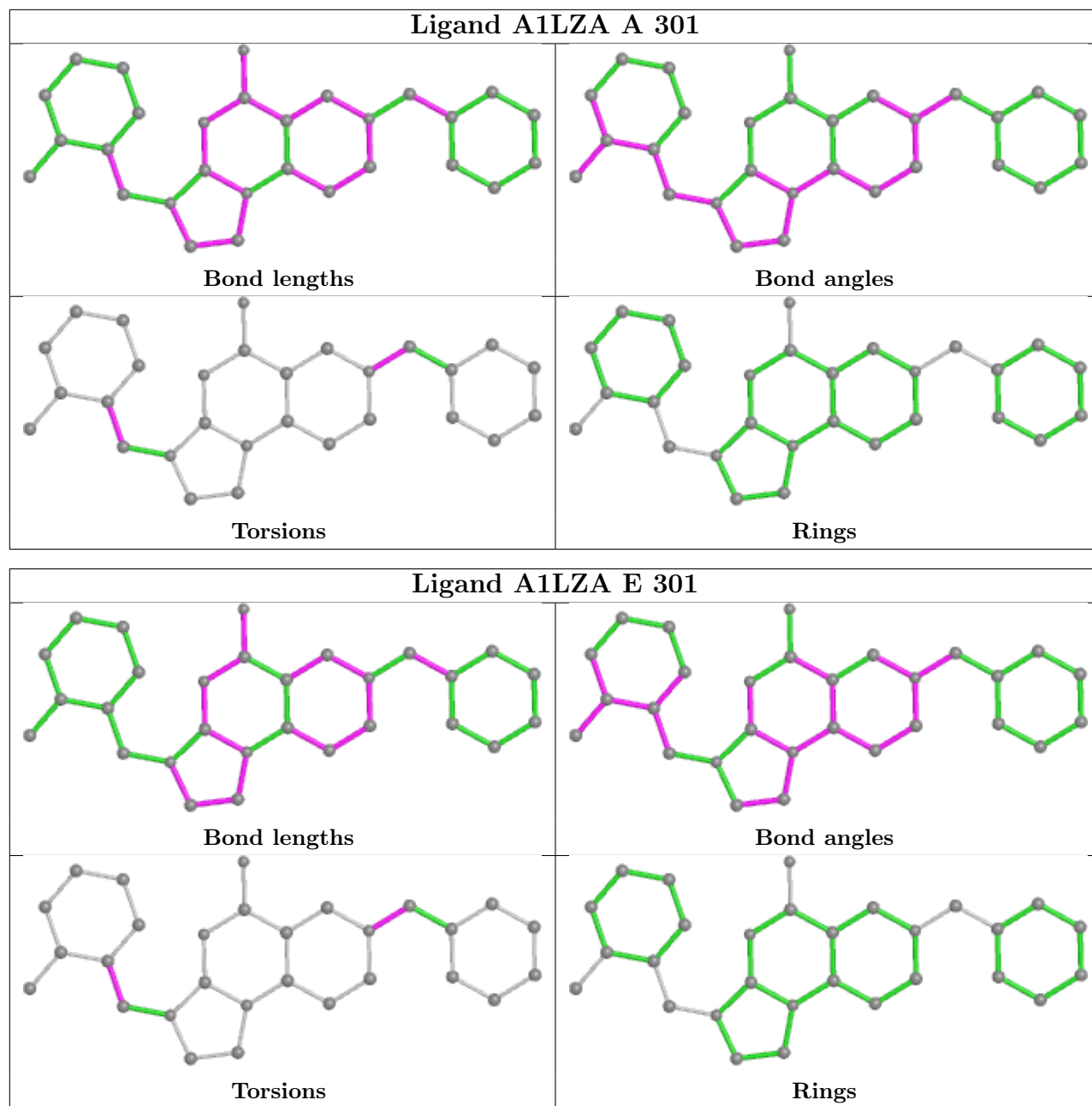


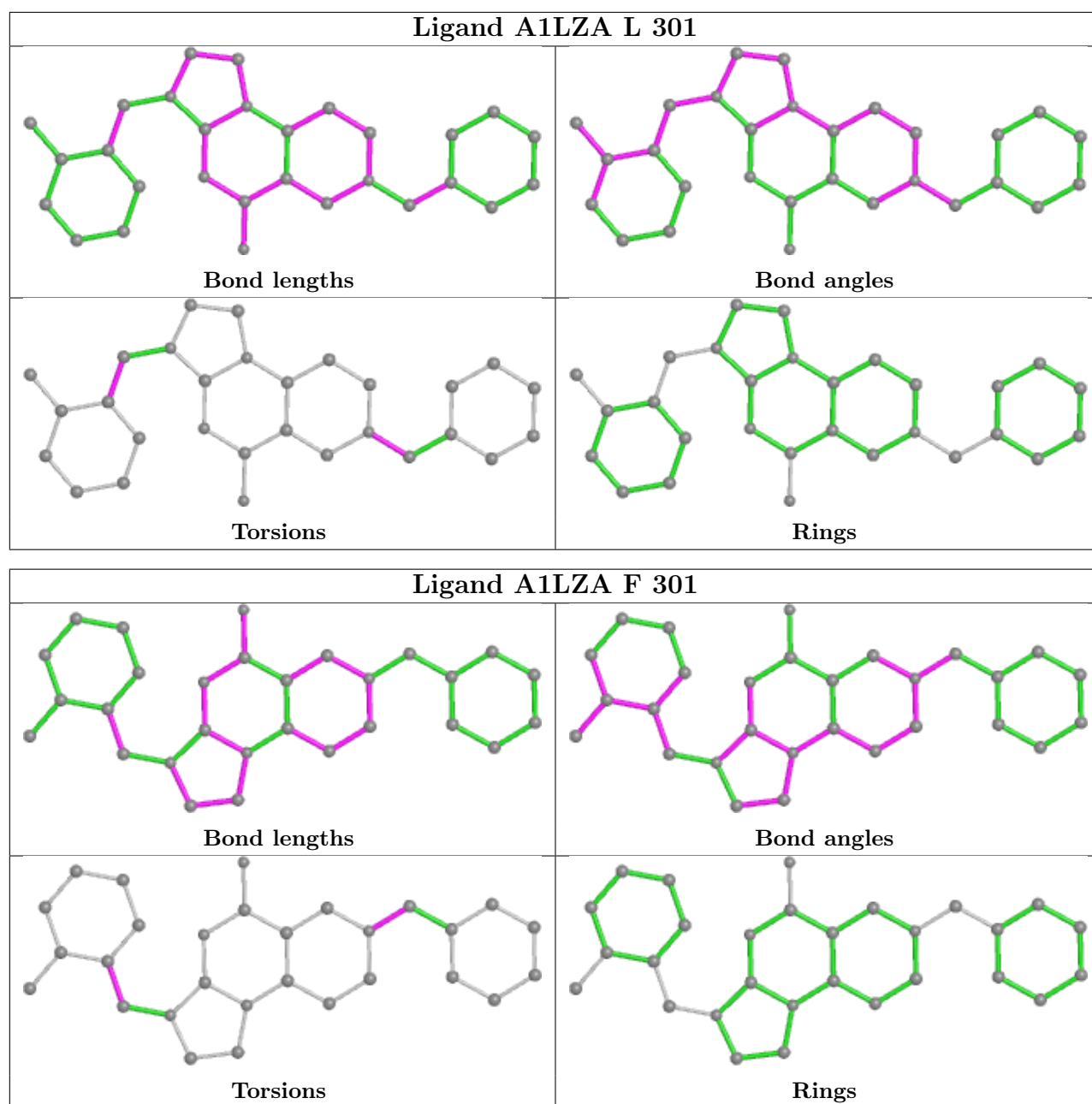












5.7 Other polymers [i](#)

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 [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	176/220 (80%)	0.26	10 (5%) 23 32	22, 33, 56, 75	0
1	B	173/220 (78%)	0.25	11 (6%) 19 26	27, 35, 55, 72	0
1	C	171/220 (77%)	0.32	8 (4%) 31 41	29, 38, 55, 69	0
1	D	171/220 (77%)	0.32	11 (6%) 19 26	27, 37, 54, 76	0
1	E	171/220 (77%)	0.17	5 (2%) 51 61	24, 33, 53, 69	0
1	F	166/220 (75%)	0.08	5 (3%) 50 59	23, 31, 46, 60	0
1	G	170/220 (77%)	0.17	7 (4%) 37 46	24, 34, 49, 64	0
1	H	166/220 (75%)	0.58	15 (9%) 9 14	33, 42, 55, 77	0
1	I	172/220 (78%)	0.36	9 (5%) 27 35	30, 39, 55, 70	0
1	J	169/220 (76%)	0.35	13 (7%) 13 18	29, 38, 55, 74	0
1	K	171/220 (77%)	0.19	6 (3%) 44 52	26, 35, 53, 75	0
1	L	170/220 (77%)	0.22	6 (3%) 44 52	21, 32, 48, 66	0
1	M	171/220 (77%)	0.19	10 (5%) 23 31	20, 31, 47, 72	0
1	N	172/220 (78%)	0.36	11 (6%) 19 26	26, 39, 54, 72	0
All	All	2389/3080 (77%)	0.27	127 (5%) 26 35	20, 36, 54, 77	0

The worst 5 of 127 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	H	58	LEU	8.8
1	M	63	VAL	5.6
1	N	63	VAL	5.2
1	H	181	SER	5.1
1	I	58	LEU	4.8

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 monosaccharides in this entry.

6.4 Ligands [i](#)

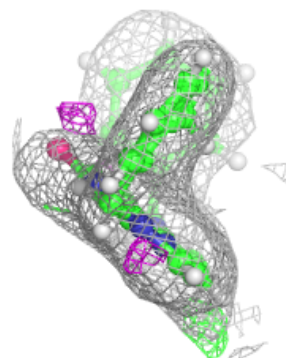
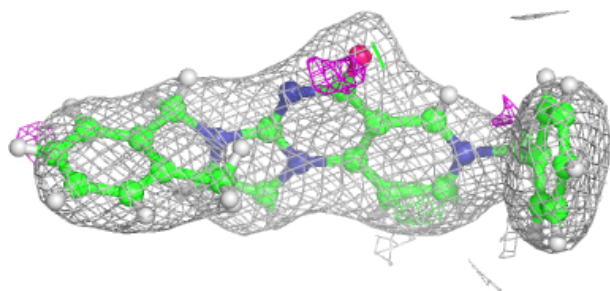
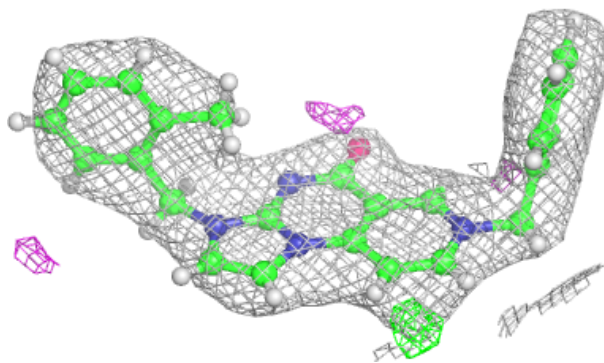
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
2	A1LZA	K	301	29/29	0.85	0.15	33,42,50,54	0
2	A1LZA	E	301	29/29	0.87	0.16	33,42,52,58	0
2	A1LZA	G	301	29/29	0.88	0.14	31,39,49,52	0
2	A1LZA	C	301	29/29	0.88	0.15	34,45,57,58	0
2	A1LZA	H	301	29/29	0.89	0.16	36,46,58,62	0
2	A1LZA	D	301	29/29	0.90	0.15	32,45,54,59	0
2	A1LZA	M	301	29/29	0.90	0.14	26,41,56,57	0
2	A1LZA	B	301	29/29	0.91	0.14	28,40,51,57	0
2	A1LZA	J	301	29/29	0.91	0.14	38,50,63,67	0
2	A1LZA	I	301	29/29	0.92	0.14	38,47,60,62	0
2	A1LZA	L	301	29/29	0.92	0.12	29,39,52,53	0
2	A1LZA	A	301	29/29	0.92	0.13	31,39,54,57	0
2	A1LZA	F	301	29/29	0.93	0.11	30,40,52,54	0
2	A1LZA	N	301	29/29	0.94	0.11	34,43,53,58	0

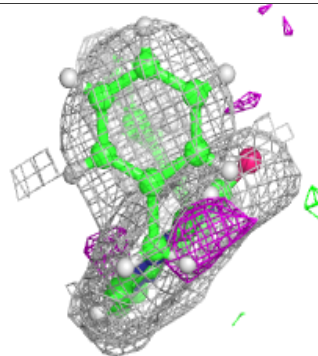
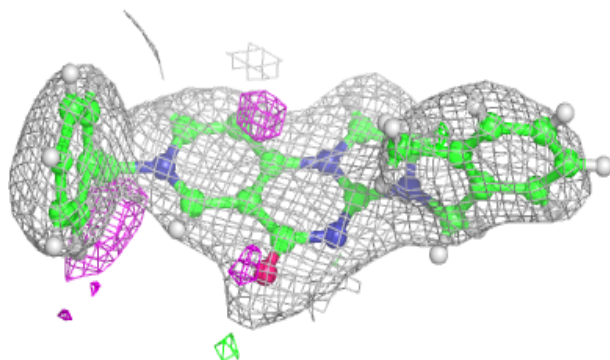
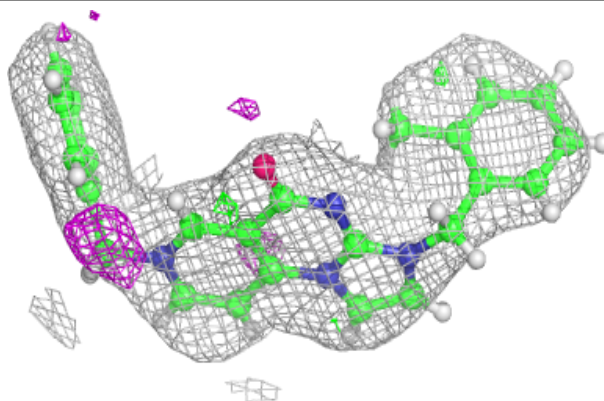
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around A1LZA K 301:

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

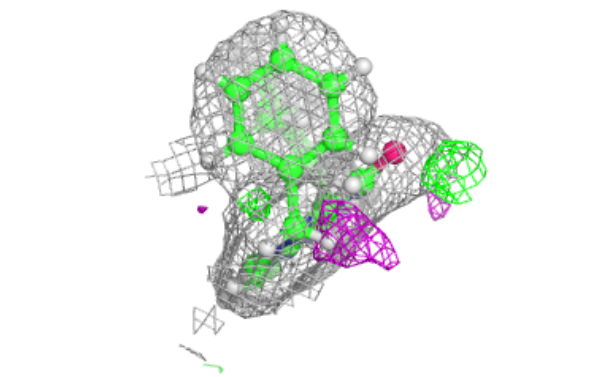
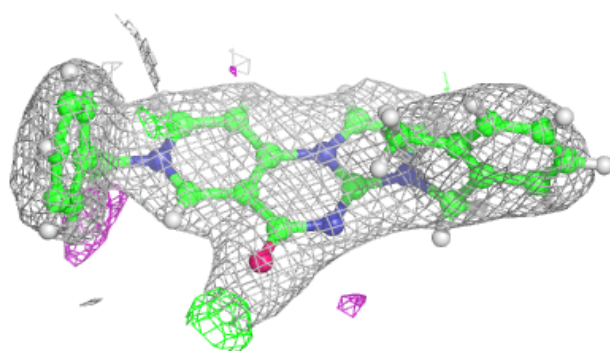
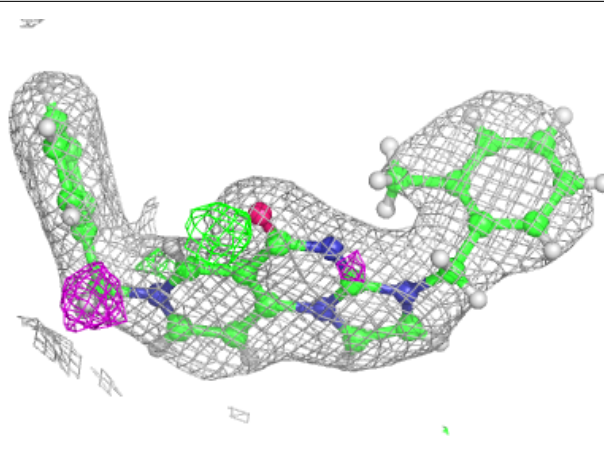
**Electron density around A1LZA E 301:**

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

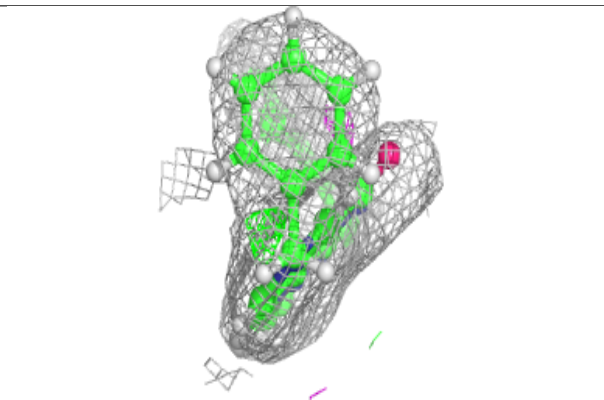
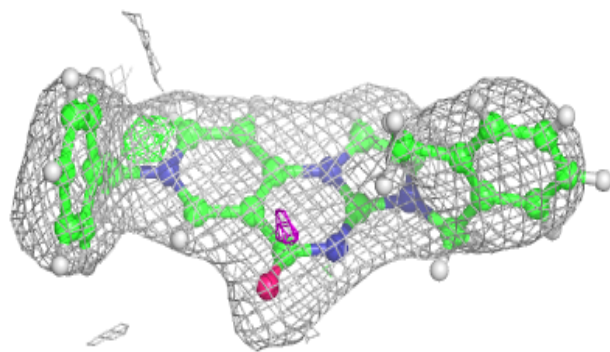
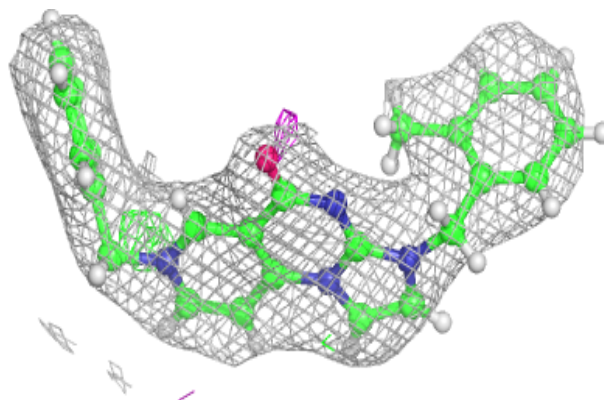


Electron density around A1LZA G 301:

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

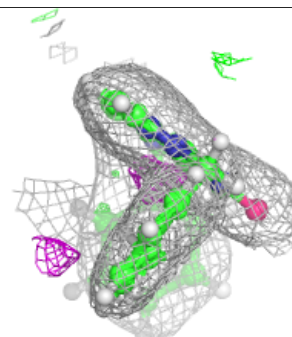
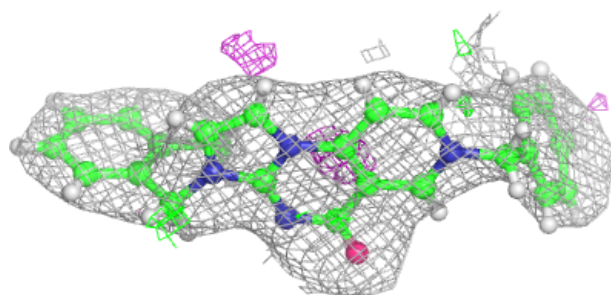
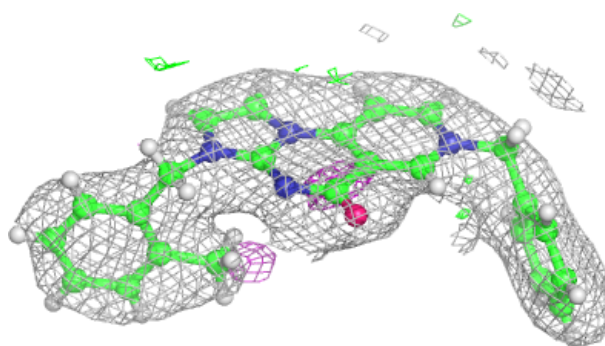
**Electron density around A1LZA C 301:**

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

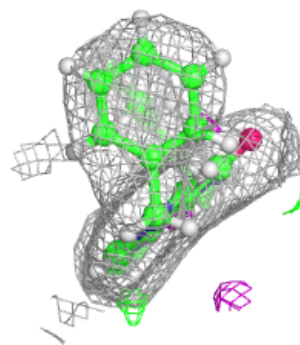
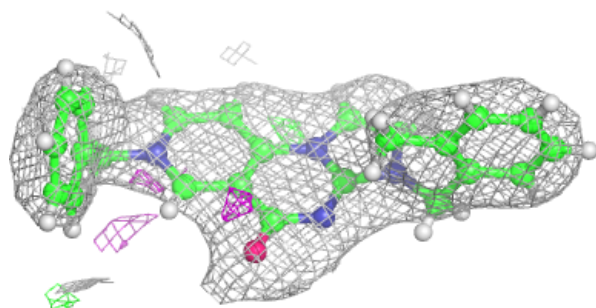
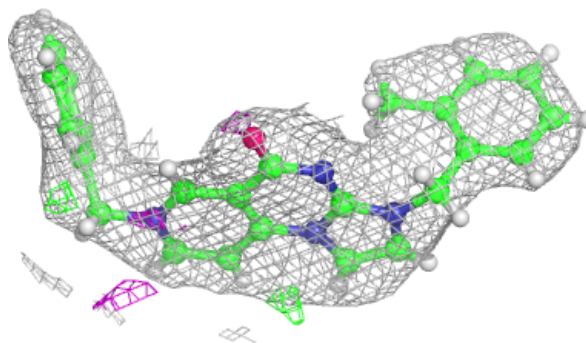


Electron density around A1LZA H 301:

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

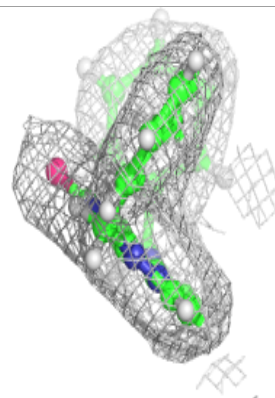
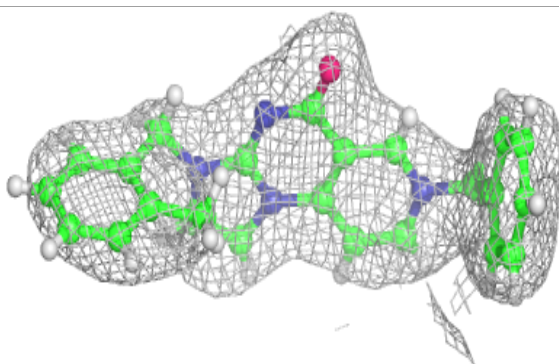
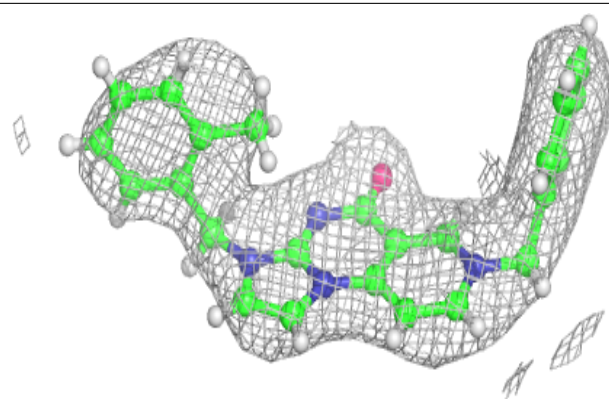
**Electron density around A1LZA D 301:**

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

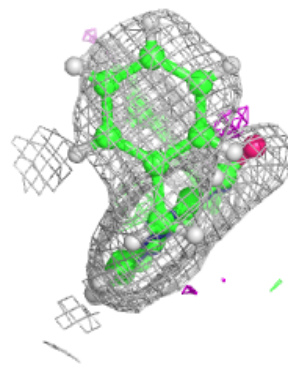
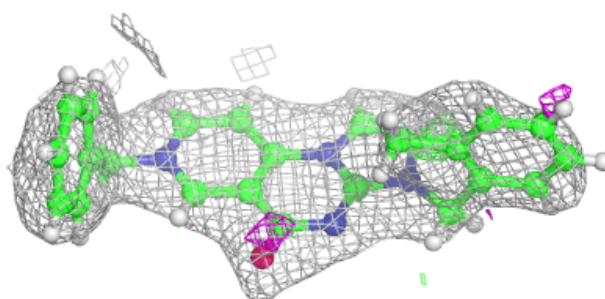
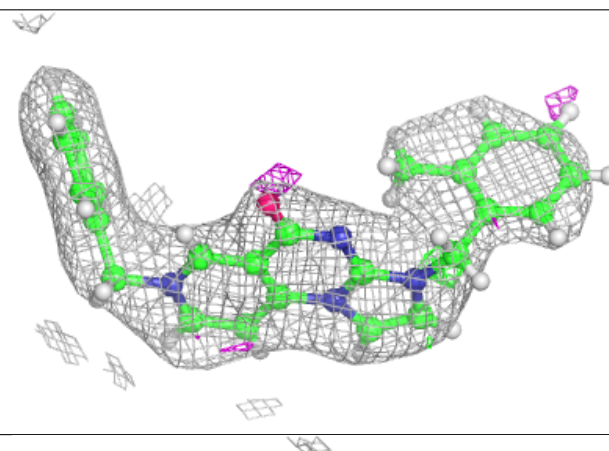


Electron density around A1LZA M 301:

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

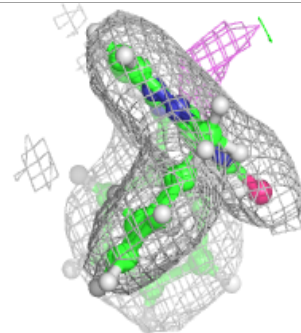
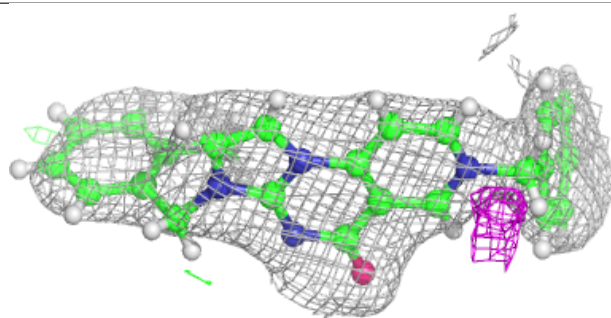
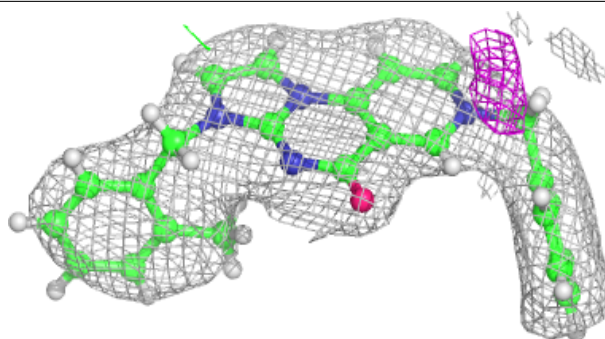
**Electron density around A1LZA B 301:**

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

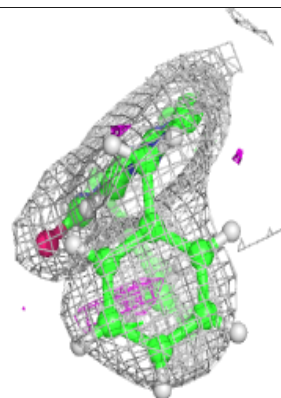
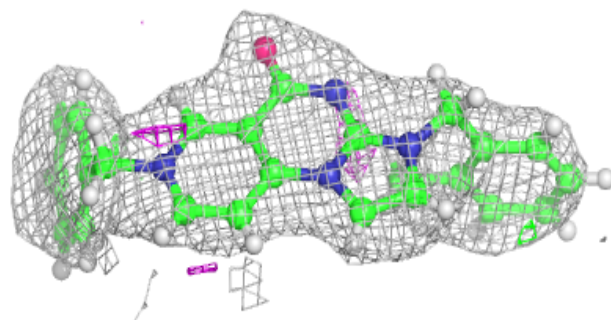
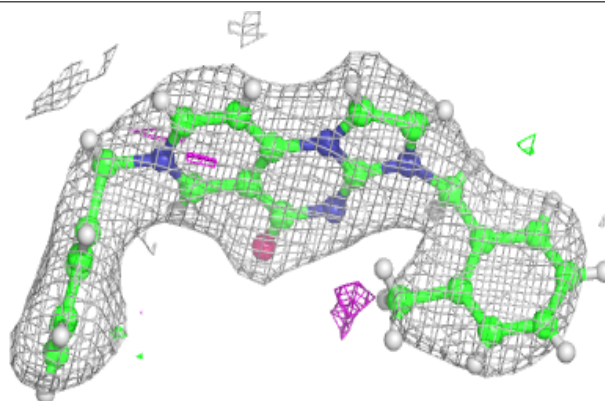


Electron density around A1LZA J 301:

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

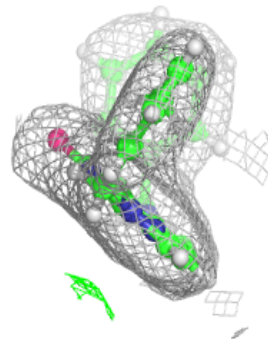
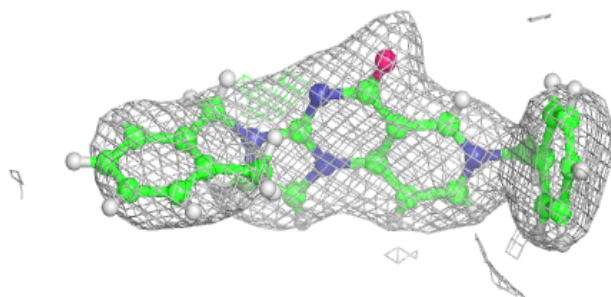
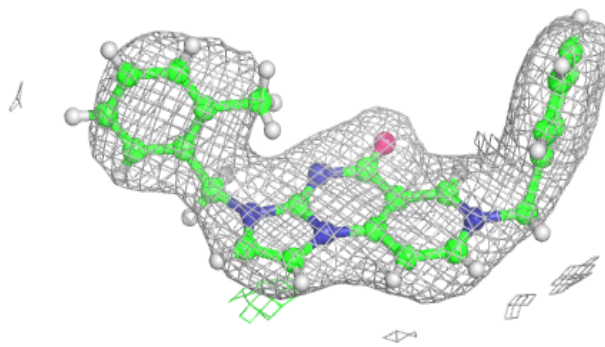
**Electron density around A1LZA I 301:**

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

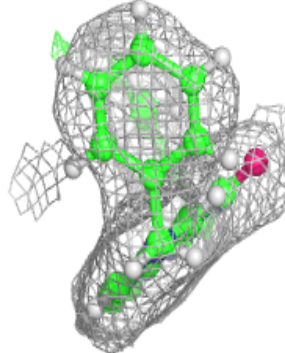
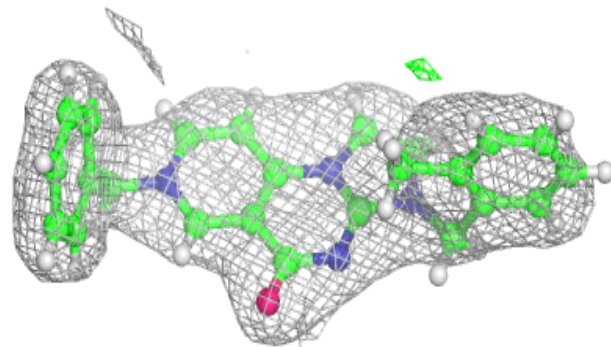
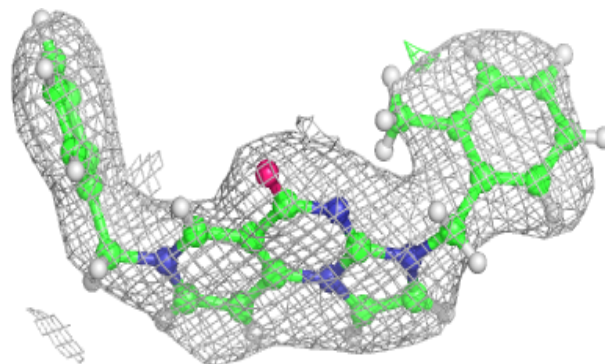


Electron density around A1LZA L 301:

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

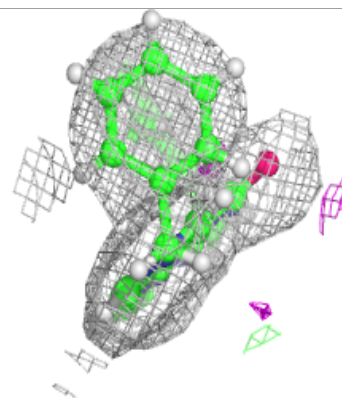
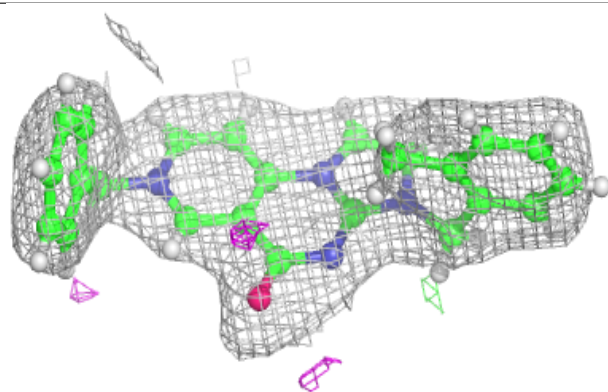
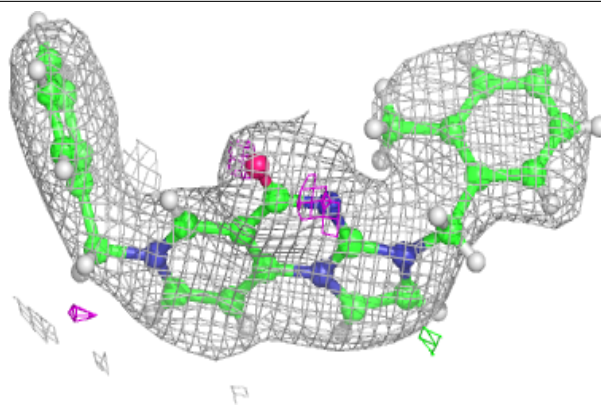
**Electron density around A1LZA A 301:**

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

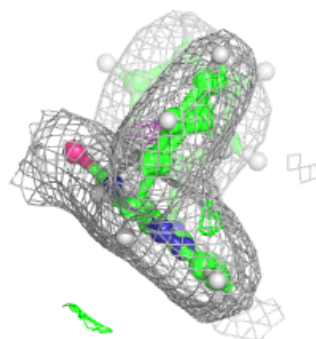
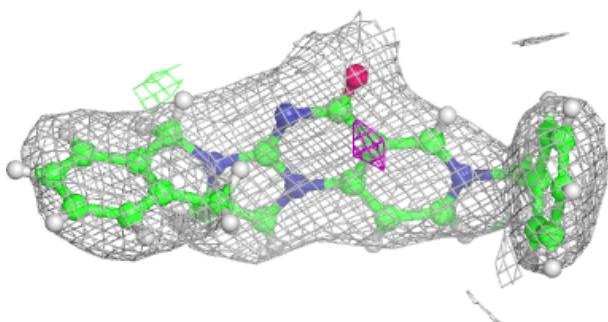
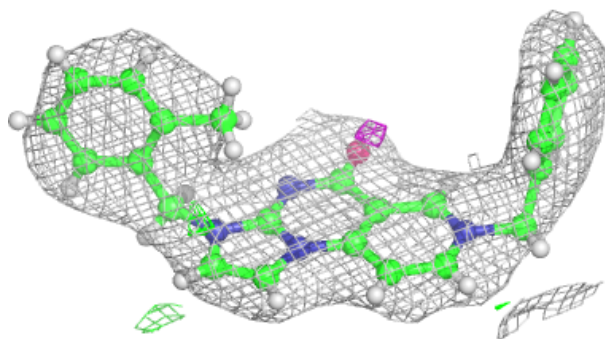


Electron density around A1LZA F 301:

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

**Electron density around A1LZA N 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.