



# wwPDB X-ray Structure Validation Summary Report ⓘ

Dec 18, 2023 – 06:27 am GMT

PDB ID : 4BN5  
Title : Structure of human SIRT3 in complex with SRT1720 inhibitor  
Authors : Nguyen, G.T.T.; Schaefer, S.; Gertz, M.; Weyand, M.; Steegborn, C.  
Deposited on : 2013-05-13  
Resolution : 3.25 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](mailto: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>.

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The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity : 4.02b-467  
Mogul : 1.8.4, CSD as541be (2020)  
Xtriage (Phenix) : 1.13  
EDS : 2.36  
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

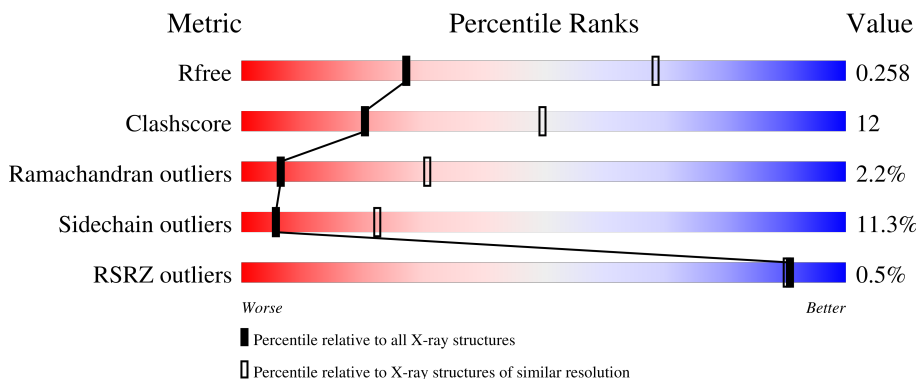
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 3.25 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	1191 (3.30-3.22)
Clashscore	141614	1251 (3.30-3.22)
Ramachandran outliers	138981	1229 (3.30-3.22)
Sidechain outliers	138945	1228 (3.30-3.22)
RSRZ outliers	127900	1154 (3.30-3.22)

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  $\geq 3$ , 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	281	 61% 30% 5% ..
1	B	281	 66% 24% 6% ..
1	C	281	 63% 30% ..
1	D	281	 64% 26% 5% ..
1	E	281	 70% 23% ..

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Mol	Chain	Length	Quality of chain
1	F	281	
1	G	281	
1	H	281	
1	I	281	
1	J	281	
1	K	281	
1	L	281	

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	SR7	F	1396	-	-	X	-
3	SR7	G	1396	-	-	X	-
3	SR7	H	1396	-	-	X	-
3	SR7	I	1396	-	-	X	-

## 2 Entry composition [i](#)

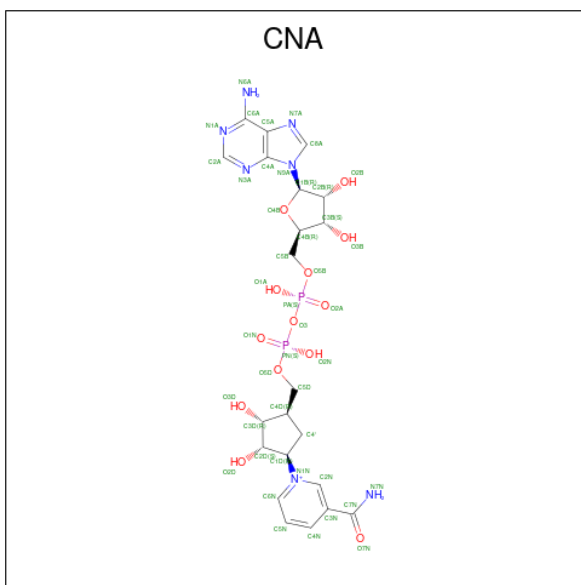
There are 5 unique types of molecules in this entry. The entry contains 26520 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 NAD-DEPENDENT PROTEIN DEACETYLASE SIRTUIN-3, MITOCHONDRIAL.

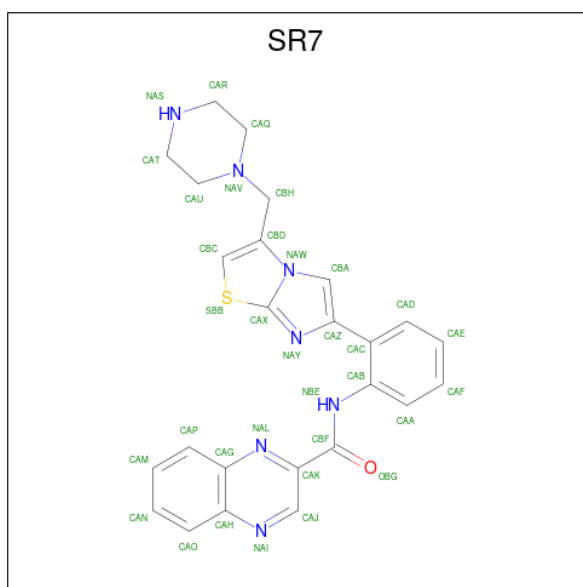
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	273	Total 2144	C 1382	N 369	O 384	S 9	0	0	0
1	B	273	Total 2144	C 1382	N 369	O 384	S 9	0	0	0
1	C	273	Total 2131	C 1372	N 369	O 381	S 9	0	0	0
1	D	272	Total 2059	C 1330	N 346	O 374	S 9	0	0	0
1	E	273	Total 2096	C 1356	N 353	O 378	S 9	0	0	0
1	F	273	Total 2144	C 1382	N 369	O 384	S 9	0	0	0
1	G	273	Total 2144	C 1382	N 369	O 384	S 9	0	0	0
1	H	273	Total 2144	C 1382	N 369	O 384	S 9	0	0	0
1	I	273	Total 2120	C 1369	N 361	O 381	S 9	0	0	0
1	J	273	Total 2144	C 1382	N 369	O 384	S 9	0	0	0
1	K	273	Total 2144	C 1382	N 369	O 384	S 9	0	0	0
1	L	273	Total 2134	C 1377	N 366	O 382	S 9	0	0	0

- Molecule 2 is CARBA-NICOTINAMIDE-ADENINE-DINUCLEOTIDE (three-letter code: CNA) (formula: C<sub>22</sub>H<sub>30</sub>N<sub>7</sub>O<sub>13</sub>P<sub>2</sub>).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	
			Total	C	N	O	P			
2	A	1	Total	44	22	7	13	2	0	0
2	B	1	Total	44	22	7	13	2	0	0
2	C	1	Total	44	22	7	13	2	0	0
2	D	1	Total	44	22	7	13	2	0	0
2	E	1	Total	44	22	7	13	2	0	0
2	F	1	Total	44	22	7	13	2	0	0
2	G	1	Total	44	22	7	13	2	0	0
2	H	1	Total	44	22	7	13	2	0	0
2	I	1	Total	44	22	7	13	2	0	0
2	J	1	Total	44	22	7	13	2	0	0
2	K	1	Total	44	22	7	13	2	0	0
2	L	1	Total	44	22	7	13	2	0	0

- Molecule 3 is N-{2-[3-(piperazin-1-ylmethyl)imidazo[2,1-b][1,3]thiazol-6-yl]phenyl}quinoxali-  
ne-2-carboxamide (three-letter code: SR7) (formula: C<sub>25</sub>H<sub>23</sub>N<sub>7</sub>OS).

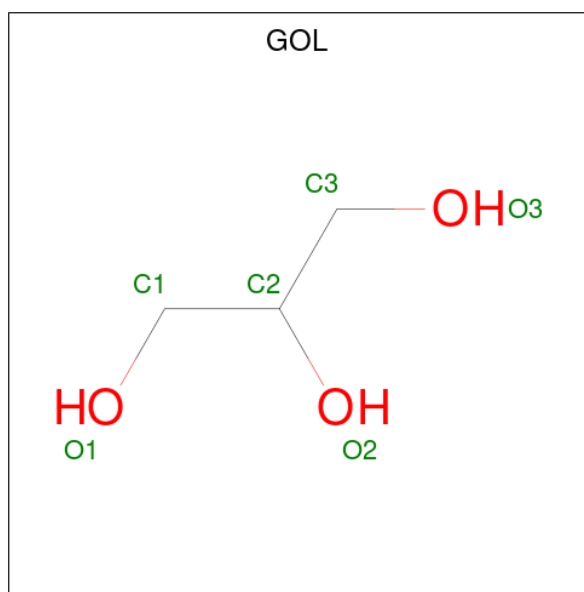


Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
			Total	C	N	O	S		
3	A	1	Total	C	N	O	S	0	0
			34	25	7	1	1		
3	B	1	Total	C	N	O	S	0	0
			34	25	7	1	1		
3	C	1	Total	C	N	O	S	0	0
			34	25	7	1	1		
3	D	1	Total	C	N	O	S	0	0
			34	25	7	1	1		
3	E	1	Total	C	N	O	S	0	0
			34	25	7	1	1		
3	F	1	Total	C	N	O	S	0	0
			34	25	7	1	1		
3	G	1	Total	C	N	O	S	0	0
			34	25	7	1	1		
3	H	1	Total	C	N	O	S	0	0
			34	25	7	1	1		
3	I	1	Total	C	N	O	S	0	0
			34	25	7	1	1		
3	J	1	Total	C	N	O	S	0	0
			34	25	7	1	1		
3	K	1	Total	C	N	O	S	0	0
			34	25	7	1	1		
3	L	1	Total	C	N	O	S	0	0
			34	25	7	1	1		

- Molecule 4 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	1	Total Zn 1 1	0	0
4	B	1	Total Zn 1 1	0	0
4	C	1	Total Zn 1 1	0	0
4	D	1	Total Zn 1 1	0	0
4	E	1	Total Zn 1 1	0	0
4	F	1	Total Zn 1 1	0	0
4	G	1	Total Zn 1 1	0	0
4	H	1	Total Zn 1 1	0	0
4	I	1	Total Zn 1 1	0	0
4	J	1	Total Zn 1 1	0	0
4	K	1	Total Zn 1 1	0	0
4	L	1	Total Zn 1 1	0	0

- Molecule 5 is GLYCEROL (three-letter code: GOL) (formula:  $C_3H_8O_3$ ).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	C	1	Total 6	C 3	O 3	0	0
5	D	1	Total 6	C 3	O 3	0	0
5	K	1	Total 6	C 3	O 3	0	0
5	L	1	Total 6	C 3	O 3	0	0

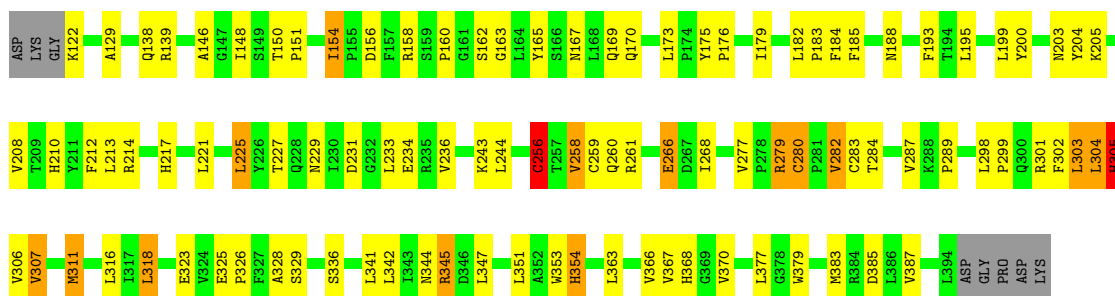


### 3 Residue-property plots

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.

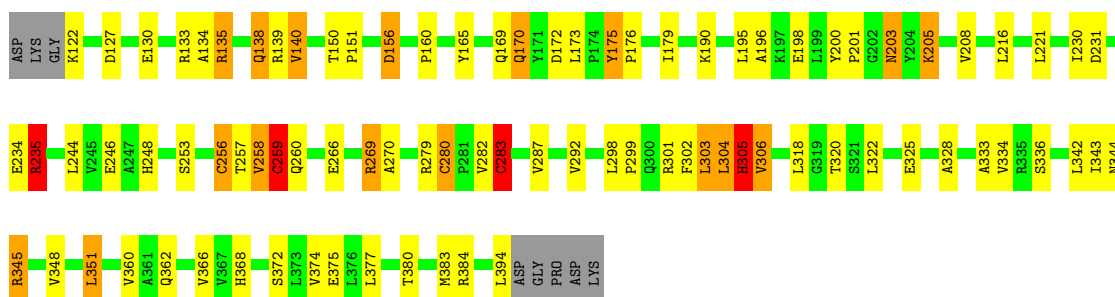
#### • Molecule 1: NAD-DEPENDENT PROTEIN DEACETYLASE SIRTUIN-3, MITOCHONDRIAL

Chain A: 



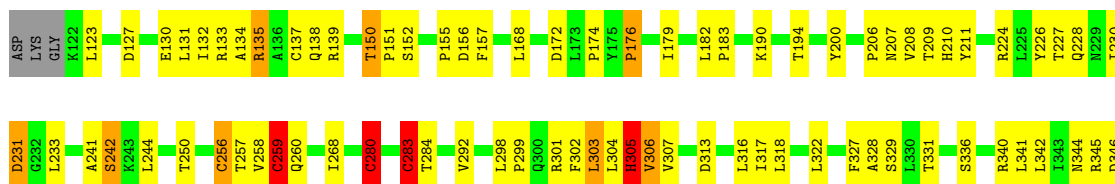
#### • Molecule 1: NAD-DEPENDENT PROTEIN DEACETYLASE SIRTUIN-3, MITOCHONDRIAL

Chain B: 



#### • Molecule 1: NAD-DEPENDENT PROTEIN DEACETYLASE SIRTUIN-3, MITOCHONDRIAL

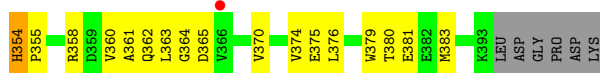
Chain C: 





- Molecule 1: NAD-DEPENDENT PROTEIN DEACETYLASE SIRTUIN-3, MITOCHONDRIAL

Chain D: 64% 26% 5% ..



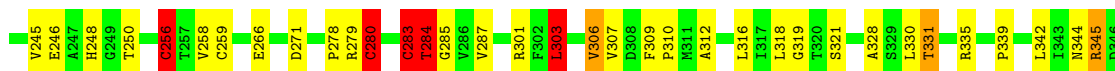
- Molecule 1: NAD-DEPENDENT PROTEIN DEACETYLASE SIRTUIN-3, MITOCHONDRIAL

Chain E: 70% 23% ..



- Molecule 1: NAD-DEPENDENT PROTEIN DEACETYLASE SIRTUIN-3, MITOCHONDRIAL

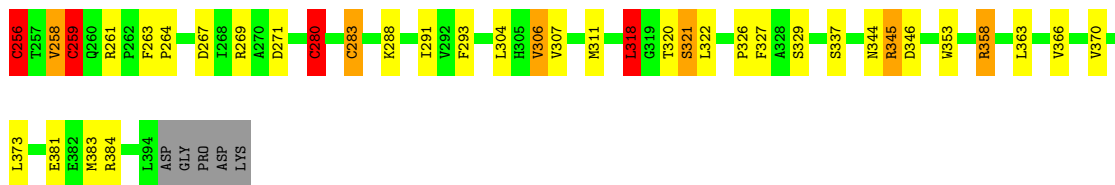
Chain F: 68% 24% ..



- Molecule 1: NAD-DEPENDENT PROTEIN DEACETYLASE SIRTUIN-3, MITOCHONDRIAL

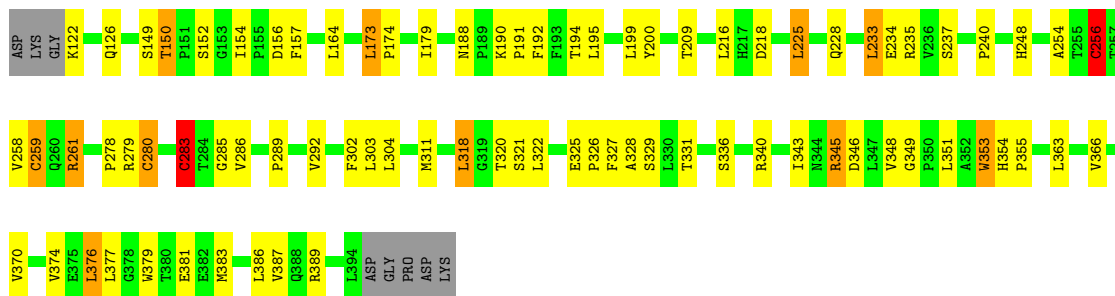
Chain G: 72% 20% ..





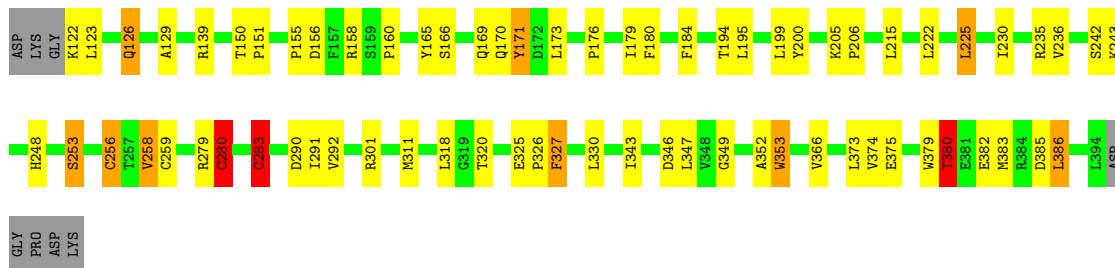
- Molecule 1: NAD-DEPENDENT PROTEIN DEACETYLASE SIRTUIN-3, MITOCHONDRIAL

Chain H: 68% 24% . . .



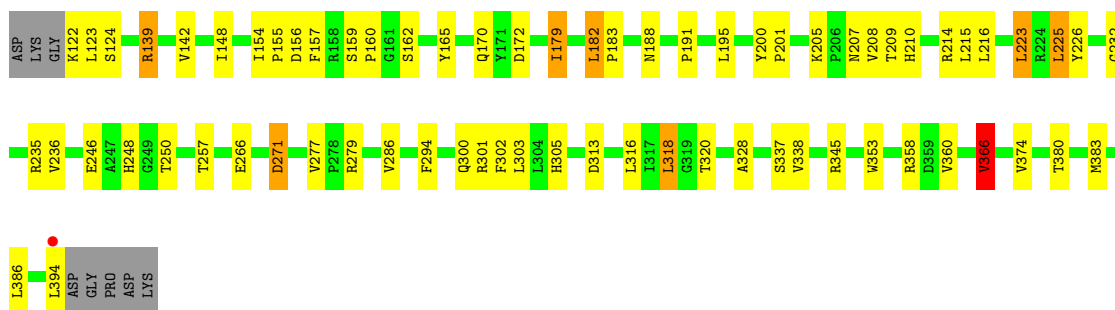
- Molecule 1: NAD-DEPENDENT PROTEIN DEACETYLASE SIRTUIN-3, MITOCHONDRIAL

Chain I: 72% 21% . . .



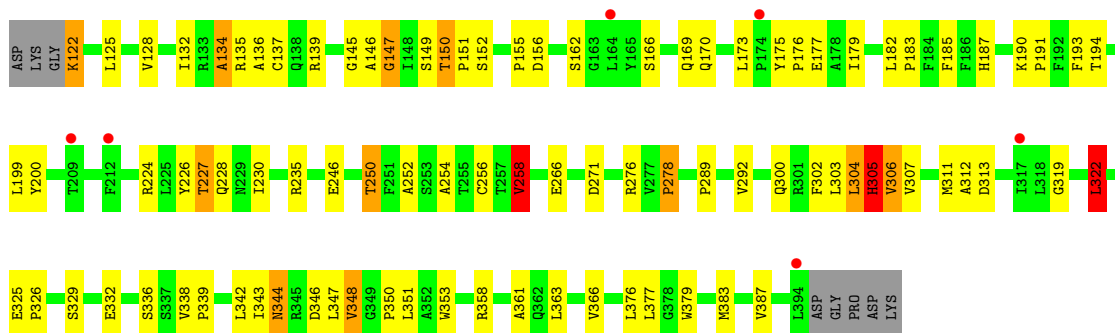
- Molecule 1: NAD-DEPENDENT PROTEIN DEACETYLASE SIRTUIN-3, MITOCHONDRIAL

Chain J: 72% 22% . .

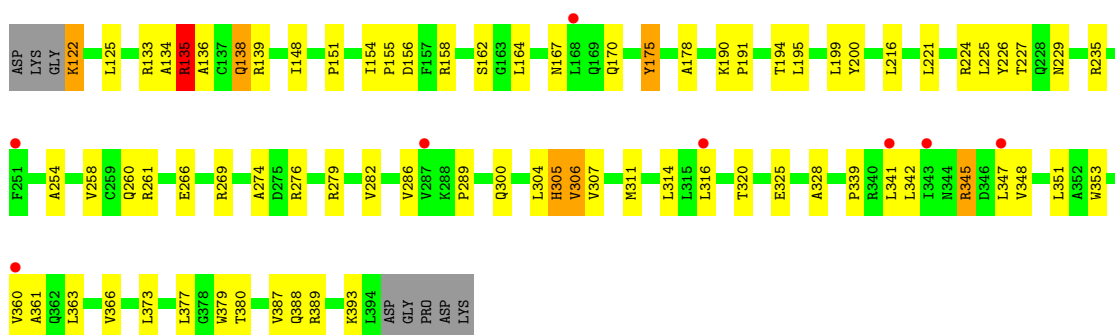


- Molecule 1: NAD-DEPENDENT PROTEIN DEACETYLASE SIRTUIN-3, MITOCHONDRIAL

Chain K: 2% 64% 28% . . .



● Molecule 1: NAD-DEPENDENT PROTEIN DEACETYLASE SIRTUIN-3, MITOCHONDRIAL



## 4 Data and refinement statistics i

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	227.82Å 246.06Å 127.34Å 90.00° 123.88° 90.00°	Depositor
Resolution (Å)	48.57 – 3.25 48.57 – 3.25	Depositor EDS
% Data completeness (in resolution range)	99.8 (48.57-3.25) 99.4 (48.57-3.25)	Depositor EDS
$R_{merge}$	0.14	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.72 (at 3.25Å)	Xtrriage
Refinement program	REFMAC 5.7.0032	Depositor
R, $R_{free}$	0.208 , 0.265 0.203 , 0.258	Depositor DCC
$R_{free}$ test set	4558 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	85.3	Xtrriage
Anisotropy	0.181	Xtrriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.30 , 45.7	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.48$ , $\langle L^2 \rangle = 0.30$	Xtrriage
Estimated twinning fraction	0.428 for -h-2*1,-k,l	Xtrriage
$F_o, F_c$ correlation	0.95	EDS
Total number of atoms	26520	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	99.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.99% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical 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: GOL, SR7, ZN, CNA

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	0.74	0/2199	0.92	8/2996 (0.3%)
1	B	0.72	0/2199	0.90	4/2996 (0.1%)
1	C	0.69	1/2184 (0.0%)	0.90	5/2975 (0.2%)
1	D	0.73	3/2110 (0.1%)	0.89	3/2883 (0.1%)
1	E	0.57	0/2150	0.79	0/2938
1	F	0.59	0/2199	0.80	6/2996 (0.2%)
1	G	0.62	1/2199 (0.0%)	0.84	5/2996 (0.2%)
1	H	0.56	0/2199	0.80	4/2996 (0.1%)
1	I	0.58	1/2175 (0.0%)	0.78	4/2968 (0.1%)
1	J	0.56	0/2199	0.77	2/2996 (0.1%)
1	K	0.48	0/2199	0.69	0/2996
1	L	0.49	0/2189	0.70	0/2984
All	All	0.62	6/26201 (0.0%)	0.82	41/35720 (0.1%)

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	A	0	1
1	B	0	2
1	D	0	2
1	E	0	2
1	K	0	2
1	L	0	1
All	All	0	10

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

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	365	ASP	CB-CG	7.46	1.67	1.51
1	C	259	CYS	CB-SG	5.79	1.92	1.82
1	I	259	CYS	CB-SG	5.51	1.91	1.82
1	D	177	GLU	CG-CD	5.22	1.59	1.51
1	G	259	CYS	CB-SG	5.13	1.91	1.82

The worst 5 of 41 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	280	CYS	CA-CB-SG	8.93	130.08	114.00
1	C	280	CYS	CA-CB-SG	8.37	129.07	114.00
1	D	280	CYS	CA-CB-SG	8.32	128.98	114.00
1	B	280	CYS	CA-CB-SG	7.87	128.17	114.00
1	A	256	CYS	CA-CB-SG	7.76	127.97	114.00

There are no chirality outliers.

5 of 10 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	304	LEU	Peptide
1	B	283	CYS	Peptide
1	B	304	LEU	Peptide
1	D	304	LEU	Peptide
1	D	305	HIS	Peptide

## 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	2144	0	2160	80	0
1	B	2144	0	2160	76	0
1	C	2131	0	2143	66	0
1	D	2059	0	2025	70	0
1	E	2096	0	2079	39	1
1	F	2144	0	2160	50	0
1	G	2144	0	2160	41	0
1	H	2144	0	2160	52	0
1	I	2120	0	2117	34	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	J	2144	0	2160	32	0
1	K	2144	0	2160	58	0
1	L	2134	0	2145	45	0
2	A	44	0	29	5	0
2	B	44	0	29	4	0
2	C	44	0	29	1	0
2	D	44	0	29	5	0
2	E	44	0	29	1	0
2	F	44	0	29	3	0
2	G	44	0	29	12	0
2	H	44	0	29	11	0
2	I	44	0	29	5	0
2	J	44	0	29	4	0
2	K	44	0	29	6	0
2	L	44	0	29	5	0
3	A	34	0	23	4	0
3	B	34	0	23	5	0
3	C	34	0	23	4	0
3	D	34	0	23	2	0
3	E	34	0	23	5	0
3	F	34	0	23	11	0
3	G	34	0	23	18	0
3	H	34	0	23	12	0
3	I	34	0	23	10	0
3	J	34	0	23	7	0
3	K	34	0	23	8	0
3	L	34	0	23	6	0
4	A	1	0	0	0	0
4	B	1	0	0	0	0
4	C	1	0	0	0	0
4	D	1	0	0	0	0
4	E	1	0	0	0	0
4	F	1	0	0	0	0
4	G	1	0	0	0	0
4	H	1	0	0	0	0
4	I	1	0	0	0	0
4	J	1	0	0	0	0
4	K	1	0	0	0	0
4	L	1	0	0	0	0
5	C	6	0	8	2	0
5	D	6	0	8	3	0
5	K	6	0	8	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
5	L	6	0	8	0	0
All	All	26520	0	26285	656	1

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 12.

The worst 5 of 656 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:C:305:HIS:CE1	1:D:305:HIS:CE1	1.88	1.58
1:A:305:HIS:CE1	1:B:305:HIS:NE2	1.85	1.43
1:A:305:HIS:NE2	1:B:305:HIS:NE2	1.68	1.36
1:C:305:HIS:NE2	1:D:305:HIS:CE1	1.84	1.35
1:A:305:HIS:NE2	1:B:305:HIS:CE1	1.96	1.31

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:305:HIS:NE2	1:E:305:HIS:NE2[2_756]	1.96	0.24

## 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	271/281 (96%)	230 (85%)	37 (14%)	4 (2%)	10	39
1	B	271/281 (96%)	231 (85%)	35 (13%)	5 (2%)	8	35
1	C	271/281 (96%)	223 (82%)	36 (13%)	12 (4%)	2	15
1	D	270/281 (96%)	227 (84%)	33 (12%)	10 (4%)	3	19
1	E	271/281 (96%)	241 (89%)	23 (8%)	7 (3%)	5	27

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	F	271/281 (96%)	239 (88%)	29 (11%)	3 (1%)	14	46
1	G	271/281 (96%)	249 (92%)	18 (7%)	4 (2%)	10	39
1	H	271/281 (96%)	244 (90%)	24 (9%)	3 (1%)	14	46
1	I	271/281 (96%)	237 (88%)	29 (11%)	5 (2%)	8	35
1	J	271/281 (96%)	246 (91%)	21 (8%)	4 (2%)	10	39
1	K	271/281 (96%)	237 (88%)	26 (10%)	8 (3%)	4	24
1	L	271/281 (96%)	237 (88%)	29 (11%)	5 (2%)	8	35
All	All	3251/3372 (96%)	2841 (87%)	340 (10%)	70 (2%)	6	31

5 of 70 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	305	HIS
1	B	305	HIS
1	C	176	PRO
1	C	242	SER
1	C	305	HIS

### 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	237/243 (98%)	210 (89%)	27 (11%)	5	22
1	B	237/243 (98%)	201 (85%)	36 (15%)	3	12
1	C	234/243 (96%)	201 (86%)	33 (14%)	3	15
1	D	219/243 (90%)	197 (90%)	22 (10%)	7	27
1	E	227/243 (93%)	204 (90%)	23 (10%)	7	27
1	F	237/243 (98%)	210 (89%)	27 (11%)	5	22
1	G	237/243 (98%)	213 (90%)	24 (10%)	7	27
1	H	237/243 (98%)	213 (90%)	24 (10%)	7	27
1	I	232/243 (96%)	205 (88%)	27 (12%)	5	22

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	J	237/243 (98%)	211 (89%)	26 (11%)	6	24
1	K	237/243 (98%)	213 (90%)	24 (10%)	7	27
1	L	235/243 (97%)	212 (90%)	23 (10%)	8	29
All	All	2806/2916 (96%)	2490 (89%)	316 (11%)	6	22

5 of 316 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	I	279	ARG
1	K	322	LEU
1	I	353	TRP
1	J	279	ARG
1	L	175	TYR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 23 such sidechains are listed below:

Mol	Chain	Res	Type
1	G	248	HIS
1	K	126	GLN
1	I	217	HIS
1	K	203	ASN
1	D	305	HIS

### 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

Of 40 ligands modelled in this entry, 12 are monoatomic - leaving 28 for Mogul analysis.

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$
3	SR7	F	1396	-	33,39,39	2.07	9 (27%)	43,55,55	2.58	16 (37%)
2	CNA	F	1395	-	42,48,48	2.06	8 (19%)	49,73,73	1.73	7 (14%)
3	SR7	E	1396	-	33,39,39	2.54	9 (27%)	43,55,55	3.03	18 (41%)
2	CNA	E	1395	-	42,48,48	2.05	10 (23%)	49,73,73	1.88	11 (22%)
2	CNA	A	1395	-	42,48,48	2.19	12 (28%)	49,73,73	1.68	8 (16%)
3	SR7	L	1397	-	33,39,39	1.92	11 (33%)	43,55,55	2.22	10 (23%)
3	SR7	A	1396	-	33,39,39	2.52	9 (27%)	43,55,55	3.04	18 (41%)
3	SR7	G	1396	-	33,39,39	2.48	10 (30%)	43,55,55	2.55	19 (44%)
2	CNA	I	1395	-	42,48,48	2.21	11 (26%)	49,73,73	1.82	9 (18%)
2	CNA	C	1395	-	42,48,48	2.07	11 (26%)	49,73,73	1.53	9 (18%)
5	GOL	L	1396	-	5,5,5	0.30	0	5,5,5	0.64	0
3	SR7	C	1397	-	33,39,39	2.07	9 (27%)	43,55,55	2.19	15 (34%)
3	SR7	J	1396	-	33,39,39	2.00	9 (27%)	43,55,55	2.53	18 (41%)
2	CNA	J	1395	-	42,48,48	2.14	11 (26%)	49,73,73	1.51	8 (16%)
3	SR7	K	1397	-	33,39,39	2.25	9 (27%)	43,55,55	1.48	10 (23%)
5	GOL	C	1396	-	5,5,5	0.39	0	5,5,5	0.93	0
3	SR7	I	1396	-	33,39,39	2.28	8 (24%)	43,55,55	2.41	15 (34%)
5	GOL	D	1395	-	5,5,5	0.35	0	5,5,5	1.17	0
2	CNA	B	1395	-	42,48,48	2.28	12 (28%)	49,73,73	1.72	9 (18%)
2	CNA	D	1394	-	42,48,48	2.20	13 (30%)	49,73,73	1.57	10 (20%)
3	SR7	H	1396	-	33,39,39	2.42	6 (18%)	43,55,55	1.95	12 (27%)
2	CNA	K	1395	-	42,48,48	2.52	15 (35%)	49,73,73	1.75	8 (16%)
2	CNA	H	1395	-	42,48,48	2.28	13 (30%)	49,73,73	2.11	9 (18%)
3	SR7	D	1396	-	33,39,39	2.12	6 (18%)	43,55,55	1.50	6 (13%)
5	GOL	K	1396	-	5,5,5	0.26	0	5,5,5	0.56	0
2	CNA	L	1395	-	42,48,48	2.37	13 (30%)	49,73,73	1.74	11 (22%)
2	CNA	G	1395	-	42,48,48	2.17	9 (21%)	49,73,73	1.96	9 (18%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
3	SR7	B	1396	-	33,39,39	2.43	10 (30%)	43,55,55	3.11	18 (41%)

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
3	SR7	F	1396	-	-	6/15/24/24	1/6/6/6
2	CNA	F	1395	-	-	13/24/62/62	0/5/5/5
3	SR7	E	1396	-	-	6/15/24/24	1/6/6/6
2	CNA	E	1395	-	-	14/24/62/62	0/5/5/5
2	CNA	A	1395	-	-	6/24/62/62	0/5/5/5
3	SR7	L	1397	-	-	7/15/24/24	1/6/6/6
3	SR7	A	1396	-	-	6/15/24/24	1/6/6/6
3	SR7	G	1396	-	-	6/15/24/24	1/6/6/6
2	CNA	I	1395	-	-	12/24/62/62	0/5/5/5
2	CNA	C	1395	-	-	4/24/62/62	0/5/5/5
5	GOL	L	1396	-	-	1/4/4/4	-
3	SR7	C	1397	-	-	6/15/24/24	0/6/6/6
3	SR7	J	1396	-	-	6/15/24/24	1/6/6/6
2	CNA	J	1395	-	-	10/24/62/62	0/5/5/5
3	SR7	K	1397	-	-	6/15/24/24	0/6/6/6
5	GOL	C	1396	-	-	2/4/4/4	-
3	SR7	I	1396	-	-	5/15/24/24	0/6/6/6
5	GOL	D	1395	-	-	4/4/4/4	-
2	CNA	B	1395	-	-	6/24/62/62	0/5/5/5
2	CNA	D	1394	-	-	4/24/62/62	0/5/5/5
3	SR7	H	1396	-	-	6/15/24/24	0/6/6/6
2	CNA	K	1395	-	-	11/24/62/62	0/5/5/5
2	CNA	H	1395	-	-	15/24/62/62	0/5/5/5
3	SR7	D	1396	-	-	2/15/24/24	1/6/6/6
5	GOL	K	1396	-	-	2/4/4/4	-
2	CNA	L	1395	-	-	14/24/62/62	0/5/5/5
2	CNA	G	1395	-	-	15/24/62/62	0/5/5/5
3	SR7	B	1396	-	-	6/15/24/24	1/6/6/6

The worst 5 of 243 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	E	1396	SR7	CBC-SBB	-8.93	1.59	1.70
3	G	1396	SR7	CBC-SBB	-8.86	1.59	1.70
3	A	1396	SR7	CBC-SBB	-8.56	1.60	1.70
3	H	1396	SR7	CBC-SBB	-8.28	1.60	1.70
2	L	1395	CNA	C3N-C7N	-8.20	1.38	1.50

The worst 5 of 283 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	E	1396	SR7	CBH-CBD-CBC	-9.32	116.99	129.46
3	B	1396	SR7	CAJ-CAK-CBF	-9.28	109.75	119.62
3	A	1396	SR7	CAJ-CAK-CBF	-9.10	109.94	119.62
3	B	1396	SR7	CAO-CAH-CAG	9.06	130.53	119.25
3	A	1396	SR7	CAO-CAH-CAG	8.28	129.56	119.25

There are no chirality outliers.

5 of 201 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	1395	CNA	C4D-C5D-O5D-PN
2	A	1395	CNA	C4'-C4D-C5D-O5D
2	A	1395	CNA	C3D-C4D-C5D-O5D
2	A	1395	CNA	C2D-C1D-N1N-C2N
2	A	1395	CNA	C2D-C1D-N1N-C6N

5 of 8 ring outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	E	1396	SR7	CAQ-CAR-CAT-CAU-NAS-NAV
3	L	1397	SR7	CAQ-CAR-CAT-CAU-NAS-NAV
3	D	1396	SR7	CAQ-CAR-CAT-CAU-NAS-NAV
3	G	1396	SR7	CAQ-CAR-CAT-CAU-NAS-NAV
3	B	1396	SR7	CAQ-CAR-CAT-CAU-NAS-NAV

27 monomers are involved in 126 short contacts:

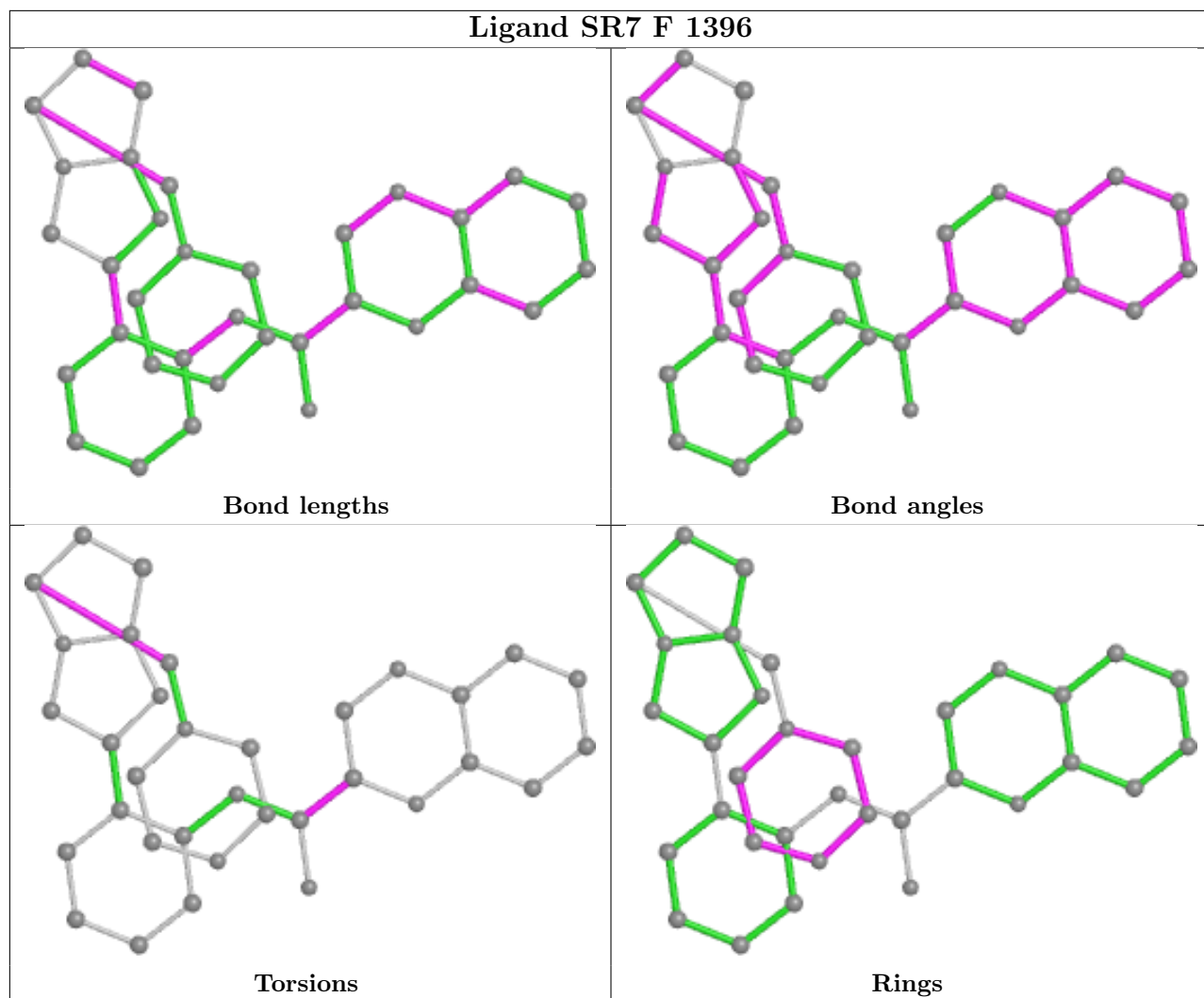
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	F	1396	SR7	11	0
2	F	1395	CNA	3	0
3	E	1396	SR7	5	0
2	E	1395	CNA	1	0

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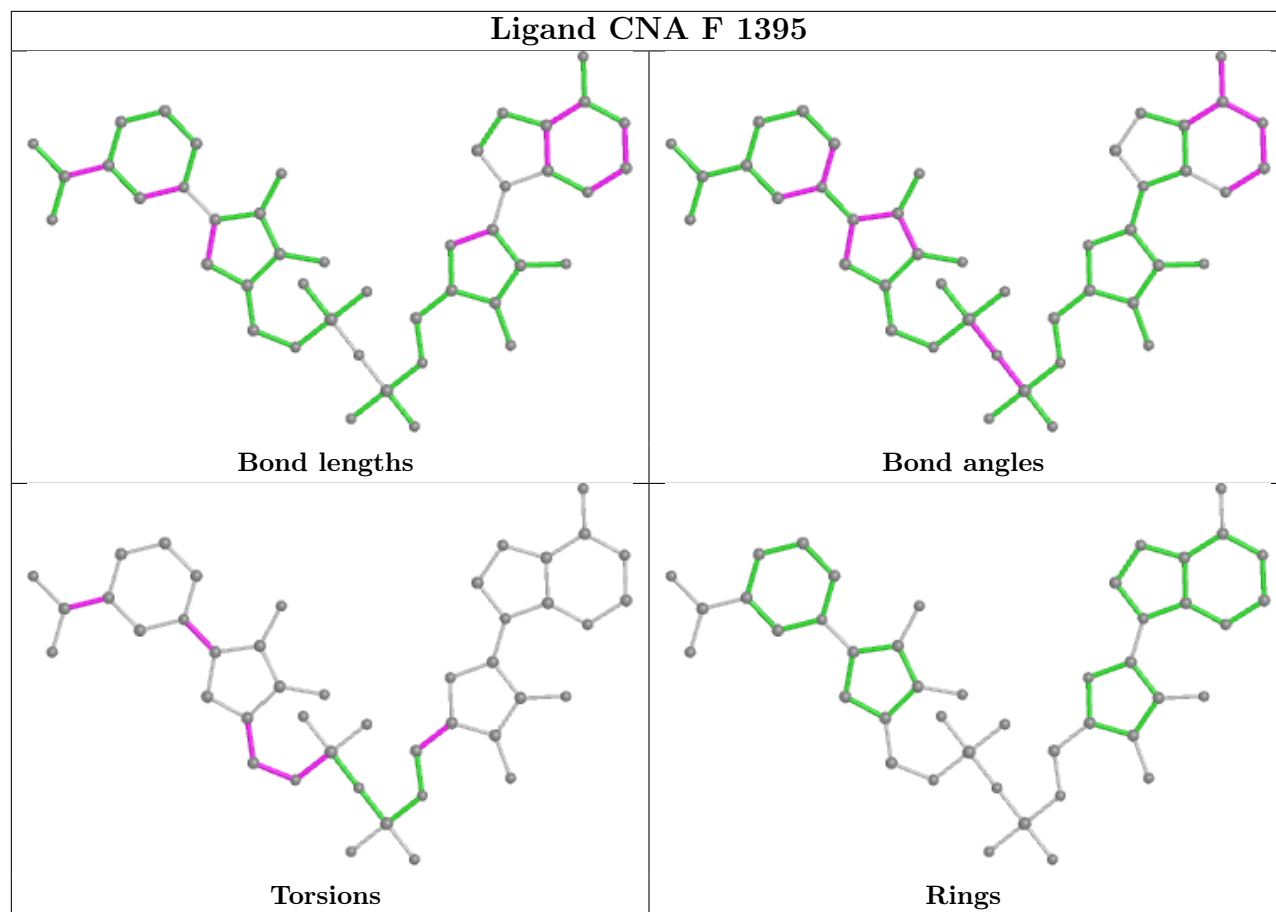
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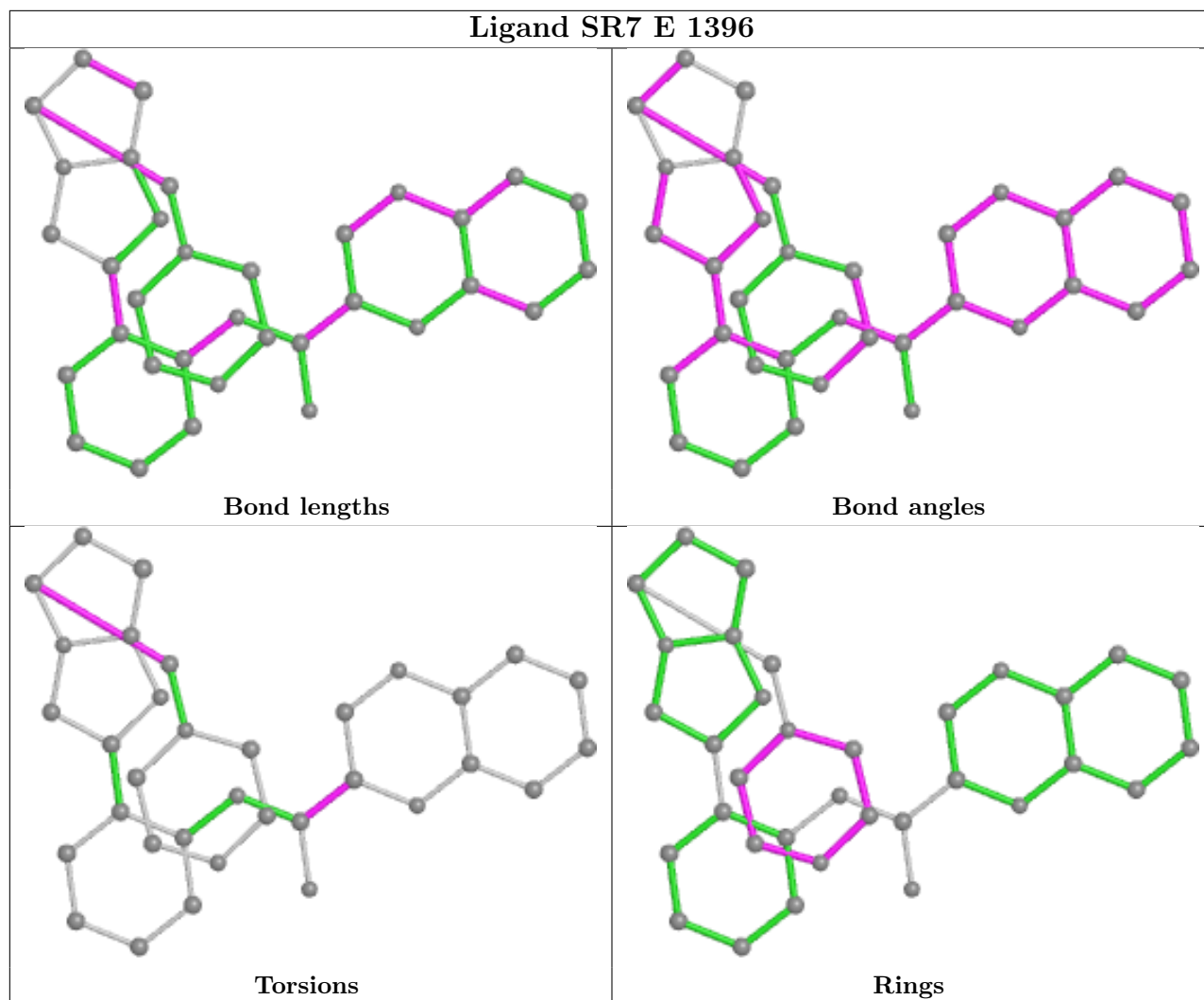
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	1395	CNA	5	0
3	L	1397	SR7	6	0
3	A	1396	SR7	4	0
3	G	1396	SR7	18	0
2	I	1395	CNA	5	0
2	C	1395	CNA	1	0
3	C	1397	SR7	4	0
3	J	1396	SR7	7	0
2	J	1395	CNA	4	0
3	K	1397	SR7	8	0
5	C	1396	GOL	2	0
3	I	1396	SR7	10	0
5	D	1395	GOL	3	0
2	B	1395	CNA	4	0
2	D	1394	CNA	5	0
3	H	1396	SR7	12	0
2	K	1395	CNA	6	0
2	H	1395	CNA	11	0
3	D	1396	SR7	2	0
5	K	1396	GOL	1	0
2	L	1395	CNA	5	0
2	G	1395	CNA	12	0
3	B	1396	SR7	5	0

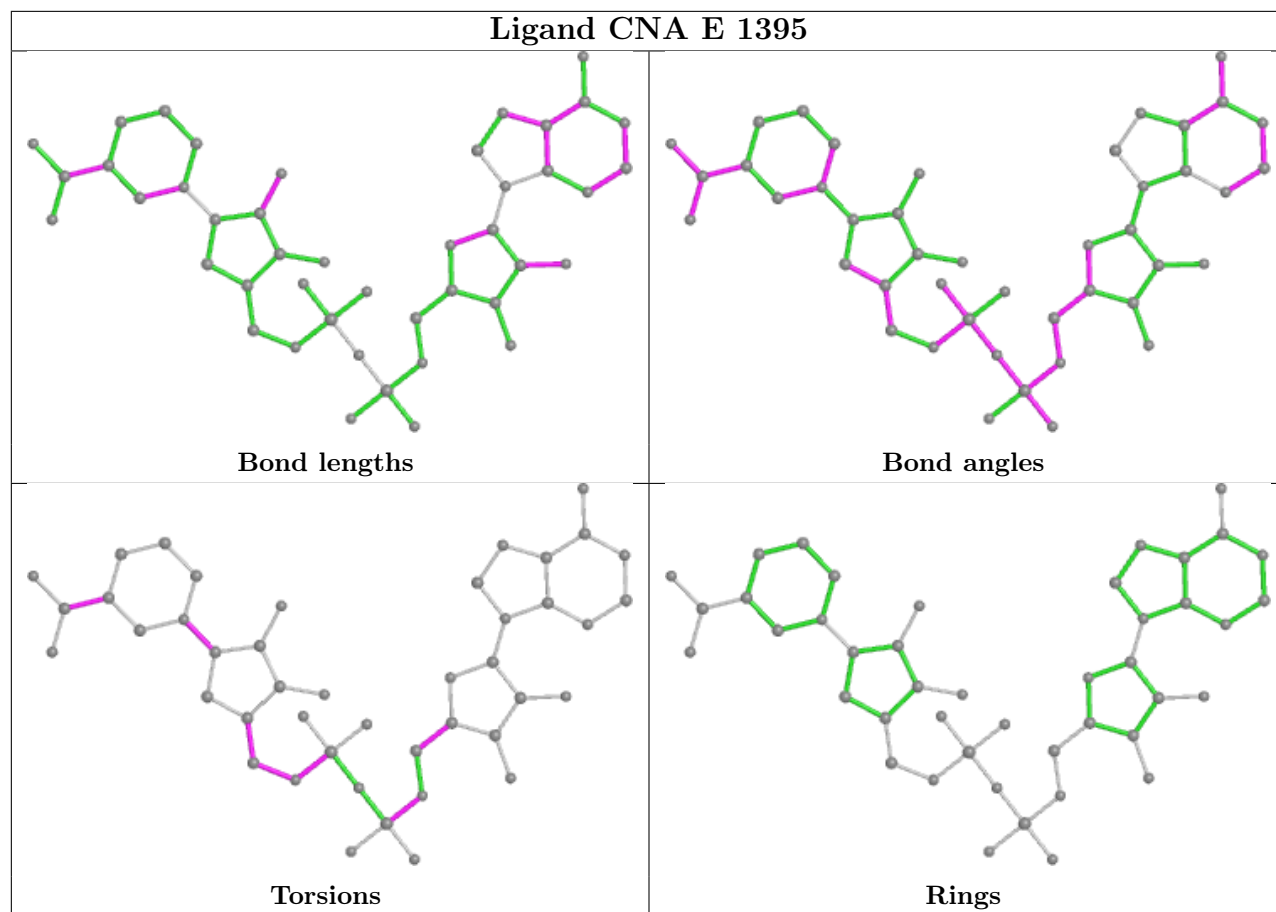
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

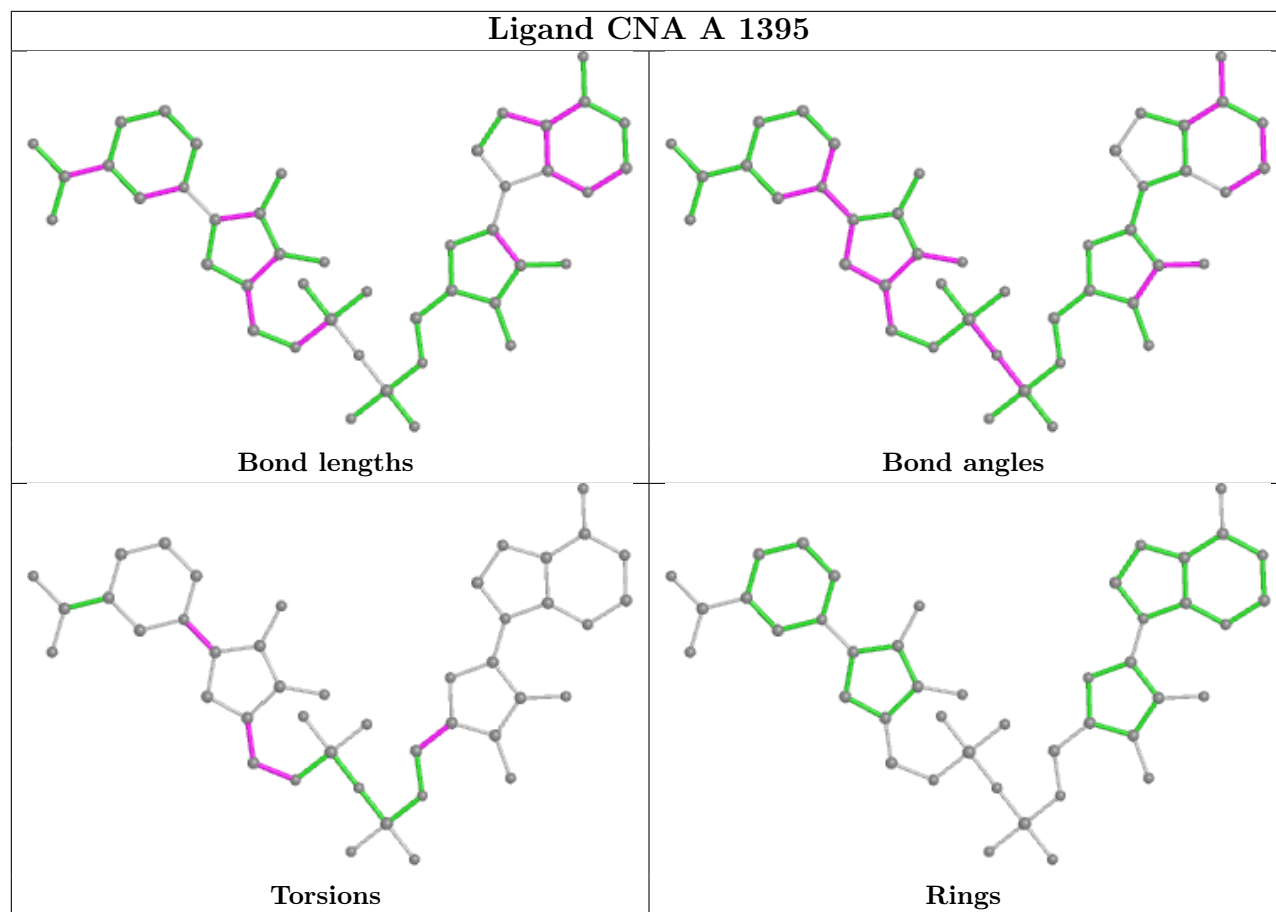


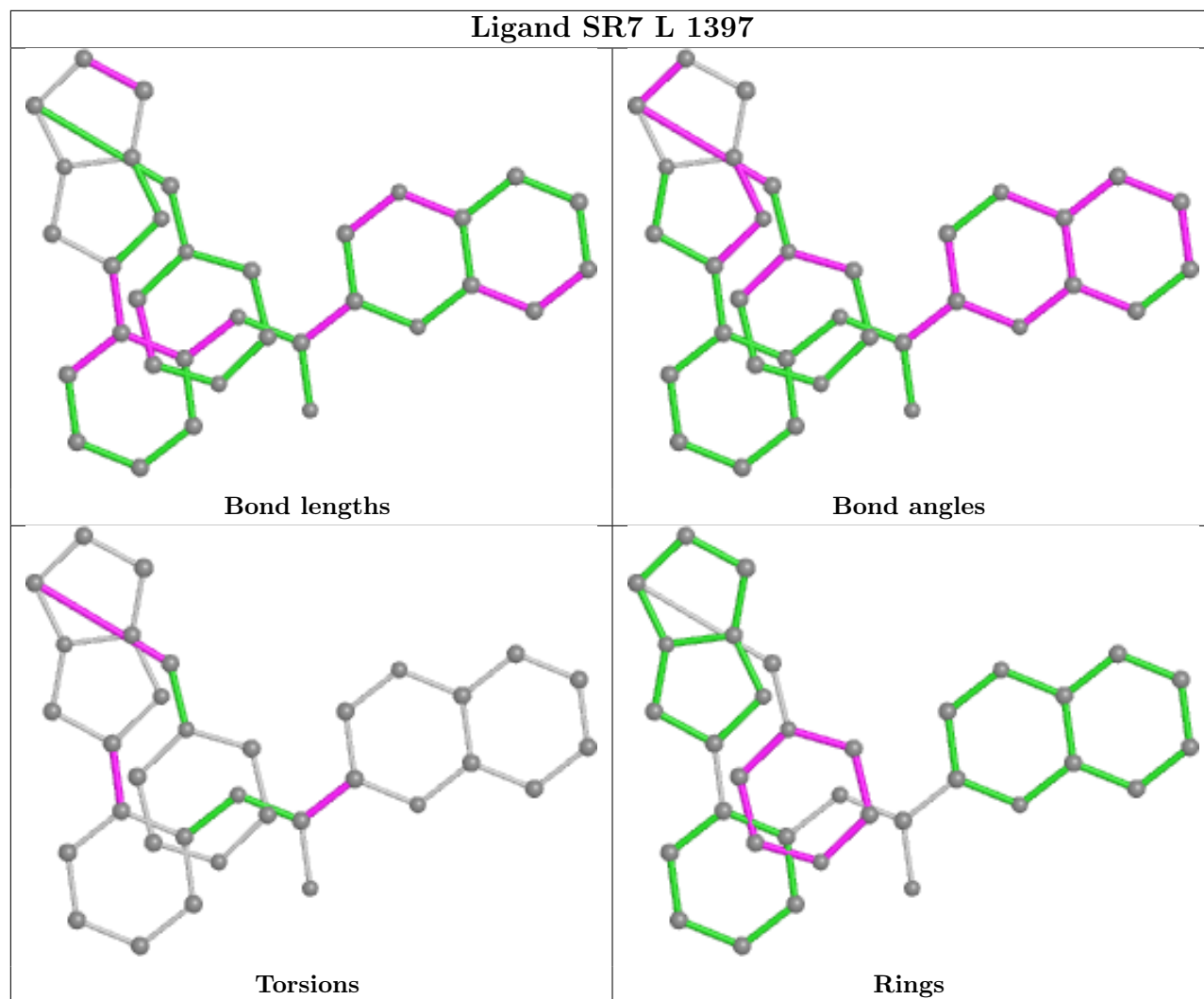


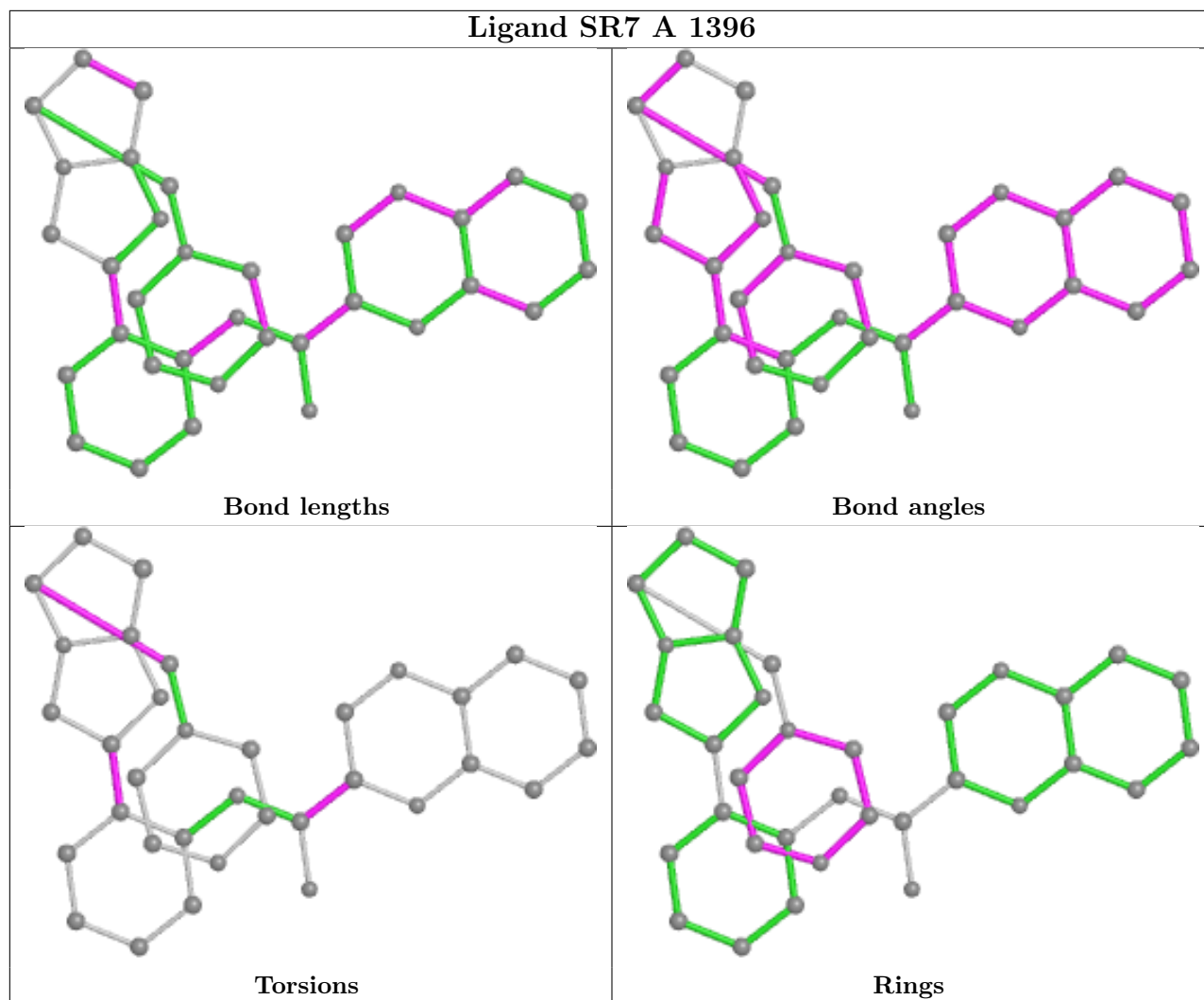


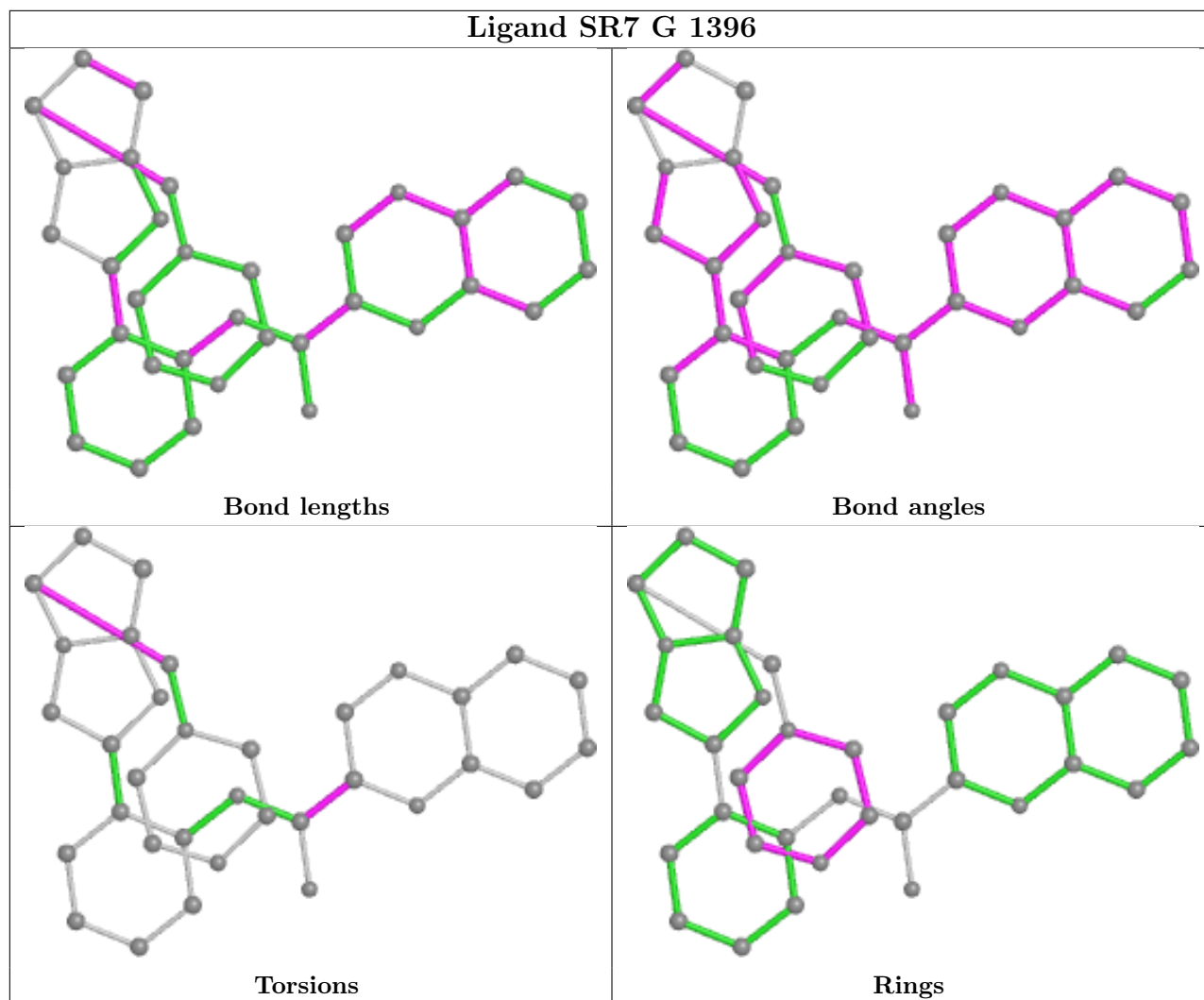


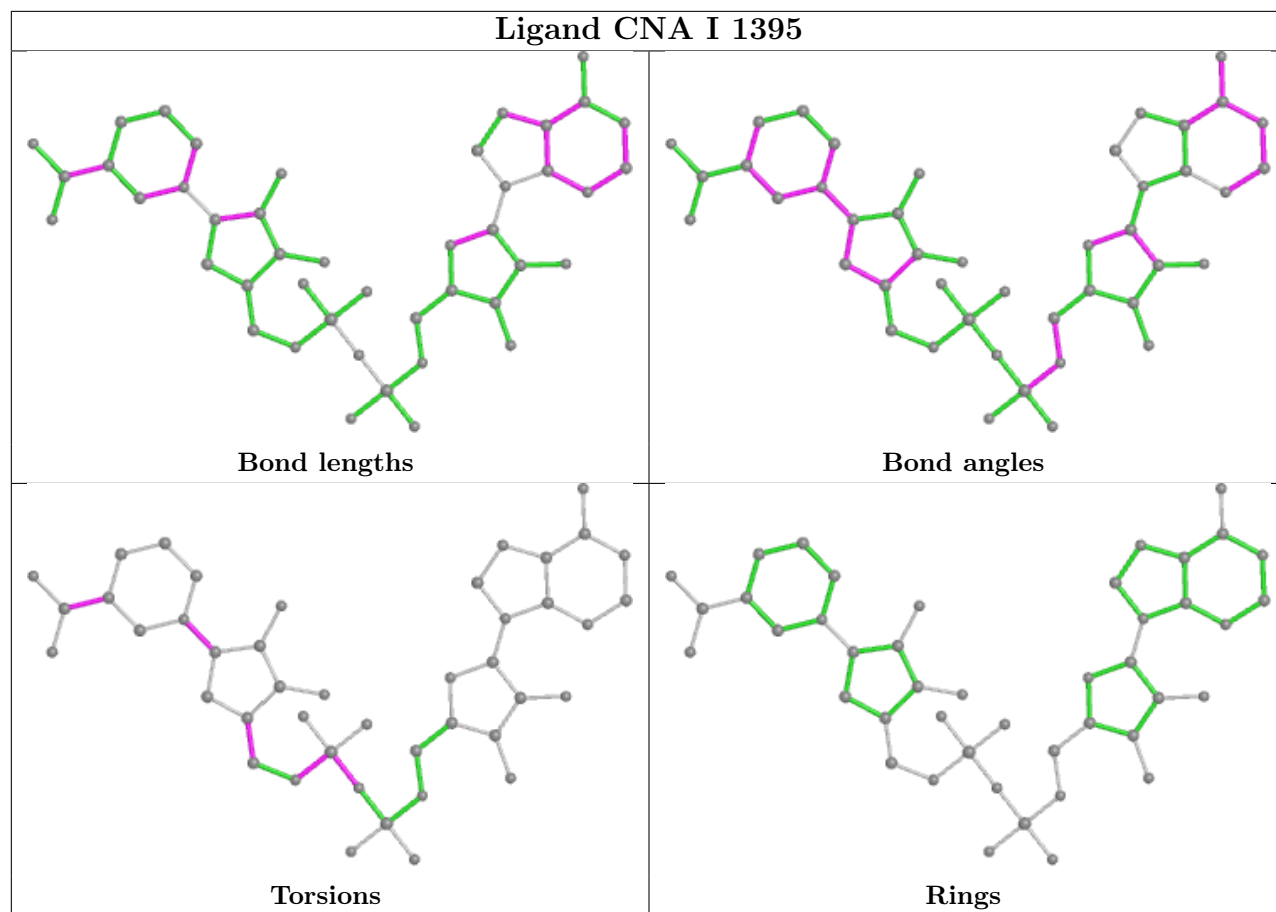




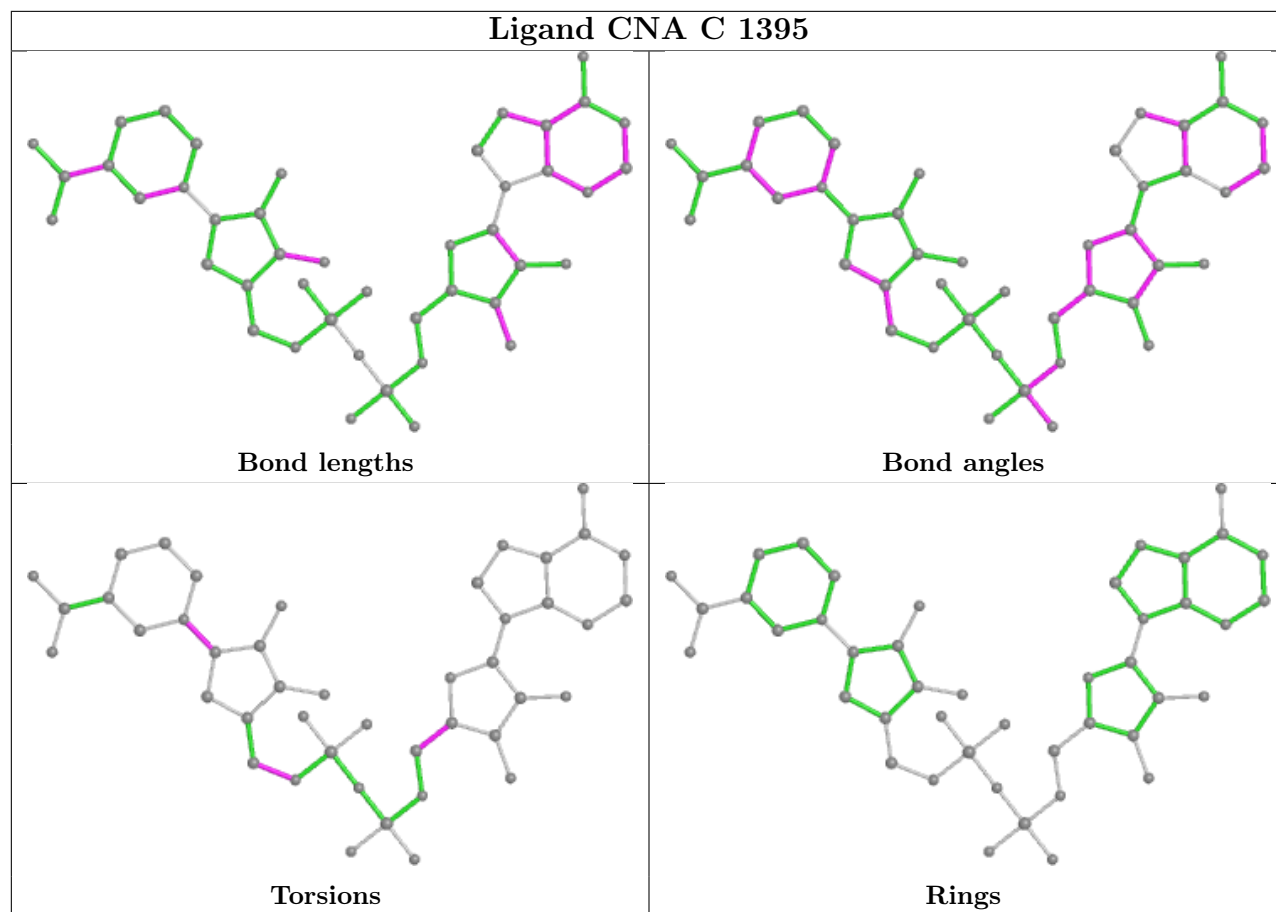


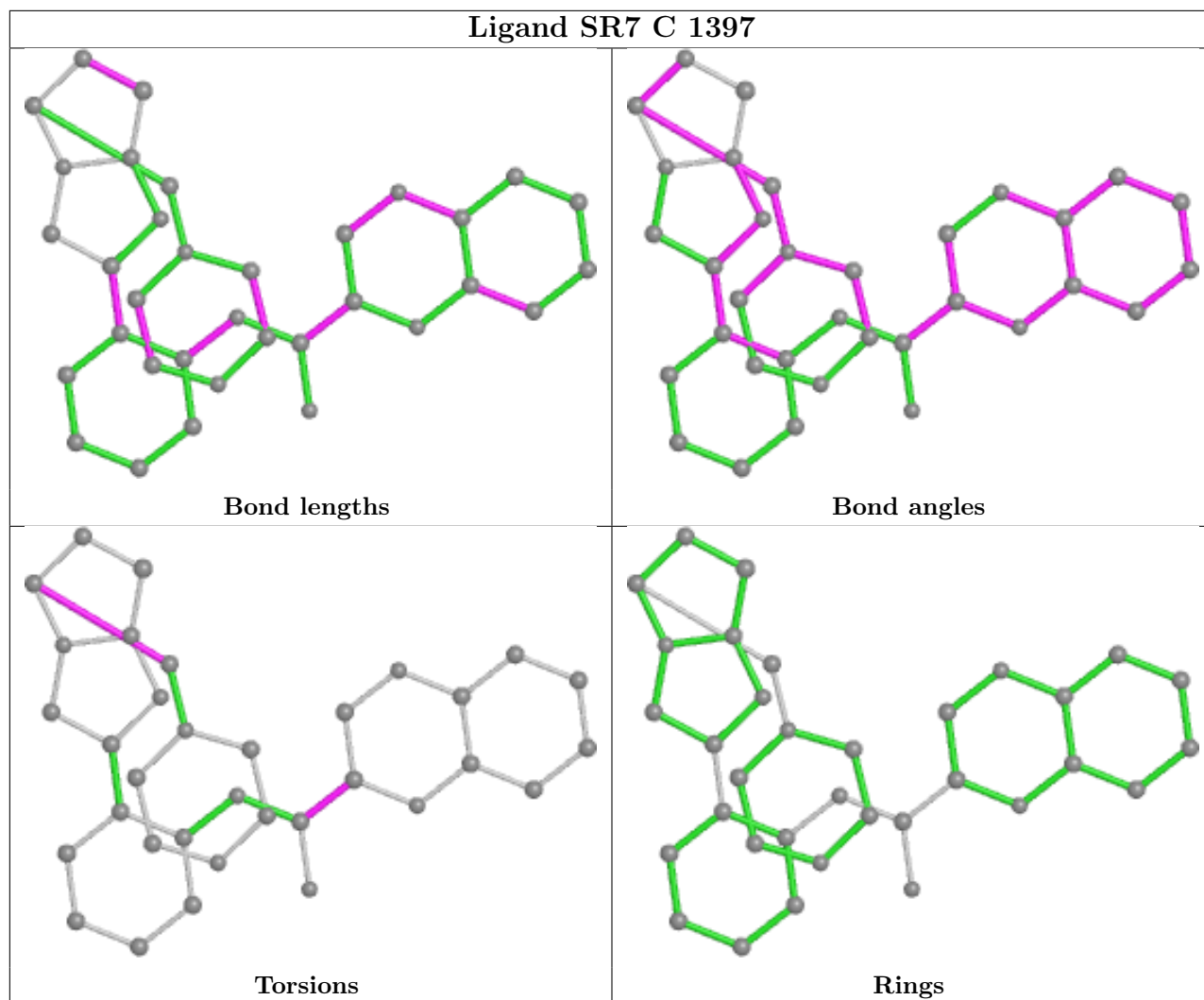


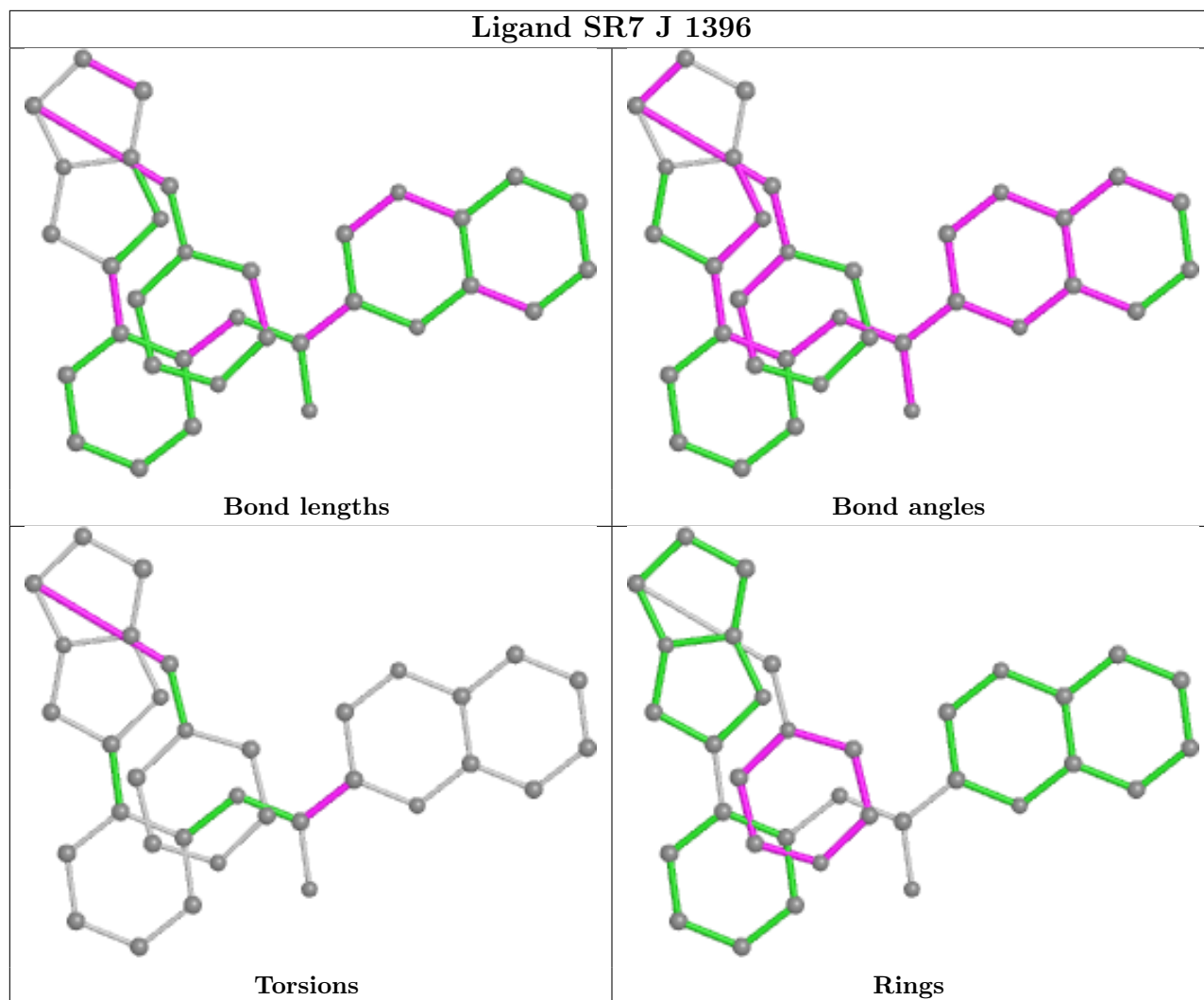


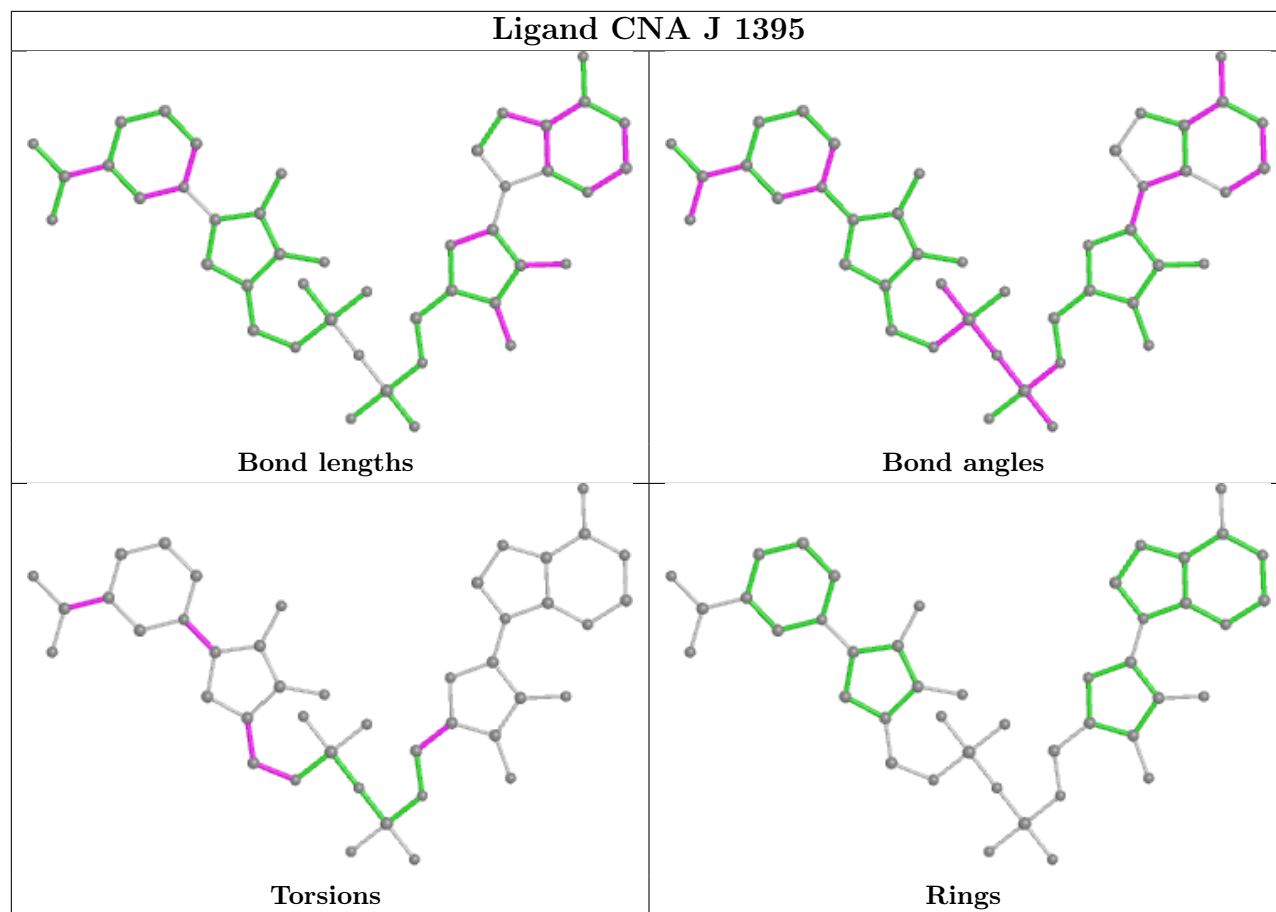


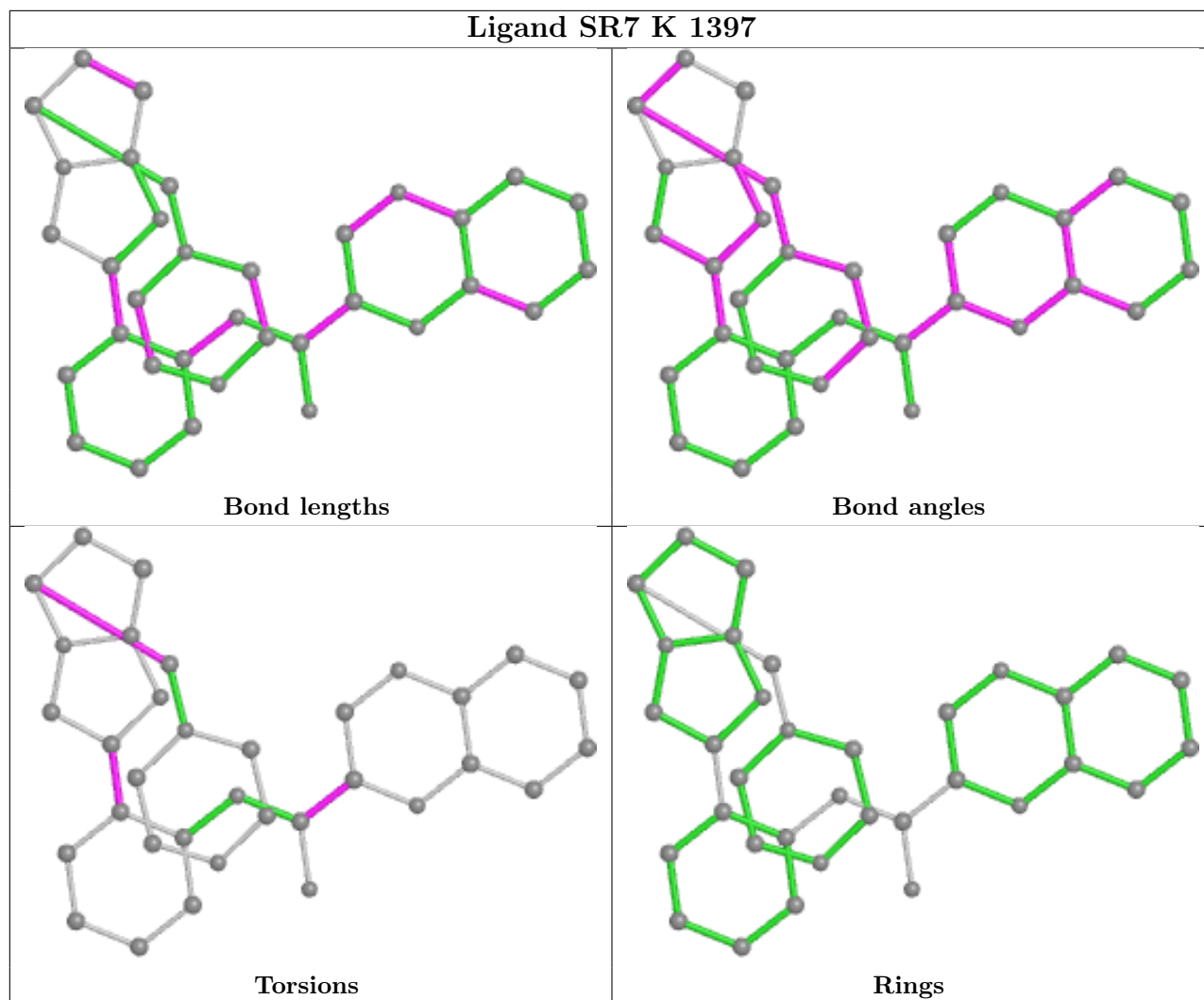


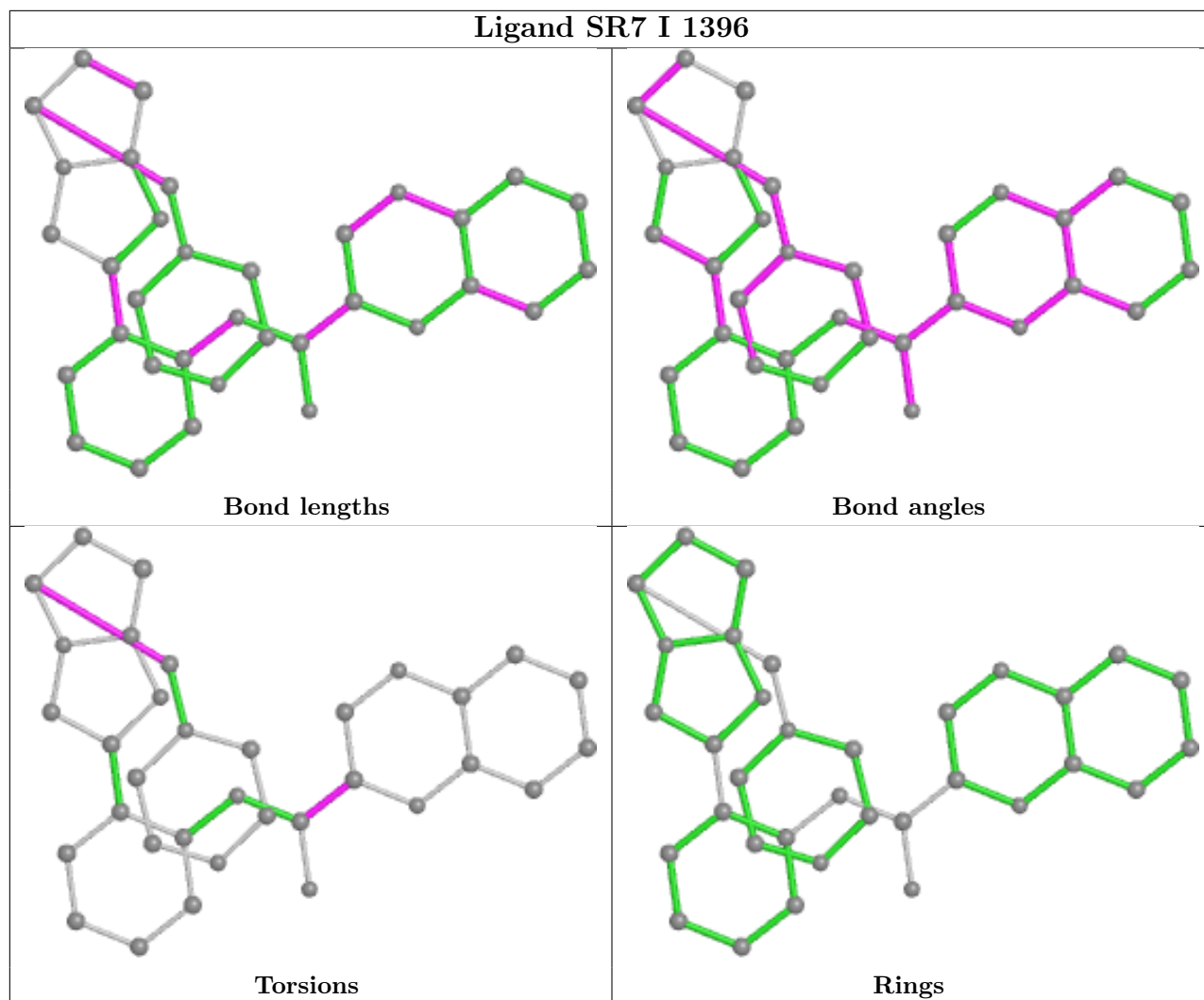


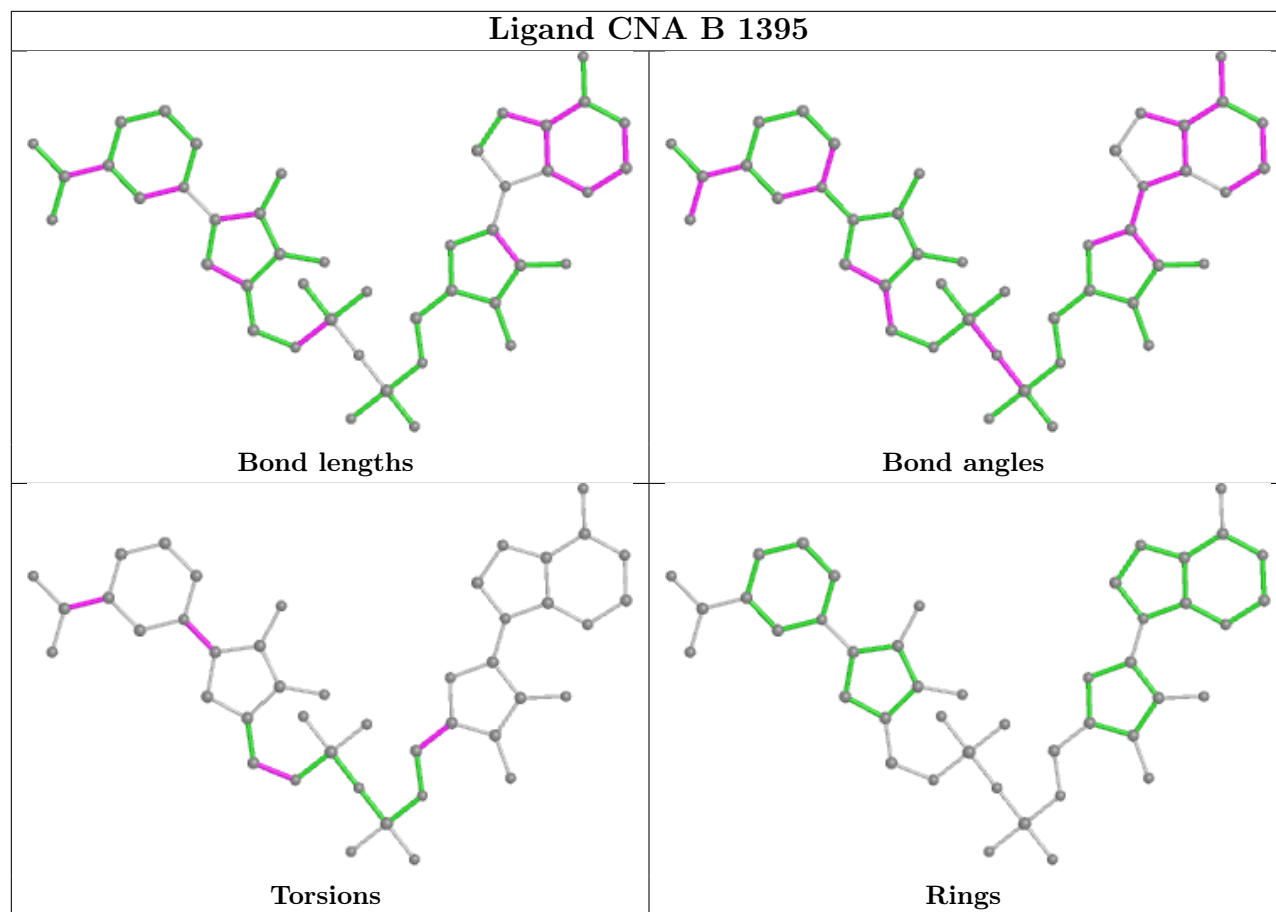


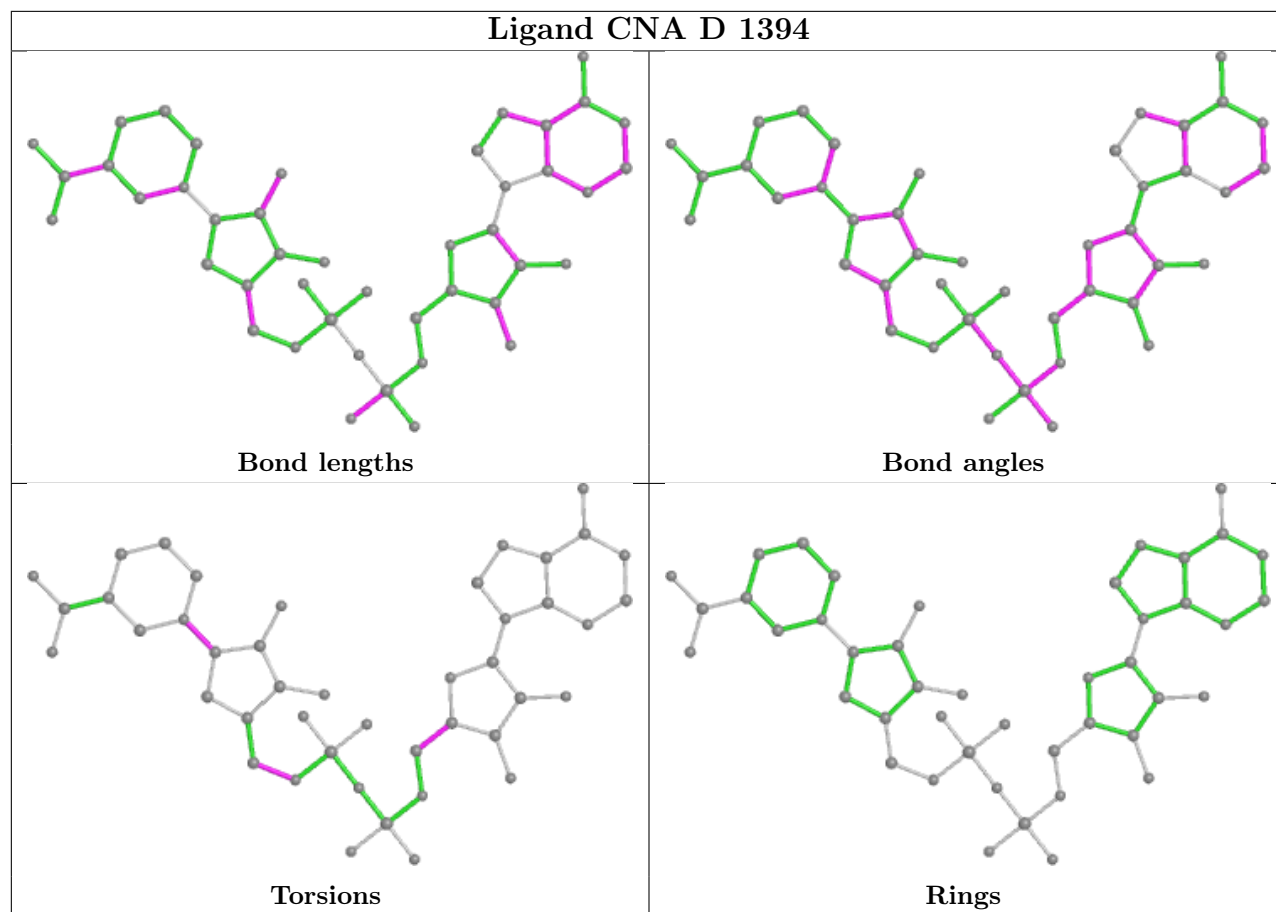




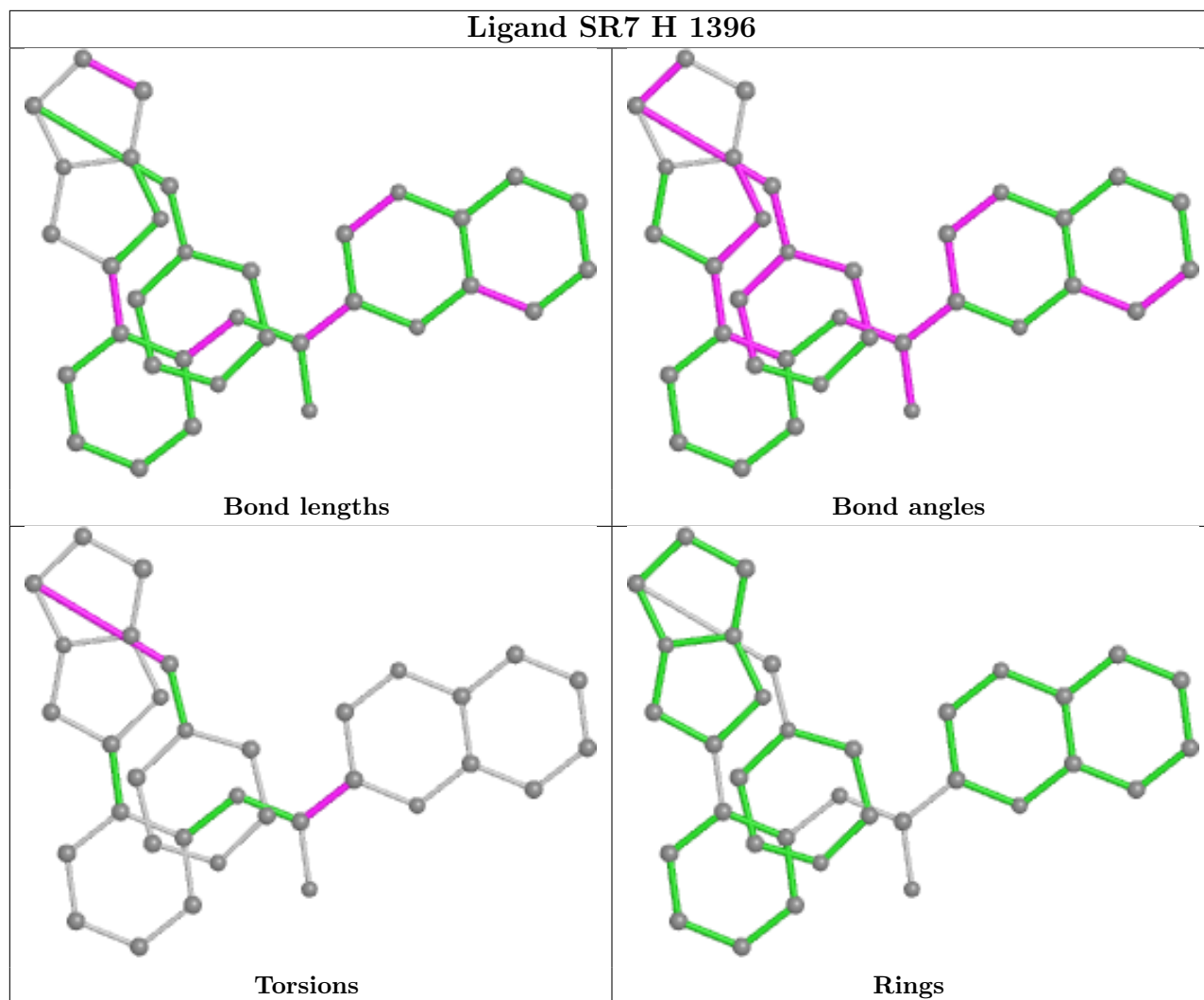


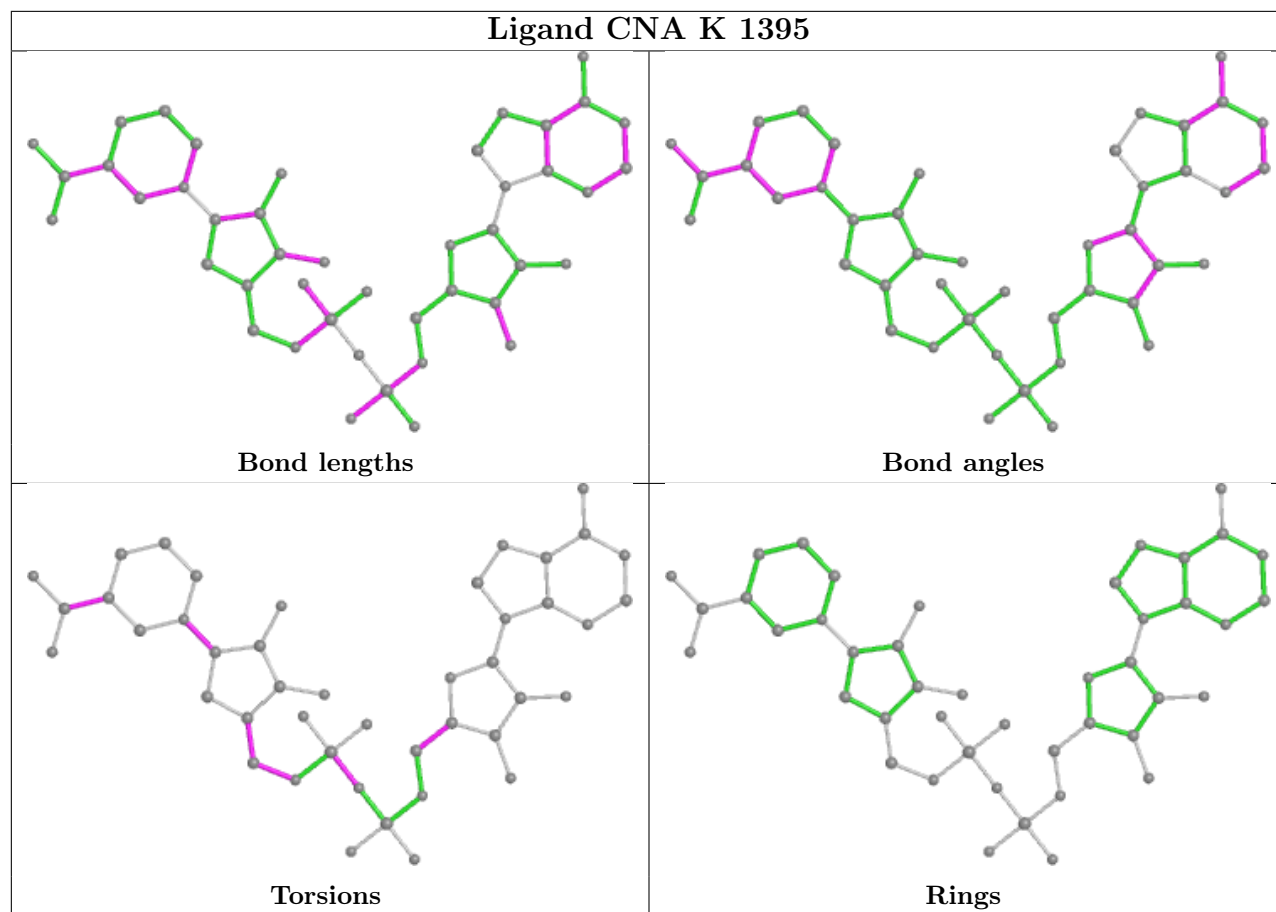


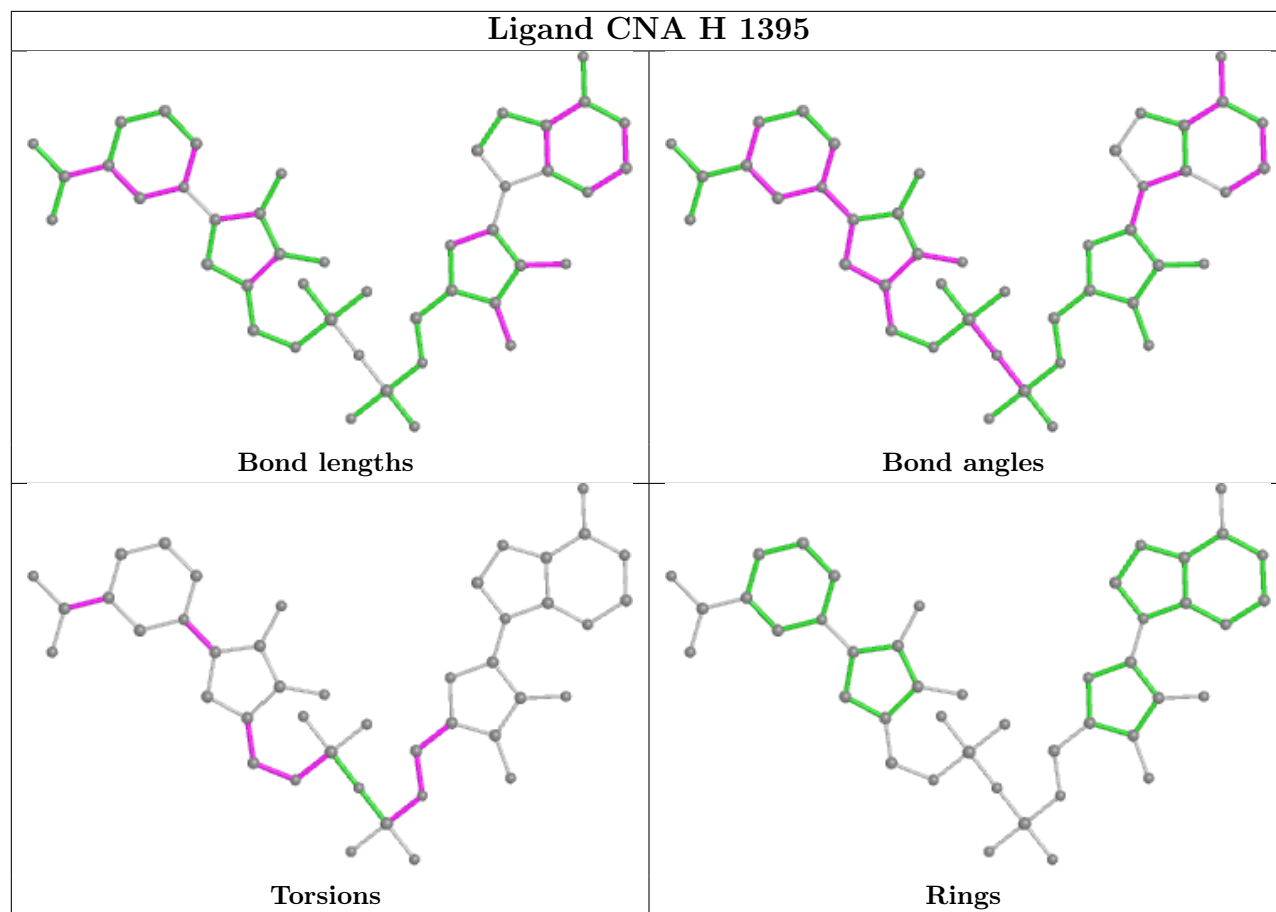


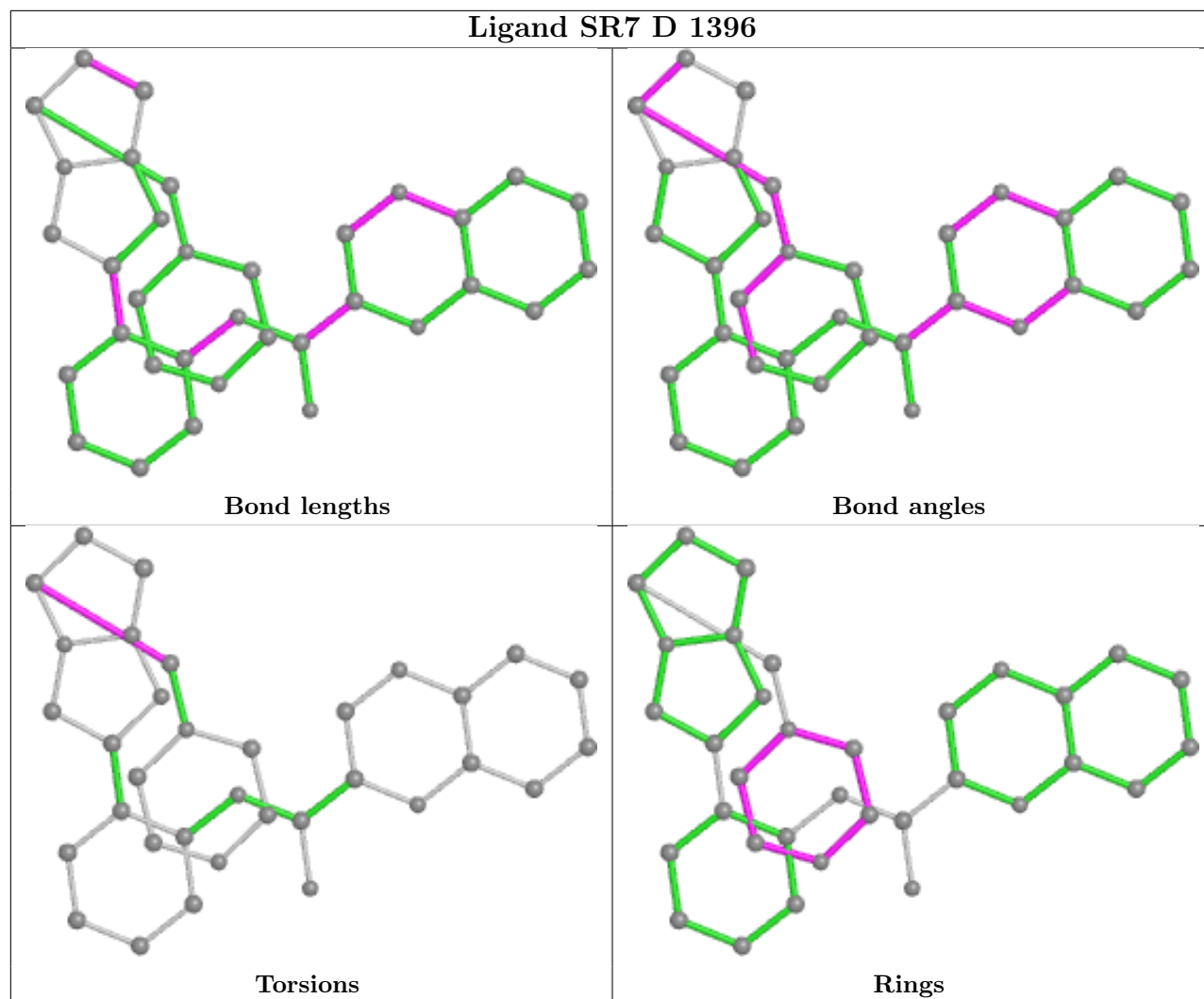


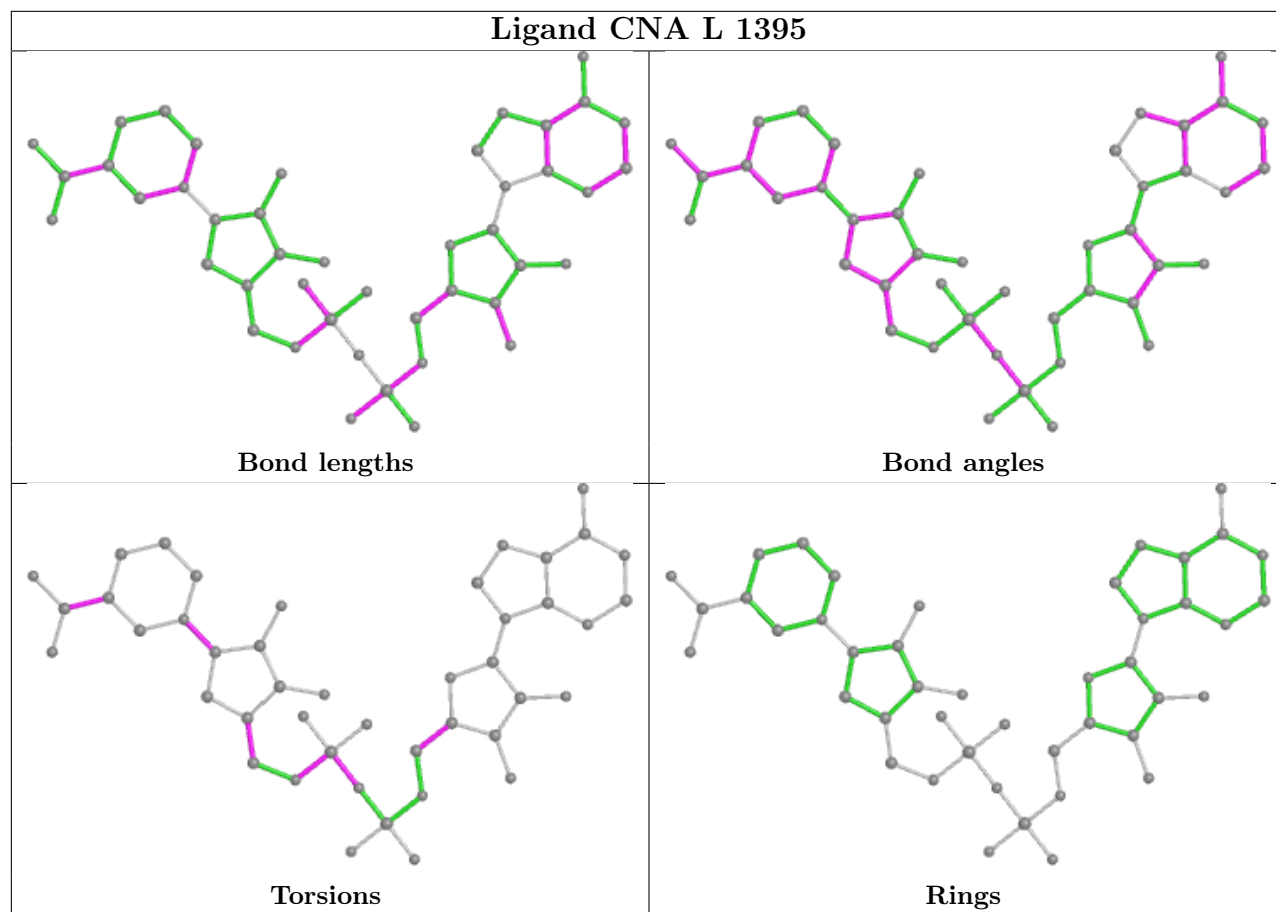


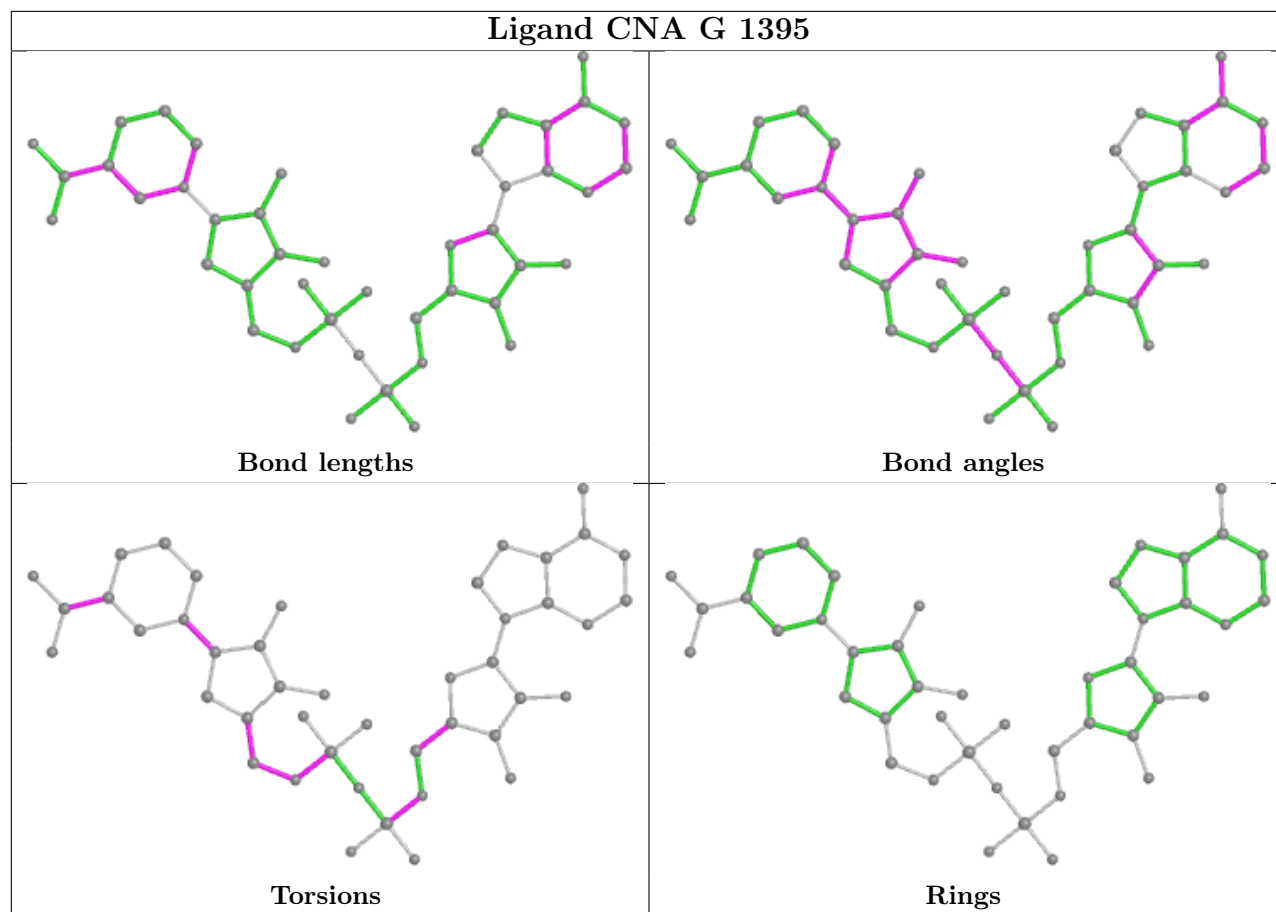


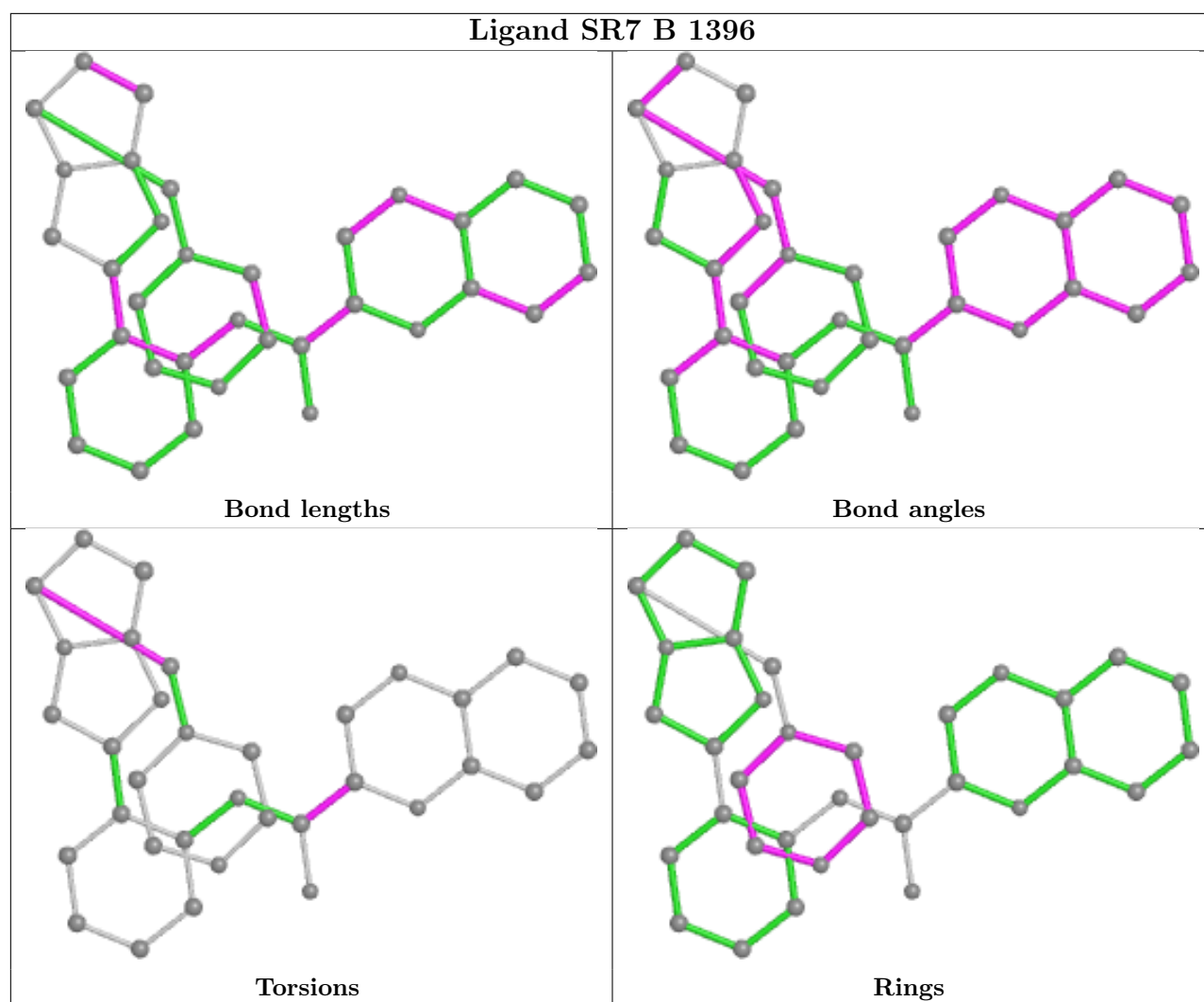












## 5.7 Other polymers [i](#)

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, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	A	273/281 (97%)	-0.10	0 100 100	56, 84, 116, 135	0
1	B	273/281 (97%)	-0.08	0 100 100	56, 81, 114, 133	0
1	C	273/281 (97%)	-0.09	0 100 100	62, 96, 131, 153	0
1	D	272/281 (96%)	-0.08	1 (0%) 92 92	64, 98, 132, 144	0
1	E	273/281 (97%)	-0.22	0 100 100	64, 87, 112, 123	0
1	F	273/281 (97%)	-0.20	1 (0%) 92 92	69, 92, 125, 139	0
1	G	273/281 (97%)	-0.18	0 100 100	66, 87, 110, 124	0
1	H	273/281 (97%)	-0.21	0 100 100	75, 101, 127, 141	0
1	I	273/281 (97%)	-0.17	0 100 100	73, 99, 127, 138	0
1	J	273/281 (97%)	-0.16	1 (0%) 92 92	68, 91, 123, 136	0
1	K	273/281 (97%)	0.05	6 (2%) 62 59	101, 132, 166, 177	0
1	L	273/281 (97%)	0.05	8 (2%) 51 50	101, 132, 168, 182	0
All	All	3275/3372 (97%)	-0.12	17 (0%) 91 90	56, 96, 145, 182	0

The worst 5 of 17 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	J	394	LEU	4.2
1	L	316	LEU	4.1
1	L	341	LEU	3.1
1	K	209	THR	3.0
1	L	360	VAL	2.8

### 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, 95<sup>th</sup> 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.

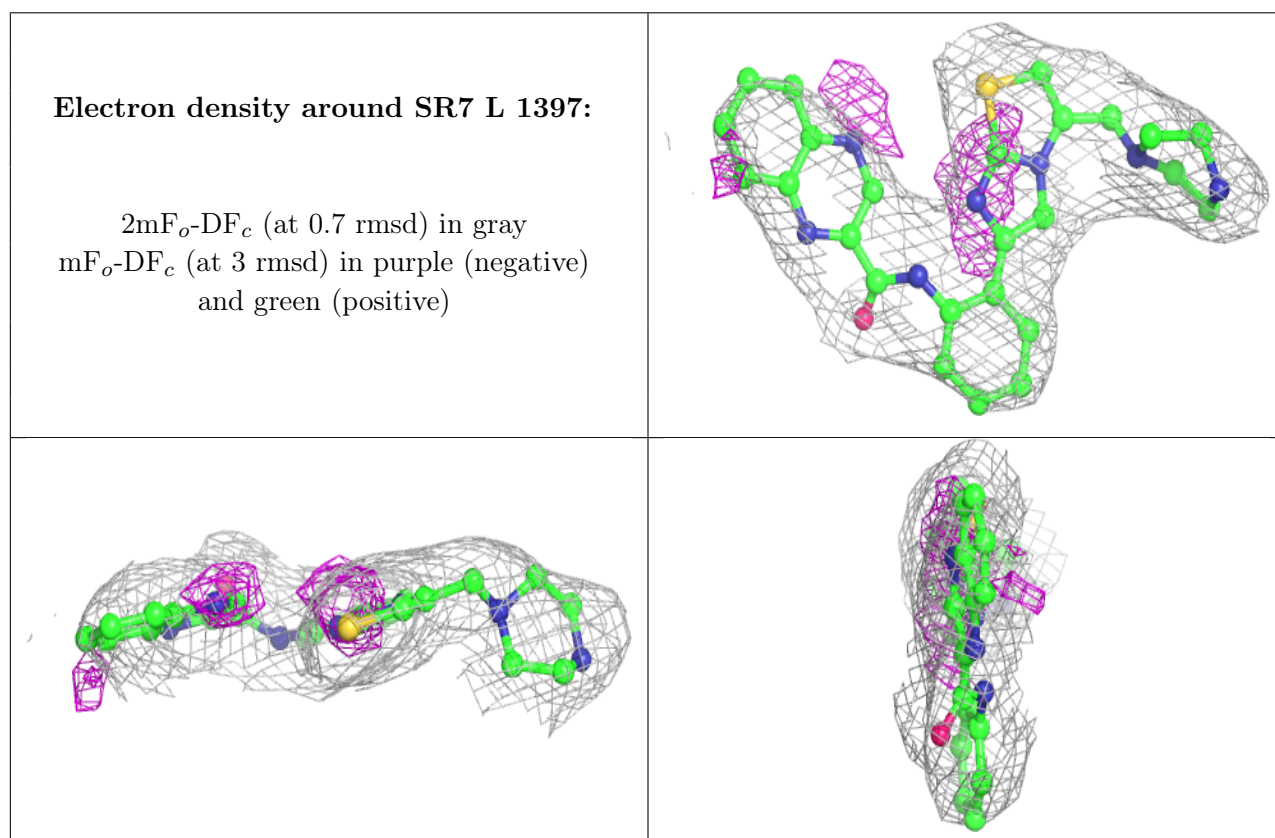
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
5	GOL	K	1396	6/6	0.90	0.30	86,86,86,86	0
3	SR7	L	1397	34/34	0.92	0.25	86,86,86,86	0
3	SR7	K	1397	34/34	0.92	0.29	86,86,86,86	0
3	SR7	J	1396	34/34	0.93	0.24	86,86,86,86	0
3	SR7	F	1396	34/34	0.94	0.26	86,86,86,86	0
2	CNA	D	1394	44/44	0.94	0.22	86,86,86,86	0
2	CNA	K	1395	44/44	0.94	0.21	86,86,86,86	0
2	CNA	L	1395	44/44	0.94	0.21	86,86,86,86	0
5	GOL	D	1395	6/6	0.94	0.40	86,86,86,86	0
3	SR7	B	1396	34/34	0.94	0.28	86,86,86,86	0
3	SR7	E	1396	34/34	0.95	0.26	86,86,86,86	0
3	SR7	A	1396	34/34	0.95	0.31	86,86,86,86	0
3	SR7	G	1396	34/34	0.95	0.29	86,86,86,86	0
2	CNA	C	1395	44/44	0.95	0.23	86,86,86,86	0
2	CNA	H	1395	44/44	0.96	0.19	86,86,86,86	0
3	SR7	H	1396	34/34	0.96	0.32	86,86,86,86	0
3	SR7	I	1396	34/34	0.96	0.25	86,86,86,86	0
2	CNA	I	1395	44/44	0.96	0.17	86,86,86,86	0
3	SR7	C	1397	34/34	0.96	0.29	86,86,86,86	0
3	SR7	D	1396	34/34	0.96	0.33	86,86,86,86	0
5	GOL	C	1396	6/6	0.96	0.34	86,86,86,86	0
2	CNA	B	1395	44/44	0.96	0.23	86,86,86,86	0
2	CNA	G	1395	44/44	0.96	0.23	86,86,86,86	0
5	GOL	L	1396	6/6	0.96	0.24	86,86,86,86	0
4	ZN	J	1397	1/1	0.97	0.10	86,86,86,86	0
2	CNA	F	1395	44/44	0.97	0.19	86,86,86,86	0
2	CNA	J	1395	44/44	0.97	0.21	86,86,86,86	0
2	CNA	A	1395	44/44	0.97	0.23	86,86,86,86	0
2	CNA	E	1395	44/44	0.97	0.19	86,86,86,86	0
4	ZN	L	1398	1/1	0.98	0.15	86,86,86,86	0
4	ZN	I	1397	1/1	0.99	0.07	86,86,86,86	0
4	ZN	A	1397	1/1	0.99	0.13	86,86,86,86	0

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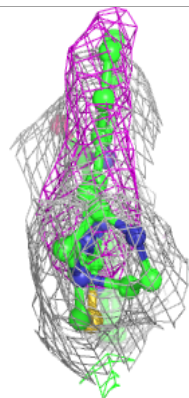
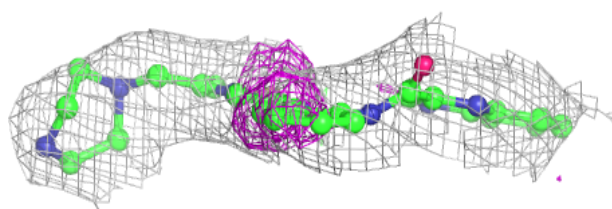
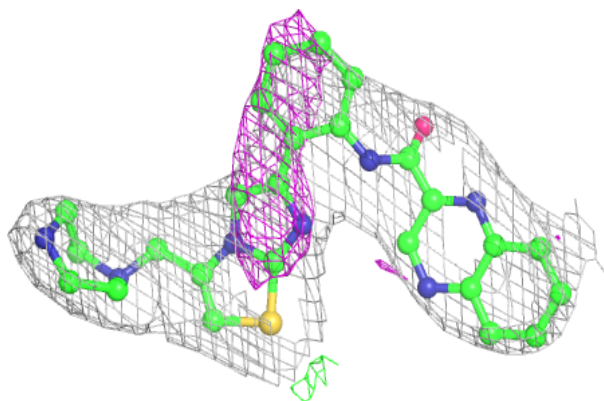
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
4	ZN	K	1398	1/1	0.99	0.14	86,86,86,86	0
4	ZN	C	1398	1/1	0.99	0.12	86,86,86,86	0
4	ZN	D	1397	1/1	0.99	0.12	86,86,86,86	0
4	ZN	E	1397	1/1	0.99	0.11	86,86,86,86	0
4	ZN	F	1397	1/1	0.99	0.07	86,86,86,86	0
4	ZN	H	1397	1/1	0.99	0.07	86,86,86,86	0
4	ZN	G	1397	1/1	1.00	0.14	86,86,86,86	0
4	ZN	B	1397	1/1	1.00	0.16	86,86,86,86	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.

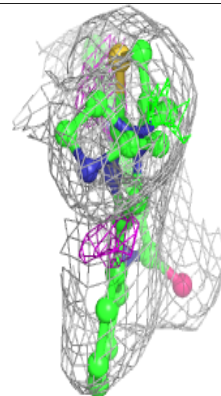
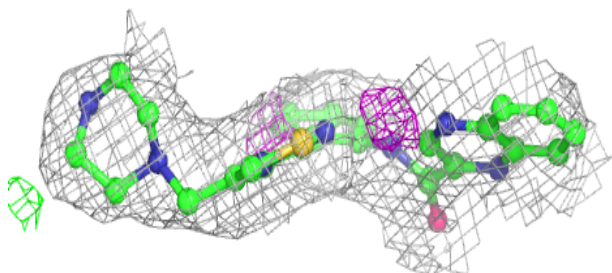
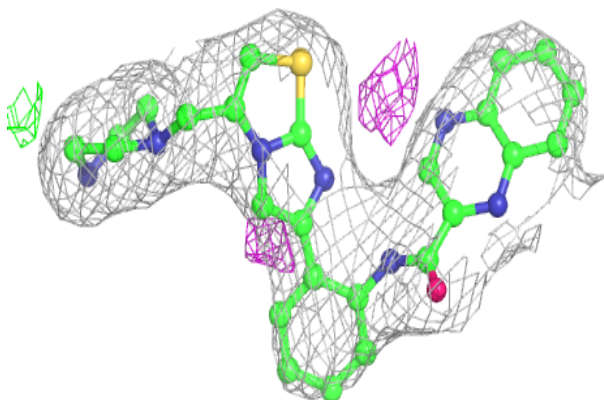


**Electron density around SR7 K 1397:**

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

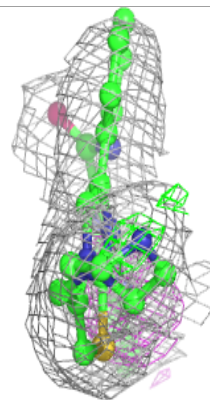
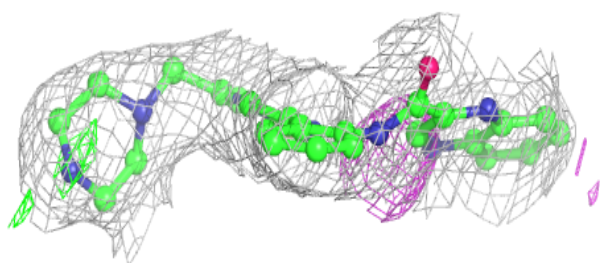
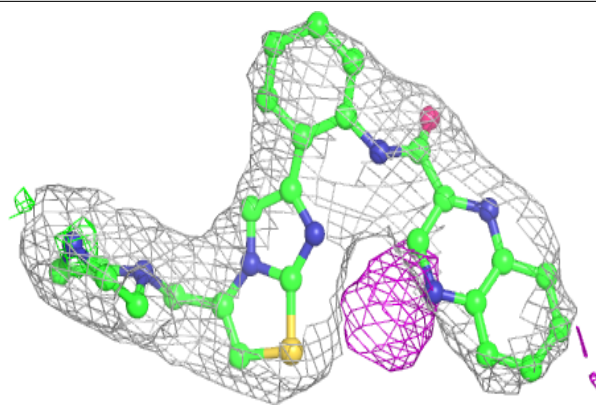
**Electron density around SR7 J 1396:**

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

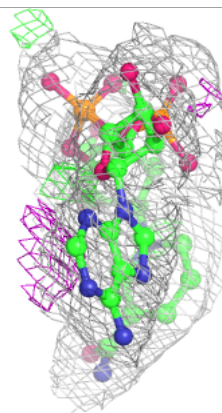
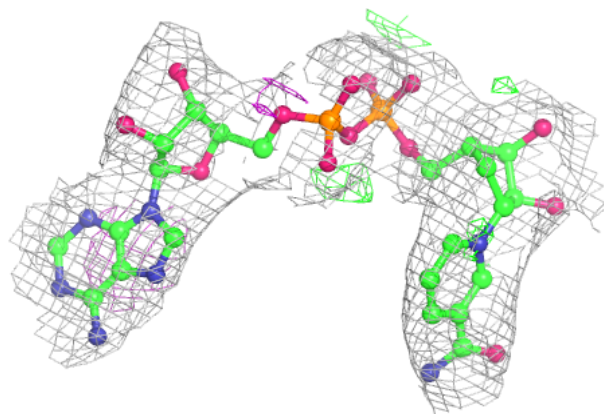


**Electron density around SR7 F 1396:**

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

**Electron density around CNA D 1394:**

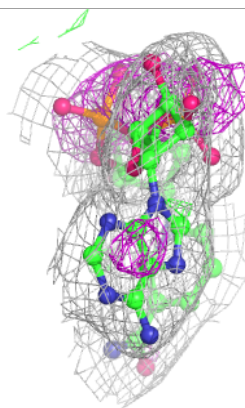
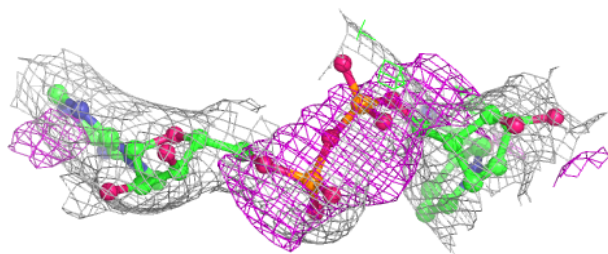
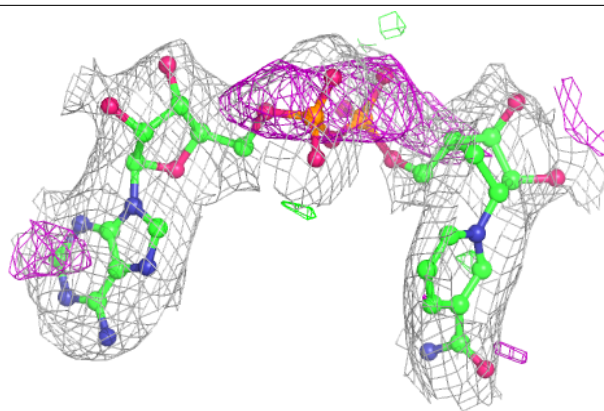
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



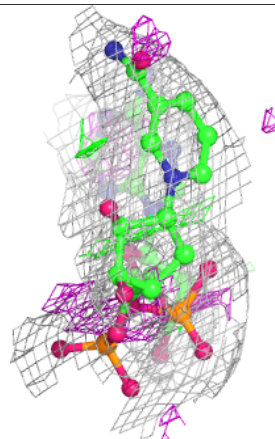
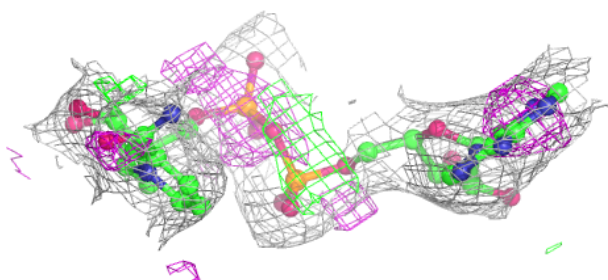
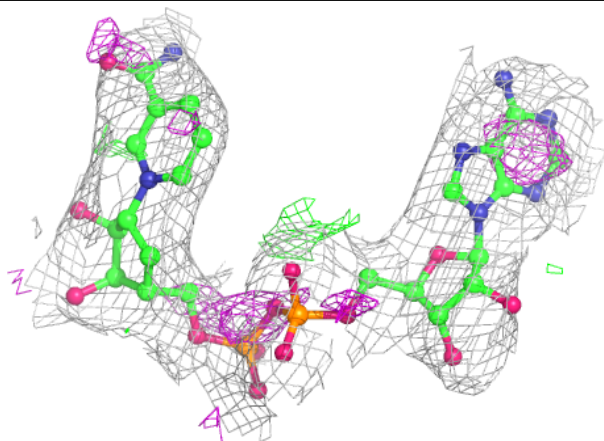


**Electron density around CNA K 1395:**

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

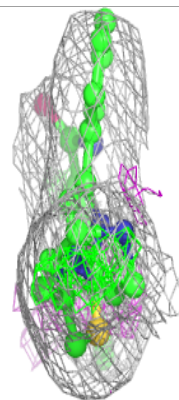
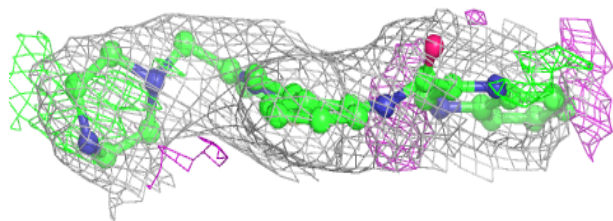
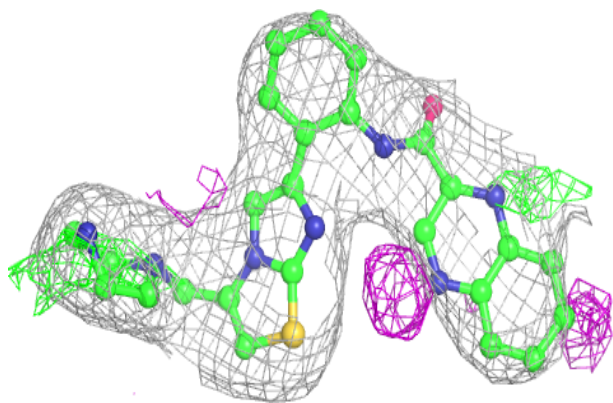
**Electron density around CNA L 1395:**

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and green (positive)

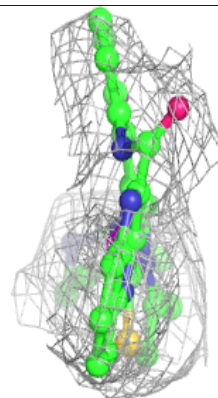
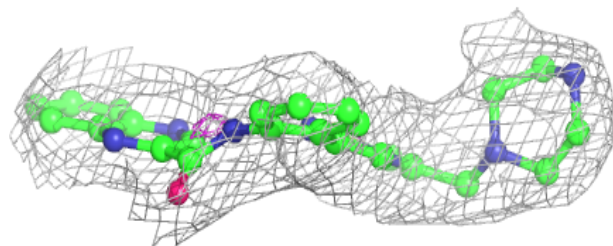
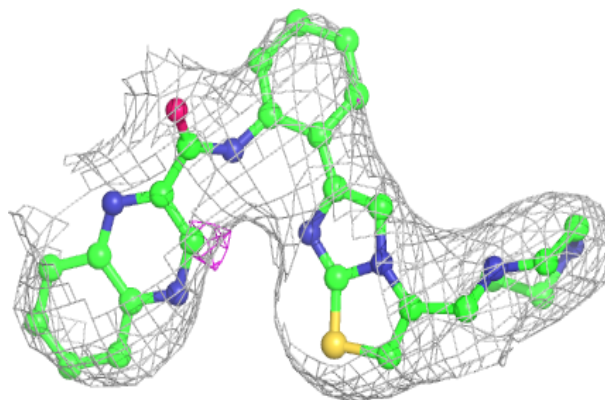


**Electron density around SR7 B 1396:**

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

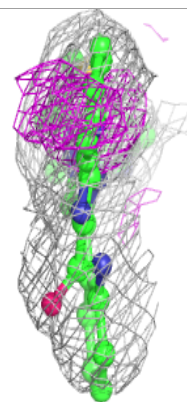
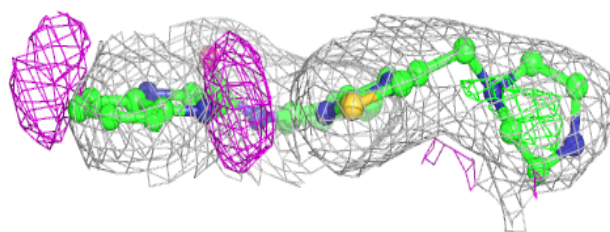
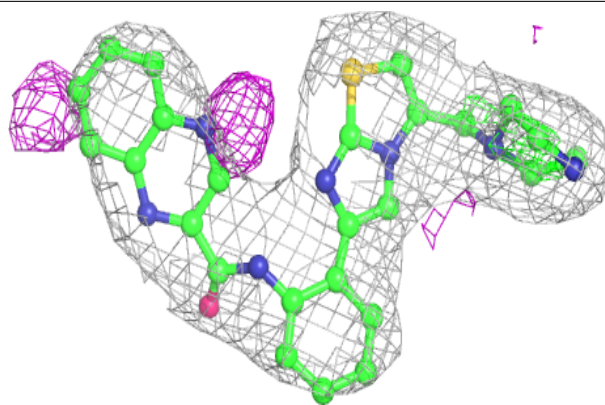
**Electron density around SR7 E 1396:**

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and green (positive)

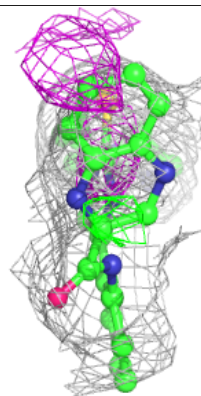
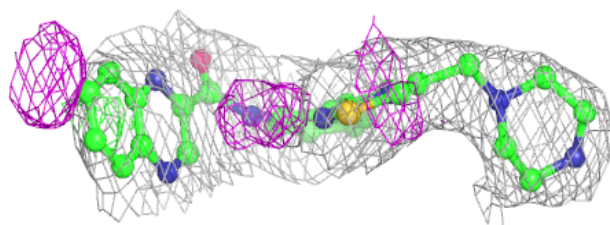
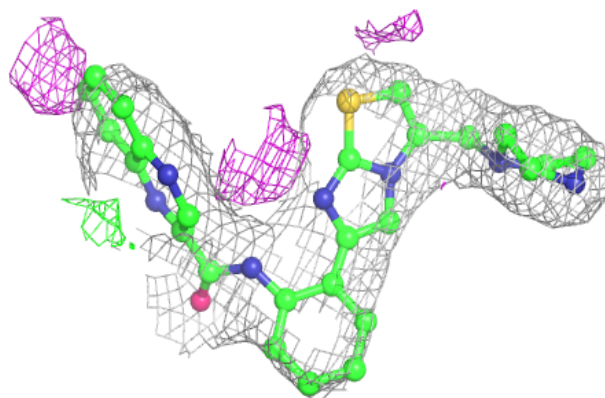


**Electron density around SR7 A 1396:**

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

**Electron density around SR7 G 1396:**

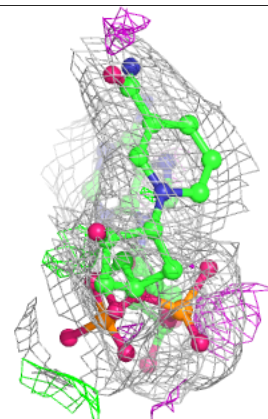
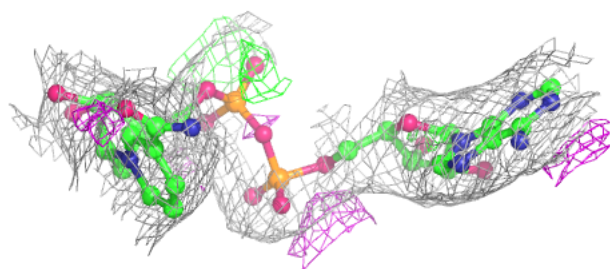
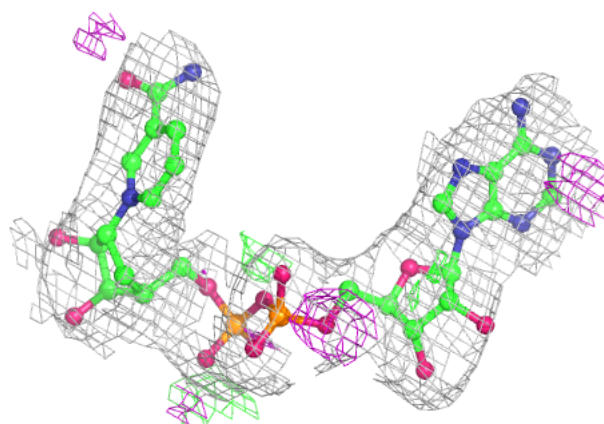
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



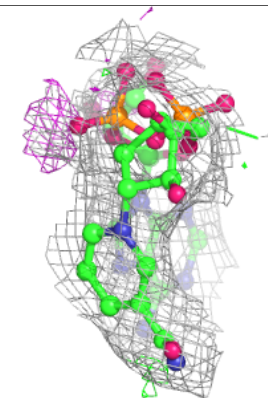
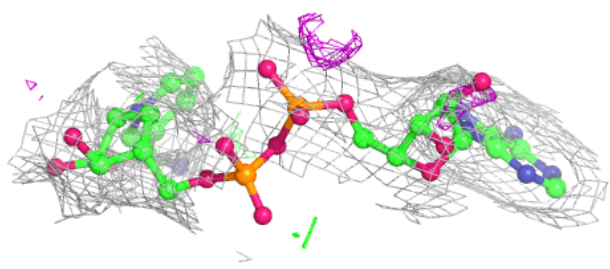
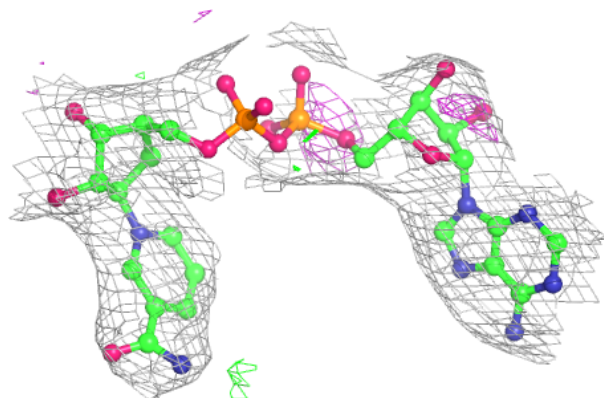


**Electron density around CNA C 1395:**

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

**Electron density around CNA H 1395:**

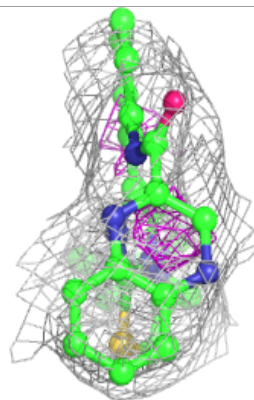
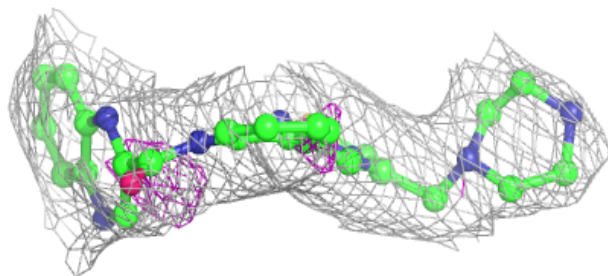
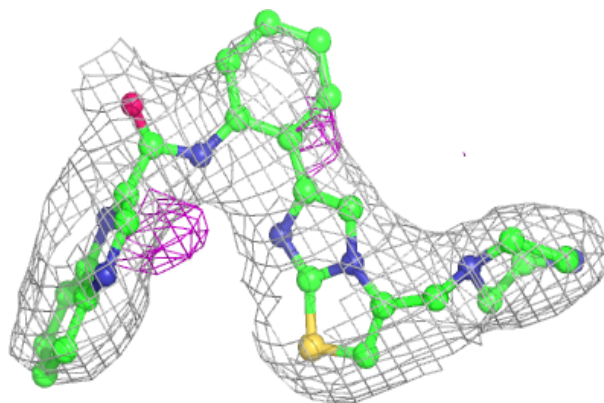
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



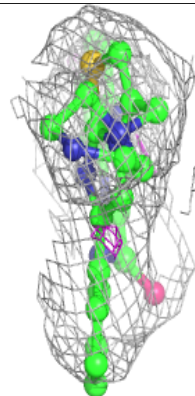
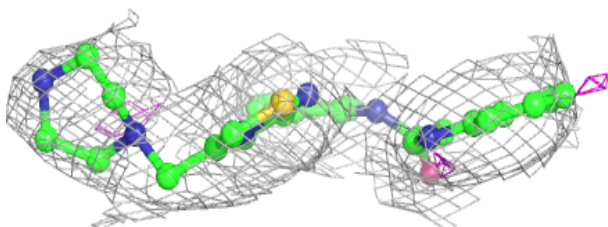
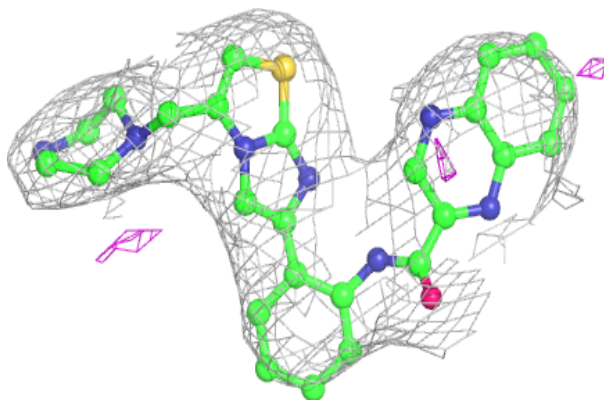


**Electron density around SR7 H 1396:**

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

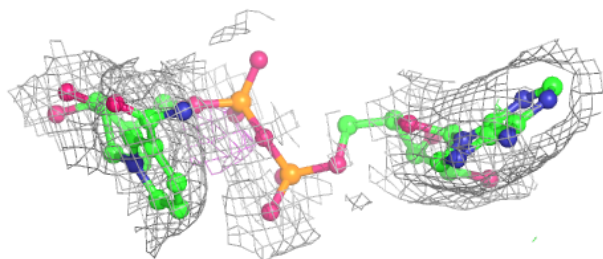
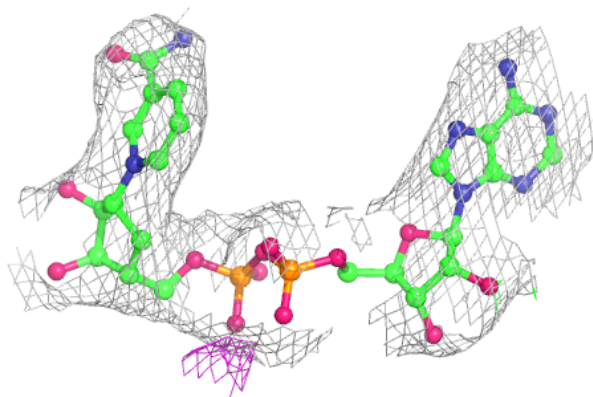
**Electron density around SR7 I 1396:**

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and green (positive)

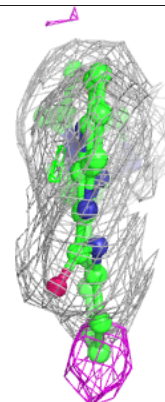
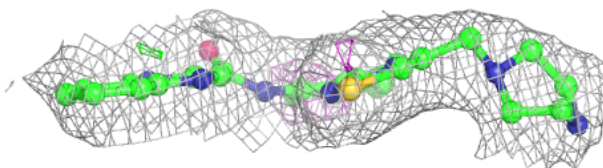
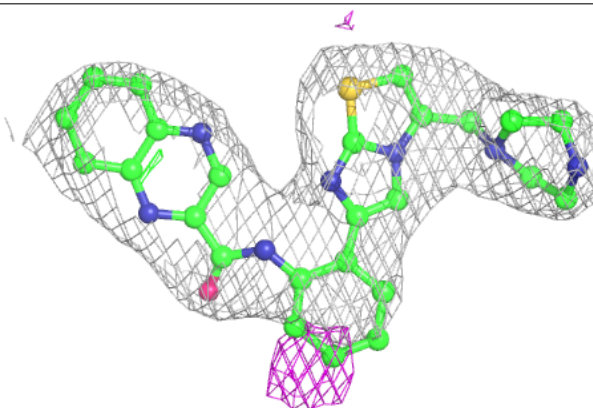


**Electron density around CNA I 1395:**

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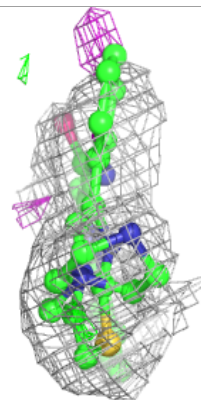
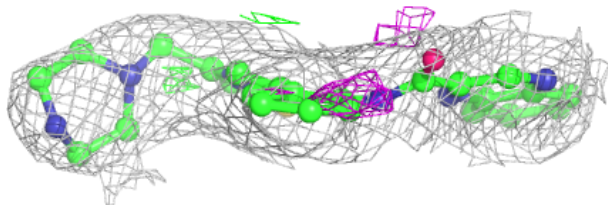
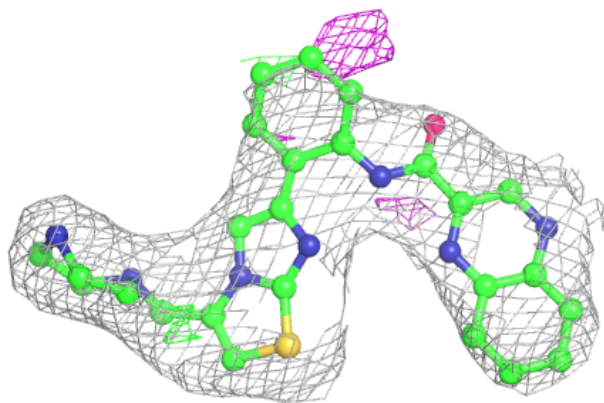
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and green (positive)

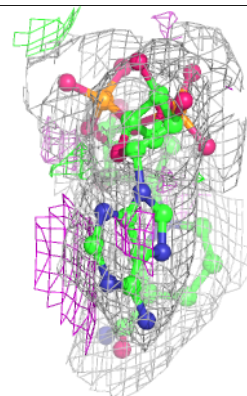
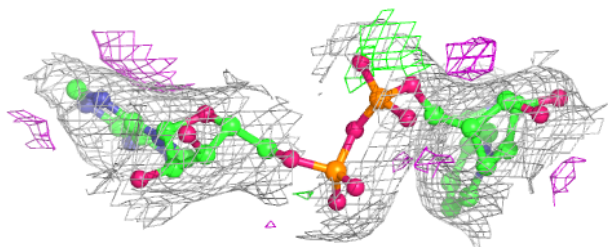
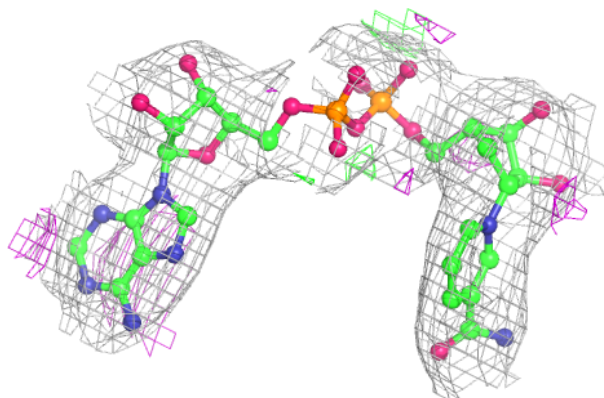


**Electron density around SR7 D 1396:**

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**Electron density around CNA B 1395:**

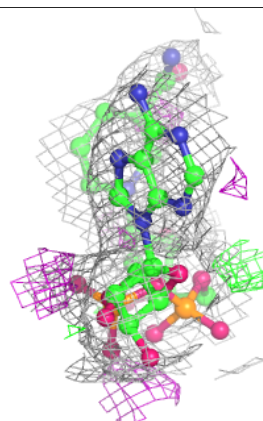
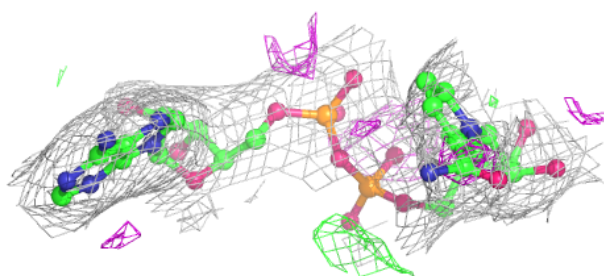
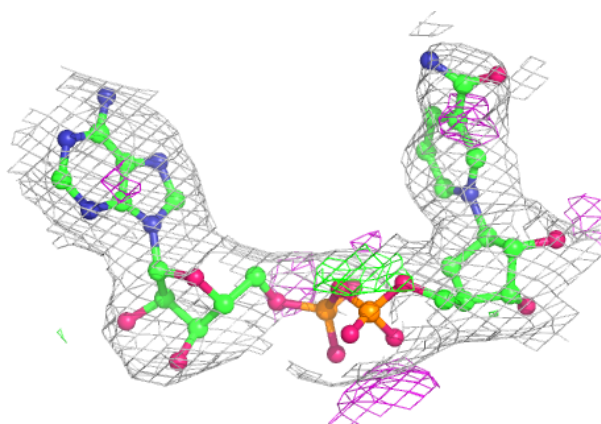
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and green (positive)



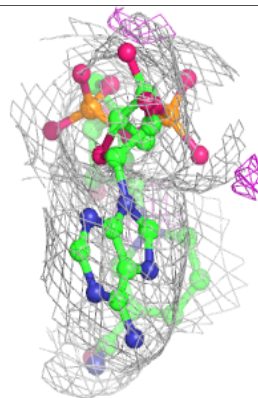
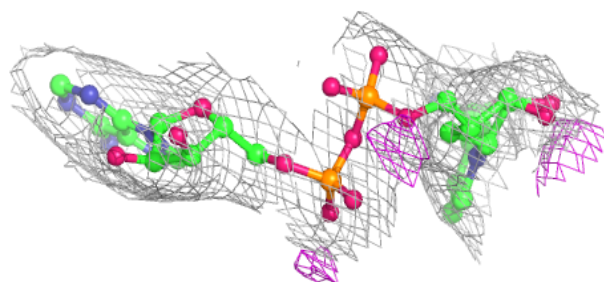
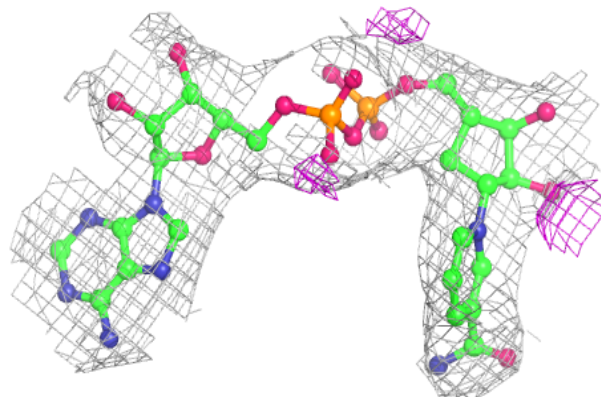


**Electron density around CNA G 1395:**

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and green (positive)

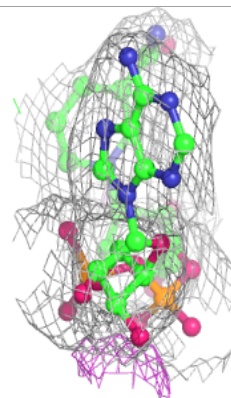
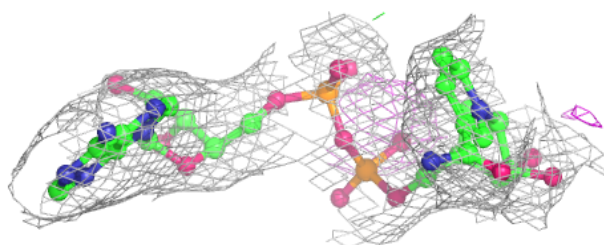
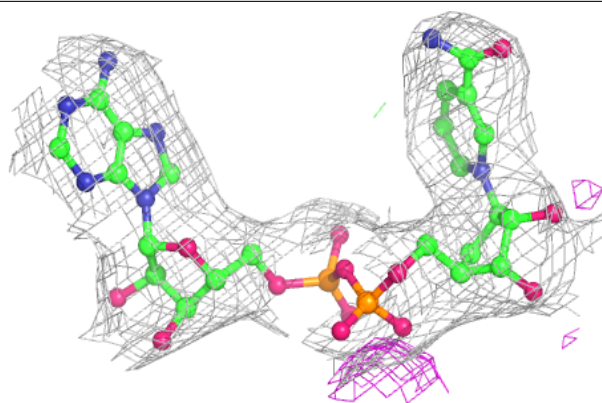
**Electron density around CNA F 1395:**

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and green (positive)

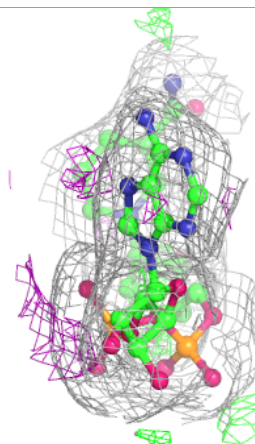
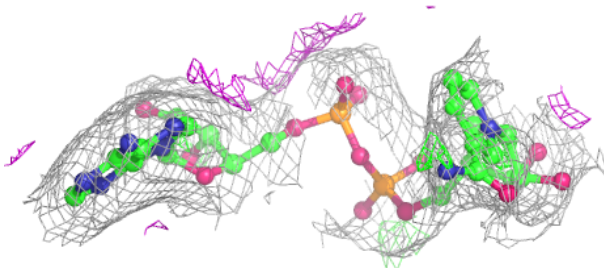
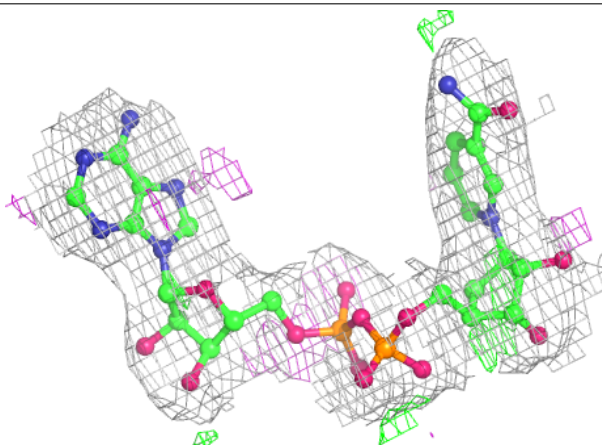


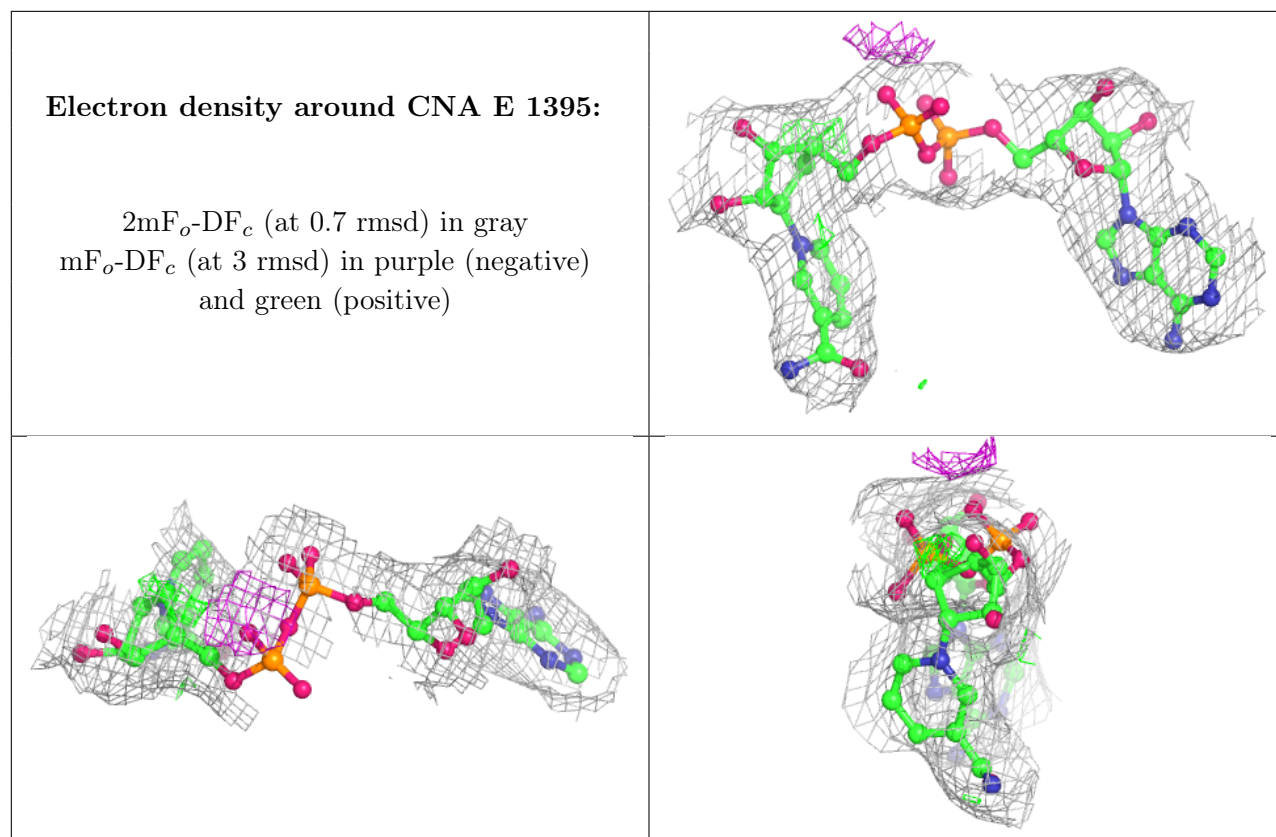
**Electron density around CNA J 1395:**

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

**Electron density around CNA A 1395:**

$2mF_o-DF_c$  (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.