



Full wwPDB X-ray Structure Validation Report ⓘ

May 13, 2020 – 05:17 am BST

PDB ID : 6CI9
Title : RMM microcompartment-associated aminopropanol dehydrogenase NADP + aminoacetone holo-structure
Authors : Mallette, E.; Kimber, M.S.
Deposited on : 2018-02-23
Resolution : 1.90 Å(reported)

This is a Full wwPDB X-ray Structure Validation 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 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 : 2.11
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) : 2.11

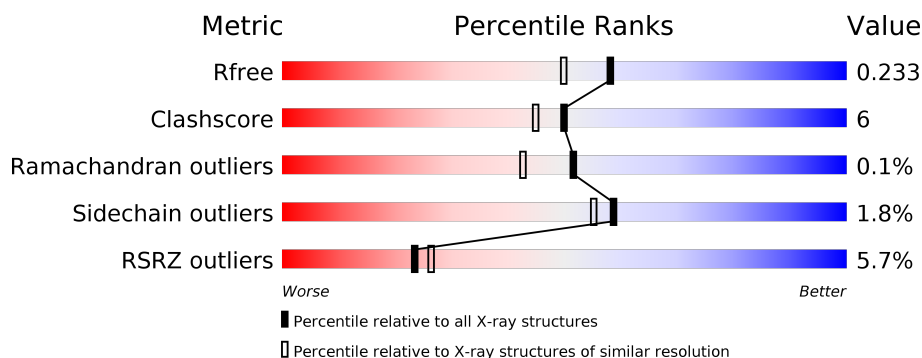
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.90 Å.

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





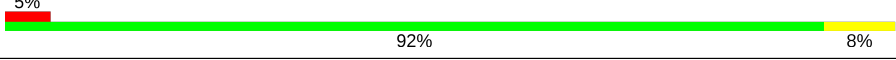
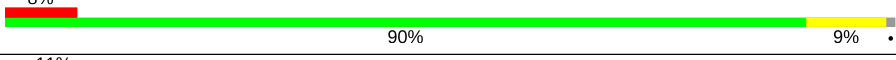
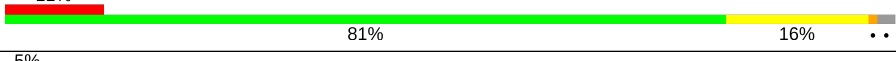
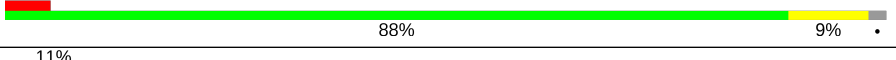
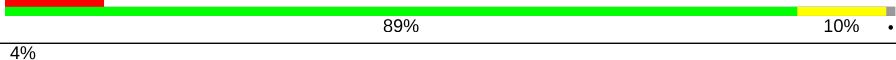
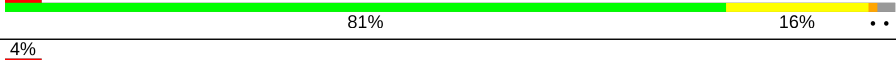

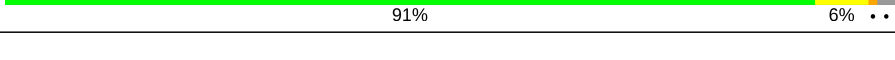
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	6207 (1.90-1.90)
Clashscore	141614	6847 (1.90-1.90)
Ramachandran outliers	138981	6760 (1.90-1.90)
Sidechain outliers	138945	6760 (1.90-1.90)
RSRZ outliers	127900	6082 (1.90-1.90)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on 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	259	<div> <div>5%</div> <div> <div></div> <div>90%</div> <div>8%</div> <div></div> </div> </div>
1	B	259	<div> <div>6%</div> <div> <div></div> <div>83%</div> <div>15%</div> <div></div> </div> </div>
1	C	259	<div> <div>5%</div> <div> <div></div> <div>87%</div> <div>12%</div> <div></div> </div> </div>
1	D	259	<div> <div>3%</div> <div> <div></div> <div>85%</div> <div>15%</div> <div></div> </div> </div>
1	E	259	<div> <div>2%</div> <div> <div></div> <div>88%</div> <div>11%</div> <div></div> </div> </div>
1	F	259	<div> <div>4%</div> <div> <div></div> <div>91%</div> <div>7%</div> <div></div> </div> </div>

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Mol	Chain	Length	Quality of chain
1	G	259	
1	H	259	
1	I	259	
1	J	259	
1	K	259	
1	L	259	
1	M	259	
1	N	259	
1	O	259	
1	P	259	

2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 33083 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.

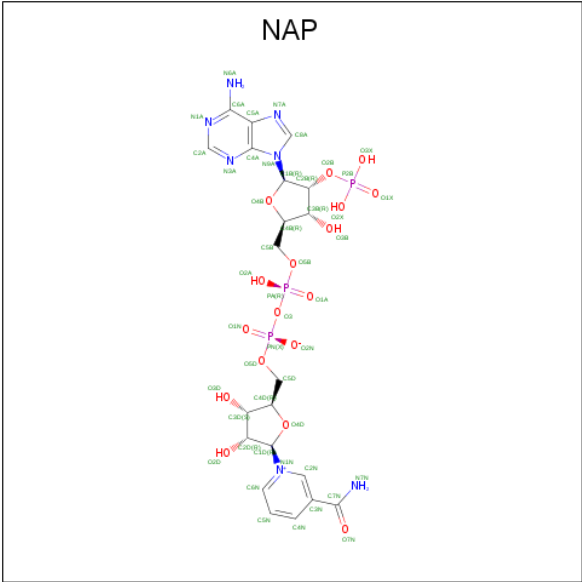
- Molecule 1 is a protein called 3-oxoacyl-[acyl-carrier-protein] reductase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	256	Total	C	N	O	S	0	0	0
			1862	1156	328	372	6			
1	B	255	Total	C	N	O	S	0	0	0
			1856	1153	327	370	6			
1	C	258	Total	C	N	O	S	0	0	0
			1875	1165	330	374	6			
1	D	259	Total	C	N	O	S	0	0	0
			1880	1168	331	375	6			
1	E	255	Total	C	N	O	S	0	0	0
			1854	1150	327	371	6			
1	F	254	Total	C	N	O	S	0	0	0
			1848	1147	326	369	6			
1	G	256	Total	C	N	O	S	0	0	0
			1862	1156	328	372	6			
1	H	253	Total	C	N	O	S	0	0	0
			1838	1141	323	368	6			
1	I	258	Total	C	N	O	S	0	0	0
			1874	1165	330	373	6			
1	J	257	Total	C	N	O	S	0	0	0
			1869	1162	329	372	6			
1	K	255	Total	C	N	O	S	0	0	0
			1854	1150	327	371	6			
1	L	253	Total	C	N	O	S	0	0	0
			1838	1141	323	368	6			
1	M	256	Total	C	N	O	S	0	0	0
			1862	1156	328	372	6			
1	N	254	Total	C	N	O	S	0	0	0
			1848	1147	326	369	6			
1	O	253	Total	C	N	O	S	0	0	0
			1838	1141	323	368	6			
1	P	255	Total	C	N	O	S	0	0	0
			1854	1150	327	371	6			

There are 32 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-1	SER	-	expression tag	UNP A0QP46
A	0	HIS	-	expression tag	UNP A0QP46
B	-1	SER	-	expression tag	UNP A0QP46
B	0	HIS	-	expression tag	UNP A0QP46
C	-1	SER	-	expression tag	UNP A0QP46
C	0	HIS	-	expression tag	UNP A0QP46
D	-1	SER	-	expression tag	UNP A0QP46
D	0	HIS	-	expression tag	UNP A0QP46
E	-1	SER	-	expression tag	UNP A0QP46
E	0	HIS	-	expression tag	UNP A0QP46
F	-1	SER	-	expression tag	UNP A0QP46
F	0	HIS	-	expression tag	UNP A0QP46
G	-1	SER	-	expression tag	UNP A0QP46
G	0	HIS	-	expression tag	UNP A0QP46
H	-1	SER	-	expression tag	UNP A0QP46
H	0	HIS	-	expression tag	UNP A0QP46
I	-1	SER	-	expression tag	UNP A0QP46
I	0	HIS	-	expression tag	UNP A0QP46
J	-1	SER	-	expression tag	UNP A0QP46
J	0	HIS	-	expression tag	UNP A0QP46
K	-1	SER	-	expression tag	UNP A0QP46
K	0	HIS	-	expression tag	UNP A0QP46
L	-1	SER	-	expression tag	UNP A0QP46
L	0	HIS	-	expression tag	UNP A0QP46
M	-1	SER	-	expression tag	UNP A0QP46
M	0	HIS	-	expression tag	UNP A0QP46
N	-1	SER	-	expression tag	UNP A0QP46
N	0	HIS	-	expression tag	UNP A0QP46
O	-1	SER	-	expression tag	UNP A0QP46
O	0	HIS	-	expression tag	UNP A0QP46
P	-1	SER	-	expression tag	UNP A0QP46
P	0	HIS	-	expression tag	UNP A0QP46

- Molecule 2 is NADP NICOTINAMIDE-ADENINE-DINUCLEOTIDE PHOSPHATE (three-letter code: NAP) (formula: C₂₁H₂₈N₇O₁₇P₃) (labeled as "Ligand of Interest" by author).



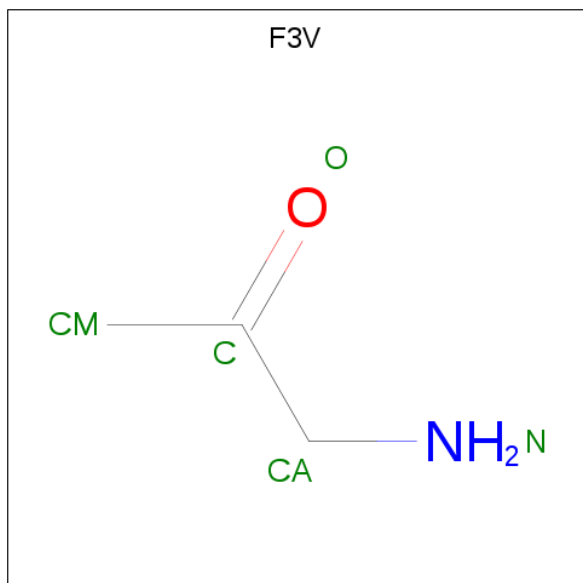
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	N	O	P	0	0
			48	21	7	17	3		
2	B	1	Total	C	N	O	P	0	0
			48	21	7	17	3		
2	C	1	Total	C	N	O	P	0	0
			48	21	7	17	3		
2	D	1	Total	C	N	O	P	0	0
			48	21	7	17	3		
2	E	1	Total	C	N	O	P	0	0
			48	21	7	17	3		
2	F	1	Total	C	N	O	P	0	0
			48	21	7	17	3		
2	G	1	Total	C	N	O	P	0	0
			48	21	7	17	3		
2	H	1	Total	C	N	O	P	0	0
			48	21	7	17	3		
2	I	1	Total	C	N	O	P	0	0
			48	21	7	17	3		
2	J	1	Total	C	N	O	P	0	0
			48	21	7	17	3		
2	K	1	Total	C	N	O	P	0	0
			48	21	7	17	3		
2	L	1	Total	C	N	O	P	0	0
			48	21	7	17	3		
2	M	1	Total	C	N	O	P	0	0
			48	21	7	17	3		
2	N	1	Total	C	N	O	P	0	0
			48	21	7	17	3		

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	O	1	Total	C	N	O	P	0	0
			48	21	7	17	3		
2	P	1	Total	C	N	O	P	0	0
			48	21	7	17	3		

- Molecule 3 is 1-aminopropan-2-one (three-letter code: F3V) (formula: C₃H₇NO) (labeled as "Ligand of Interest" by author).



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

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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	J	1	Total	C	N	O	0	0
			5	3	1	1		
3	K	1	Total	C	N	O	0	0
			5	3	1	1		
3	L	1	Total	C	N	O	0	0
			5	3	1	1		
3	M	1	Total	C	N	O	0	0
			5	3	1	1		
3	N	1	Total	C	N	O	0	0
			5	3	1	1		
3	O	1	Total	C	N	O	0	0
			5	3	1	1		
3	P	1	Total	C	N	O	0	0
			5	3	1	1		

- Molecule 4 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	P	1	Total	Cl	0	0
			1	1		
4	G	1	Total	Cl	0	0
			1	1		
4	J	1	Total	Cl	0	0
			1	1		
4	D	1	Total	Cl	0	0
			1	1		
4	K	1	Total	Cl	0	0
			1	1		
4	E	1	Total	Cl	0	0
			1	1		
4	H	1	Total	Cl	0	0
			1	1		
4	B	1	Total	Cl	0	0
			1	1		
4	I	1	Total	Cl	0	0
			1	1		
4	C	1	Total	Cl	0	0
			1	1		
4	A	2	Total	Cl	0	0
			2	2		
4	N	1	Total	Cl	0	0
			1	1		

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	O	1	Total 1	Cl 1	0	0
4	L	1	Total 1	Cl 1	0	0
4	F	1	Total 1	Cl 1	0	0
4	M	1	Total 1	Cl 1	0	0

- Molecule 5 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	J	1	Total 1	Mg 1	0	0
5	H	1	Total 1	Mg 1	0	0
5	C	1	Total 1	Mg 1	0	0
5	A	1	Total 1	Mg 1	0	0
5	O	1	Total 1	Mg 1	0	0
5	L	1	Total 1	Mg 1	0	0
5	F	1	Total 1	Mg 1	0	0
5	M	1	Total 1	Mg 1	0	0

- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	223	Total 223	O 223	0	0
6	B	180	Total 180	O 180	0	0
6	C	189	Total 189	O 189	0	0
6	D	191	Total 191	O 191	0	0
6	E	202	Total 202	O 202	0	0

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	F	203	Total 203	O 203	0	0
6	G	186	Total 186	O 186	0	0
6	H	209	Total 209	O 209	0	0
6	I	106	Total 106	O 106	0	0
6	J	113	Total 113	O 113	0	0
6	K	96	Total 96	O 96	0	0
6	L	123	Total 123	O 123	0	0
6	M	111	Total 111	O 111	0	0
6	N	118	Total 118	O 118	0	0
6	O	132	Total 132	O 132	0	0
6	P	116	Total 116	O 116	0	0

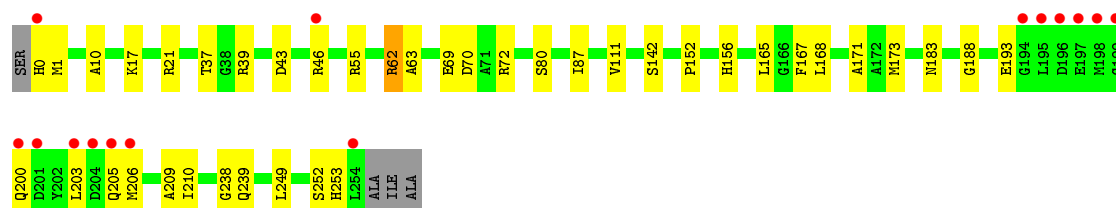
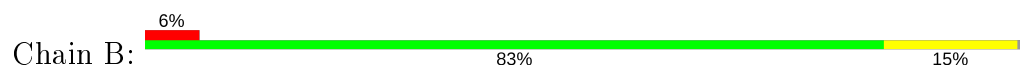
3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA and DNA 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.

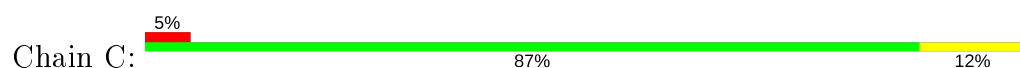
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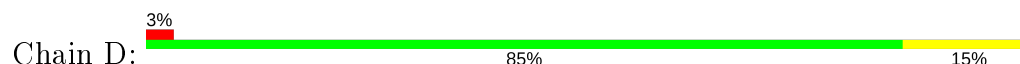
- Molecule 1: 3-oxoacyl-[acyl-carrier-protein] reductase



- Molecule 1: 3-oxoacyl-[acyl-carrier-protein] reductase

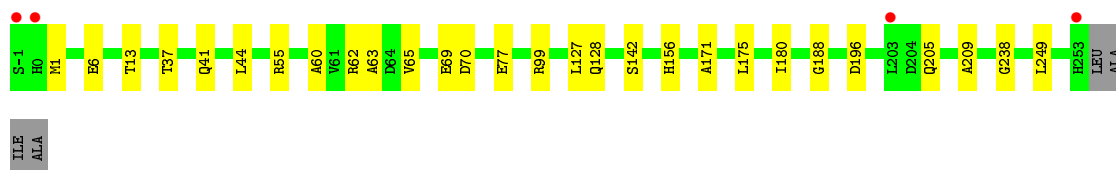
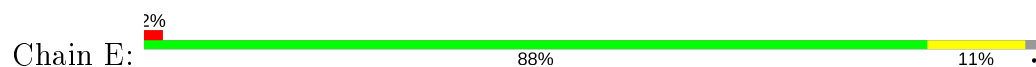


- Molecule 1: 3-oxoacyl-[acyl-carrier-protein] reductase





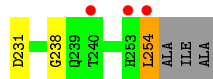
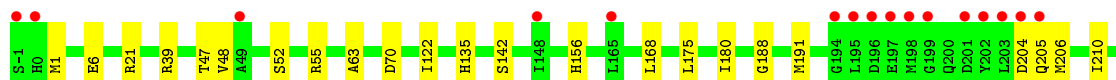
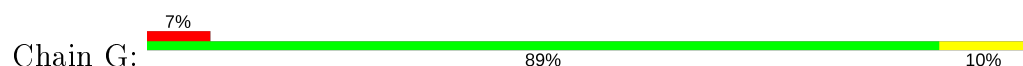
- Molecule 1: 3-oxoacyl-[acyl-carrier-protein] reductase



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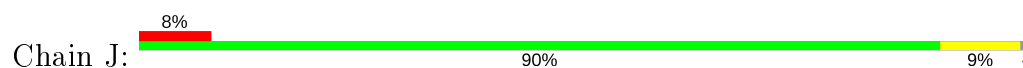
- Molecule 1: 3-oxoacyl-[acyl-carrier-protein] reductase

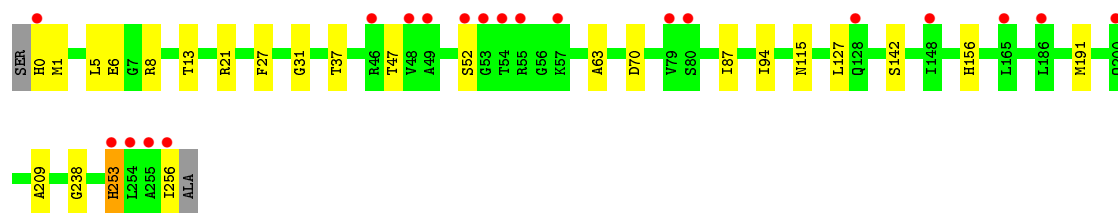


- Molecule 1: 3-oxoacyl-[acyl-carrier-protein] reductase

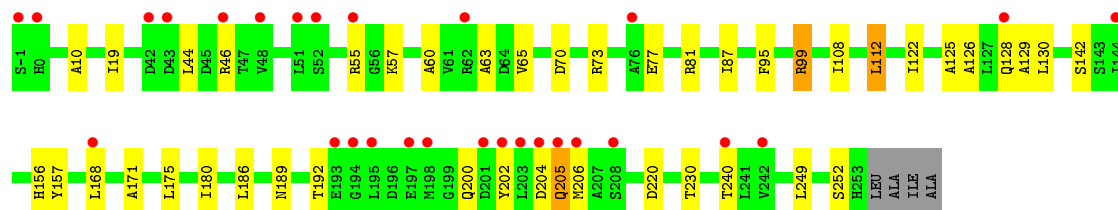
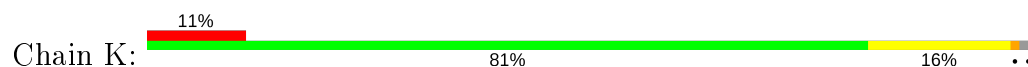


- Molecule 1: 3-oxoacyl-[acyl-carrier-protein] reductase

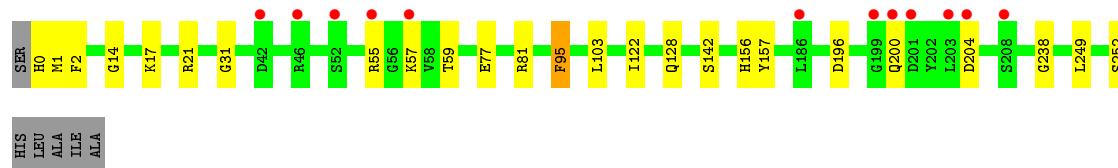
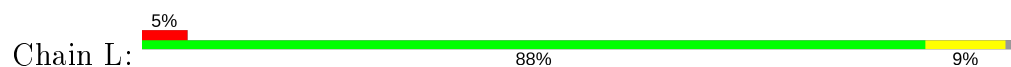




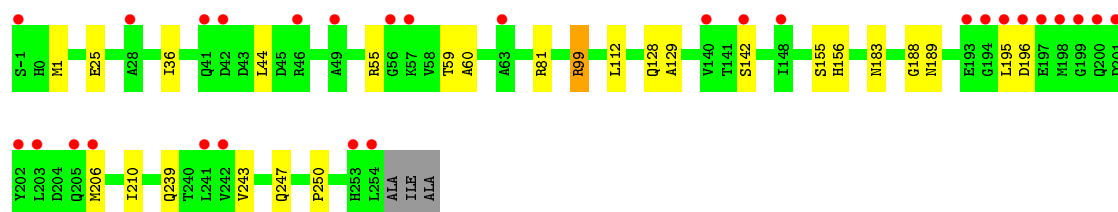
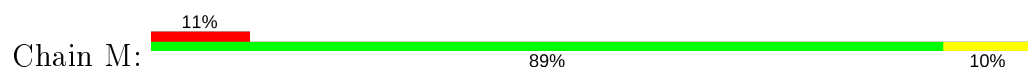
- Molecule 1: 3-oxoacyl-[acyl-carrier-protein] reductase



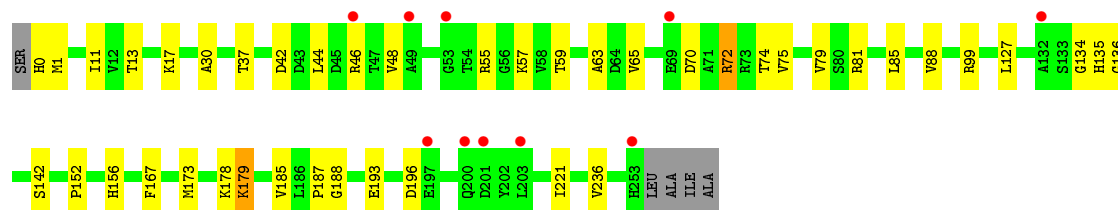
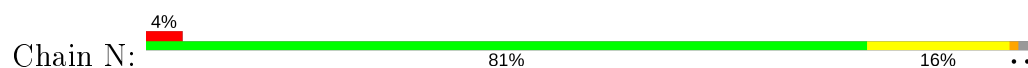
- Molecule 1: 3-oxoacyl-[acyl-carrier-protein] reductase



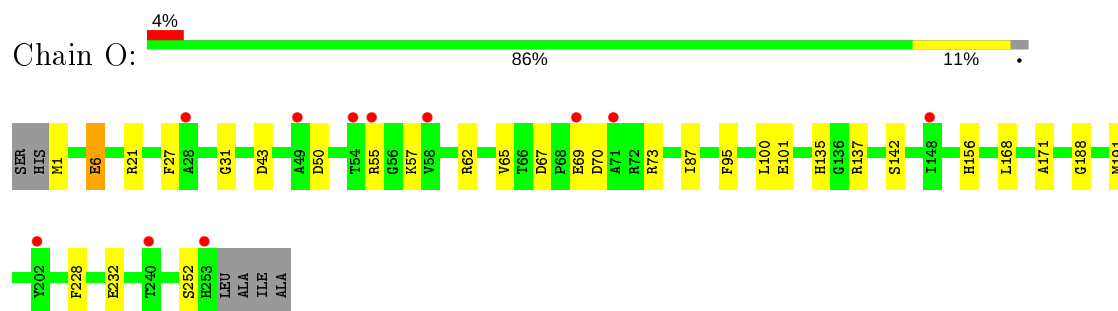
- Molecule 1: 3-oxoacyl-[acyl-carrier-protein] reductase



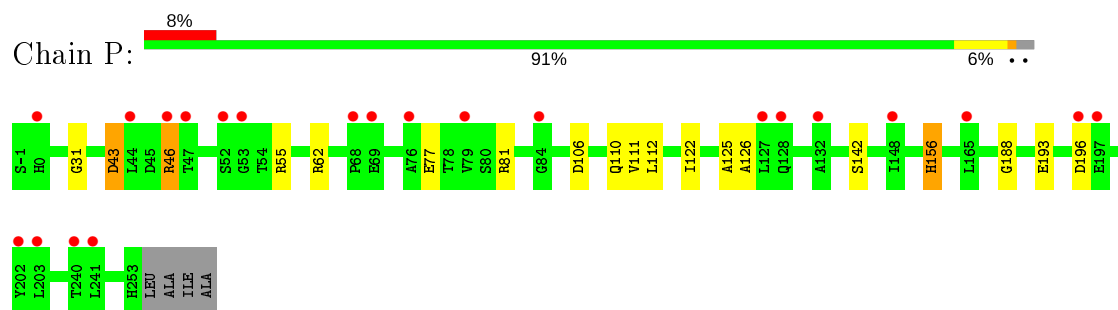
- Molecule 1: 3-oxoacyl-[acyl-carrier-protein] reductase



- Molecule 1: 3-oxoacyl-[acyl-carrier-protein] reductase



- Molecule 1: 3-oxoacyl-[acyl-carrier-protein] reductase



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	131.77Å 129.06Å 145.79Å 90.00° 107.88° 90.00°	Depositor
Resolution (Å)	48.49 – 1.90 48.49 – 1.54	Depositor EDS
% Data completeness (in resolution range)	99.5 (48.49-1.90) 81.4 (48.49-1.54)	Depositor EDS
R_{merge}	0.14	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.17 (at 1.54Å)	Xtriage
Refinement program	PHENIX 1.12 _2829	Depositor
R, R_{free}	0.204 , 0.233 0.203 , 0.233	Depositor DCC
R_{free} test set	27768 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å ²)	25.3	Xtriage
Anisotropy	0.042	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.36 , 45.4	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	33083	wwPDB-VP
Average B, all atoms (Å ²)	40.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 47.84 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 9.3678e-05. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

¹Intensities estimated from amplitudes.

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

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: NAP, MG, F3V, CL

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	0.44	0/1889	0.61	1/2568 (0.0%)
1	B	0.41	0/1883	0.58	0/2560
1	C	0.45	0/1902	0.59	1/2586 (0.0%)
1	D	0.42	0/1907	0.59	1/2593 (0.0%)
1	E	0.41	0/1881	0.58	0/2557
1	F	0.42	0/1875	0.58	1/2549 (0.0%)
1	G	0.39	0/1889	0.58	1/2568 (0.0%)
1	H	0.42	0/1864	0.56	1/2534 (0.0%)
1	I	0.32	0/1901	0.52	0/2585
1	J	0.32	0/1896	0.49	0/2578
1	K	0.32	0/1881	0.52	0/2557
1	L	0.31	0/1864	0.51	0/2534
1	M	0.32	0/1889	0.50	0/2568
1	N	0.33	0/1875	0.52	0/2549
1	O	0.32	0/1864	0.50	0/2534
1	P	0.31	0/1881	0.50	0/2557
All	All	0.37	0/30141	0.55	6/40977 (0.0%)

There are no bond length outliers.

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	173	MET	CG-SD-CE	-7.41	88.35	100.20
1	F	168	LEU	CA-CB-CG	6.33	129.87	115.30
1	D	168	LEU	CA-CB-CG	5.51	127.97	115.30
1	H	168	LEU	CA-CB-CG	5.49	127.92	115.30
1	C	168	LEU	CA-CB-CG	5.43	127.78	115.30
1	G	168	LEU	CA-CB-CG	5.01	126.82	115.30

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	1862	0	1848	22	0
1	B	1856	0	1843	38	0
1	C	1875	0	1864	26	0
1	D	1880	0	1869	37	0
1	E	1854	0	1837	22	0
1	F	1848	0	1832	13	0
1	G	1862	0	1848	20	0
1	H	1838	0	1825	14	0
1	I	1874	0	1864	19	0
1	J	1869	0	1859	19	0
1	K	1854	0	1837	37	0
1	L	1838	0	1825	20	0
1	M	1862	0	1848	23	0
1	N	1848	0	1832	46	0
1	O	1838	0	1825	20	0
1	P	1854	0	1837	13	0
2	A	48	0	25	2	0
2	B	48	0	25	3	0
2	C	48	0	25	1	0
2	D	48	0	25	2	0
2	E	48	0	25	2	0
2	F	48	0	25	2	0
2	G	48	0	25	2	0
2	H	48	0	25	1	0
2	I	48	0	25	3	0
2	J	48	0	25	1	0
2	K	48	0	25	2	0
2	L	48	0	25	2	0
2	M	48	0	25	2	0
2	N	48	0	25	5	0
2	O	48	0	25	3	0
2	P	48	0	25	2	0
3	A	5	0	0	0	0
3	B	5	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	C	5	0	0	0	0
3	D	5	0	0	0	0
3	E	5	0	0	0	0
3	F	5	0	0	0	0
3	G	5	0	0	0	0
3	H	5	0	0	0	0
3	I	5	0	0	0	0
3	J	5	0	0	0	0
3	K	5	0	0	0	0
3	L	5	0	0	0	0
3	M	5	0	0	0	0
3	N	5	0	0	0	0
3	O	5	0	0	0	0
3	P	5	0	0	0	0
4	A	2	0	0	1	0
4	B	1	0	0	1	0
4	C	1	0	0	1	0
4	D	1	0	0	1	0
4	E	1	0	0	1	0
4	F	1	0	0	1	0
4	G	1	0	0	1	0
4	H	1	0	0	1	0
4	I	1	0	0	1	0
4	J	1	0	0	1	0
4	K	1	0	0	1	0
4	L	1	0	0	1	0
4	M	1	0	0	1	0
4	N	1	0	0	1	0
4	O	1	0	0	1	0
4	P	1	0	0	1	0
5	A	1	0	0	0	0
5	C	1	0	0	0	0
5	F	1	0	0	0	0
5	H	1	0	0	0	0
5	J	1	0	0	0	0
5	L	1	0	0	0	0
5	M	1	0	0	0	0
5	O	1	0	0	0	0
6	A	223	0	0	6	1
6	B	180	0	0	11	0
6	C	189	0	0	3	2
6	D	191	0	0	10	1

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
6	E	202	0	0	10	0
6	F	203	0	0	2	1
6	G	186	0	0	10	0
6	H	209	0	0	2	1
6	I	106	0	0	5	0
6	J	113	0	0	2	0
6	K	96	0	0	8	0
6	L	123	0	0	6	0
6	M	111	0	0	5	0
6	N	118	0	0	9	0
6	O	132	0	0	4	0
6	P	116	0	0	4	0
All	All	33083	0	29893	352	3

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 6.

All (352) 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:N:134:GLY:H	1:N:179:LYS:NZ	1.35	1.23
1:N:134:GLY:N	1:N:179:LYS:NZ	1.94	1.14
1:E:99:ARG:NH1	6:E:401:HOH:O	1.83	1.10
1:N:134:GLY:N	1:N:179:LYS:HZ3	1.50	1.02
1:B:17:LYS:NZ	6:B:401:HOH:O	1.94	1.00
1:N:134:GLY:CA	1:N:179:LYS:HZ3	1.77	0.97
1:B:55:ARG:NH2	6:B:402:HOH:O	1.99	0.95
1:K:128:GLN:NE2	6:K:403:HOH:O	1.98	0.94
1:M:1:MET:O	6:M:401:HOH:O	1.88	0.92
1:G:39:ARG:O	6:G:401:HOH:O	1.89	0.90
1:M:55:ARG:HH12	1:N:0:HIS:N	1.70	0.90
1:E:55:ARG:NH2	6:E:407:HOH:O	2.03	0.90
1:E:69:GLU:OE2	6:E:402:HOH:O	1.91	0.89
1:K:128:GLN:OE1	6:K:401:HOH:O	1.91	0.89
6:G:403:HOH:O	1:H:0:HIS:N	2.05	0.89
1:B:0:HIS:N	6:B:403:HOH:O	2.07	0.88
1:L:103:LEU:O	6:L:401:HOH:O	1.90	0.87
1:K:108:ILE:O	1:K:112:LEU:HD12	1.74	0.87
1:K:220:ASP:OD2	6:K:402:HOH:O	1.92	0.86
1:G:52:SER:O	6:G:402:HOH:O	1.93	0.86
1:A:103:LEU:O	6:A:401:HOH:O	1.95	0.84

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:41:GLN:H	1:D:62:ARG:HH21	1.23	0.83
1:E:1:MET:O	6:E:403:HOH:O	1.99	0.81
1:N:1:MET:O	6:N:401:HOH:O	1.98	0.80
1:G:48:VAL:O	6:G:404:HOH:O	2.00	0.79
1:N:135:HIS:N	1:N:179:LYS:HD3	1.96	0.79
1:N:30:ALA:O	6:N:402:HOH:O	2.00	0.79
1:D:191:MET:SD	6:D:456:HOH:O	2.41	0.78
1:D:33:ASP:OD1	6:D:402:HOH:O	2.02	0.78
1:J:94:ILE:H	1:J:115:ASN:HD21	1.28	0.77
1:E:65:VAL:O	6:E:405:HOH:O	2.03	0.76
1:E:6:GLU:OE2	6:E:404:HOH:O	2.03	0.76
2:I:301:NAP:O1X	6:I:401:HOH:O	2.03	0.76
1:E:77:GLU:OE2	6:E:406:HOH:O	2.03	0.76
1:P:122:ILE:O	6:P:401:HOH:O	2.03	0.76
1:N:48:VAL:O	6:N:403:HOH:O	2.02	0.76
1:J:52:SER:O	6:J:401:HOH:O	2.03	0.76
1:N:134:GLY:H	1:N:179:LYS:HZ1	1.30	0.76
1:A:1:MET:O	6:A:402:HOH:O	2.01	0.76
1:P:43:ASP:HA	1:P:46:ARG:HD3	1.68	0.75
1:N:72:ARG:O	6:N:404:HOH:O	2.02	0.75
1:H:189:ASN:HD22	1:H:247:GLN:HE22	1.34	0.75
1:M:55:ARG:HH12	1:N:0:HIS:H3	1.34	0.75
1:O:6:GLU:OE2	1:O:55:ARG:HD3	1.87	0.74
1:A:254:LEU:HD22	1:C:205:GLN:HE21	1.49	0.74
1:D:55:ARG:NH1	6:D:403:HOH:O	2.06	0.73
1:L:1:MET:O	6:L:402:HOH:O	2.05	0.73
1:I:0:HIS:N	1:L:55:ARG:HH12	1.86	0.73
1:B:62:ARG:NH1	6:B:409:HOH:O	2.21	0.73
4:A:303:CL:CL	4:D:303:CL:CL	2.81	0.73
1:J:1:MET:O	6:J:402:HOH:O	2.07	0.72
1:M:59:THR:OG1	6:M:402:HOH:O	2.06	0.72
1:D:41:GLN:NE2	6:D:401:HOH:O	1.96	0.72
1:O:101:GLU:OE1	6:O:402:HOH:O	2.09	0.71
1:N:193:GLU:OE1	6:N:408:HOH:O	2.10	0.70
1:N:59:THR:OG1	6:N:407:HOH:O	2.07	0.70
1:E:128:GLN:HG2	6:E:437:HOH:O	1.90	0.70
1:O:62:ARG:O	1:O:73:ARG:NH2	2.25	0.70
1:C:1:MET:O	6:C:402:HOH:O	2.09	0.70
1:G:1:MET:O	6:G:405:HOH:O	2.09	0.70
1:A:100:LEU:HD22	1:D:127:LEU:HD11	1.73	0.70
1:F:252:SER:HB3	1:H:206:MET:HE2	1.74	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:37:THR:O	6:B:404:HOH:O	2.09	0.70
1:D:110:GLN:OE1	6:D:404:HOH:O	2.10	0.70
1:O:1:MET:O	6:O:403:HOH:O	2.11	0.69
1:I:59:THR:OG1	6:I:402:HOH:O	2.11	0.68
1:I:62:ARG:NE	6:I:405:HOH:O	2.25	0.67
1:P:196:ASP:OD2	6:P:402:HOH:O	2.13	0.67
1:A:254:LEU:CD2	1:C:205:GLN:HE21	2.08	0.66
1:N:136:GLY:H	1:N:179:LYS:CD	2.09	0.66
1:E:127:LEU:HD21	1:E:175:LEU:HD22	1.76	0.66
1:M:196:ASP:OD1	6:M:403:HOH:O	2.15	0.65
1:P:125:ALA:N	6:P:401:HOH:O	2.29	0.65
1:D:67:ASP:OD1	6:D:405:HOH:O	2.14	0.65
1:O:6:GLU:HG2	1:O:31:GLY:HA3	1.79	0.65
2:B:301:NAP:H2A	6:B:440:HOH:O	1.94	0.65
1:L:21:ARG:HD3	6:L:506:HOH:O	1.96	0.64
1:P:31:GLY:HA2	1:P:55:ARG:HG2	1.80	0.64
1:B:69:GLU:OE1	6:B:405:HOH:O	2.14	0.64
1:D:82:HIS:HE1	6:D:438:HOH:O	1.79	0.64
1:B:142:SER:O	2:B:301:NAP:H6N	1.98	0.63
4:F:303:CL:CL	4:G:303:CL:CL	2.90	0.63
1:N:136:GLY:H	1:N:179:LYS:HD3	1.63	0.63
1:H:101:GLU:OE1	6:H:402:HOH:O	2.16	0.63
1:C:50:ASP:OD2	6:C:403:HOH:O	2.16	0.63
1:N:134:GLY:N	1:N:179:LYS:HZ2	1.94	0.62
1:I:0:HIS:H1	1:L:55:ARG:HH12	1.44	0.62
1:F:252:SER:HB3	1:H:206:MET:CE	2.29	0.62
1:L:17:LYS:NZ	6:L:403:HOH:O	2.26	0.62
1:B:69:GLU:HG2	1:B:72:ARG:HH21	1.64	0.61
1:B:206:MET:HE1	1:D:251:GLU:HG2	1.81	0.61
4:E:303:CL:CL	4:H:303:CL:CL	2.92	0.61
1:C:55:ARG:CZ	1:D:-1:SER:HB2	2.31	0.61
1:G:142:SER:O	2:G:301:NAP:H6N	2.01	0.61
1:B:1:MET:O	6:B:406:HOH:O	2.16	0.60
1:J:6:GLU:HG3	1:J:31:GLY:HA3	1.82	0.60
1:H:111:VAL:HG21	1:H:156:HIS:CD2	2.36	0.60
1:B:183:ASN:HD22	1:B:239:GLN:H	1.47	0.60
1:A:142:SER:O	2:A:301:NAP:H6N	2.01	0.60
1:G:191:MET:SD	6:G:535:HOH:O	2.57	0.60
1:N:42:ASP:O	1:N:46:ARG:HG2	2.01	0.60
1:K:77:GLU:O	1:K:81:ARG:HG3	2.01	0.60
1:K:65:VAL:HA	6:K:460:HOH:O	2.01	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:125:ALA:O	6:K:401:HOH:O	2.17	0.59
1:P:142:SER:O	2:P:301:NAP:H6N	2.01	0.59
1:B:55:ARG:HG3	6:B:412:HOH:O	2.01	0.59
1:B:209:ALA:HB1	1:B:253:HIS:CD2	2.38	0.59
1:I:142:SER:O	2:I:301:NAP:H6N	2.03	0.59
1:E:41:GLN:HE21	1:E:62:ARG:NH1	2.01	0.58
1:B:188:GLY:O	2:B:301:NAP:H4N	2.02	0.58
1:I:254:LEU:HD13	1:K:205:GLN:HA	1.85	0.58
4:N:303:CL:CL	4:O:303:CL:CL	2.95	0.58
1:L:31:GLY:HA2	1:L:55:ARG:HG2	1.86	0.58
1:D:142:SER:O	2:D:301:NAP:H6N	2.03	0.57
4:B:303:CL:CL	4:C:303:CL:CL	2.97	0.57
1:M:112:LEU:HD21	1:P:112:LEU:HD12	1.86	0.57
1:N:63:ALA:HB1	1:N:70:ASP:HB3	1.86	0.57
1:G:135:HIS:O	6:G:407:HOH:O	2.17	0.57
1:E:142:SER:O	2:E:301:NAP:H6N	2.05	0.57
1:D:67:ASP:OD2	6:D:406:HOH:O	2.17	0.56
1:K:57:LYS:HG2	1:N:81:ARG:O	2.05	0.56
1:O:43:ASP:O	6:O:404:HOH:O	2.18	0.56
1:D:171:ALA:O	1:D:175:LEU:HG	2.06	0.56
1:N:135:HIS:CA	1:N:179:LYS:HD3	2.35	0.56
1:E:205:GLN:NE2	6:E:412:HOH:O	2.33	0.56
1:H:6:GLU:OE2	1:H:55:ARG:HD2	2.04	0.56
1:F:142:SER:O	2:F:301:NAP:H6N	2.05	0.56
1:M:155:SER:HB3	6:M:413:HOH:O	2.03	0.56
1:N:44:LEU:O	1:N:48:VAL:HG12	2.06	0.56
1:P:77:GLU:O	1:P:81:ARG:HG3	2.05	0.56
1:D:6:GLU:O	6:D:407:HOH:O	2.18	0.56
1:B:152:PRO:HD2	1:D:255:ALA:HA	1.88	0.55
1:L:142:SER:O	2:L:301:NAP:H6N	2.07	0.55
1:C:183:ASN:HD22	1:C:239:GLN:H	1.55	0.55
1:M:206:MET:O	1:M:210:ILE:HG13	2.06	0.55
1:C:77:GLU:O	1:C:81:ARG:HG3	2.07	0.55
1:G:188:GLY:O	2:G:301:NAP:H4N	2.06	0.54
4:K:303:CL:CL	4:L:303:CL:CL	2.99	0.54
1:F:9:SER:OG	1:F:82:HIS:HD2	1.90	0.54
1:N:127:LEU:HD21	1:N:178:LYS:HD3	1.90	0.54
1:D:41:GLN:HB2	1:D:62:ARG:HE	1.73	0.54
1:G:254:LEU:HD23	1:G:254:LEU:H	1.72	0.54
1:E:55:ARG:CZ	6:E:407:HOH:O	2.48	0.53
1:C:173:MET:HE1	1:D:255:ALA:HB1	1.91	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:0:HIS:N	6:L:409:HOH:O	2.40	0.53
1:B:205:GLN:NE2	1:D:252:SER:OG	2.42	0.53
1:K:142:SER:O	2:K:301:NAP:H6N	2.09	0.53
1:K:128:GLN:CD	6:K:401:HOH:O	2.41	0.53
1:N:17:LYS:NZ	6:N:405:HOH:O	2.03	0.53
1:E:238:GLY:HA3	1:F:249:LEU:HD11	1.90	0.53
1:A:254:LEU:HD22	1:C:205:GLN:NE2	2.23	0.53
1:K:128:GLN:NE2	6:K:401:HOH:O	2.42	0.53
1:P:126:ALA:N	6:P:401:HOH:O	2.07	0.52
1:H:142:SER:O	2:H:301:NAP:H6N	2.10	0.52
1:N:178:LYS:O	1:N:179:LYS:HB3	2.07	0.52
1:K:175:LEU:HB3	1:K:180:ILE:HB	1.91	0.52
1:I:254:LEU:HD22	1:K:205:GLN:HB2	1.91	0.52
1:M:36:ILE:HD12	1:M:44:LEU:HD23	1.92	0.52
1:D:183:ASN:HD22	1:D:239:GLN:H	1.57	0.51
1:B:173:MET:HE1	1:C:151:TYR:HA	1.93	0.51
1:C:43:ASP:OD2	1:C:46:ARG:NH2	2.42	0.51
1:I:65:VAL:O	6:I:403:HOH:O	2.19	0.51
1:K:63:ALA:HB1	1:K:70:ASP:HB3	1.92	0.51
1:E:188:GLY:O	2:E:301:NAP:H4N	2.10	0.51
1:B:167:PHE:HE1	1:C:100:LEU:HD13	1.76	0.51
1:A:188:GLY:O	2:A:301:NAP:H4N	2.10	0.51
1:B:80:SER:OG	6:B:407:HOH:O	2.19	0.51
1:J:142:SER:O	2:J:301:NAP:H6N	2.11	0.51
1:P:106:ASP:O	1:P:110:GLN:HG2	2.11	0.51
1:B:17:LYS:NZ	1:B:43:ASP:OD2	2.36	0.50
1:D:5:LEU:O	1:D:8:ARG:HG3	2.11	0.50
1:N:134:GLY:C	1:N:179:LYS:HD3	2.32	0.50
1:P:188:GLY:O	2:P:301:NAP:H4N	2.12	0.50
1:A:202:TYR:HD1	1:A:203:LEU:HD12	1.75	0.50
1:K:202:TYR:HA	1:K:205:GLN:HE21	1.77	0.50
1:F:1:MET:O	6:F:401:HOH:O	2.18	0.50
1:J:0:HIS:N	1:K:55:ARG:HH21	2.10	0.50
1:G:63:ALA:HB1	1:G:70:ASP:HB3	1.93	0.50
1:I:0:HIS:N	1:L:55:ARG:NH1	2.59	0.50
1:A:-1:SER:HB3	1:B:55:ARG:HE	1.77	0.50
1:A:248:VAL:O	6:A:403:HOH:O	2.19	0.50
1:K:200:GLN:HG3	1:K:204:ASP:OD2	2.12	0.50
1:M:189:ASN:HD22	1:M:195:LEU:HD21	1.77	0.49
1:A:249:LEU:HD11	1:B:238:GLY:HA3	1.94	0.49
1:C:142:SER:O	2:C:301:NAP:H6N	2.13	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:6:GLU:OE1	1:G:55:ARG:NE	2.46	0.49
1:M:128:GLN:OE1	1:M:129:ALA:N	2.41	0.49
1:M:250:PRO:HG3	1:N:173:MET:HE3	1.93	0.49
4:M:303:CL:CL	4:P:303:CL:CL	3.04	0.49
1:B:193:GLU:OE1	6:B:408:HOH:O	2.20	0.49
1:D:149:THR:HG22	6:D:442:HOH:O	2.12	0.49
1:O:142:SER:O	2:O:301:NAP:H6N	2.13	0.49
1:H:144:ILE:HG12	1:H:188:GLY:HA2	1.93	0.48
1:K:189:ASN:CG	1:K:206:MET:HG3	2.33	0.48
1:O:137:ARG:HD2	1:O:228:PHE:O	2.12	0.48
1:J:21:ARG:HH11	1:J:47:THR:HG23	1.78	0.48
1:O:27:PHE:HE1	1:O:87:ILE:HD13	1.79	0.48
1:M:183:ASN:HD22	1:M:239:GLN:H	1.61	0.48
1:A:238:GLY:HA3	1:B:249:LEU:HD11	1.96	0.48
1:D:252:SER:OG	1:D:253:HIS:N	2.47	0.48
1:H:63:ALA:HB1	1:H:70:ASP:HB3	1.96	0.48
1:O:232:GLU:N	1:O:232:GLU:OE2	2.47	0.48
1:G:238:GLY:HA3	1:H:249:LEU:HD11	1.96	0.47
1:N:65:VAL:HA	6:N:413:HOH:O	2.14	0.47
1:M:142:SER:O	2:M:301:NAP:H6N	2.14	0.47
1:O:27:PHE:CE1	1:O:87:ILE:HD13	2.49	0.47
1:B:205:GLN:NE2	1:D:254:LEU:H	2.12	0.47
1:K:168:LEU:HA	1:K:171:ALA:HB3	1.95	0.47
1:G:206:MET:O	1:G:210:ILE:HG13	2.15	0.47
1:N:142:SER:O	2:N:301:NAP:H6N	2.15	0.47
1:D:106:ASP:O	1:D:110:GLN:HG2	2.15	0.47
1:D:21:ARG:HD2	1:D:47:THR:HG23	1.95	0.47
1:D:41:GLN:HB2	1:D:62:ARG:NE	2.30	0.47
1:J:209:ALA:HA	1:J:256:ILE:HD13	1.97	0.47
1:A:173:MET:CE	1:D:150:GLY:HA3	2.45	0.47
1:E:13:THR:HA	1:E:37:THR:OG1	2.13	0.47
1:A:252:SER:HB3	1:C:206:MET:HE2	1.97	0.47
1:A:149:THR:HA	6:A:468:HOH:O	2.15	0.46
1:C:249:LEU:HD11	1:D:238:GLY:HA3	1.98	0.46
1:J:238:GLY:HA3	1:K:249:LEU:HD11	1.96	0.46
1:B:63:ALA:HB1	1:B:70:ASP:HB3	1.97	0.46
1:I:1:MET:CE	1:L:2:PHE:HB2	2.46	0.46
1:F:178:LYS:HD3	6:F:521:HOH:O	2.15	0.46
1:L:59:THR:HB	1:L:81:ARG:NH1	2.31	0.46
1:M:59:THR:HB	1:M:81:ARG:NH1	2.30	0.46
1:C:55:ARG:NE	1:D:-1:SER:HB2	2.31	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:115:ASN:HD22	1:J:115:ASN:N	2.12	0.46
1:I:210:ILE:HG12	1:I:247:GLN:HB2	1.98	0.46
1:B:21:ARG:NH1	1:B:46:ARG:NH1	2.63	0.45
1:E:171:ALA:O	1:E:175:LEU:HG	2.16	0.45
1:O:67:ASP:HB3	1:O:70:ASP:HB2	1.97	0.45
1:C:253:HIS:CD2	1:C:253:HIS:H	2.35	0.45
1:D:65:VAL:HG22	2:D:301:NAP:N1A	2.31	0.45
1:G:175:LEU:HB3	1:G:180:ILE:HB	1.98	0.45
1:A:253:HIS:HD2	6:A:564:HOH:O	1.98	0.45
1:B:183:ASN:ND2	1:B:239:GLN:H	2.14	0.45
1:N:13:THR:HA	1:N:37:THR:OG1	2.17	0.45
1:A:170:THR:HA	1:A:173:MET:HE3	1.99	0.45
1:B:173:MET:CE	1:C:152:PRO:HD3	2.47	0.45
1:L:200:GLN:NE2	1:L:204:ASP:OD1	2.48	0.45
1:M:188:GLY:O	2:M:301:NAP:H4N	2.16	0.45
2:N:301:NAP:H2A	6:N:437:HOH:O	2.16	0.45
1:K:95:PHE:HB3	1:K:157:TYR:CE1	2.52	0.45
1:M:25:GLU:OE1	6:M:404:HOH:O	2.20	0.45
1:N:134:GLY:H	1:N:179:LYS:HZ3	1.16	0.45
1:D:31:GLY:HA2	1:D:55:ARG:HD2	1.97	0.45
1:I:91:ASN:O	2:I:301:NAP:H4D	2.17	0.45
1:M:210:ILE:HG12	1:M:247:GLN:HB2	1.98	0.45
1:A:165:LEU:HA	1:A:168:LEU:HG	1.98	0.44
1:E:175:LEU:HB3	1:E:180:ILE:HB	1.99	0.44
1:D:175:LEU:HB3	1:D:180:ILE:HB	1.99	0.44
4:I:303:CL:CL	4:J:303:CL:CL	3.09	0.44
1:N:179:LYS:HB3	1:N:179:LYS:HE2	1.69	0.44
1:K:122:ILE:HA	1:K:122:ILE:HD12	1.86	0.44
1:N:187:PRO:HB2	2:N:301:NAP:C5N	2.48	0.44
1:O:168:LEU:HA	1:O:171:ALA:HB3	1.99	0.44
1:G:231:ASP:OD2	6:G:408:HOH:O	2.21	0.44
1:I:249:LEU:HD11	1:L:238:GLY:HA3	1.98	0.44
1:E:44:LEU:HD22	1:E:60:ALA:HB1	1.99	0.44
1:G:21:ARG:HD2	1:G:47:THR:HG23	1.99	0.44
1:G:55:ARG:NH1	6:G:403:HOH:O	1.95	0.44
1:M:44:LEU:HD22	1:M:60:ALA:HB1	2.00	0.44
1:N:188:GLY:O	2:N:301:NAP:H4N	2.17	0.44
1:N:65:VAL:HG22	2:N:301:NAP:N1A	2.33	0.44
1:A:0:HIS:NE2	6:A:408:HOH:O	2.36	0.44
1:M:247:GLN:O	1:M:250:PRO:HD2	2.17	0.44
1:A:55:ARG:NH1	1:B:0:HIS:N	2.66	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:63:ALA:HB1	1:D:70:ASP:HB3	2.00	0.43
1:H:10:ALA:HA	1:H:87:ILE:O	2.18	0.43
1:J:13:THR:HA	1:J:37:THR:OG1	2.18	0.43
1:K:128:GLN:NE2	1:K:129:ALA:H	2.16	0.43
1:K:99:ARG:HD2	1:K:99:ARG:HA	1.75	0.43
1:F:31:GLY:HA2	1:F:55:ARG:HG2	2.00	0.43
1:G:205:GLN:NE2	6:G:423:HOH:O	2.51	0.43
1:K:108:ILE:HG23	1:K:112:LEU:CD1	2.48	0.43
1:L:77:GLU:O	1:L:81:ARG:HG3	2.18	0.43
1:N:99:ARG:NH1	1:N:152:PRO:HB3	2.32	0.43
1:E:63:ALA:HB1	1:E:70:ASP:HB3	1.99	0.43
1:J:5:LEU:O	1:J:8:ARG:HG3	2.19	0.43
1:K:19:ILE:HG13	1:K:192:THR:HG21	2.00	0.43
1:N:99:ARG:HH12	1:N:152:PRO:CB	2.32	0.43
1:J:94:ILE:H	1:J:115:ASN:ND2	2.07	0.43
1:M:243:VAL:HG13	1:N:236:VAL:HG22	2.00	0.43
1:P:193:GLU:O	1:P:196:ASP:HB2	2.18	0.43
1:I:95:PHE:HB3	1:I:157:TYR:CE1	2.54	0.43
1:B:200:GLN:HA	1:B:203:LEU:HB2	2.01	0.43
1:A:252:SER:HB3	1:C:206:MET:CE	2.49	0.43
1:F:113:GLY:HA2	1:F:117:LYS:HG3	2.00	0.43
1:P:111:VAL:HG21	1:P:156:HIS:CD2	2.53	0.43
1:D:254:LEU:HG	1:D:257:ALA:C	2.39	0.43
1:H:197:GLU:HG3	6:H:602:HOH:O	2.19	0.43
1:J:21:ARG:NH1	1:J:47:THR:HG23	2.34	0.43
1:B:165:LEU:HA	1:B:168:LEU:HG	2.01	0.43
1:L:128:GLN:HG2	6:L:450:HOH:O	2.18	0.43
1:B:39:ARG:HA	1:B:62:ARG:HH11	1.84	0.43
1:I:13:THR:HA	1:I:37:THR:OG1	2.19	0.42
1:K:126:ALA:O	1:K:130:LEU:HG	2.19	0.42
1:O:21:ARG:HH22	1:O:50:ASP:HB3	1.84	0.42
1:C:6:GLU:HG3	6:C:428:HOH:O	2.18	0.42
1:J:127:LEU:HA	1:J:127:LEU:HD12	1.89	0.42
1:D:9:SER:OG	1:D:82:HIS:HD2	2.02	0.42
1:E:249:LEU:HD11	1:F:238:GLY:HA3	2.00	0.42
1:C:183:ASN:ND2	1:C:239:GLN:H	2.18	0.42
1:N:136:GLY:N	1:N:179:LYS:HD3	2.31	0.42
1:O:188:GLY:O	2:O:301:NAP:H4N	2.18	0.42
1:B:168:LEU:HA	1:B:171:ALA:HB3	2.01	0.42
1:B:10:ALA:HA	1:B:87:ILE:O	2.19	0.42
1:M:99:ARG:HB3	1:M:99:ARG:HE	1.64	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:188:GLY:O	2:F:301:NAP:H4N	2.20	0.42
1:N:75:VAL:O	1:N:79:VAL:HG23	2.19	0.42
1:E:209:ALA:HB2	1:G:254:LEU:HD21	2.01	0.42
1:B:206:MET:O	1:B:210:ILE:HG13	2.20	0.42
1:F:111:VAL:HG21	1:F:156:HIS:CD2	2.55	0.42
1:G:122:ILE:HA	1:G:122:ILE:HD12	1.92	0.42
1:J:253:HIS:O	1:J:256:ILE:HD12	2.19	0.42
1:K:65:VAL:HG22	2:K:301:NAP:N1A	2.36	0.41
1:M:206:MET:SD	1:O:252:SER:HB3	2.60	0.41
1:I:22:GLY:HA3	1:I:218:VAL:HB	2.03	0.41
1:K:186:LEU:HD13	1:K:240:THR:HB	2.02	0.41
1:O:65:VAL:HG22	2:O:301:NAP:N1A	2.35	0.41
1:C:10:ALA:HA	1:C:87:ILE:O	2.20	0.41
1:I:65:VAL:HA	6:I:468:HOH:O	2.19	0.41
1:C:185:VAL:HG11	1:C:221:ILE:HG23	2.03	0.41
1:J:27:PHE:CE1	1:J:87:ILE:HD13	2.56	0.41
1:F:9:SER:OG	1:F:82:HIS:CD2	2.72	0.41
1:H:202:TYR:CE1	1:H:206:MET:HG3	2.55	0.41
1:N:57:LYS:HB2	1:N:57:LYS:HE3	1.92	0.41
1:C:55:ARG:HE	1:C:55:ARG:HB2	1.61	0.41
1:I:238:GLY:HA3	1:L:249:LEU:HD11	2.01	0.41
1:N:99:ARG:HH12	1:N:152:PRO:HB3	1.85	0.41
1:B:205:GLN:HG2	1:B:205:GLN:O	2.21	0.41
1:J:1:MET:HE1	1:K:230:THR:HG22	2.02	0.41
1:O:67:ASP:OD2	1:O:69:GLU:HG2	2.21	0.41
1:D:113:GLY:HA2	1:D:117:LYS:HB2	2.02	0.41
1:J:63:ALA:HB1	1:J:70:ASP:HB3	2.03	0.41
1:O:57:LYS:NZ	6:O:407:HOH:O	2.39	0.41
1:B:111:VAL:HG21	1:B:156:HIS:CD2	2.56	0.40
1:N:85:LEU:HD11	1:N:88:VAL:HG23	2.02	0.40
1:C:253:HIS:CG	1:C:254:LEU:H	2.39	0.40
1:K:202:TYR:C	1:K:205:GLN:HB3	2.41	0.40
1:N:11:ILE:HD13	1:N:74:THR:HG22	2.03	0.40
1:N:167:PHE:HE2	1:O:100:LEU:HD13	1.85	0.40
1:K:10:ALA:HA	1:K:87:ILE:O	2.21	0.40
1:I:252:SER:HB3	1:K:206:MET:SD	2.61	0.40
1:K:44:LEU:HD22	1:K:60:ALA:HB1	2.02	0.40
1:K:73:ARG:O	1:K:77:GLU:HG2	2.21	0.40
1:L:122:ILE:HA	1:L:122:ILE:HD12	1.90	0.40
1:L:14:GLY:HA2	2:L:301:NAP:H1B	2.03	0.40
1:N:185:VAL:HG11	1:N:221:ILE:HG23	2.03	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:200:GLN:N	6:K:405:HOH:O	2.29	0.40
1:C:144:ILE:HG12	1:C:188:GLY:HA2	2.04	0.40
1:L:95:PHE:HB3	1:L:157:TYR:CE1	2.57	0.40

All (3) 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)
6:A:577:HOH:O	6:C:558:HOH:O[2_948]	1.96	0.24
6:C:582:HOH:O	6:D:534:HOH:O[2_958]	2.14	0.06
6:F:470:HOH:O	6:H:566:HOH:O[2_859]	2.16	0.04

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	254/259 (98%)	244 (96%)	10 (4%)	0	100	100
1	B	253/259 (98%)	246 (97%)	7 (3%)	0	100	100
1	C	256/259 (99%)	244 (95%)	11 (4%)	1 (0%)	34	24
1	D	257/259 (99%)	246 (96%)	11 (4%)	0	100	100
1	E	253/259 (98%)	246 (97%)	7 (3%)	0	100	100
1	F	252/259 (97%)	241 (96%)	11 (4%)	0	100	100
1	G	254/259 (98%)	245 (96%)	9 (4%)	0	100	100
1	H	251/259 (97%)	240 (96%)	11 (4%)	0	100	100
1	I	256/259 (99%)	245 (96%)	11 (4%)	0	100	100
1	J	255/259 (98%)	243 (95%)	11 (4%)	1 (0%)	34	24
1	K	253/259 (98%)	243 (96%)	9 (4%)	1 (0%)	34	24
1	L	251/259 (97%)	243 (97%)	8 (3%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	M	254/259 (98%)	242 (95%)	12 (5%)	0	100	100
1	N	252/259 (97%)	240 (95%)	12 (5%)	0	100	100
1	O	251/259 (97%)	242 (96%)	9 (4%)	0	100	100
1	P	253/259 (98%)	241 (95%)	12 (5%)	0	100	100
All	All	4055/4144 (98%)	3891 (96%)	161 (4%)	3 (0%)	51	43

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	J	253	HIS
1	K	205	GLN
1	C	253	HIS

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	193/194 (100%)	192 (100%)	1 (0%)	88	89
1	B	192/194 (99%)	190 (99%)	2 (1%)	76	76
1	C	194/194 (100%)	188 (97%)	6 (3%)	40	32
1	D	194/194 (100%)	191 (98%)	3 (2%)	65	62
1	E	192/194 (99%)	190 (99%)	2 (1%)	76	76
1	F	191/194 (98%)	187 (98%)	4 (2%)	53	48
1	G	193/194 (100%)	190 (98%)	3 (2%)	62	60
1	H	190/194 (98%)	187 (98%)	3 (2%)	62	60
1	I	193/194 (100%)	190 (98%)	3 (2%)	62	60
1	J	193/194 (100%)	191 (99%)	2 (1%)	76	76
1	K	192/194 (99%)	187 (97%)	5 (3%)	46	39
1	L	190/194 (98%)	185 (97%)	5 (3%)	46	39
1	M	193/194 (100%)	191 (99%)	2 (1%)	76	76

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	N	191/194 (98%)	186 (97%)	5 (3%)	46	39
1	O	190/194 (98%)	185 (97%)	5 (3%)	46	39
1	P	192/194 (99%)	188 (98%)	4 (2%)	53	48
All	All	3073/3104 (99%)	3018 (98%)	55 (2%)	59	55

All (55) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	156	HIS
1	B	62	ARG
1	B	252	SER
1	C	55	ARG
1	C	95	PHE
1	C	135	HIS
1	C	156	HIS
1	C	179	LYS
1	C	191	MET
1	D	55	ARG
1	D	62	ARG
1	D	156	HIS
1	E	156	HIS
1	E	196	ASP
1	F	95	PHE
1	F	99	ARG
1	F	156	HIS
1	F	200	GLN
1	G	156	HIS
1	G	204	ASP
1	G	254	LEU
1	H	95	PHE
1	H	135	HIS
1	H	191	MET
1	I	1	MET
1	I	135	HIS
1	I	156	HIS
1	J	156	HIS
1	J	191	MET
1	K	46	ARG
1	K	99	ARG
1	K	112	LEU
1	K	156	HIS

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Mol	Chain	Res	Type
1	K	252	SER
1	L	57	LYS
1	L	95	PHE
1	L	156	HIS
1	L	196	ASP
1	L	252	SER
1	M	99	ARG
1	M	156	HIS
1	N	55	ARG
1	N	72	ARG
1	N	156	HIS
1	N	179	LYS
1	N	196	ASP
1	O	6	GLU
1	O	95	PHE
1	O	135	HIS
1	O	156	HIS
1	O	191	MET
1	P	43	ASP
1	P	46	ARG
1	P	62	ARG
1	P	156	HIS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (22) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	29	ASN
1	B	183	ASN
1	B	205	GLN
1	B	253	HIS
1	C	183	ASN
1	C	189	ASN
1	C	200	GLN
1	C	205	GLN
1	D	82	HIS
1	D	183	ASN
1	D	239	GLN
1	E	41	GLN
1	E	239	GLN
1	F	82	HIS
1	F	253	HIS
1	G	91	ASN

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Mol	Chain	Res	Type
1	G	135	HIS
1	H	247	GLN
1	J	115	ASN
1	L	189	ASN
1	M	183	ASN
1	M	189	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

5.6 Ligand geometry ⓘ

Of 57 ligands modelled in this entry, 25 are monoatomic - leaving 32 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	F3V	L	302	-	4,4,4	0.79	0	3,4,4	2.02	1 (33%)
3	F3V	M	302	-	4,4,4	0.84	0	3,4,4	2.22	1 (33%)
3	F3V	F	302	-	4,4,4	0.85	0	3,4,4	1.72	1 (33%)
3	F3V	D	302	-	4,4,4	0.86	0	3,4,4	1.17	0
3	F3V	G	302	-	4,4,4	0.91	0	3,4,4	1.63	1 (33%)
3	F3V	E	302	-	4,4,4	1.07	0	3,4,4	2.28	2 (66%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
3	F3V	B	302	-	4,4,4	0.78	0	3,4,4	3.01	2 (66%)
2	NAP	A	301	-	45,52,52	2.75	16 (35%)	56,80,80	1.37	6 (10%)
2	NAP	N	301	-	45,52,52	2.79	16 (35%)	56,80,80	1.45	8 (14%)
2	NAP	H	301	5	45,52,52	2.57	15 (33%)	56,80,80	1.48	8 (14%)
2	NAP	F	301	-	45,52,52	2.74	16 (35%)	56,80,80	1.41	9 (16%)
2	NAP	O	301	5	45,52,52	2.61	17 (37%)	56,80,80	1.29	6 (10%)
3	F3V	A	302	-	4,4,4	0.70	0	3,4,4	2.15	2 (66%)
3	F3V	J	302	-	4,4,4	0.83	0	3,4,4	1.53	1 (33%)
2	NAP	C	301	5	45,52,52	2.50	15 (33%)	56,80,80	1.56	8 (14%)
3	F3V	P	302	-	4,4,4	0.82	0	3,4,4	2.07	1 (33%)
2	NAP	K	301	-	45,52,52	2.75	17 (37%)	56,80,80	1.35	5 (8%)
3	F3V	H	302	-	4,4,4	0.67	0	3,4,4	2.48	2 (66%)
3	F3V	K	302	-	4,4,4	0.86	0	3,4,4	2.16	1 (33%)
3	F3V	I	302	-	4,4,4	0.80	0	3,4,4	2.77	2 (66%)
3	F3V	C	302	-	4,4,4	0.78	0	3,4,4	1.54	1 (33%)
2	NAP	M	301	-	45,52,52	2.82	16 (35%)	56,80,80	1.30	8 (14%)
2	NAP	I	301	-	45,52,52	2.75	17 (37%)	56,80,80	1.35	7 (12%)
2	NAP	E	301	-	45,52,52	2.74	17 (37%)	56,80,80	1.41	7 (12%)
2	NAP	L	301	-	45,52,52	2.75	17 (37%)	56,80,80	1.35	7 (12%)
3	F3V	N	302	-	4,4,4	0.98	0	3,4,4	1.80	1 (33%)
3	F3V	O	302	-	4,4,4	0.73	0	3,4,4	1.85	1 (33%)
2	NAP	B	301	-	45,52,52	2.82	15 (33%)	56,80,80	1.33	10 (17%)
2	NAP	G	301	-	45,52,52	2.67	16 (35%)	56,80,80	1.28	5 (8%)
2	NAP	J	301	5	45,52,52	2.72	18 (40%)	56,80,80	1.35	8 (14%)
2	NAP	P	301	-	45,52,52	2.71	16 (35%)	56,80,80	1.33	6 (10%)
2	NAP	D	301	-	45,52,52	2.70	17 (37%)	56,80,80	1.45	9 (16%)

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	F3V	L	302	-	-	0/1/2/2	-
3	F3V	M	302	-	-	0/1/2/2	-
3	F3V	F	302	-	-	0/1/2/2	-
3	F3V	D	302	-	-	0/1/2/2	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	F3V	G	302	-	-	0/1/2/2	-
3	F3V	E	302	-	-	0/1/2/2	-
3	F3V	B	302	-	-	0/1/2/2	-
2	NAP	A	301	-	-	5/31/67/67	0/5/5/5
2	NAP	N	301	-	-	3/31/67/67	0/5/5/5
2	NAP	H	301	5	-	3/31/67/67	0/5/5/5
2	NAP	F	301	-	-	3/31/67/67	0/5/5/5
2	NAP	O	301	5	-	2/31/67/67	0/5/5/5
3	F3V	A	302	-	-	0/1/2/2	-
3	F3V	J	302	-	-	0/1/2/2	-
2	NAP	C	301	5	-	3/31/67/67	0/5/5/5
3	F3V	P	302	-	-	0/1/2/2	-
2	NAP	K	301	-	-	4/31/67/67	0/5/5/5
3	F3V	H	302	-	-	0/1/2/2	-
3	F3V	K	302	-	-	0/1/2/2	-
3	F3V	I	302	-	-	0/1/2/2	-
3	F3V	C	302	-	-	0/1/2/2	-
2	NAP	M	301	-	-	6/31/67/67	0/5/5/5
2	NAP	I	301	-	-	3/31/67/67	0/5/5/5
2	NAP	E	301	-	-	2/31/67/67	0/5/5/5
2	NAP	L	301	-	-	4/31/67/67	0/5/5/5
3	F3V	N	302	-	-	0/1/2/2	-
3	F3V	O	302	-	-	0/1/2/2	-
2	NAP	B	301	-	-	2/31/67/67	0/5/5/5
2	NAP	G	301	-	-	4/31/67/67	0/5/5/5
2	NAP	J	301	5	-	5/31/67/67	0/5/5/5
2	NAP	P	301	-	-	5/31/67/67	0/5/5/5
2	NAP	D	301	-	-	5/31/67/67	0/5/5/5

All (261) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	301	NAP	C7N-N7N	9.26	1.50	1.33
2	G	301	NAP	C7N-N7N	9.01	1.50	1.33
2	N	301	NAP	C7N-N7N	8.87	1.49	1.33
2	J	301	NAP	C7N-N7N	8.86	1.49	1.33
2	M	301	NAP	C7N-N7N	8.85	1.49	1.33
2	B	301	NAP	C7N-N7N	8.83	1.49	1.33
2	O	301	NAP	C7N-N7N	8.76	1.49	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	L	301	NAP	C7N-N7N	8.74	1.49	1.33
2	I	301	NAP	C7N-N7N	8.70	1.49	1.33
2	E	301	NAP	C7N-N7N	8.67	1.49	1.33
2	P	301	NAP	C7N-N7N	8.67	1.49	1.33
2	F	301	NAP	C7N-N7N	8.61	1.49	1.33
2	K	301	NAP	C7N-N7N	8.52	1.49	1.33
2	A	301	NAP	C7N-N7N	8.50	1.49	1.33
2	H	301	NAP	C7N-N7N	8.22	1.48	1.33
2	C	301	NAP	C7N-N7N	8.11	1.48	1.33
2	B	301	NAP	O4D-C1D	7.37	1.51	1.41
2	A	301	NAP	O4D-C1D	7.14	1.51	1.41
2	F	301	NAP	O4D-C1D	7.13	1.51	1.41
2	D	301	NAP	O4D-C1D	7.09	1.51	1.41
2	K	301	NAP	O4D-C1D	7.04	1.50	1.41
2	N	301	NAP	O4D-C1D	7.02	1.50	1.41
2	E	301	NAP	O4D-C1D	7.01	1.50	1.41
2	P	301	NAP	O4D-C1D	6.92	1.50	1.41
2	M	301	NAP	O4D-C1D	6.92	1.50	1.41
2	L	301	NAP	O4D-C1D	6.90	1.50	1.41
2	I	301	NAP	O4D-C1D	6.76	1.50	1.41
2	O	301	NAP	O4D-C1D	6.73	1.50	1.41
2	J	301	NAP	O4D-C1D	6.65	1.50	1.41
2	G	301	NAP	O4D-C1D	6.53	1.50	1.41
2	C	301	NAP	O4D-C1D	6.39	1.50	1.41
2	H	301	NAP	O4D-C1D	6.17	1.49	1.41
2	B	301	NAP	C3N-C7N	6.03	1.59	1.50
2	M	301	NAP	C3N-C7N	5.77	1.59	1.50
2	K	301	NAP	C3N-C7N	5.64	1.59	1.50
2	N	301	NAP	C3N-C7N	5.60	1.59	1.50
2	M	301	NAP	O4B-C1B	5.59	1.48	1.41
2	F	301	NAP	O4B-C1B	5.56	1.48	1.41
2	L	301	NAP	O4B-C1B	5.53	1.48	1.41
2	L	301	NAP	C3N-C7N	5.48	1.58	1.50
2	I	301	NAP	O4B-C1B	5.45	1.48	1.41
2	N	301	NAP	O4B-C1B	5.44	1.48	1.41
2	E	301	NAP	O4B-C1B	5.42	1.48	1.41
2	A	301	NAP	C3N-C7N	5.40	1.58	1.50
2	I	301	NAP	C3N-C7N	5.36	1.58	1.50
2	K	301	NAP	O4B-C1B	5.32	1.48	1.41
2	A	301	NAP	O4B-C1B	5.23	1.48	1.41
2	H	301	NAP	P2B-O2B	5.21	1.69	1.59
2	J	301	NAP	O4B-C1B	5.20	1.48	1.41

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	301	NAP	O4B-C1B	5.19	1.48	1.41
2	P	301	NAP	O4B-C1B	5.17	1.48	1.41
2	J	301	NAP	C3N-C7N	5.13	1.58	1.50
2	P	301	NAP	C3N-C7N	5.13	1.58	1.50
2	M	301	NAP	P2B-O2B	5.11	1.69	1.59
2	F	301	NAP	P2B-O2B	5.09	1.68	1.59
2	L	301	NAP	P2B-O2B	5.09	1.68	1.59
2	B	301	NAP	O4B-C1B	5.06	1.48	1.41
2	G	301	NAP	O4B-C1B	5.03	1.48	1.41
2	J	301	NAP	P2B-O2B	5.01	1.68	1.59
2	B	301	NAP	P2B-O2B	5.00	1.68	1.59
2	F	301	NAP	C3N-C7N	4.95	1.58	1.50
2	H	301	NAP	O4B-C1B	4.85	1.47	1.41
2	E	301	NAP	C3N-C7N	4.85	1.57	1.50
2	A	301	NAP	P2B-O2B	4.83	1.68	1.59
2	P	301	NAP	P2B-O2B	4.80	1.68	1.59
2	G	301	NAP	C2D-C1D	-4.76	1.46	1.53
2	H	301	NAP	C3N-C7N	4.75	1.57	1.50
2	M	301	NAP	C2D-C1D	-4.74	1.46	1.53
2	E	301	NAP	P2B-O2B	4.72	1.68	1.59
2	G	301	NAP	C3N-C7N	4.72	1.57	1.50
2	B	301	NAP	C2D-C1D	-4.71	1.46	1.53
2	O	301	NAP	O4B-C1B	4.69	1.47	1.41
2	C	301	NAP	P2B-O2B	4.65	1.68	1.59
2	I	301	NAP	C2D-C1D	-4.64	1.46	1.53
2	A	301	NAP	C2D-C1D	-4.61	1.46	1.53
2	G	301	NAP	P2B-O2B	4.60	1.68	1.59
2	O	301	NAP	C3N-C7N	4.60	1.57	1.50
2	N	301	NAP	C2N-N1N	4.56	1.40	1.35
2	I	301	NAP	P2B-O2B	4.55	1.67	1.59
2	K	301	NAP	P2B-O2B	4.54	1.67	1.59
2	F	301	NAP	C2D-C1D	-4.50	1.46	1.53
2	N	301	NAP	P2B-O2B	4.49	1.67	1.59
2	C	301	NAP	C3N-C7N	4.47	1.57	1.50
2	K	301	NAP	C2D-C1D	-4.47	1.47	1.53
2	C	301	NAP	O4B-C1B	4.43	1.47	1.41
2	P	301	NAP	C2D-C1D	-4.42	1.47	1.53
2	O	301	NAP	C2D-C1D	-4.37	1.47	1.53
2	D	301	NAP	C2D-C1D	-4.37	1.47	1.53
2	D	301	NAP	P2B-O2B	4.35	1.67	1.59
2	E	301	NAP	C2D-C1D	-4.35	1.47	1.53
2	E	301	NAP	C2N-N1N	4.32	1.40	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	301	NAP	C2N-N1N	4.31	1.40	1.35
2	L	301	NAP	C2D-C1D	-4.30	1.47	1.53
2	N	301	NAP	C2D-C1D	-4.30	1.47	1.53
2	J	301	NAP	C2D-C1D	-4.25	1.47	1.53
2	D	301	NAP	C3N-C7N	4.23	1.56	1.50
2	O	301	NAP	P2B-O2B	4.22	1.67	1.59
2	B	301	NAP	C2N-N1N	4.22	1.40	1.35
2	I	301	NAP	C2N-N1N	4.16	1.40	1.35
2	M	301	NAP	C2N-N1N	4.14	1.40	1.35
2	F	301	NAP	C2N-N1N	4.09	1.39	1.35
2	C	301	NAP	C2N-N1N	4.08	1.39	1.35
2	P	301	NAP	C2N-N1N	4.05	1.39	1.35
2	L	301	NAP	C2N-N1N	4.00	1.39	1.35
2	K	301	NAP	C2N-N1N	3.98	1.39	1.35
2	J	301	NAP	C2N-N1N	3.92	1.39	1.35
2	H	301	NAP	C2N-N1N	3.83	1.39	1.35
2	D	301	NAP	C2N-N1N	3.76	1.39	1.35
2	H	301	NAP	C6A-N6A	3.75	1.47	1.34
2	O	301	NAP	C6A-N6A	3.74	1.47	1.34
2	J	301	NAP	C6A-N6A	3.66	1.47	1.34
2	H	301	NAP	C2D-C1D	-3.66	1.48	1.53
2	O	301	NAP	C2N-N1N	3.65	1.39	1.35
2	C	301	NAP	C2D-C1D	-3.65	1.48	1.53
2	I	301	NAP	C6A-N6A	3.57	1.47	1.34
2	B	301	NAP	C6A-N6A	3.52	1.46	1.34
2	A	301	NAP	C6A-N6A	3.49	1.46	1.34
2	G	301	NAP	C2N-N1N	3.48	1.39	1.35
2	K	301	NAP	C6A-N6A	3.46	1.46	1.34
2	M	301	NAP	C6A-N6A	3.44	1.46	1.34
2	L	301	NAP	C6A-N6A	3.43	1.46	1.34
2	N	301	NAP	C6A-N6A	3.43	1.46	1.34
2	B	301	NAP	O4D-C4D	3.40	1.52	1.45
2	P	301	NAP	C6A-N6A	3.40	1.46	1.34
2	F	301	NAP	C6A-N6A	3.39	1.46	1.34
2	E	301	NAP	C6A-N6A	3.39	1.46	1.34
2	G	301	NAP	C6A-N6A	3.36	1.46	1.34
2	E	301	NAP	O4D-C4D	3.34	1.52	1.45
2	C	301	NAP	C6A-N6A	3.32	1.46	1.34
2	N	301	NAP	O4D-C4D	3.29	1.52	1.45
2	M	301	NAP	O4D-C4D	3.25	1.52	1.45
2	K	301	NAP	O4D-C4D	3.25	1.52	1.45
2	N	301	NAP	C2N-C3N	3.21	1.44	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	G	301	NAP	O4B-C4B	3.14	1.52	1.45
2	L	301	NAP	O4D-C4D	3.14	1.52	1.45
2	J	301	NAP	O4D-C4D	3.12	1.52	1.45
2	D	301	NAP	O4B-C4B	3.07	1.51	1.45
2	I	301	NAP	C2N-C3N	3.07	1.43	1.39
2	D	301	NAP	O4D-C4D	3.06	1.51	1.45
2	H	301	NAP	C2N-C3N	3.05	1.43	1.39
2	A	301	NAP	O4B-C4B	3.05	1.51	1.45
2	D	301	NAP	C6A-N6A	3.03	1.45	1.34
2	P	301	NAP	O4B-C4B	3.02	1.51	1.45
2	P	301	NAP	O4D-C4D	3.02	1.51	1.45
2	J	301	NAP	C2N-C3N	3.00	1.43	1.39
2	K	301	NAP	O4B-C4B	2.99	1.51	1.45
2	D	301	NAP	C4A-N3A	-2.99	1.31	1.35
2	M	301	NAP	O4B-C4B	2.99	1.51	1.45
2	F	301	NAP	C2N-C3N	2.98	1.43	1.39
2	I	301	NAP	O4B-C4B	2.98	1.51	1.45
2	E	301	NAP	C3B-C2B	-2.97	1.46	1.52
2	N	301	NAP	C3B-C2B	-2.97	1.46	1.52
2	F	301	NAP	C3D-C4D	-2.96	1.45	1.53
2	G	301	NAP	O4D-C4D	2.96	1.51	1.45
2	O	301	NAP	O4D-C4D	2.94	1.51	1.45
2	M	301	NAP	C3D-C4D	-2.94	1.45	1.53
2	G	301	NAP	C3B-C2B	-2.93	1.46	1.52
2	D	301	NAP	C3B-C2B	-2.91	1.46	1.52
2	E	301	NAP	C2N-C3N	2.91	1.43	1.39
2	N	301	NAP	O4B-C4B	2.90	1.51	1.45
2	O	301	NAP	O4B-C4B	2.89	1.51	1.45
2	I	301	NAP	O4D-C4D	2.89	1.51	1.45
2	K	301	NAP	C3B-C2B	-2.87	1.46	1.52
2	B	301	NAP	O4B-C4B	2.86	1.51	1.45
2	L	301	NAP	C2N-C3N	2.86	1.43	1.39
2	E	301	NAP	O4B-C4B	2.85	1.51	1.45
2	K	301	NAP	C2N-C3N	2.85	1.43	1.39
2	M	301	NAP	C2N-C3N	2.84	1.43	1.39
2	L	301	NAP	O4B-C4B	2.84	1.51	1.45
2	J	301	NAP	O4B-C4B	2.84	1.51	1.45
2	G	301	NAP	C3D-C4D	-2.83	1.45	1.53
2	K	301	NAP	C3D-C4D	-2.82	1.45	1.53
2	B	301	NAP	C2N-C3N	2.82	1.43	1.39
2	H	301	NAP	O4D-C4D	2.80	1.51	1.45
2	B	301	NAP	C3B-C2B	-2.77	1.46	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	301	NAP	O4D-C4D	2.77	1.51	1.45
2	A	301	NAP	O4D-C4D	2.77	1.51	1.45
2	A	301	NAP	C3D-C4D	-2.76	1.45	1.53
2	P	301	NAP	C3D-C4D	-2.74	1.46	1.53
2	O	301	NAP	C3B-C2B	-2.74	1.46	1.52
2	L	301	NAP	C3D-C4D	-2.73	1.46	1.53
2	C	301	NAP	C2N-C3N	2.72	1.43	1.39
2	F	301	NAP	C3B-C2B	-2.72	1.46	1.52
2	A	301	NAP	C4A-N3A	-2.71	1.31	1.35
2	I	301	NAP	C3B-C2B	-2.70	1.46	1.52
2	I	301	NAP	C2D-C3D	-2.69	1.46	1.53
2	G	301	NAP	C4A-N3A	-2.69	1.31	1.35
2	F	301	NAP	O4D-C4D	2.68	1.51	1.45
2	P	301	NAP	C2N-C3N	2.68	1.43	1.39
2	H	301	NAP	O4B-C4B	2.66	1.51	1.45
2	B	301	NAP	C3D-C4D	-2.65	1.46	1.53
2	P	301	NAP	C2D-C3D	-2.64	1.46	1.53
2	F	301	NAP	O4B-C4B	2.64	1.50	1.45
2	E	301	NAP	C3D-C4D	-2.64	1.46	1.53
2	M	301	NAP	C2D-C3D	-2.59	1.46	1.53
2	K	301	NAP	C2D-C3D	-2.57	1.46	1.53
2	N	301	NAP	C3D-C4D	-2.56	1.46	1.53
2	D	301	NAP	C2D-C3D	-2.55	1.46	1.53
2	A	301	NAP	C3B-C2B	-2.55	1.47	1.52
2	M	301	NAP	C3B-C2B	-2.54	1.47	1.52
2	D	301	NAP	C3D-C4D	-2.53	1.46	1.53
2	A	301	NAP	C2N-C3N	2.53	1.42	1.39
2	I	301	NAP	C3D-C4D	-2.52	1.46	1.53
2	P	301	NAP	C3B-C2B	-2.52	1.47	1.52
2	C	301	NAP	C2D-C3D	-2.51	1.46	1.53
2	L	301	NAP	C3B-C2B	-2.50	1.47	1.52
2	C	301	NAP	C3B-C2B	-2.48	1.47	1.52
2	I	301	NAP	O3D-C3D	2.45	1.48	1.43
2	B	301	NAP	C2D-C3D	-2.44	1.46	1.53
2	C	301	NAP	O4B-C4B	2.43	1.50	1.45
2	N	301	NAP	C2D-C3D	-2.43	1.46	1.53
2	F	301	NAP	C4A-N3A	-2.41	1.32	1.35
2	O	301	NAP	C2D-C3D	-2.40	1.46	1.53
2	H	301	NAP	C2D-C3D	-2.37	1.46	1.53
2	J	301	NAP	C2D-C3D	-2.36	1.46	1.53
2	J	301	NAP	C3B-C2B	-2.34	1.47	1.52
2	J	301	NAP	C3D-C4D	-2.33	1.47	1.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	J	301	NAP	O3D-C3D	2.32	1.48	1.43
2	E	301	NAP	C2D-C3D	-2.31	1.47	1.53
2	O	301	NAP	C2N-C3N	2.31	1.42	1.39
2	A	301	NAP	O3D-C3D	2.30	1.48	1.43
2	L	301	NAP	C2D-C3D	-2.29	1.47	1.53
2	H	301	NAP	C3B-C2B	-2.27	1.47	1.52
2	P	301	NAP	C3B-C4B	-2.27	1.47	1.53
2	O	301	NAP	C3D-C4D	-2.25	1.47	1.53
2	G	301	NAP	O3D-C3D	2.24	1.48	1.43
2	E	301	NAP	C3B-C4B	-2.22	1.47	1.53
2	G	301	NAP	C2D-C3D	-2.20	1.47	1.53
2	O	301	NAP	O3D-C3D	2.20	1.48	1.43
2	I	301	NAP	C4A-N3A	-2.19	1.32	1.35
2	C	301	NAP	C4A-N3A	-2.19	1.32	1.35
2	K	301	NAP	O3D-C3D	2.19	1.48	1.43
2	K	301	NAP	C3B-C4B	-2.18	1.47	1.53
2	H	301	NAP	O3D-C3D	2.16	1.48	1.43
2	J	301	NAP	C4A-N3A	-2.14	1.32	1.35
2	G	301	NAP	C2N-C3N	2.14	1.42	1.39
2	E	301	NAP	O3D-C3D	2.14	1.48	1.43
2	H	301	NAP	C3D-C4D	-2.13	1.47	1.53
2	P	301	NAP	O3D-C3D	2.12	1.48	1.43
2	M	301	NAP	PA-O5B	2.12	1.67	1.59
2	N	301	NAP	C3B-C4B	-2.12	1.47	1.53
2	O	301	NAP	C3B-C4B	-2.12	1.47	1.53
2	D	301	NAP	C2N-C3N	2.11	1.42	1.39
2	J	301	NAP	C3B-C4B	-2.11	1.47	1.53
2	L	301	NAP	C3B-C4B	-2.11	1.47	1.53
2	A	301	NAP	C3B-C4B	-2.10	1.47	1.53
2	F	301	NAP	C3B-C4B	-2.10	1.47	1.53
2	M	301	NAP	C4A-N3A	-2.09	1.32	1.35
2	I	301	NAP	C3B-C4B	-2.08	1.47	1.53
2	C	301	NAP	C3B-C4B	-2.08	1.47	1.53
2	N	301	NAP	C4A-N3A	-2.08	1.32	1.35
2	B	301	NAP	C3B-C4B	-2.07	1.47	1.53
2	D	301	NAP	O3D-C3D	2.07	1.47	1.43
2	E	301	NAP	C4A-N3A	-2.06	1.32	1.35
2	L	301	NAP	O3D-C3D	2.05	1.47	1.43
2	L	301	NAP	PA-O5B	2.05	1.67	1.59
2	K	301	NAP	C4A-N3A	-2.03	1.32	1.35
2	D	301	NAP	C3B-C4B	-2.03	1.47	1.53
2	F	301	NAP	C2D-C3D	-2.03	1.47	1.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	O	301	NAP	C4A-N3A	-2.01	1.32	1.35
2	J	301	NAP	PA-O5B	2.01	1.67	1.59

All (137) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	301	NAP	N3A-C2A-N1A	-5.77	119.66	128.68
2	D	301	NAP	N3A-C2A-N1A	-4.49	121.65	128.68
2	A	301	NAP	N3A-C2A-N1A	-4.38	121.83	128.68
2	E	301	NAP	N3A-C2A-N1A	-4.31	121.94	128.68
2	K	301	NAP	N3A-C2A-N1A	-4.26	122.02	128.68
2	F	301	NAP	N3A-C2A-N1A	-4.21	122.09	128.68
2	N	301	NAP	N3A-C2A-N1A	-4.20	122.11	128.68
2	I	301	NAP	N3A-C2A-N1A	-4.17	122.16	128.68
2	O	301	NAP	N3A-C2A-N1A	-4.17	122.17	128.68
2	H	301	NAP	N3A-C2A-N1A	-4.15	122.20	128.68
2	A	301	NAP	C4A-C5A-N7A	-4.13	105.09	109.40
2	H	301	NAP	C4A-C5A-N7A	-4.13	105.10	109.40
2	L	301	NAP	N3A-C2A-N1A	-4.10	122.26	128.68
2	J	301	NAP	N3A-C2A-N1A	-4.07	122.32	128.68
2	P	301	NAP	N3A-C2A-N1A	-4.06	122.34	128.68
2	M	301	NAP	N3A-C2A-N1A	-4.05	122.35	128.68
2	O	301	NAP	C4A-C5A-N7A	-3.94	105.30	109.40
2	A	301	NAP	C1B-N9A-C4A	-3.93	119.74	126.64
2	I	301	NAP	C4A-C5A-N7A	-3.91	105.33	109.40
2	N	301	NAP	C4A-C5A-N7A	-3.90	105.33	109.40
2	B	301	NAP	N3A-C2A-N1A	-3.87	122.63	128.68
2	E	301	NAP	C4A-C5A-N7A	-3.85	105.39	109.40
2	F	301	NAP	C4A-C5A-N7A	-3.84	105.40	109.40
2	G	301	NAP	N3A-C2A-N1A	-3.83	122.69	128.68
3	B	302	F3V	O-C-CA	-3.80	118.61	121.31
2	K	301	NAP	C1B-N9A-C4A	-3.75	120.06	126.64
2	C	301	NAP	C1B-N9A-C4A	-3.74	120.06	126.64
2	L	301	NAP	C4A-C5A-N7A	-3.74	105.50	109.40
2	B	301	NAP	C4A-C5A-N7A	-3.72	105.52	109.40
2	J	301	NAP	C4A-C5A-N7A	-3.69	105.56	109.40
2	G	301	NAP	C1B-N9A-C4A	-3.64	120.25	126.64
2	C	301	NAP	C4A-C5A-N7A	-3.56	105.69	109.40
3	B	302	F3V	CM-C-CA	3.56	121.04	115.26
3	I	302	F3V	CM-C-CA	3.54	121.02	115.26
2	D	301	NAP	C1B-N9A-C4A	-3.54	120.42	126.64
2	N	301	NAP	C1B-N9A-C4A	-3.51	120.47	126.64

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	M	301	NAP	C4A-C5A-N7A	-3.50	105.75	109.40
2	F	301	NAP	C1B-N9A-C4A	-3.48	120.53	126.64
2	K	301	NAP	C4A-C5A-N7A	-3.46	105.79	109.40
2	P	301	NAP	C4A-C5A-N7A	-3.44	105.81	109.40
2	G	301	NAP	C4A-C5A-N7A	-3.38	105.87	109.40
2	J	301	NAP	C1B-N9A-C4A	-3.32	120.80	126.64
2	L	301	NAP	C1B-N9A-C4A	-3.32	120.81	126.64
3	H	302	F3V	CM-C-CA	3.31	120.63	115.26
3	E	302	F3V	CM-C-CA	3.29	120.61	115.26
2	M	301	NAP	C1B-N9A-C4A	-3.26	120.92	126.64
2	D	301	NAP	C3N-C7N-N7N	3.24	121.64	117.75
3	M	302	F3V	CM-C-CA	3.23	120.51	115.26
3	I	302	F3V	O-C-CA	-3.18	119.04	121.31
3	K	302	F3V	CM-C-CA	3.16	120.39	115.26
2	P	301	NAP	C1B-N9A-C4A	-3.13	121.14	126.64
3	A	302	F3V	CM-C-CA	3.04	120.20	115.26
2	H	301	NAP	C1B-N9A-C4A	-2.98	121.41	126.64
2	B	301	NAP	C1B-N9A-C4A	-2.98	121.41	126.64
3	L	302	F3V	CM-C-CA	2.97	120.08	115.26
3	P	302	F3V	CM-C-CA	2.96	120.07	115.26
2	I	301	NAP	C1B-N9A-C4A	-2.96	121.44	126.64
3	N	302	F3V	CM-C-CA	2.93	120.01	115.26
2	H	301	NAP	O4D-C1D-C2D	-2.91	102.68	106.93
3	O	302	F3V	CM-C-CA	2.87	119.92	115.26
2	N	301	NAP	C3N-C7N-N7N	2.83	121.14	117.75
2	E	301	NAP	C6N-N1N-C2N	-2.82	119.40	121.97
2	C	301	NAP	O4D-C1D-C2D	-2.82	102.81	106.93
2	D	301	NAP	C4A-C5A-N7A	-2.81	106.47	109.40
2	F	301	NAP	C2D-C3D-C4D	2.79	108.07	102.64
2	N	301	NAP	C3D-C2D-C1D	2.79	105.18	100.98
2	M	301	NAP	PN-O3-PA	-2.77	123.31	132.83
2	E	301	NAP	C3D-C2D-C1D	2.75	105.12	100.98
2	E	301	NAP	C2N-C3N-C4N	2.75	121.37	118.26
2	H	301	NAP	C2D-C3D-C4D	2.69	107.87	102.64
2	N	301	NAP	C2D-C3D-C4D	2.69	107.86	102.64
2	N	301	NAP	C6N-N1N-C2N	-2.68	119.53	121.97
3	F	302	F3V	CM-C-CA	2.68	119.61	115.26
3	H	302	F3V	O-C-CA	-2.67	119.41	121.31
2	B	301	NAP	O3D-C3D-C4D	-2.63	103.44	111.05
2	F	301	NAP	O3D-C3D-C4D	-2.63	103.44	111.05
3	G	302	F3V	CM-C-CA	2.61	119.50	115.26
2	E	301	NAP	C1B-N9A-C4A	-2.59	122.08	126.64

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	L	301	NAP	C2D-C3D-C4D	2.57	107.63	102.64
2	J	301	NAP	C3N-C7N-N7N	2.55	120.82	117.75
2	J	301	NAP	C6N-N1N-C2N	-2.55	119.65	121.97
2	L	301	NAP	PN-O3-PA	-2.54	124.10	132.83
3	J	302	F3V	CM-C-CA	2.52	119.35	115.26
2	L	301	NAP	C6N-N1N-C2N	-2.51	119.69	121.97
2	E	301	NAP	C2D-C3D-C4D	2.50	107.50	102.64
2	D	301	NAP	PN-O3-PA	-2.50	124.26	132.83
2	H	301	NAP	C2N-C3N-C4N	2.49	121.09	118.26
2	C	301	NAP	O3D-C3D-C4D	-2.49	103.84	111.05
2	O	301	NAP	C2D-C3D-C4D	2.47	107.44	102.64
2	J	301	NAP	C2N-C3N-C4N	2.45	121.03	118.26
2	B	301	NAP	C3D-C2D-C1D	2.44	104.66	100.98
2	J	301	NAP	C2D-C3D-C4D	2.43	107.37	102.64
2	O	301	NAP	C2N-C3N-C4N	2.40	120.98	118.26
2	C	301	NAP	C2D-C3D-C4D	2.40	107.31	102.64
2	O	301	NAP	C1B-N9A-C4A	-2.40	122.43	126.64
2	H	301	NAP	C6N-N1N-C2N	-2.39	119.79	121.97
2	P	301	NAP	PN-O3-PA	-2.38	124.65	132.83
2	F	301	NAP	C3N-C7N-N7N	2.37	120.60	117.75
2	F	301	NAP	C6N-N1N-C2N	-2.37	119.82	121.97
2	B	301	NAP	C3N-C7N-N7N	2.34	120.56	117.75
2	O	301	NAP	PN-O3-PA	-2.31	124.89	132.83
2	C	301	NAP	C2A-N1A-C6A	2.31	122.70	118.75
3	C	302	F3V	CM-C-CA	2.29	118.97	115.26
2	M	301	NAP	O3D-C3D-C4D	-2.28	104.45	111.05
2	K	301	NAP	C6N-N1N-C2N	-2.28	119.89	121.97
2	I	301	NAP	C2D-C3D-C4D	2.26	107.03	102.64
2	A	301	NAP	O3D-C3D-C4D	-2.25	104.53	111.05
2	A	301	NAP	C3N-C7N-N7N	2.25	120.45	117.75
2	I	301	NAP	C3N-C7N-N7N	2.25	120.44	117.75
2	M	301	NAP	C3N-C7N-N7N	2.23	120.42	117.75
2	B	301	NAP	O7N-C7N-N7N	-2.20	119.46	122.58
2	D	301	NAP	C2D-C3D-C4D	2.19	106.89	102.64
2	F	301	NAP	C2B-C3B-C4B	2.18	106.72	101.99
2	D	301	NAP	O7N-C7N-C3N	-2.17	117.03	119.63
2	M	301	NAP	C2D-C3D-C4D	2.14	106.80	102.64
2	D	301	NAP	C5B-C4B-C3B	-2.13	107.20	115.18
2	N	301	NAP	PN-O3-PA	-2.10	125.60	132.83
3	A	302	F3V	O-C-CA	-2.09	119.82	121.31
2	G	301	NAP	C2D-C3D-C4D	2.09	106.70	102.64
2	P	301	NAP	C6N-N1N-C2N	-2.08	120.08	121.97

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	301	NAP	C2D-C3D-C4D	2.08	106.68	102.64
2	G	301	NAP	O3D-C3D-C4D	-2.07	105.07	111.05
2	I	301	NAP	C6N-N1N-C2N	-2.06	120.09	121.97
3	E	302	F3V	O-C-CA	-2.06	119.84	121.31
2	P	301	NAP	C2D-C3D-C4D	2.06	106.65	102.64
2	M	301	NAP	C2B-C3B-C4B	2.06	106.47	101.99
2	A	301	NAP	C2D-C3D-C4D	2.06	106.64	102.64
2	I	301	NAP	C2N-C3N-C4N	2.05	120.58	118.26
2	L	301	NAP	C2B-C3B-C4B	2.05	106.45	101.99
2	B	301	NAP	C6N-N1N-C2N	-2.05	120.11	121.97
2	C	301	NAP	O3X-P2B-O2X	2.05	115.45	107.64
2	B	301	NAP	PN-O3-PA	-2.04	125.81	132.83
2	F	301	NAP	PN-O3-PA	-2.04	125.82	132.83
2	D	301	NAP	O3D-C3D-C4D	-2.03	105.18	111.05
2	K	301	NAP	PN-O3-PA	-2.03	125.87	132.83
2	H	301	NAP	O4B-C4B-C3B	2.02	109.11	105.11
2	J	301	NAP	C3D-C2D-C1D	2.01	104.00	100.98

There are no chirality outliers.

All (59) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	301	NAP	C2B-O2B-P2B-O1X
2	A	301	NAP	C2B-O2B-P2B-O2X
2	N	301	NAP	C2B-O2B-P2B-O1X
2	N	301	NAP	C2B-O2B-P2B-O2X
2	H	301	NAP	C2B-O2B-P2B-O1X
2	F	301	NAP	C2B-O2B-P2B-O1X
2	F	301	NAP	C2B-O2B-P2B-O2X
2	O	301	NAP	C2B-O2B-P2B-O1X
2	C	301	NAP	C2B-O2B-P2B-O1X
2	K	301	NAP	C2B-O2B-P2B-O1X
2	M	301	NAP	C5B-O5B-PA-O3
2	M	301	NAP	C2B-O2B-P2B-O1X
2	I	301	NAP	C2B-O2B-P2B-O1X
2	L	301	NAP	C2B-O2B-P2B-O1X
2	L	301	NAP	C2B-O2B-P2B-O2X
2	B	301	NAP	C2B-O2B-P2B-O2X
2	G	301	NAP	C2B-O2B-P2B-O1X
2	J	301	NAP	C2B-O2B-P2B-O1X
2	P	301	NAP	C2B-O2B-P2B-O1X
2	D	301	NAP	C2B-O2B-P2B-O1X

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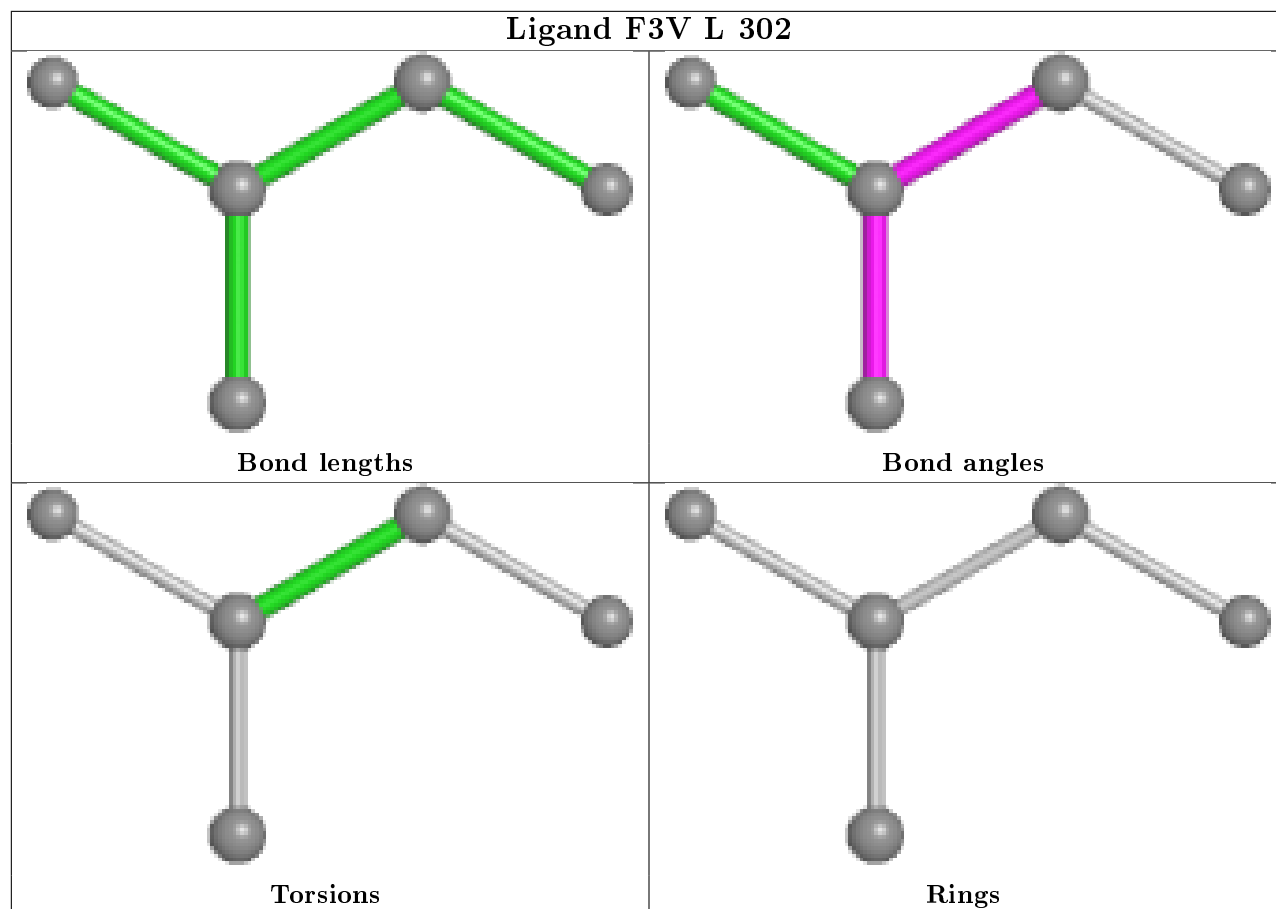
Mol	Chain	Res	Type	Atoms
2	A	301	NAP	O4D-C4D-C5D-O5D
2	A	301	NAP	C3D-C4D-C5D-O5D
2	K	301	NAP	O4D-C4D-C5D-O5D
2	M	301	NAP	O4D-C4D-C5D-O5D
2	P	301	NAP	O4D-C4D-C5D-O5D
2	D	301	NAP	O4D-C4D-C5D-O5D
2	I	301	NAP	C2B-O2B-P2B-O2X
2	E	301	NAP	C2B-O2B-P2B-O2X
2	J	301	NAP	C2B-O2B-P2B-O2X
2	P	301	NAP	C2B-O2B-P2B-O2X
2	D	301	NAP	C2B-O2B-P2B-O2X
2	M	301	NAP	C5B-O5B-PA-O2A
2	M	301	NAP	C3D-C4D-C5D-O5D
2	G	301	NAP	O4D-C4D-C5D-O5D
2	O	301	NAP	O4B-C4B-C5B-O5B
2	K	301	NAP	C3D-C4D-C5D-O5D
2	H	301	NAP	O4D-C4D-C5D-O5D
2	M	301	NAP	O4B-C4B-C5B-O5B
2	C	301	NAP	O4D-C4D-C5D-O5D
2	D	301	NAP	O4B-C4B-C5B-O5B
2	L	301	NAP	O4D-C4D-C5D-O5D
2	P	301	NAP	C3D-C4D-C5D-O5D
2	C	301	NAP	O4B-C4B-C5B-O5B
2	J	301	NAP	O4B-C4B-C5B-O5B
2	G	301	NAP	C2B-O2B-P2B-O2X
2	J	301	NAP	C5B-O5B-PA-O3
2	N	301	NAP	O4B-C4B-C5B-O5B
2	K	301	NAP	O4B-C4B-C5B-O5B
2	I	301	NAP	O4B-C4B-C5B-O5B
2	B	301	NAP	O4B-C4B-C5B-O5B
2	P	301	NAP	O4B-C4B-C5B-O5B
2	D	301	NAP	C3D-C4D-C5D-O5D
2	J	301	NAP	C5D-O5D-PN-O1N
2	A	301	NAP	O4B-C4B-C5B-O5B
2	H	301	NAP	O4B-C4B-C5B-O5B
2	F	301	NAP	O4B-C4B-C5B-O5B
2	E	301	NAP	O4B-C4B-C5B-O5B
2	L	301	NAP	O4B-C4B-C5B-O5B
2	G	301	NAP	O4B-C4B-C5B-O5B

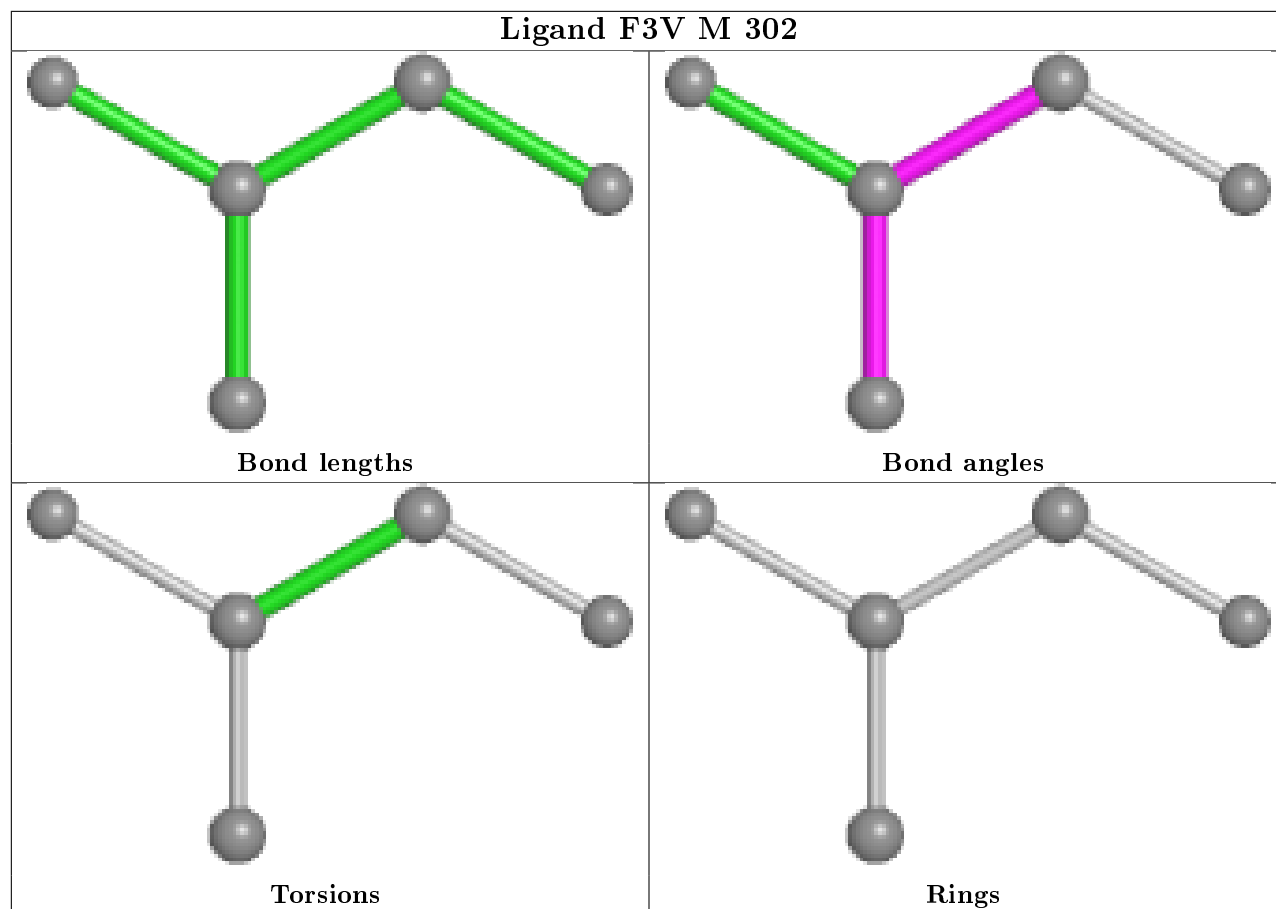
There are no ring outliers.

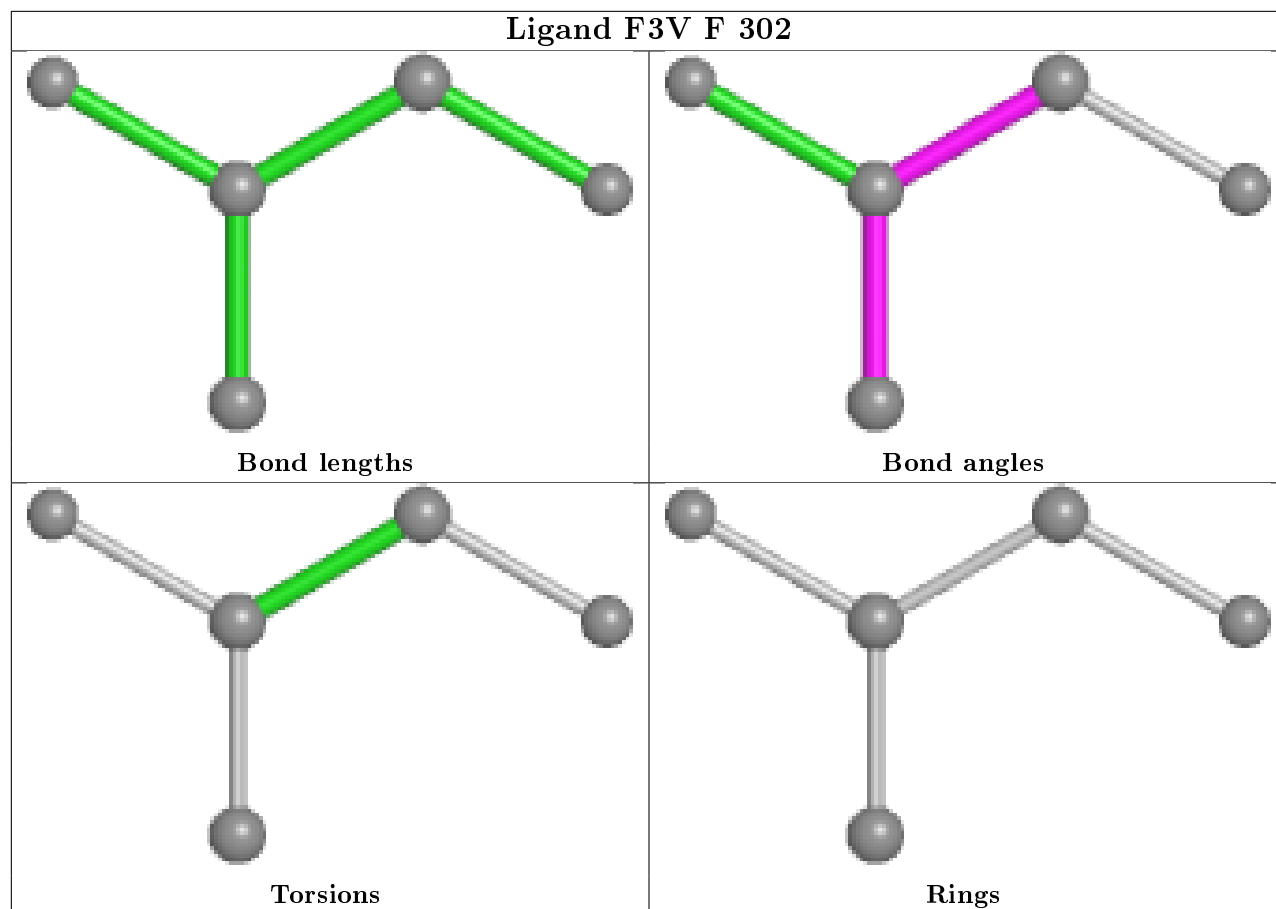
16 monomers are involved in 35 short contacts:

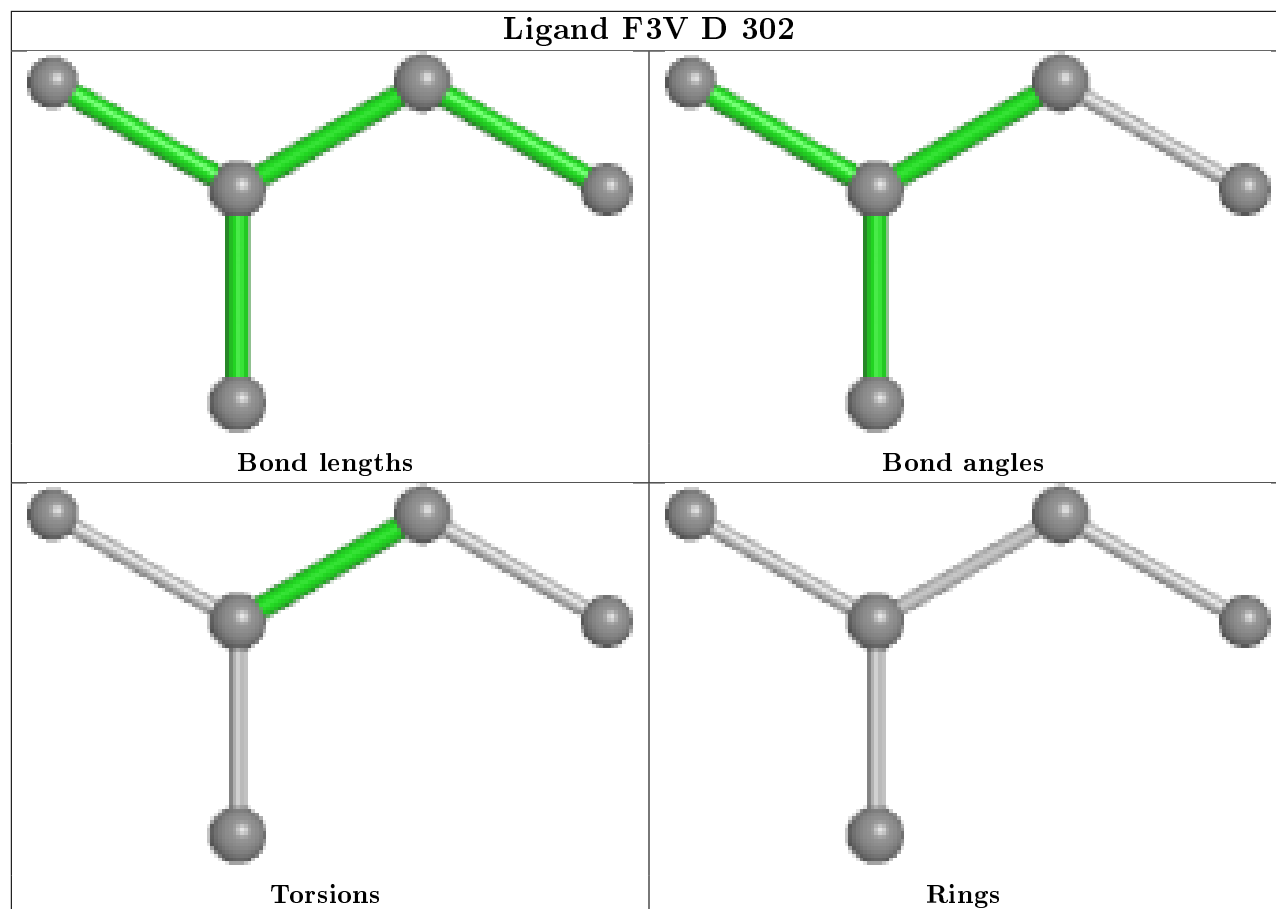
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	301	NAP	2	0
2	N	301	NAP	5	0
2	H	301	NAP	1	0
2	F	301	NAP	2	0
2	O	301	NAP	3	0
2	C	301	NAP	1	0
2	K	301	NAP	2	0
2	M	301	NAP	2	0
2	I	301	NAP	3	0
2	E	301	NAP	2	0
2	L	301	NAP	2	0
2	B	301	NAP	3	0
2	G	301	NAP	2	0
2	J	301	NAP	1	0
2	P	301	NAP	2	0
2	D	301	NAP	2	0

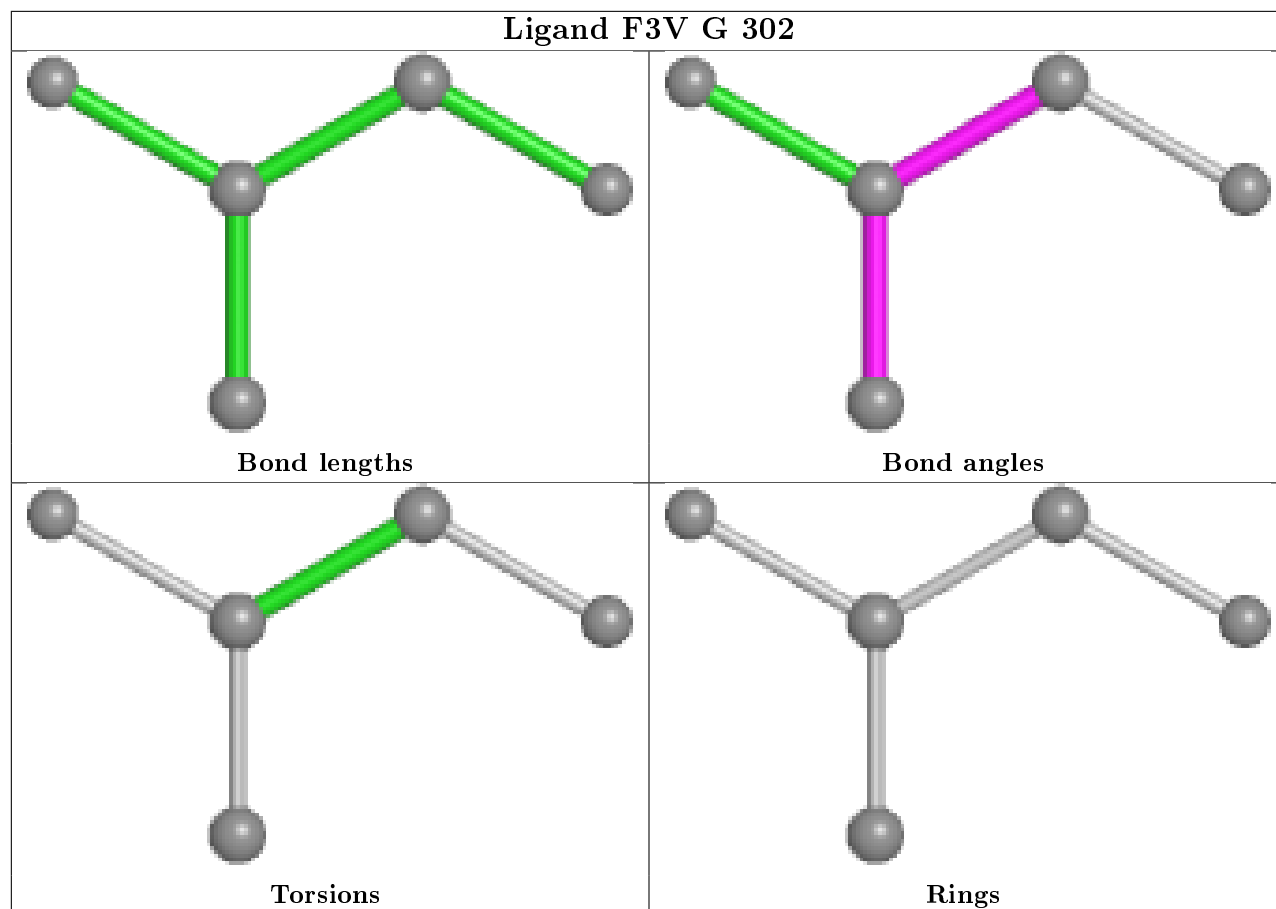
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

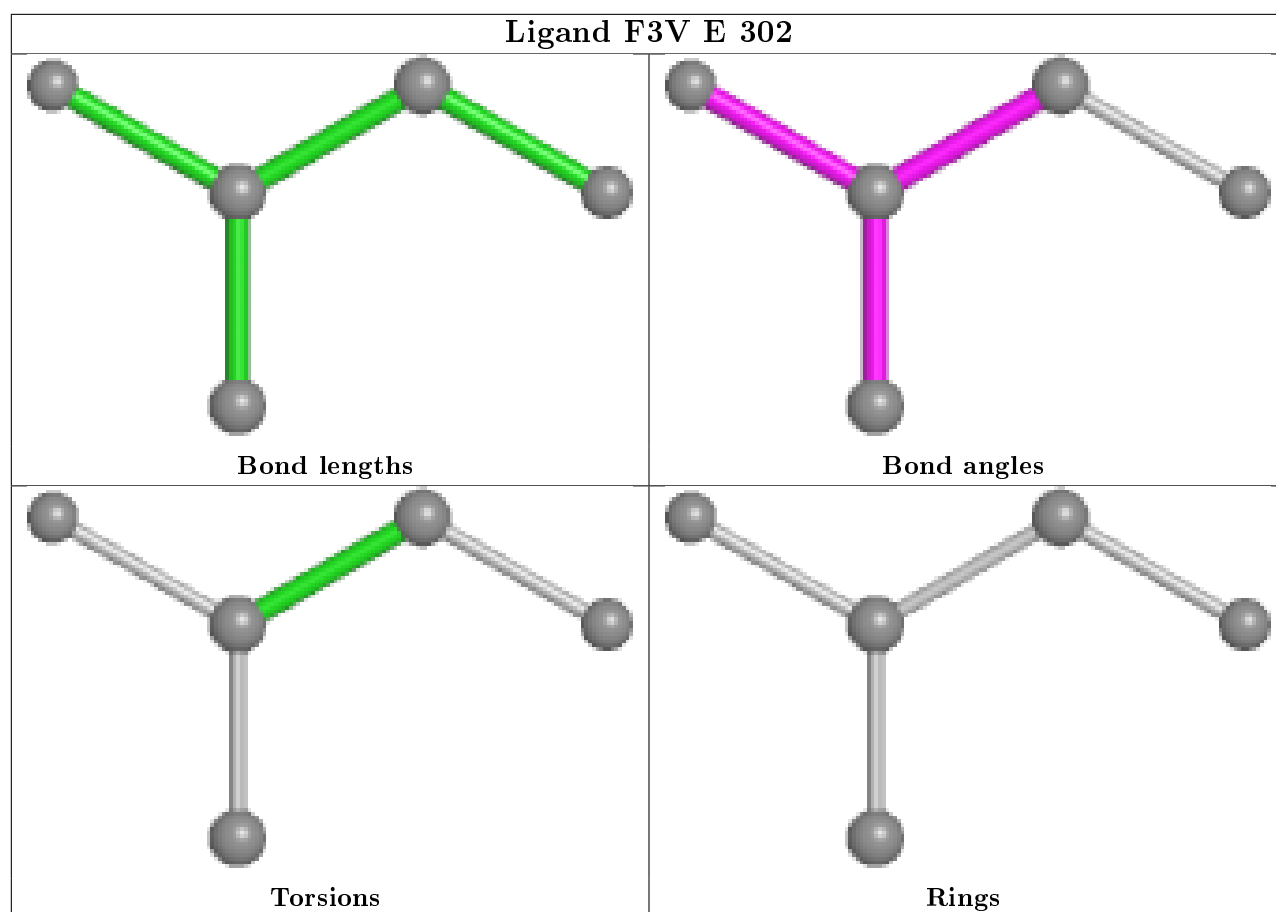


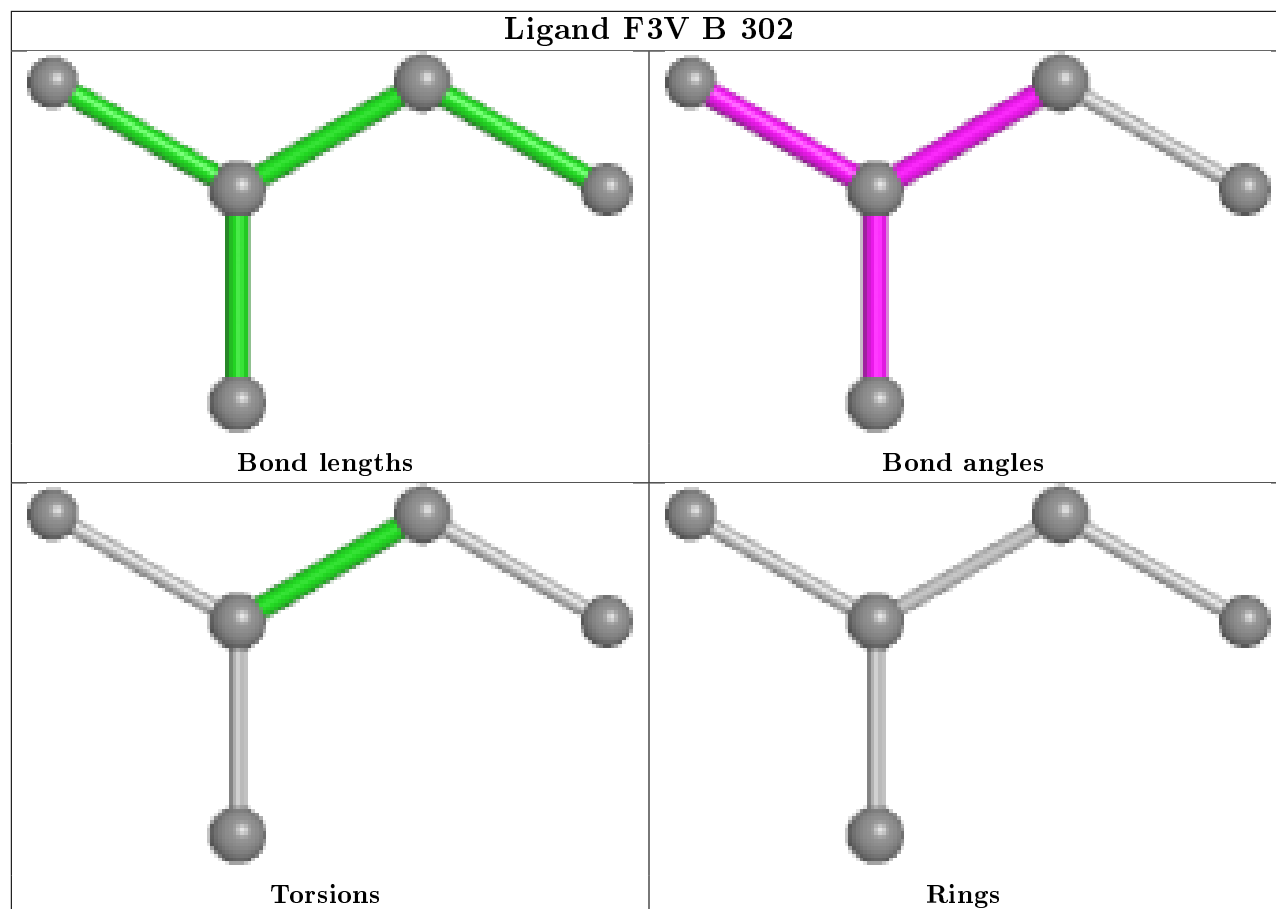


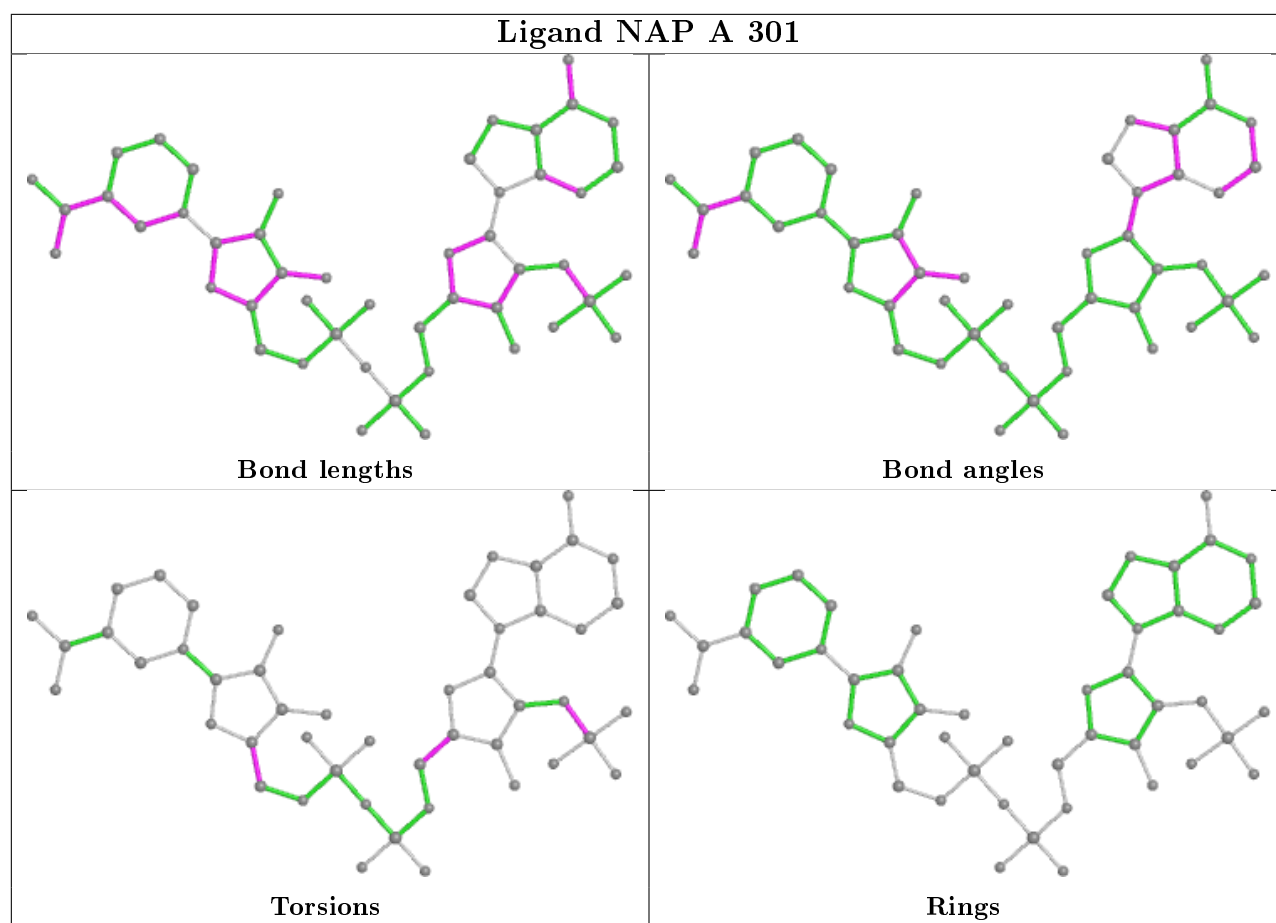


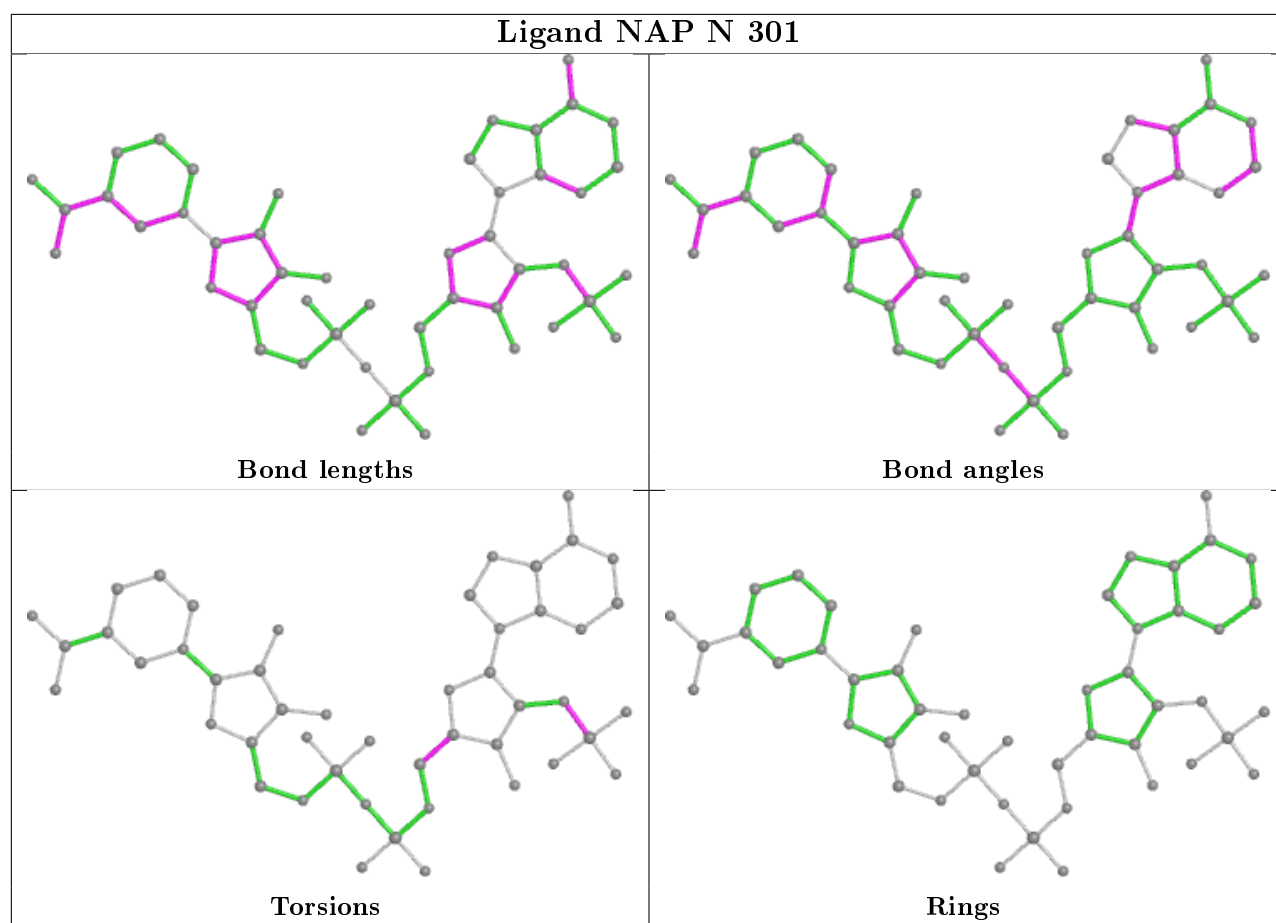


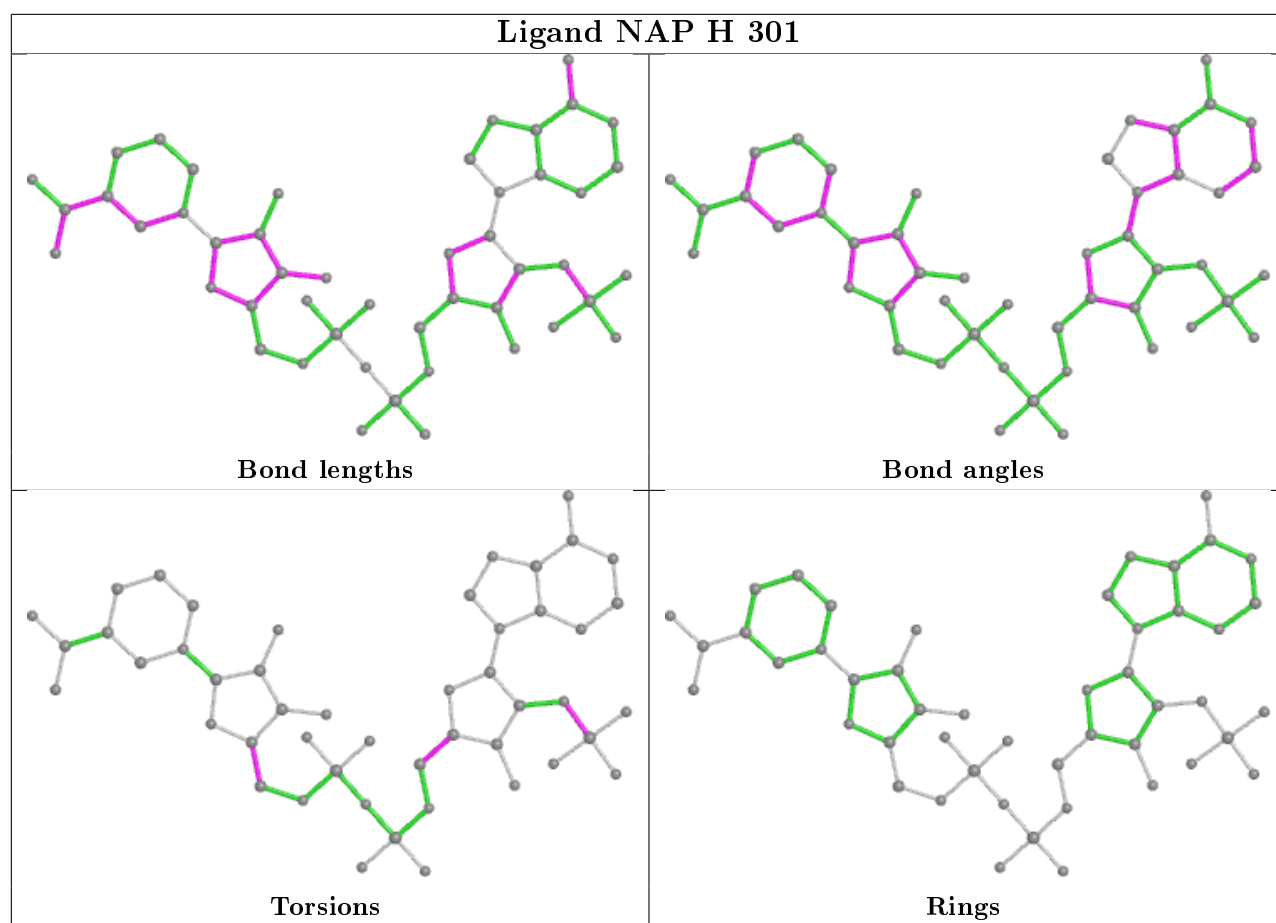


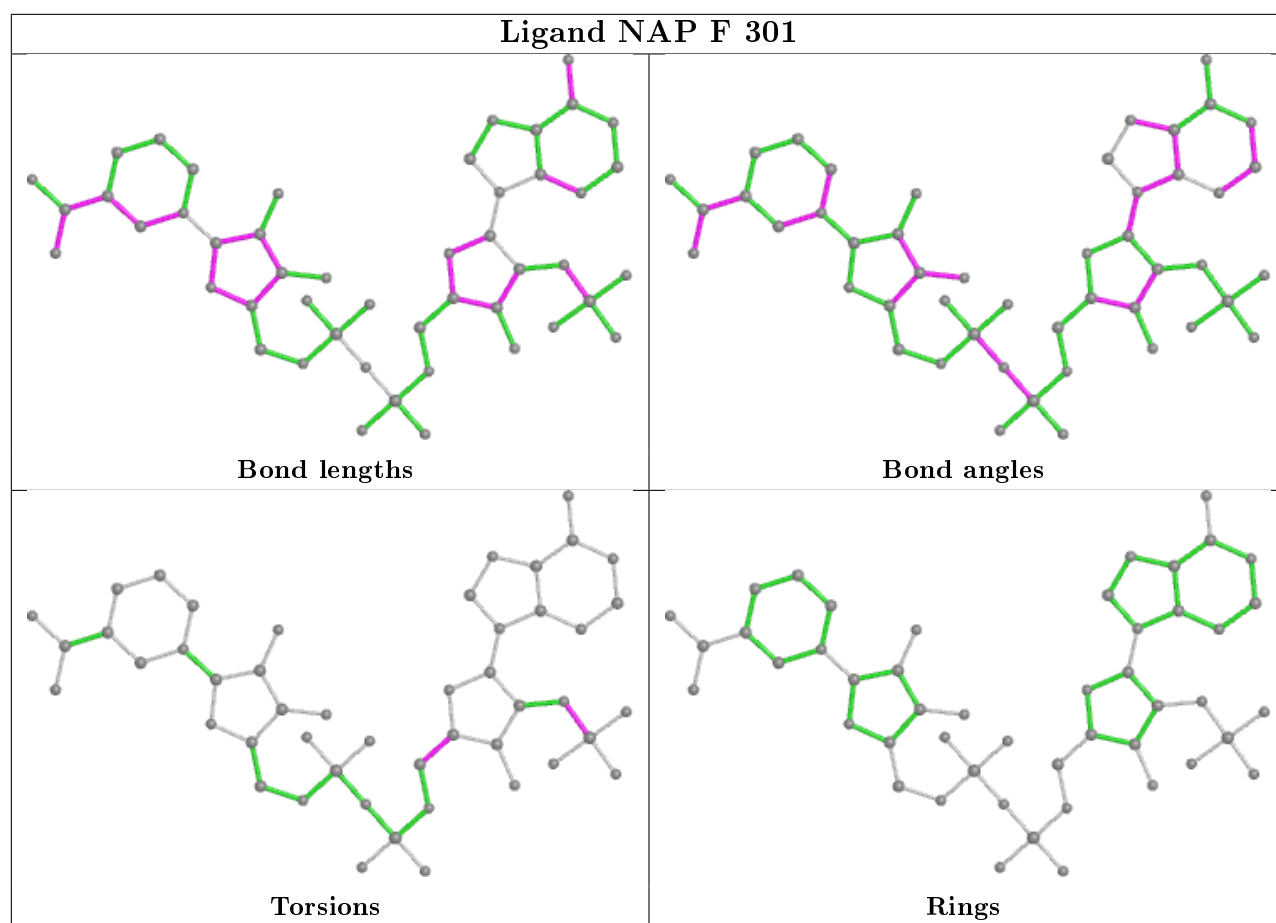


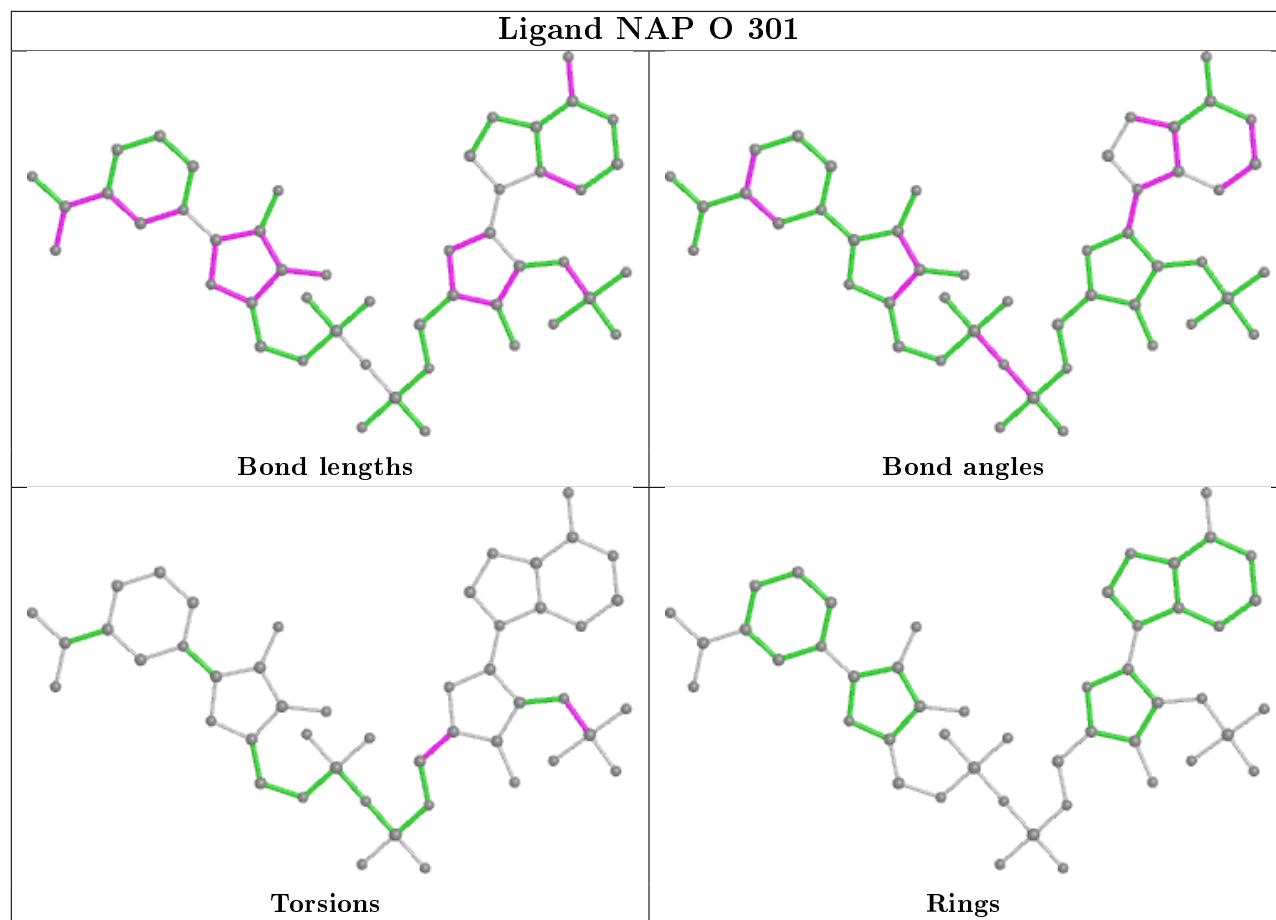


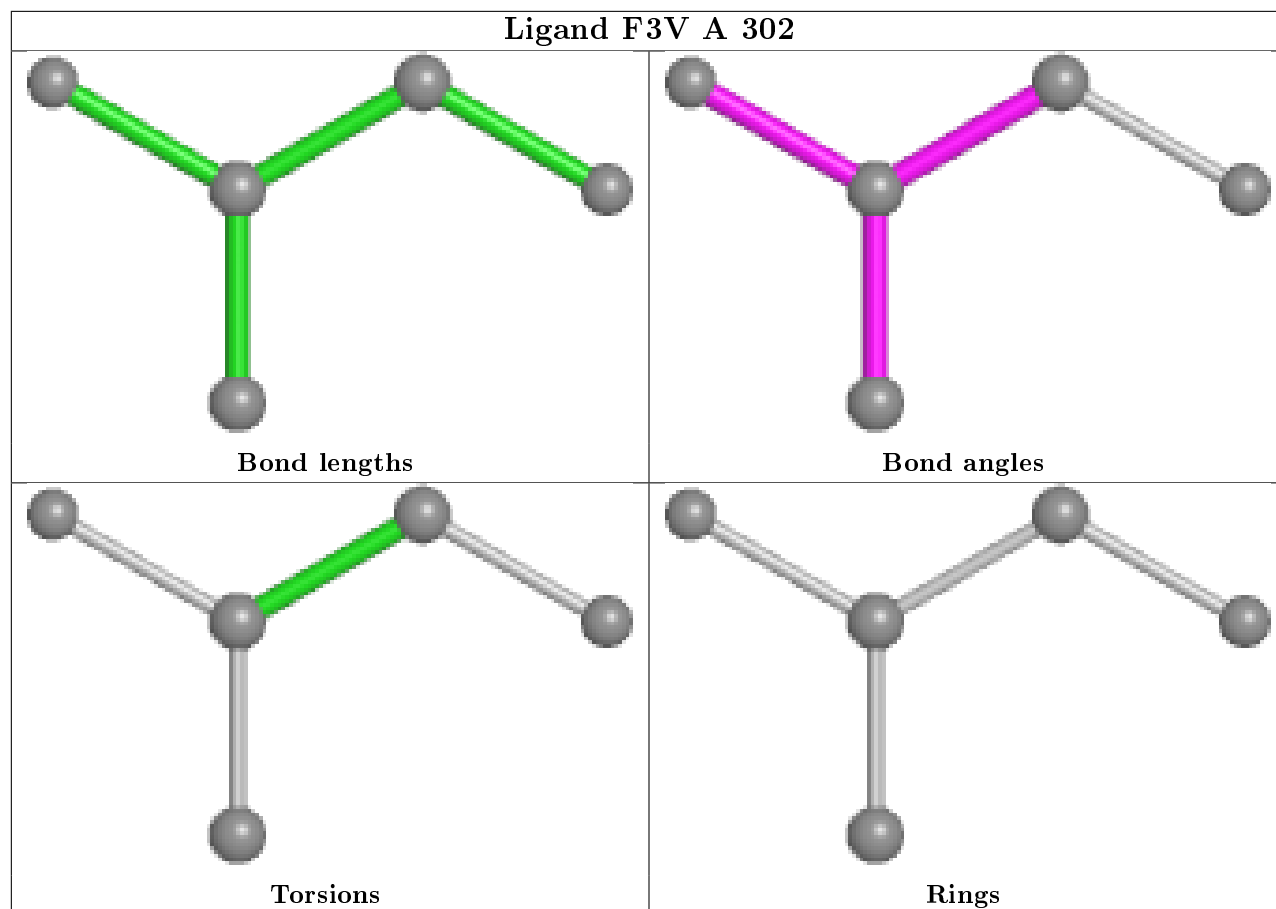


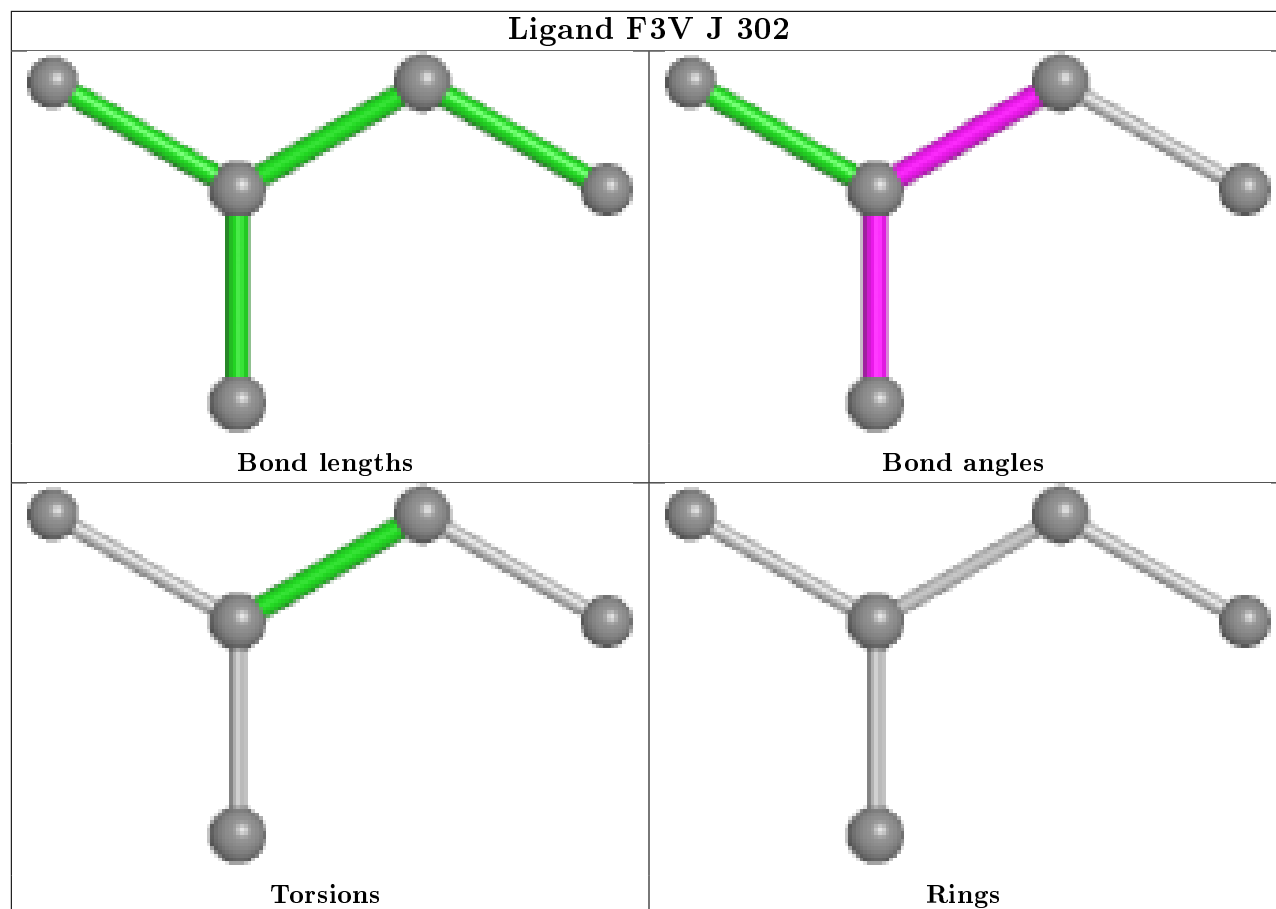


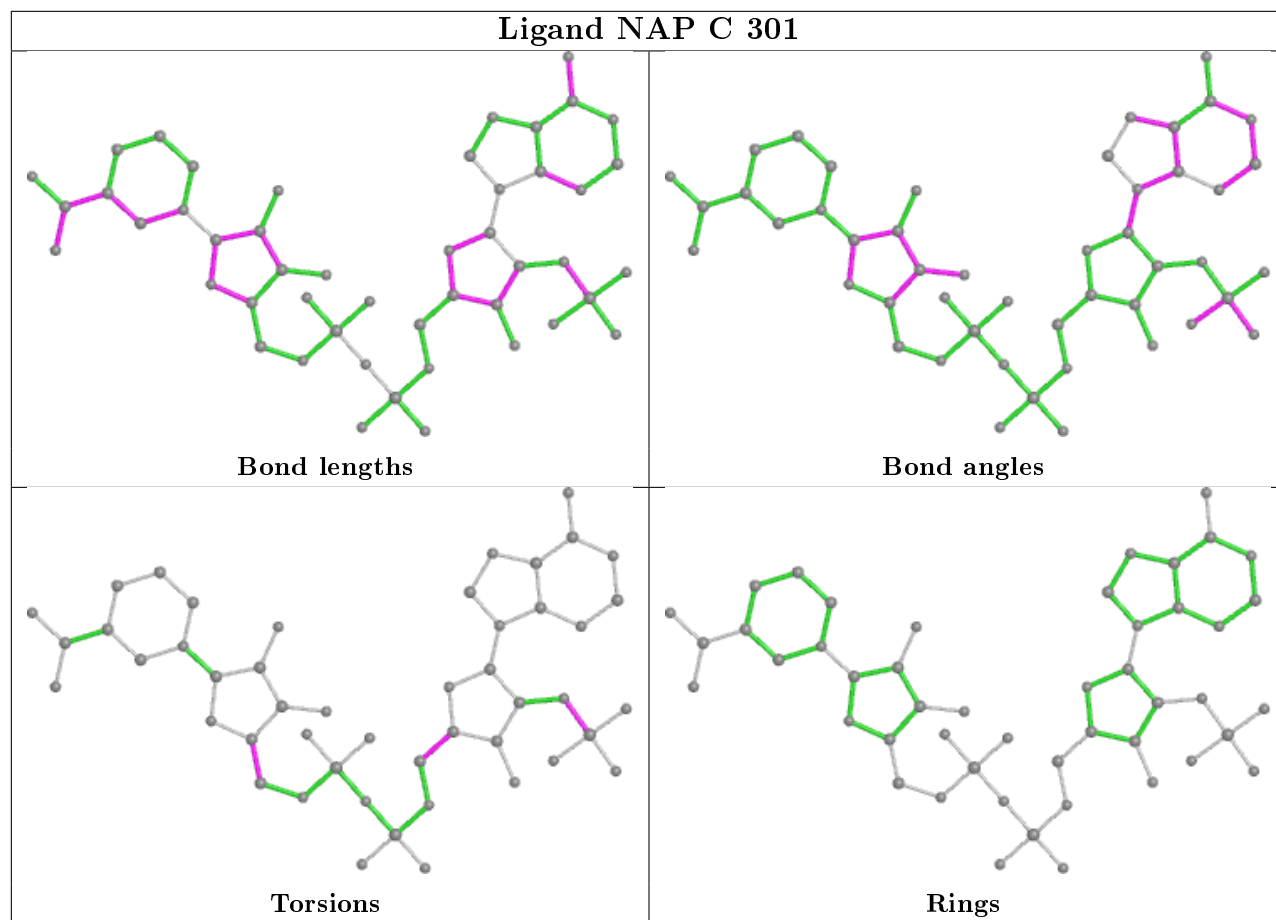


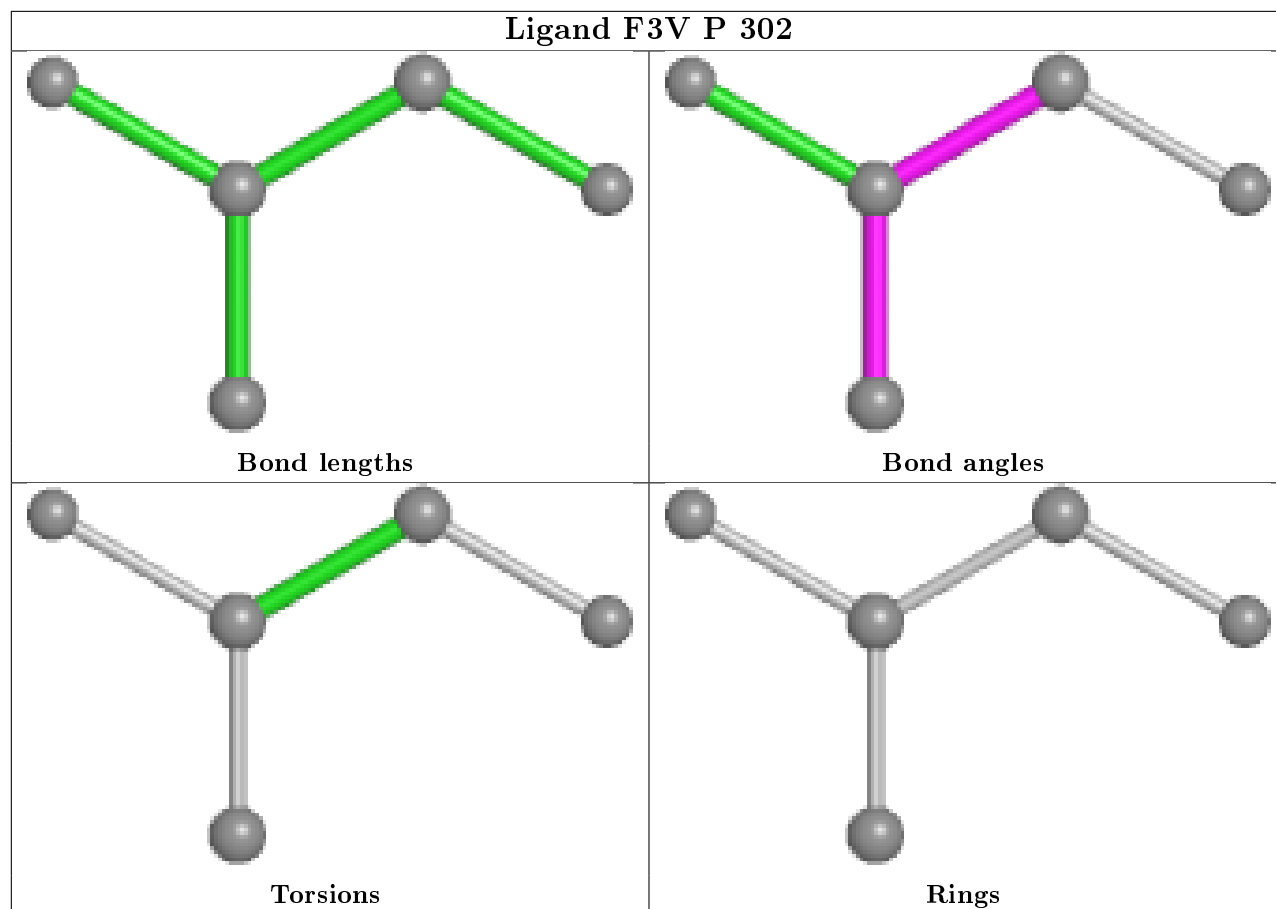


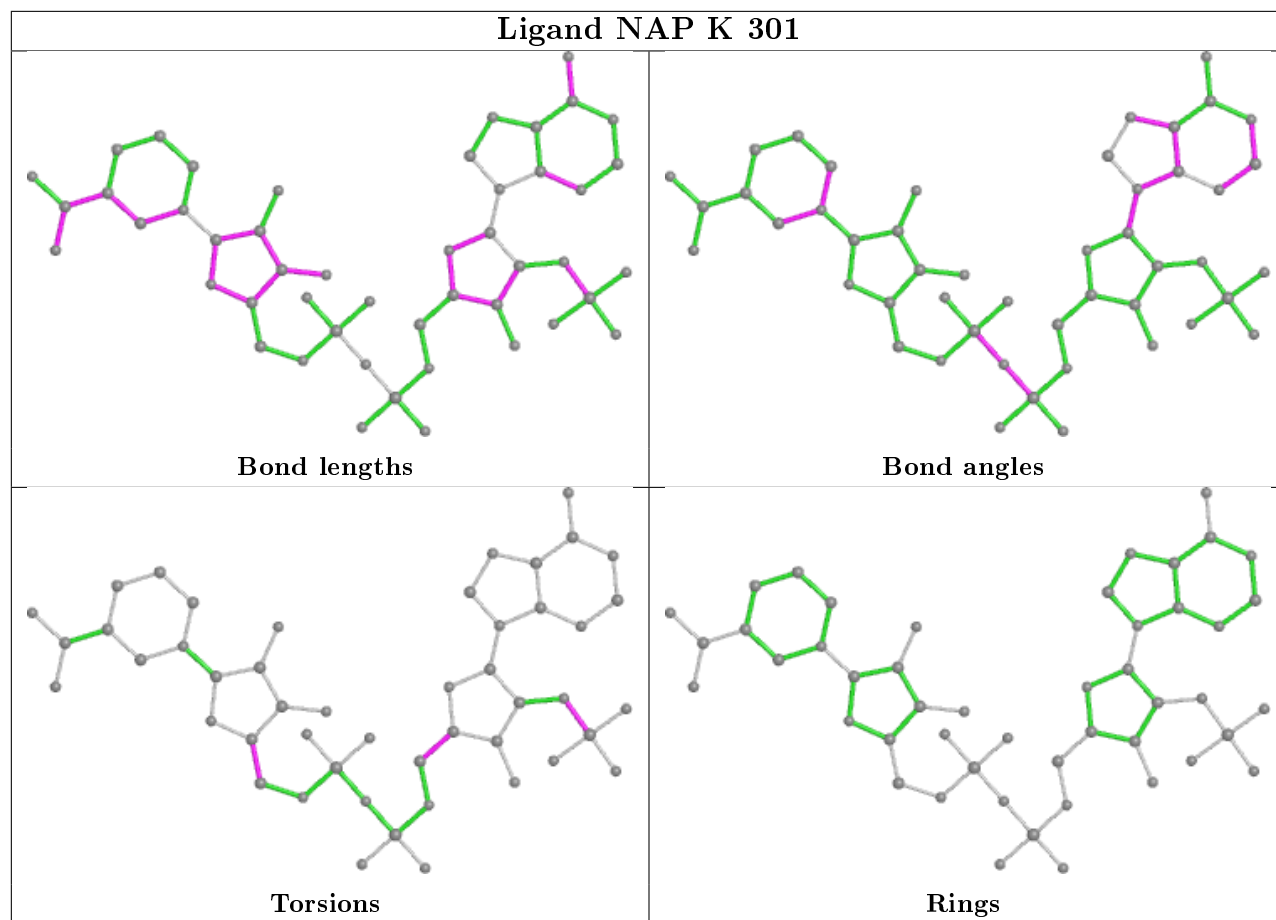


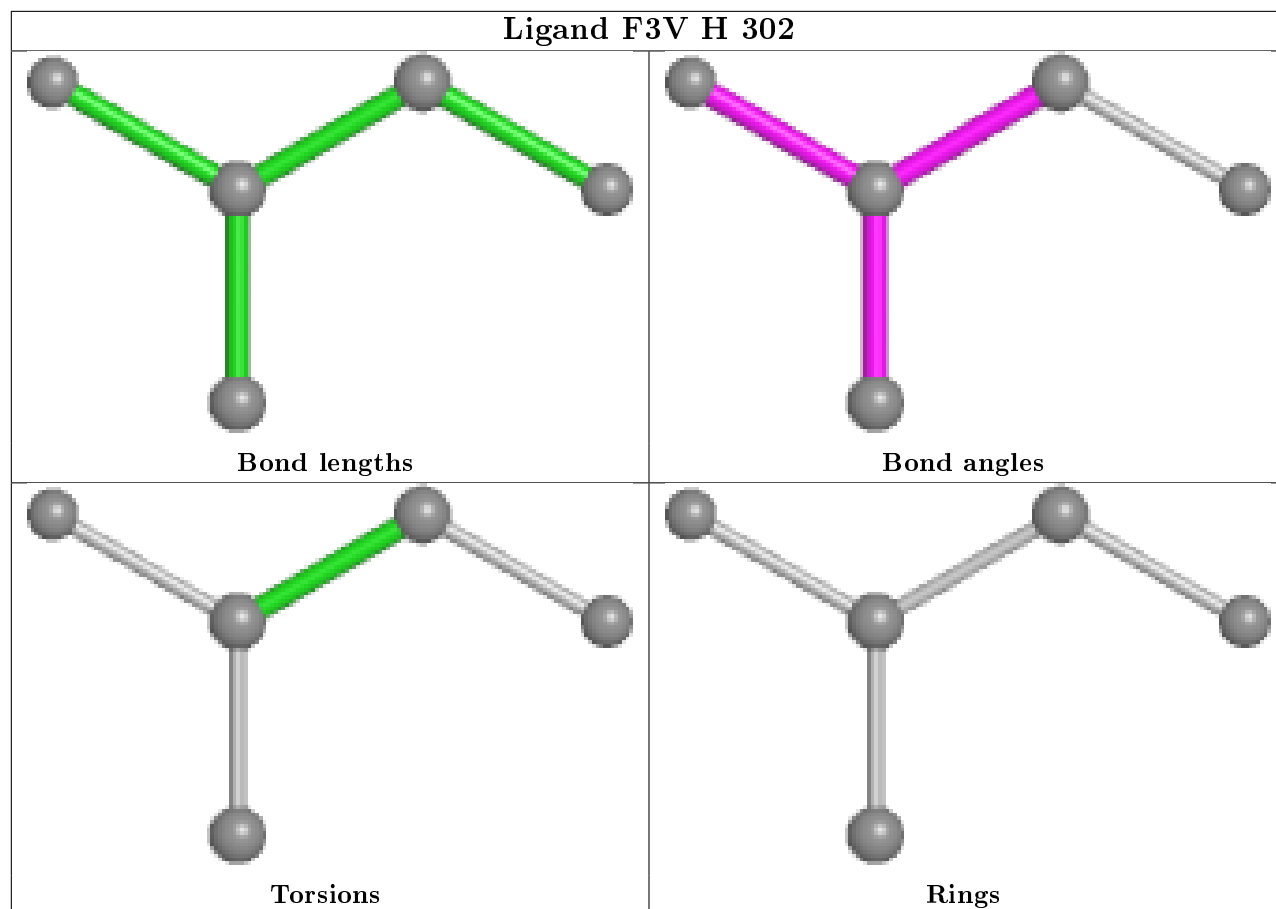


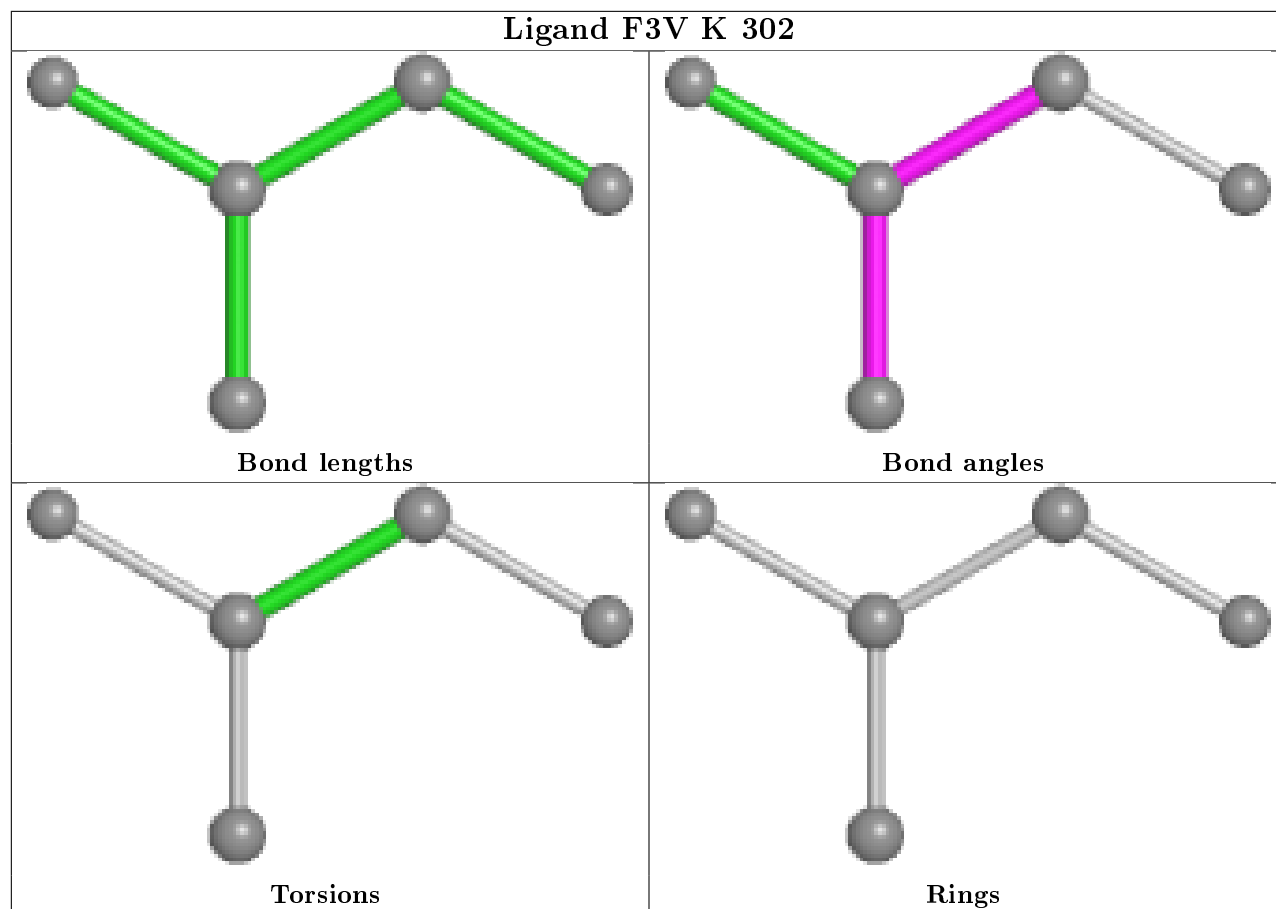


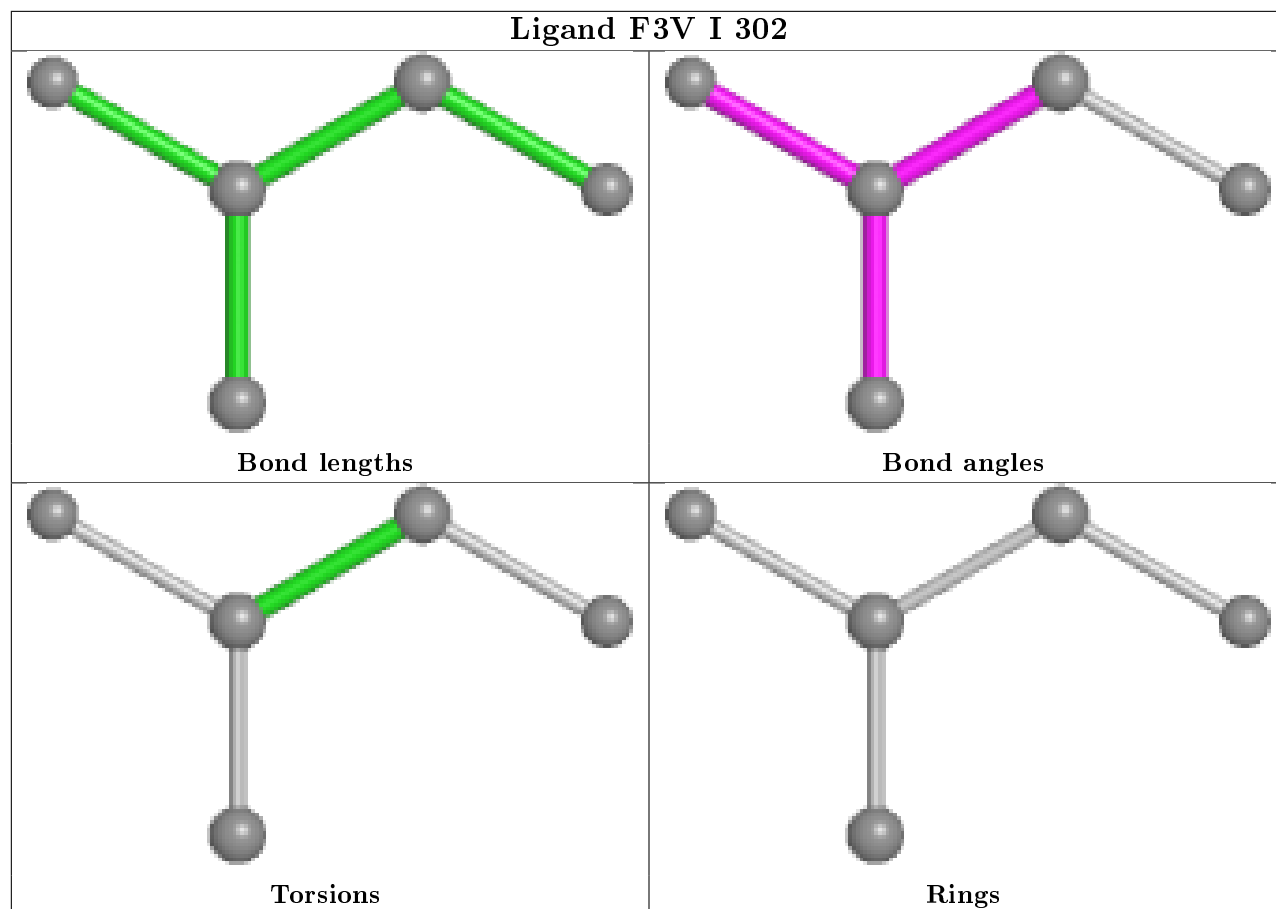


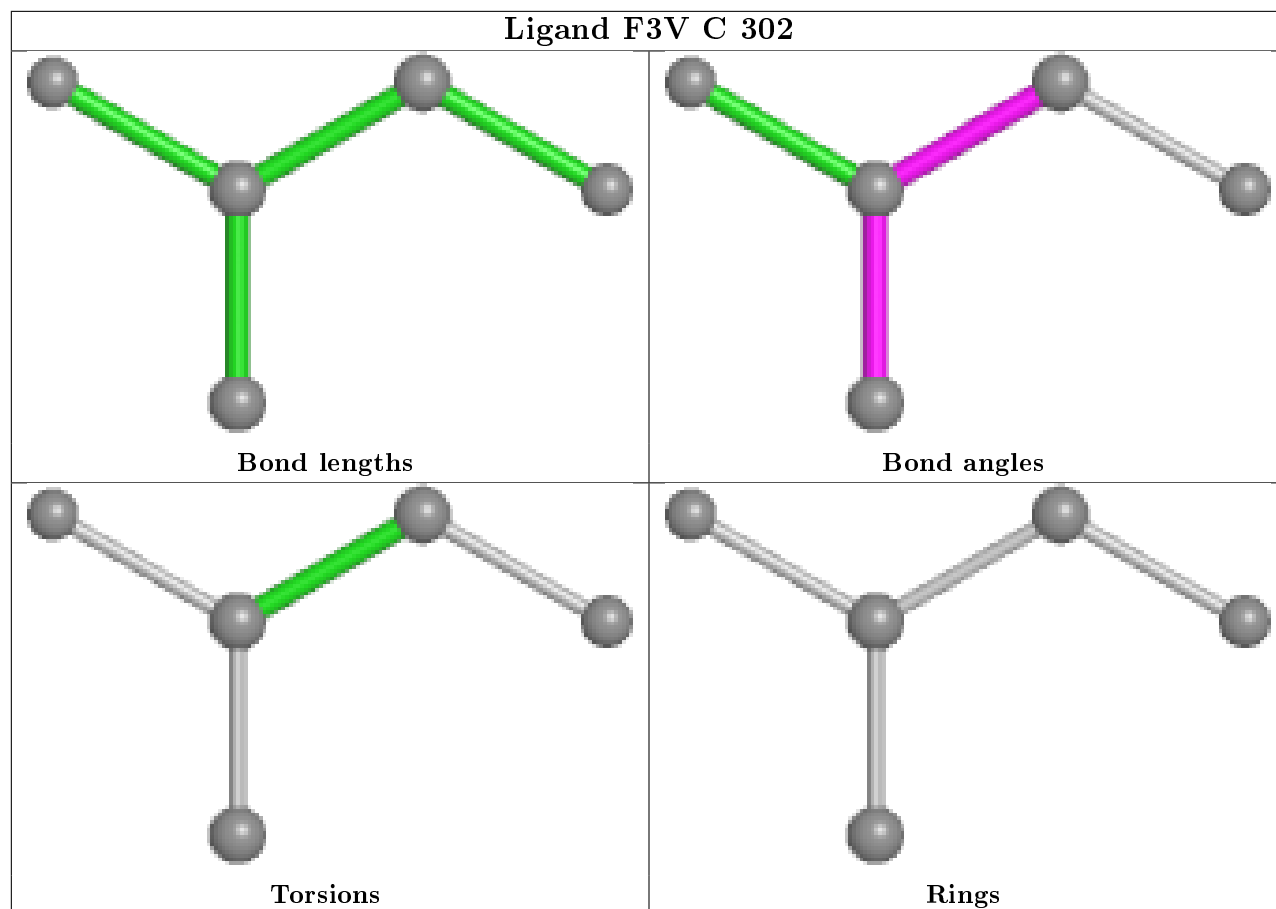


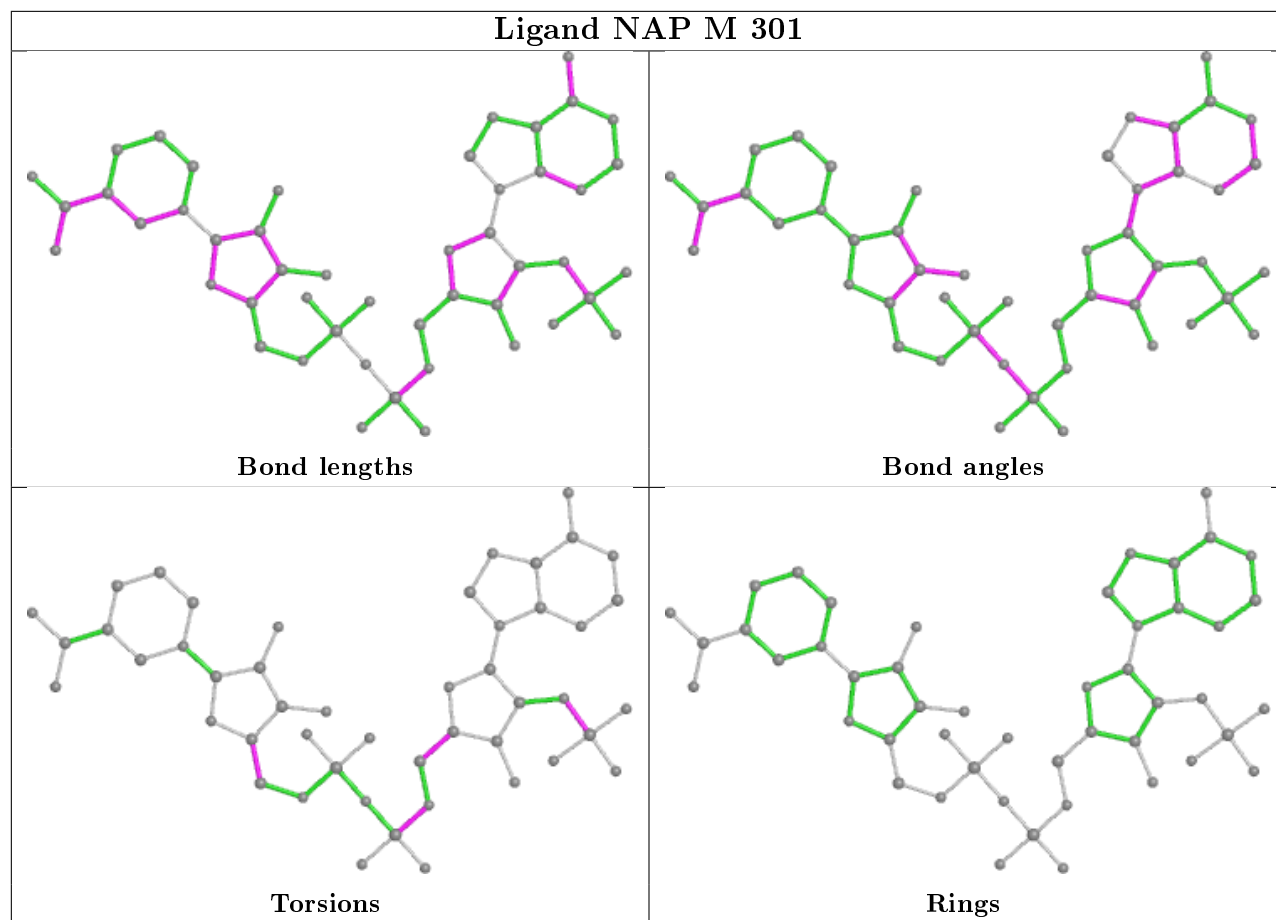


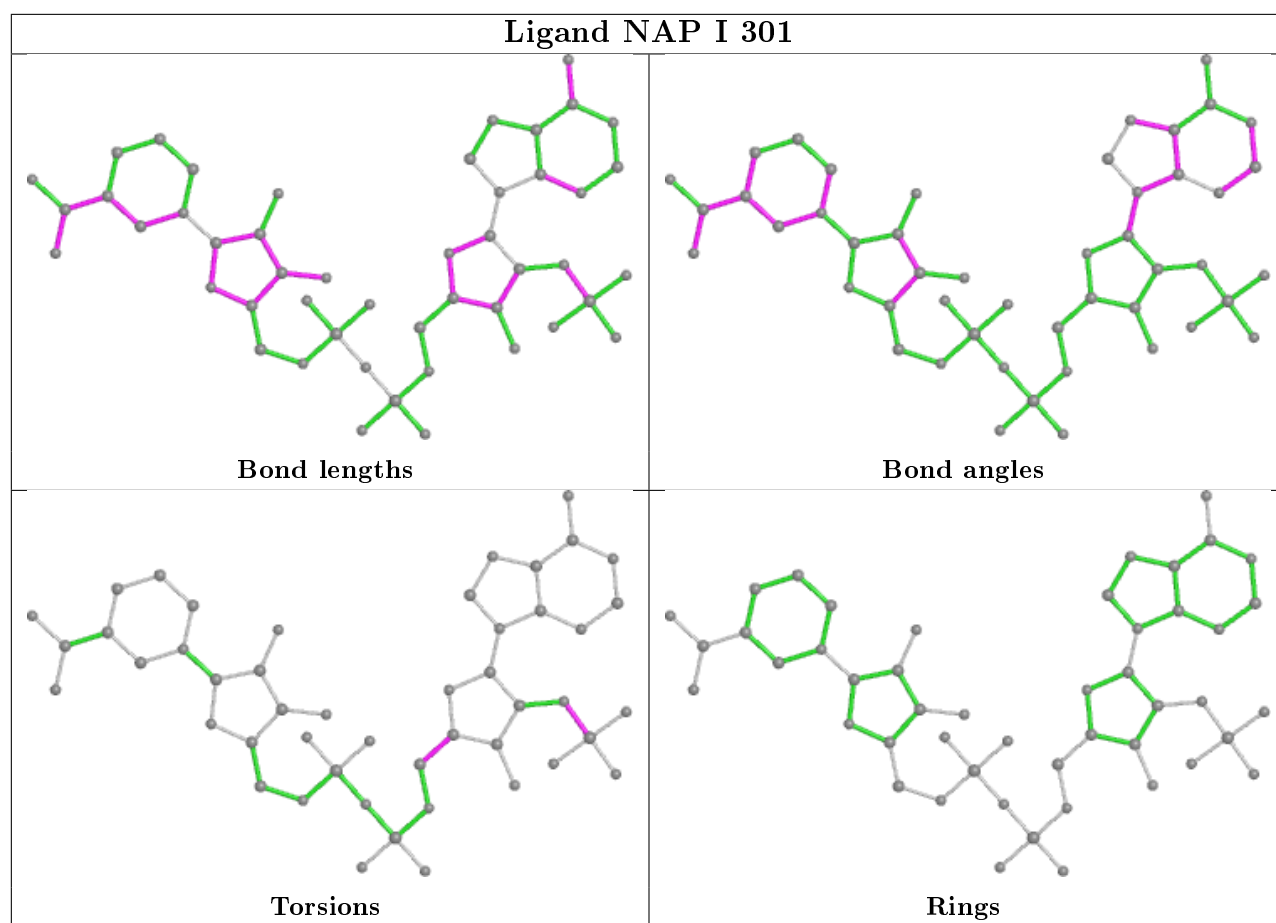


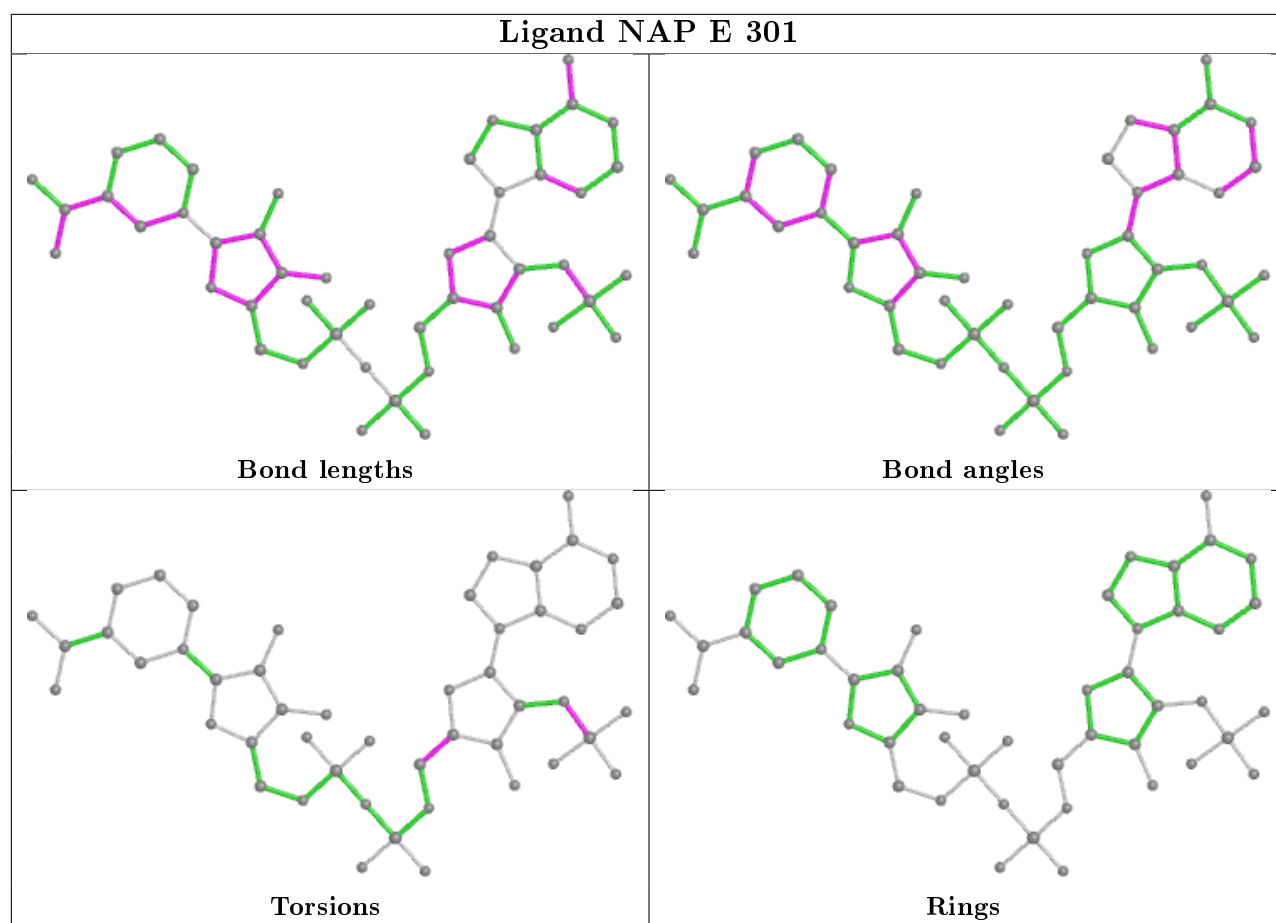


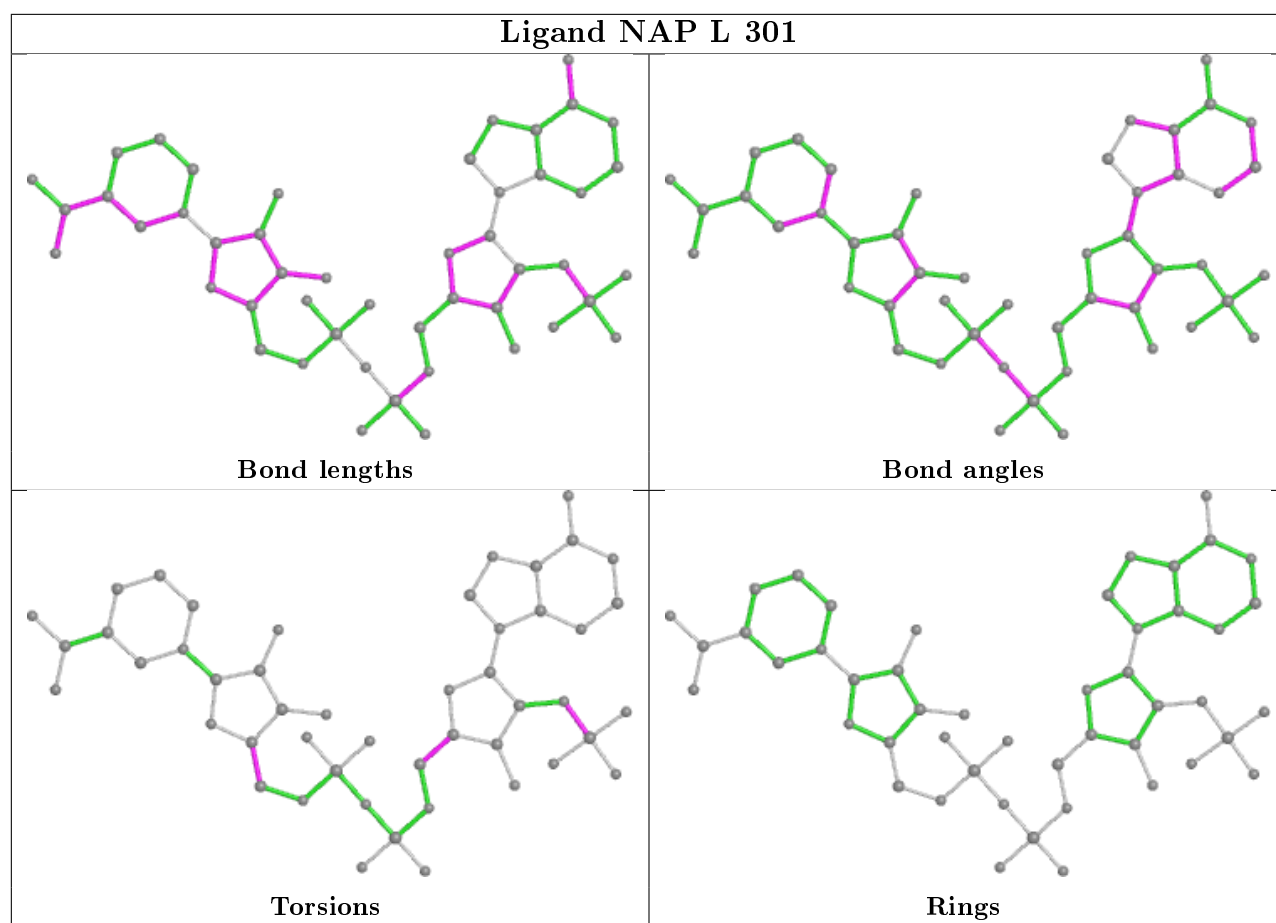


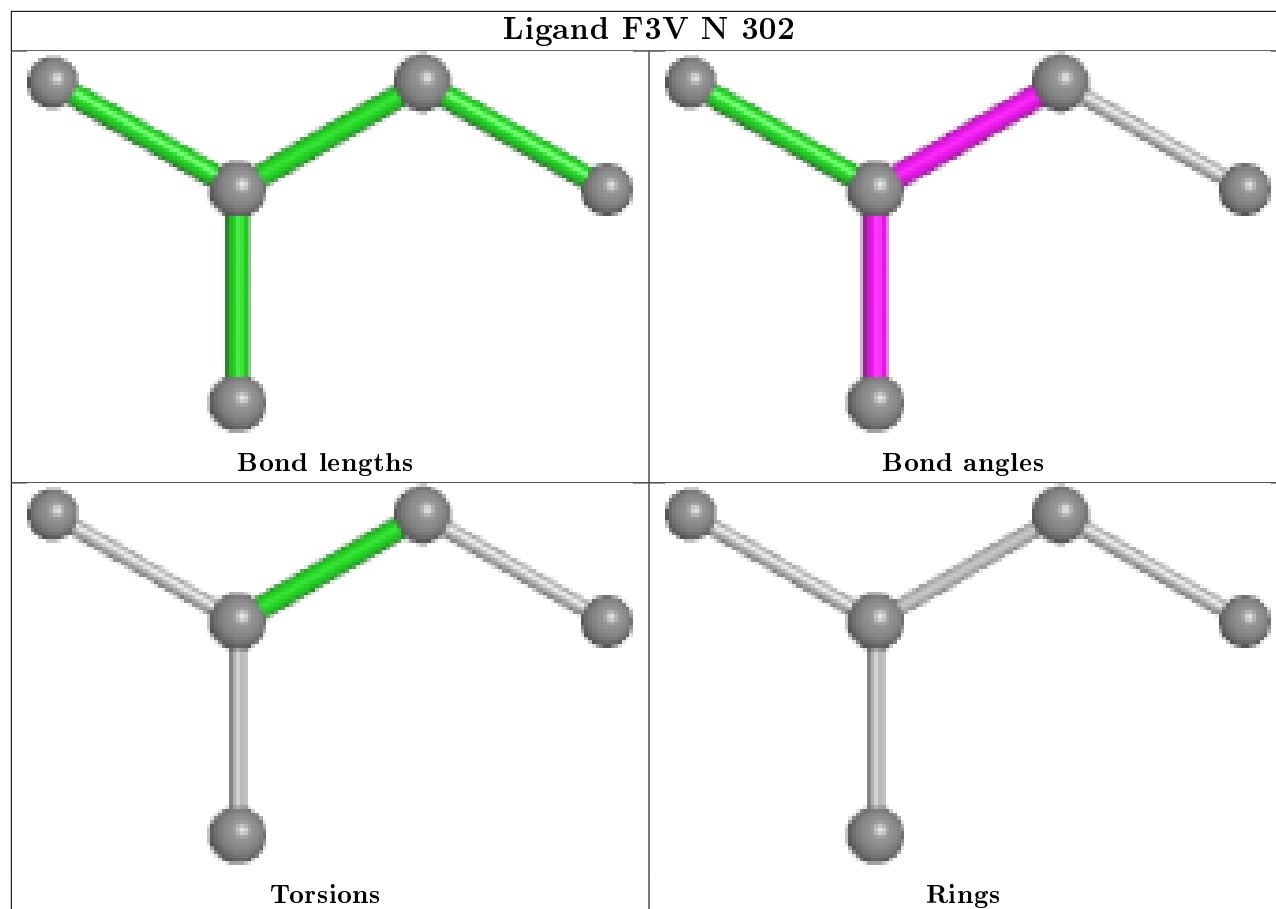


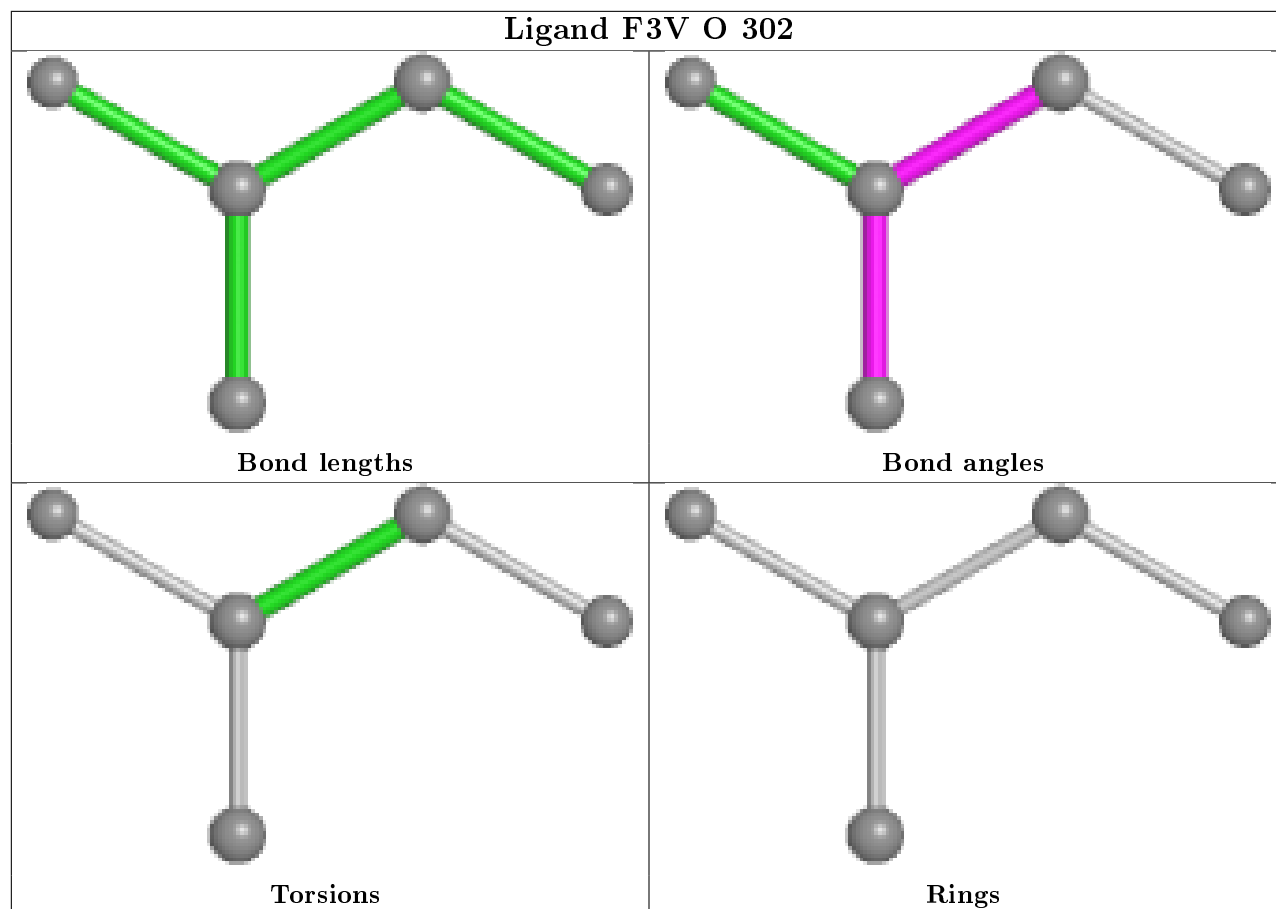


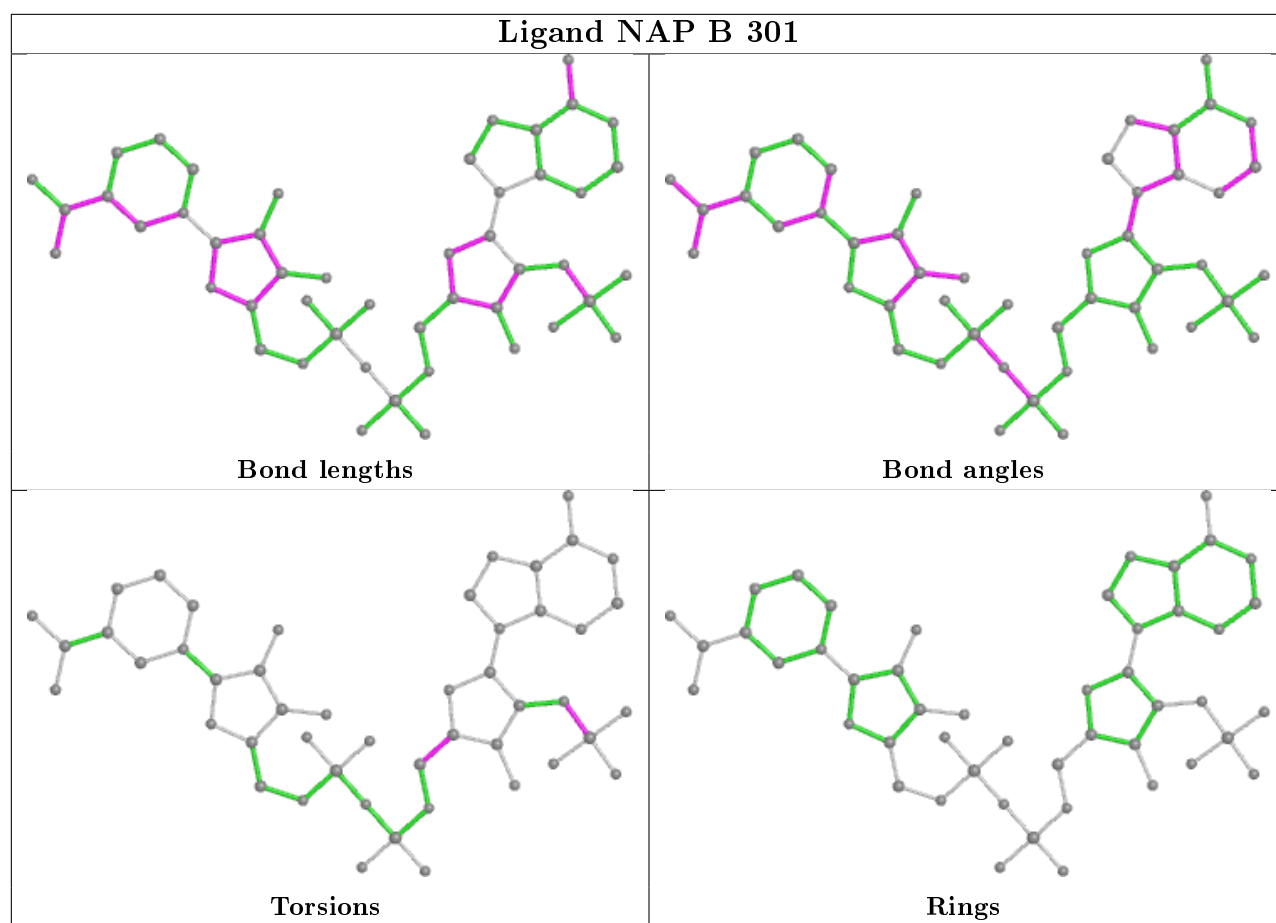


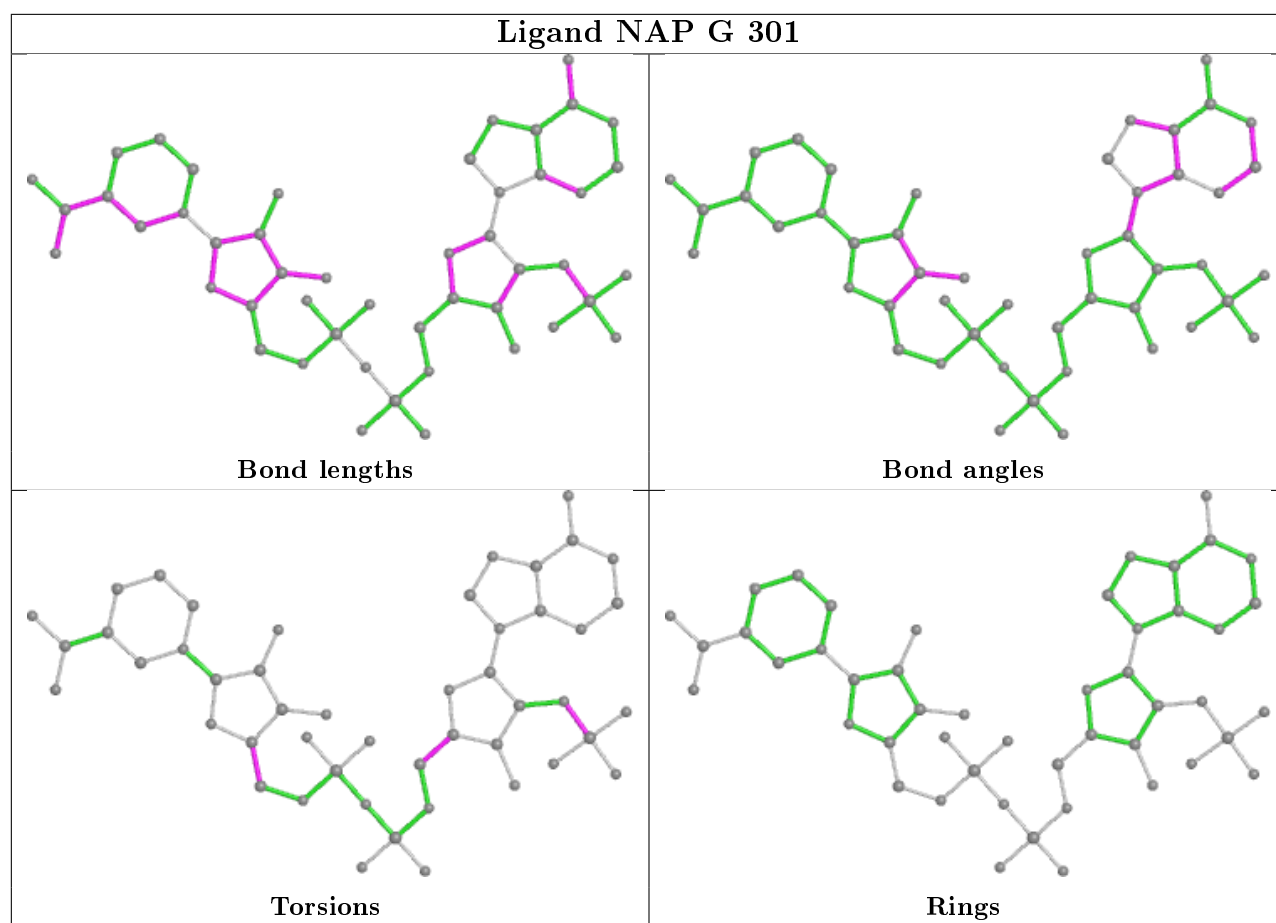


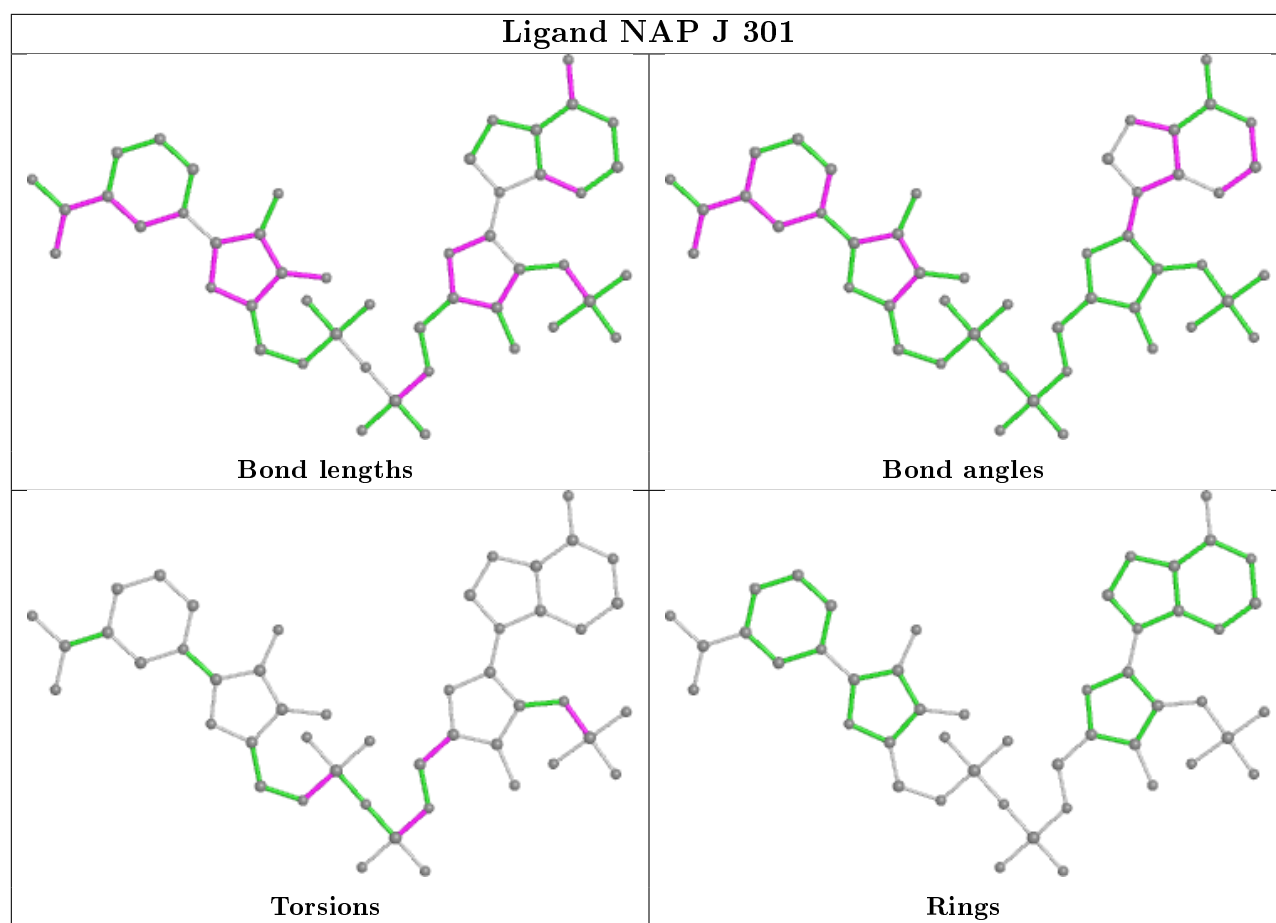


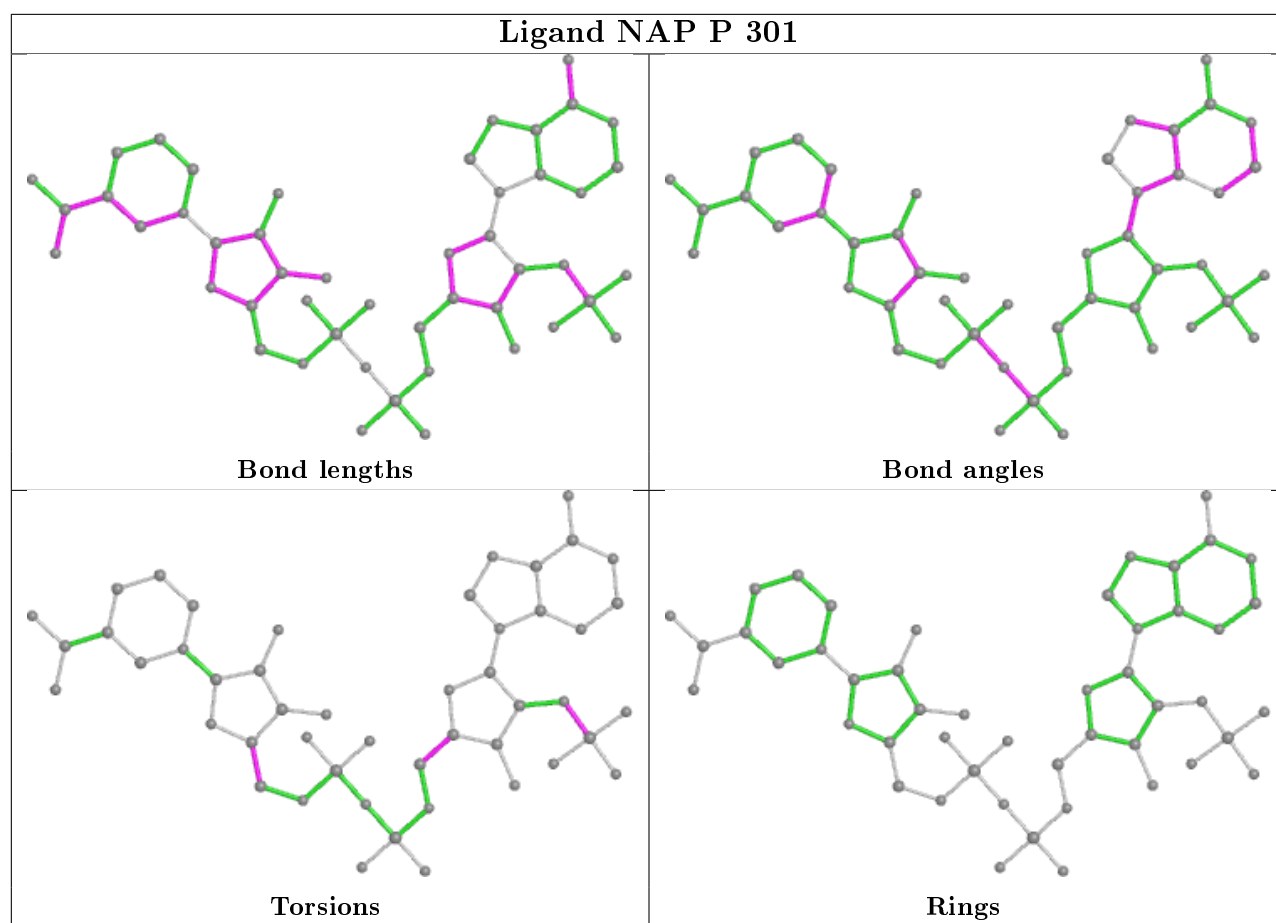


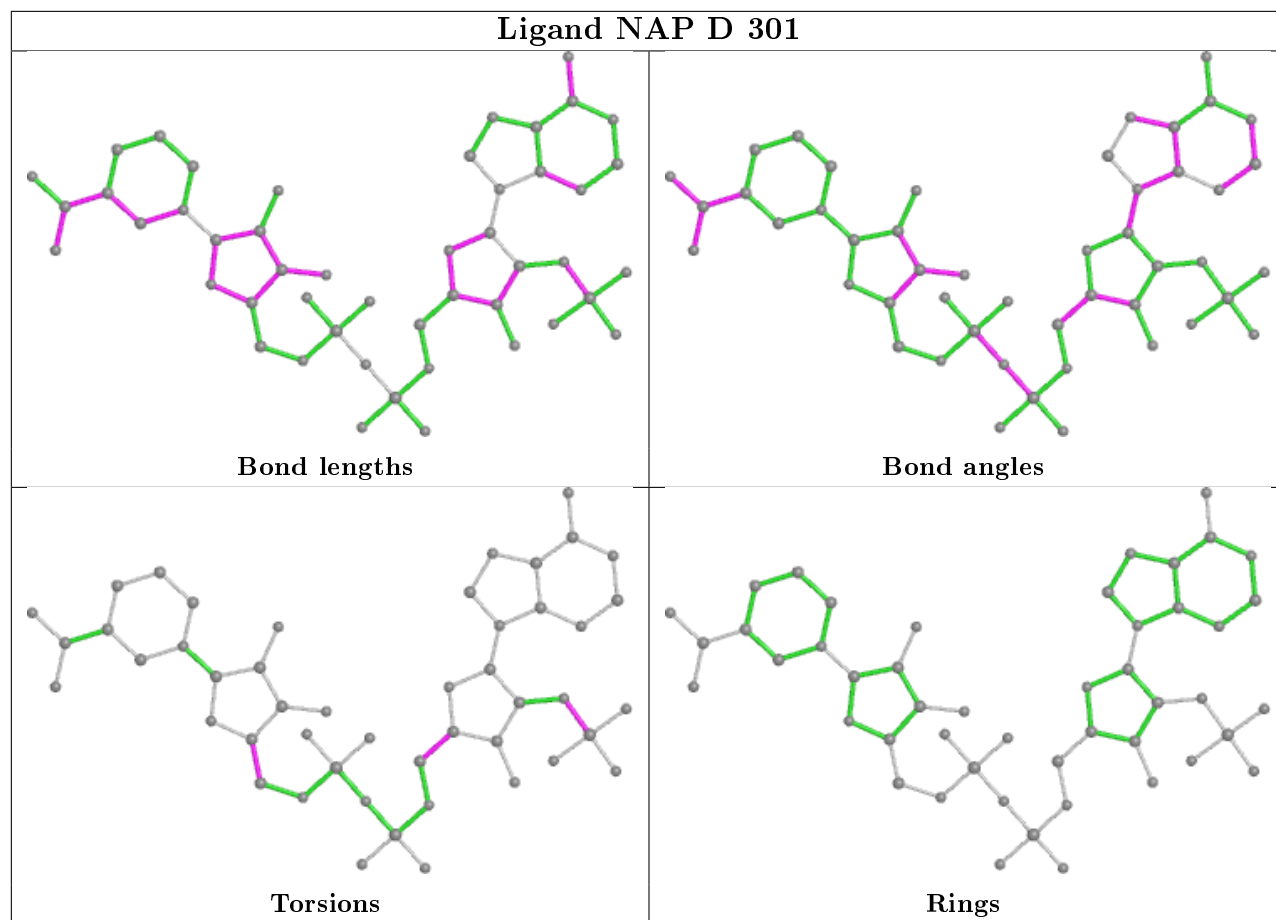












5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	256/259 (98%)	-0.02	14 (5%) 25 28	13, 26, 67, 97	0
1	B	255/259 (98%)	0.12	15 (5%) 22 25	18, 33, 67, 102	0
1	C	258/259 (99%)	0.22	13 (5%) 28 32	19, 32, 51, 81	0
1	D	259/259 (100%)	0.27	8 (3%) 49 51	18, 34, 50, 84	0
1	E	255/259 (98%)	-0.00	4 (1%) 72 74	17, 31, 54, 67	0
1	F	254/259 (98%)	0.14	11 (4%) 35 38	16, 28, 56, 79	0
1	G	256/259 (98%)	0.34	19 (7%) 14 16	20, 35, 61, 71	0
1	H	253/259 (97%)	0.01	3 (1%) 79 81	18, 30, 49, 63	0
1	I	258/259 (99%)	0.32	13 (5%) 28 32	27, 43, 67, 81	0
1	J	257/259 (99%)	0.59	20 (7%) 13 14	29, 44, 72, 105	0
1	K	255/259 (98%)	0.48	28 (10%) 5 6	27, 47, 79, 106	0
1	L	253/259 (97%)	0.22	12 (4%) 31 34	28, 41, 66, 82	0
1	M	256/259 (98%)	0.54	29 (11%) 5 5	27, 45, 81, 110	0
1	N	254/259 (98%)	0.19	10 (3%) 39 42	29, 47, 67, 79	0
1	O	253/259 (97%)	0.31	11 (4%) 35 38	30, 45, 64, 76	0
1	P	255/259 (98%)	0.51	22 (8%) 10 12	29, 42, 67, 93	0
All	All	4087/4144 (98%)	0.26	232 (5%) 23 26	13, 38, 66, 110	0

All (232) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	J	254	LEU	12.3
1	D	254	LEU	11.4
1	B	203	LEU	11.3
1	J	253	HIS	8.5
1	K	205	GLN	8.5

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Mol	Chain	Res	Type	RSRZ
1	I	254	LEU	8.3
1	K	203	LEU	8.1
1	M	203	LEU	8.0
1	J	255	ALA	7.8
1	M	198	MET	7.1
1	G	203	LEU	6.9
1	I	257	ALA	6.7
1	C	256	ILE	6.4
1	D	255	ALA	6.3
1	C	254	LEU	6.2
1	M	197	GLU	6.0
1	K	128	GLN	5.9
1	H	0	HIS	5.7
1	M	206	MET	5.6
1	A	203	LEU	5.5
1	M	205	GLN	5.5
1	M	194	GLY	5.4
1	M	254	LEU	5.3
1	C	253	HIS	5.2
1	P	203	LEU	5.2
1	I	256	ILE	5.2
1	D	257	ALA	5.1
1	I	253	HIS	5.1
1	A	254	LEU	5.0
1	K	-1	SER	4.9
1	K	197	GLU	4.8
1	L	203	LEU	4.8
1	O	253	HIS	4.8
1	B	198	MET	4.7
1	O	49	ALA	4.7
1	G	201	ASP	4.6
1	J	0	HIS	4.6
1	F	203	LEU	4.6
1	M	201	ASP	4.5
1	J	256	ILE	4.5
1	K	195	LEU	4.4
1	B	197	GLU	4.4
1	G	254	LEU	4.4
1	M	-1	SER	4.3
1	C	255	ALA	4.3
1	I	0	HIS	4.2
1	M	196	ASP	4.0

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Mol	Chain	Res	Type	RSRZ
1	J	49	ALA	3.9
1	A	201	ASP	3.9
1	C	-1	SER	3.9
1	D	256	ILE	3.8
1	J	52	SER	3.8
1	B	195	LEU	3.8
1	M	202	TYR	3.7
1	E	-1	SER	3.7
1	G	194	GLY	3.7
1	E	203	LEU	3.7
1	N	201	ASP	3.6
1	E	253	HIS	3.6
1	I	255	ALA	3.5
1	K	206	MET	3.5
1	K	194	GLY	3.5
1	B	194	GLY	3.5
1	M	42	ASP	3.4
1	I	53	GLY	3.4
1	A	193	GLU	3.4
1	P	46	ARG	3.4
1	B	200	GLN	3.4
1	P	148	ILE	3.3
1	F	197	GLU	3.3
1	M	200	GLN	3.3
1	A	-1	SER	3.2
1	K	52	SER	3.2
1	P	79	VAL	3.2
1	J	80	SER	3.2
1	G	199	GLY	3.2
1	J	55	ARG	3.1
1	G	197	GLU	3.1
1	K	42	ASP	3.1
1	J	53	GLY	3.1
1	J	57	LYS	3.1
1	I	46	ARG	3.1
1	D	-1	SER	3.1
1	K	48	VAL	3.1
1	M	148	ILE	3.1
1	A	202	TYR	3.1
1	P	53	GLY	3.0
1	C	53	GLY	3.0
1	P	127	LEU	3.0

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Mol	Chain	Res	Type	RSRZ
1	C	0	HIS	3.0
1	M	195	LEU	3.0
1	E	0	HIS	3.0
1	F	201	ASP	3.0
1	L	186	LEU	3.0
1	G	49	ALA	3.0
1	K	201	ASP	3.0
1	N	203	LEU	2.9
1	M	46	ARG	2.9
1	P	76	ALA	2.9
1	J	54	THR	2.9
1	H	201	ASP	2.9
1	M	193	GLU	2.9
1	B	0	HIS	2.9
1	B	206	MET	2.9
1	A	205	GLN	2.9
1	J	200	GLN	2.9
1	L	204	ASP	2.9
1	K	202	TYR	2.8
1	M	56	GLY	2.8
1	A	200	GLN	2.8
1	G	202	TYR	2.8
1	J	79	VAL	2.8
1	L	201	ASP	2.8
1	J	148	ILE	2.8
1	L	46	ARG	2.8
1	P	52	SER	2.8
1	M	140	VAL	2.8
1	N	49	ALA	2.7
1	P	47	THR	2.7
1	G	165	LEU	2.7
1	G	204	ASP	2.7
1	B	205	GLN	2.7
1	C	52	SER	2.7
1	K	0	HIS	2.7
1	D	42	ASP	2.7
1	D	0	HIS	2.7
1	K	204	ASP	2.7
1	J	46	ARG	2.7
1	N	46	ARG	2.7
1	N	253	HIS	2.7
1	C	55	ARG	2.6

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Mol	Chain	Res	Type	RSRZ
1	M	253	HIS	2.6
1	K	51	LEU	2.6
1	P	165	LEU	2.6
1	A	206	MET	2.6
1	B	254	LEU	2.6
1	G	195	LEU	2.6
1	O	54	THR	2.6
1	A	194	GLY	2.6
1	I	148	ILE	2.6
1	K	193	GLU	2.6
1	G	148	ILE	2.6
1	A	89	CYS	2.6
1	G	196	ASP	2.6
1	K	168	LEU	2.5
1	P	241	LEU	2.5
1	A	253	HIS	2.5
1	G	0	HIS	2.5
1	I	165	LEU	2.5
1	P	128	GLN	2.5
1	K	43	ASP	2.5
1	L	199	GLY	2.5
1	B	204	ASP	2.5
1	G	-1	SER	2.5
1	C	242	VAL	2.5
1	F	46	ARG	2.5
1	J	186	LEU	2.5
1	O	202	TYR	2.5
1	K	208	SER	2.5
1	F	242	VAL	2.5
1	C	200	GLN	2.5
1	F	42	ASP	2.5
1	I	203	LEU	2.5
1	B	199	GLY	2.4
1	L	57	LYS	2.4
1	M	49	ALA	2.4
1	B	196	ASP	2.4
1	N	197	GLU	2.4
1	L	208	SER	2.4
1	N	132	ALA	2.4
1	G	198	MET	2.4
1	P	197	GLU	2.4
1	F	49	ALA	2.4

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Mol	Chain	Res	Type	RSRZ
1	P	196	ASP	2.4
1	G	253	HIS	2.4
1	F	140	VAL	2.4
1	L	55	ARG	2.3
1	A	198	MET	2.3
1	O	148	ILE	2.3
1	O	69	GLU	2.3
1	K	76	ALA	2.3
1	K	46	ARG	2.3
1	K	62	ARG	2.3
1	O	58	VAL	2.3
1	M	63	ALA	2.3
1	P	132	ALA	2.3
1	N	69	GLU	2.3
1	P	44	LEU	2.3
1	J	48	VAL	2.3
1	O	240	THR	2.3
1	C	165	LEU	2.3
1	M	241	LEU	2.3
1	B	46	ARG	2.3
1	H	53	GLY	2.2
1	M	142	SER	2.2
1	P	84	GLY	2.2
1	P	202	TYR	2.2
1	O	71	ALA	2.2
1	L	52	SER	2.2
1	J	128	GLN	2.2
1	N	200	GLN	2.2
1	L	42	ASP	2.2
1	F	142	SER	2.2
1	N	53	GLY	2.2
1	M	57	LYS	2.2
1	F	198	MET	2.2
1	M	28	ALA	2.2
1	O	28	ALA	2.2
1	B	201	ASP	2.2
1	G	205	GLN	2.2
1	M	242	VAL	2.2
1	C	186	LEU	2.1
1	I	197	GLU	2.1
1	L	200	GLN	2.1
1	A	204	ASP	2.1

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Mol	Chain	Res	Type	RSRZ
1	O	55	ARG	2.1
1	P	0	HIS	2.1
1	P	69	GLU	2.1
1	M	199	GLY	2.1
1	K	242	VAL	2.1
1	K	198	MET	2.0
1	I	42	ASP	2.0
1	M	41	GLN	2.0
1	D	46	ARG	2.0
1	P	68	PRO	2.0
1	F	200	GLN	2.0
1	J	165	LEU	2.0
1	K	144	ILE	2.0
1	G	240	THR	2.0
1	K	240	THR	2.0
1	P	240	THR	2.0
1	K	55	ARG	2.0

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 carbohydrates 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
5	MG	F	304	1/1	0.59	0.11	52,52,52,52	0
5	MG	O	304	1/1	0.70	0.18	45,45,45,45	0
3	F3V	M	302	5/5	0.76	0.15	66,68,68,68	0
5	MG	J	304	1/1	0.79	0.09	42,42,42,42	0
5	MG	H	304	1/1	0.79	0.11	28,28,28,28	0
3	F3V	E	302	5/5	0.83	0.11	25,27,31,33	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
3	F3V	N	302	5/5	0.83	0.11	42,43,44,45	0
3	F3V	B	302	5/5	0.83	0.14	38,42,44,46	0
3	F3V	G	302	5/5	0.84	0.11	39,39,40,41	0
2	NAP	M	301	48/48	0.84	0.13	42,53,62,63	48
4	CL	A	304	1/1	0.86	0.10	82,82,82,82	0
5	MG	M	304	1/1	0.87	0.13	71,71,71,71	0
2	NAP	B	301	48/48	0.87	0.13	24,32,41,42	48
3	F3V	I	302	5/5	0.87	0.15	44,44,47,48	0
2	NAP	G	301	48/48	0.87	0.12	19,27,32,32	48
2	NAP	I	301	48/48	0.88	0.12	31,37,43,46	48
5	MG	C	304	1/1	0.88	0.08	24,24,24,24	0
3	F3V	P	302	5/5	0.88	0.19	45,47,49,50	0
2	NAP	K	301	48/48	0.88	0.12	35,38,42,44	48
3	F3V	F	302	5/5	0.89	0.12	35,39,41,42	0
2	NAP	N	301	48/48	0.89	0.11	31,41,51,52	48
2	NAP	P	301	48/48	0.89	0.11	32,35,41,45	48
3	F3V	C	302	5/5	0.90	0.17	24,24,26,26	0
2	NAP	E	301	48/48	0.90	0.11	20,27,32,34	48
2	NAP	L	301	48/48	0.90	0.10	32,45,49,51	0
4	CL	P	303	1/1	0.90	0.14	49,49,49,49	0
4	CL	J	303	1/1	0.90	0.18	56,56,56,56	0
3	F3V	K	302	5/5	0.91	0.12	45,46,48,50	0
2	NAP	F	301	48/48	0.91	0.10	17,32,38,41	48
4	CL	O	303	1/1	0.91	0.08	47,47,47,47	0
3	F3V	D	302	5/5	0.91	0.11	22,23,23,26	0
2	NAP	A	301	48/48	0.91	0.10	16,29,34,36	48
4	CL	E	303	1/1	0.91	0.07	36,36,36,36	0
4	CL	M	303	1/1	0.91	0.15	53,53,53,53	0
2	NAP	D	301	48/48	0.91	0.10	17,22,27,30	0
5	MG	A	305	1/1	0.92	0.04	43,43,43,43	0
4	CL	L	303	1/1	0.92	0.15	52,52,52,52	0
2	NAP	J	301	48/48	0.92	0.11	28,34,36,38	0
3	F3V	L	302	5/5	0.93	0.09	47,50,52,53	0
2	NAP	H	301	48/48	0.93	0.10	12,18,24,25	0
2	NAP	O	301	48/48	0.93	0.09	31,35,42,45	0
5	MG	L	304	1/1	0.93	0.06	66,66,66,66	0
3	F3V	H	302	5/5	0.93	0.14	23,24,24,26	0
4	CL	I	303	1/1	0.93	0.39	65,65,65,65	0
4	CL	F	303	1/1	0.93	0.07	33,33,33,33	0
3	F3V	A	302	5/5	0.93	0.12	35,36,37,37	0
3	F3V	J	302	5/5	0.93	0.13	43,45,45,46	0
4	CL	K	303	1/1	0.93	0.08	57,57,57,57	0

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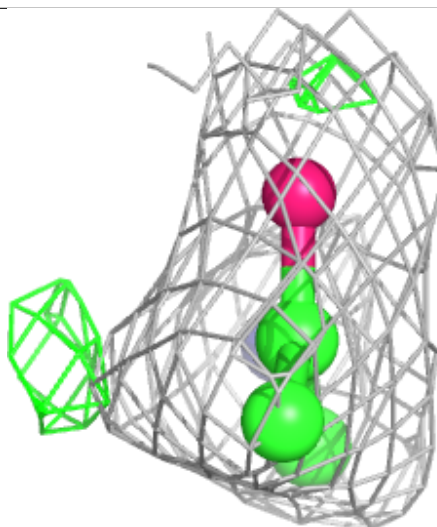
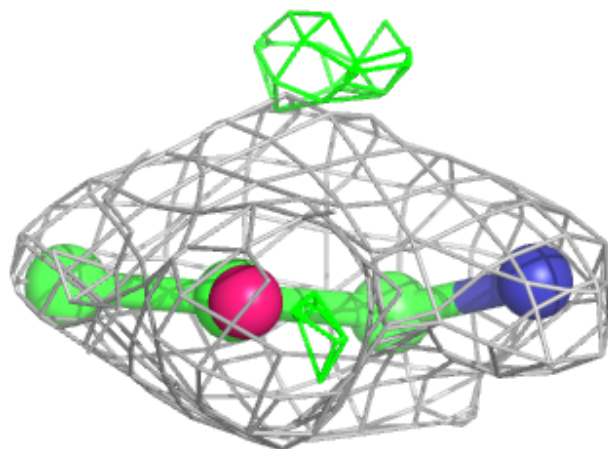
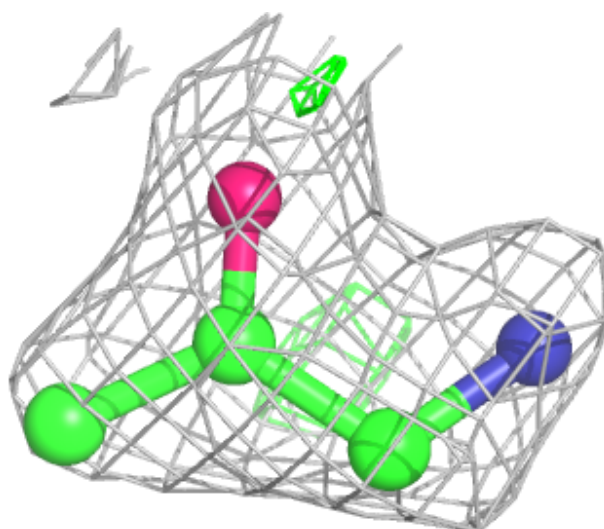
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
2	NAP	C	301	48/48	0.93	0.10	12,19,25,32	0
4	CL	A	303	1/1	0.94	0.07	31,31,31,31	0
4	CL	C	303	1/1	0.94	0.06	31,31,31,31	0
4	CL	N	303	1/1	0.95	0.09	47,47,47,47	0
4	CL	B	303	1/1	0.95	0.09	37,37,37,37	0
3	F3V	O	302	5/5	0.95	0.14	35,35,39,40	0
4	CL	D	303	1/1	0.96	0.06	33,33,33,33	0
4	CL	H	303	1/1	0.96	0.07	34,34,34,34	0
4	CL	G	303	1/1	0.97	0.07	33,33,33,33	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.

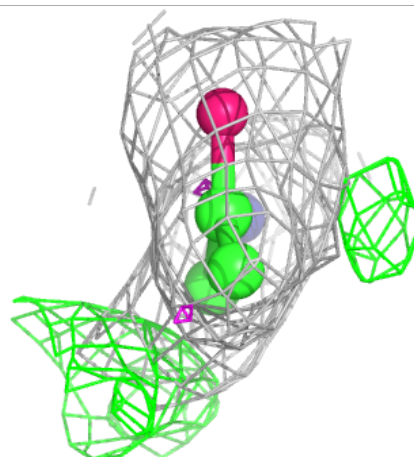
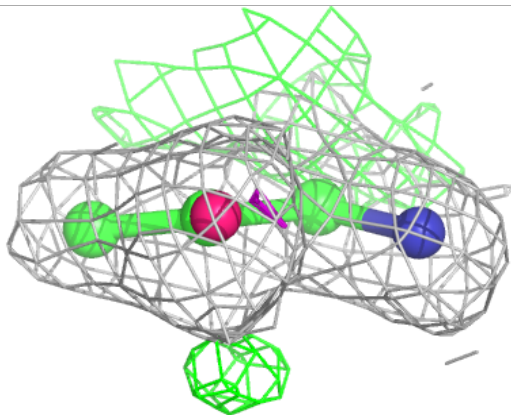
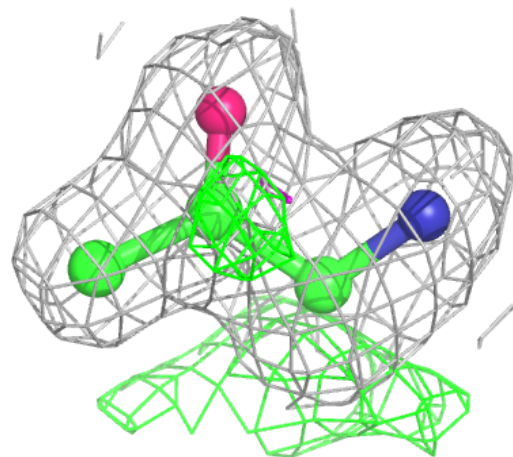
Electron density around F3V M 302:

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



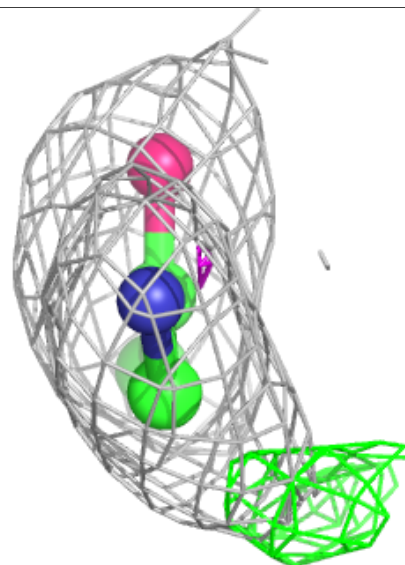
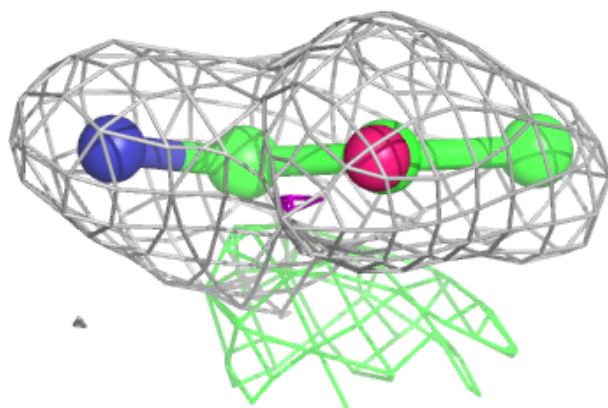
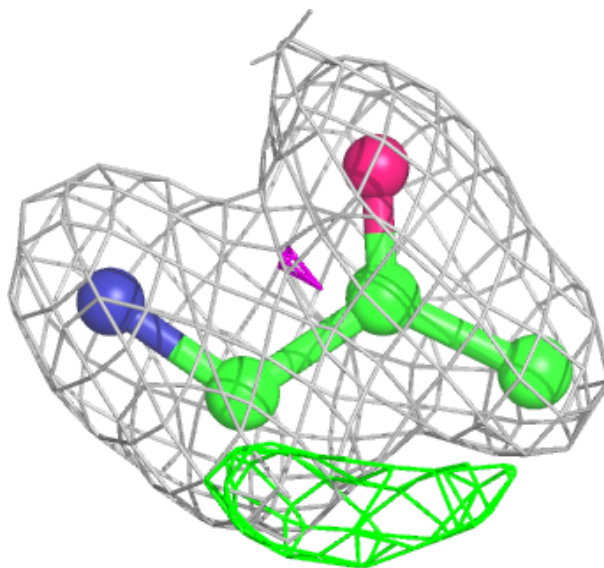
Electron density around F3V E 302:

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



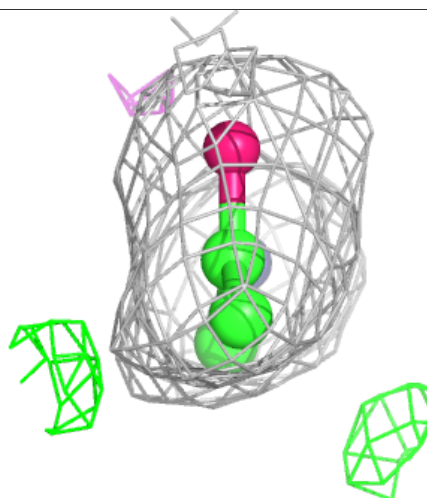
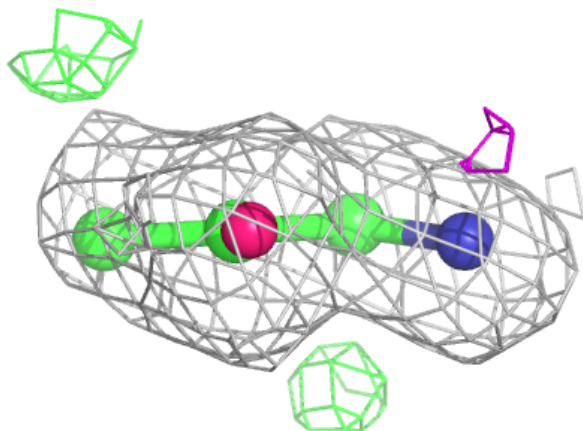
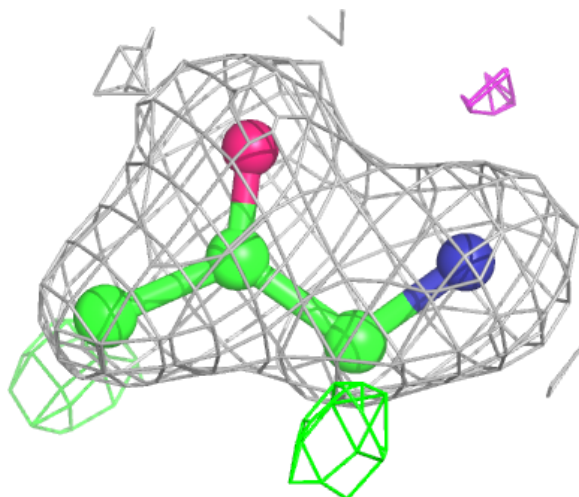
Electron density around F3V N 302:

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



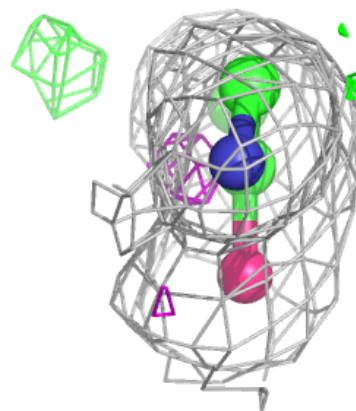
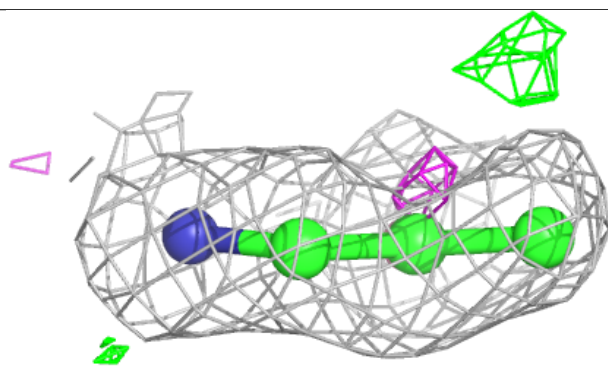
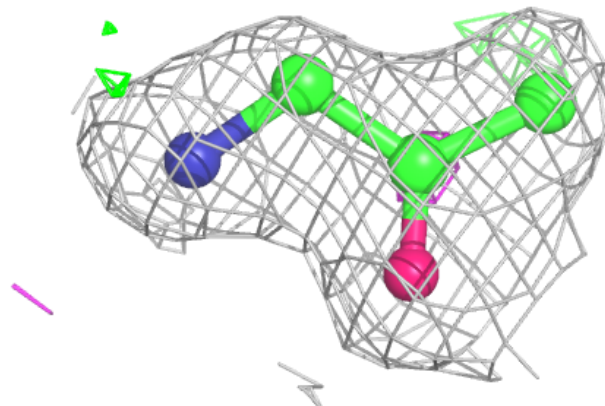
Electron density around F3V B 302:

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



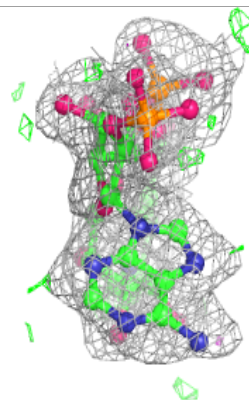
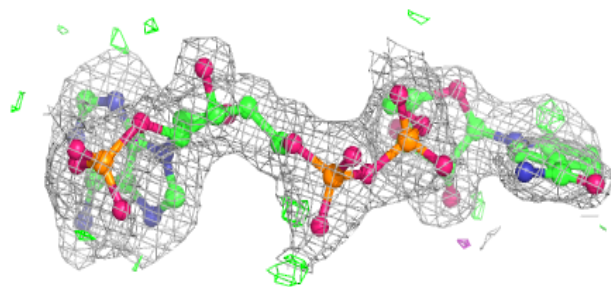
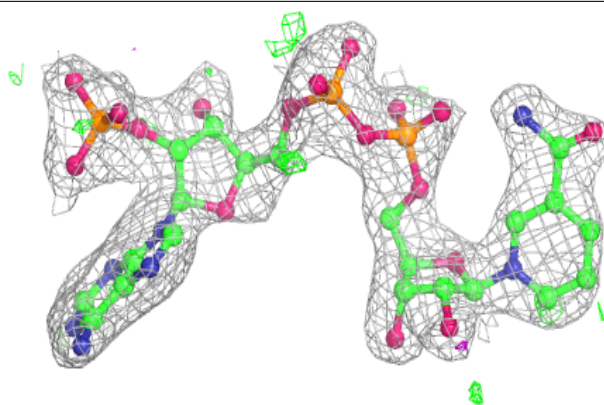
Electron density around F3V G 302:

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

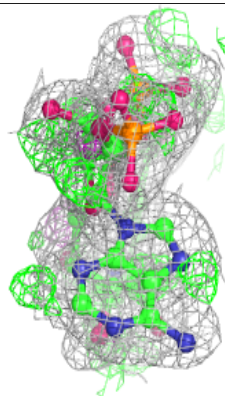
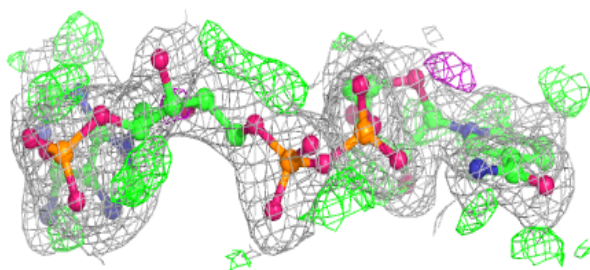
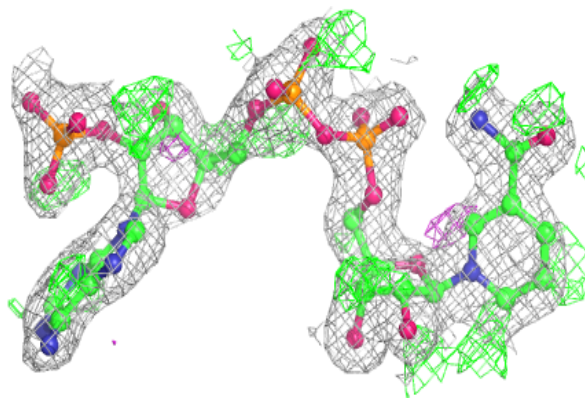


Electron density around NAP M 301:

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

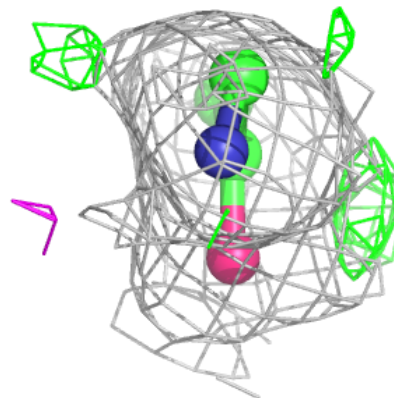
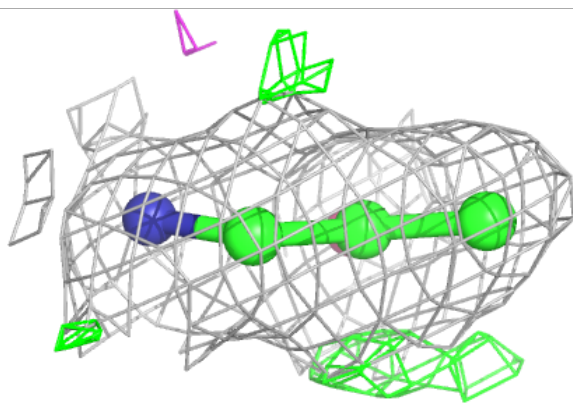
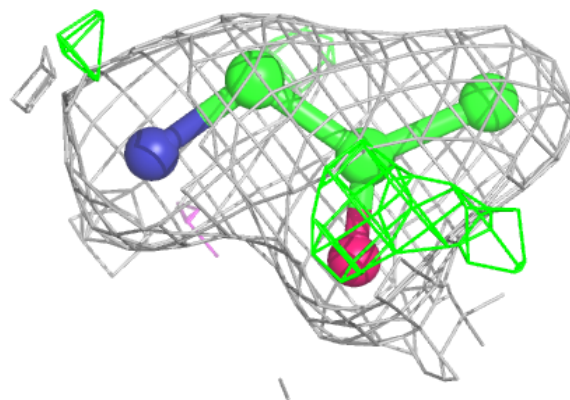
**Electron density around NAP B 301:**

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



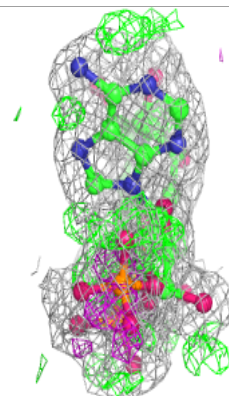
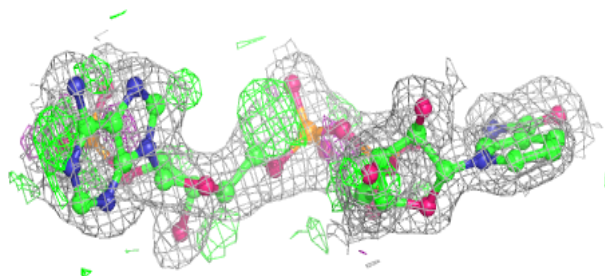
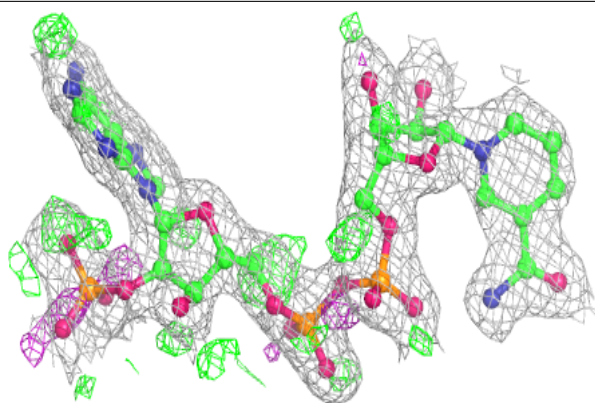
Electron density around F3V I 302:

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and green (positive)

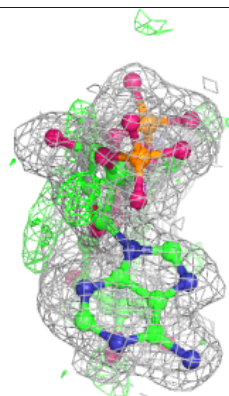
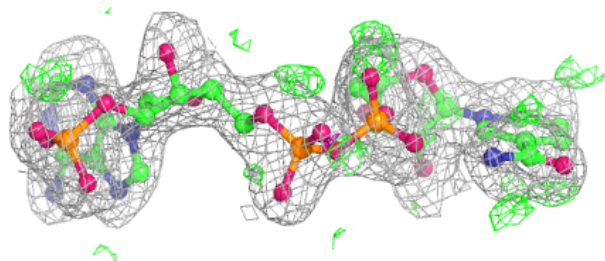
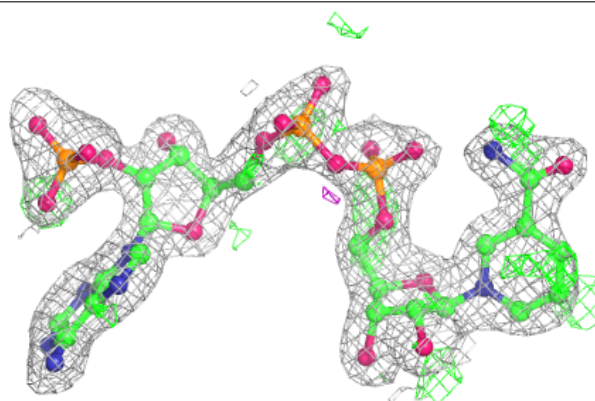


Electron density around NAP G 301:

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and green (positive)

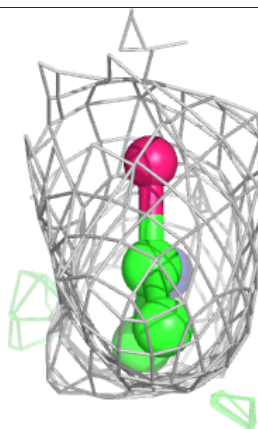
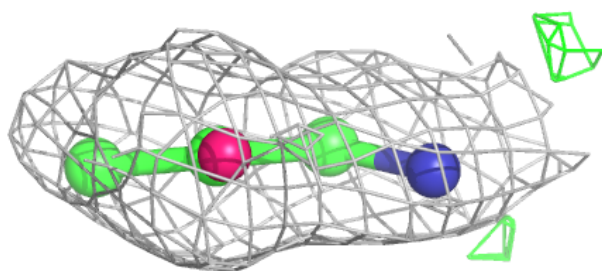
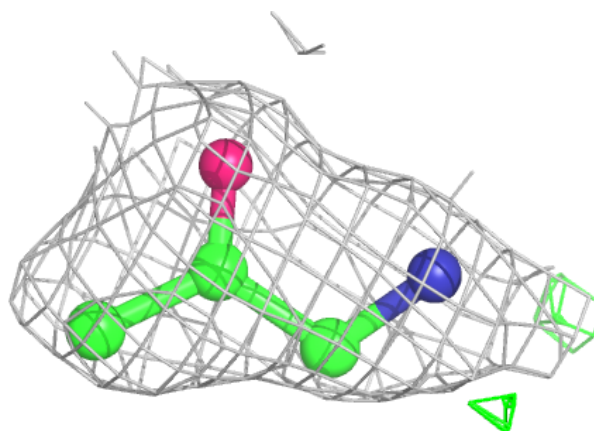
**Electron density around NAP I 301:**

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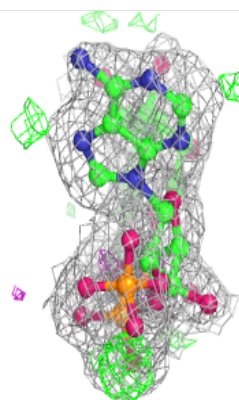
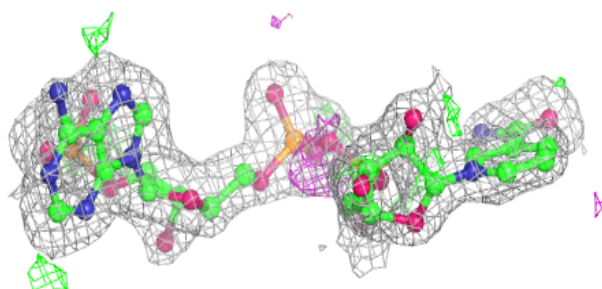
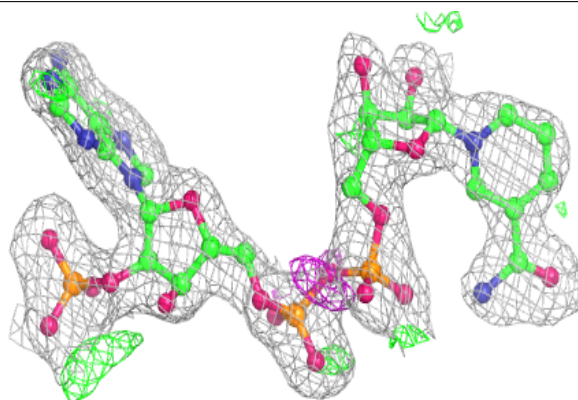


Electron density around F3V P 302:

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

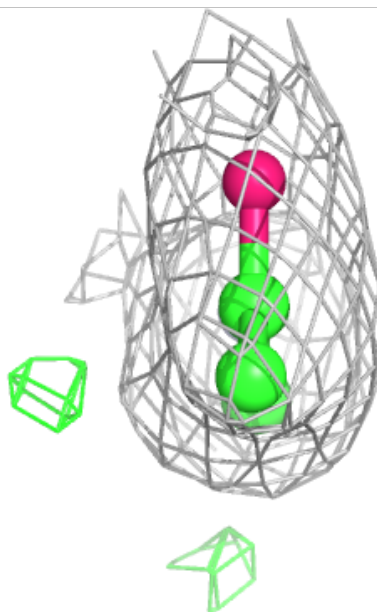
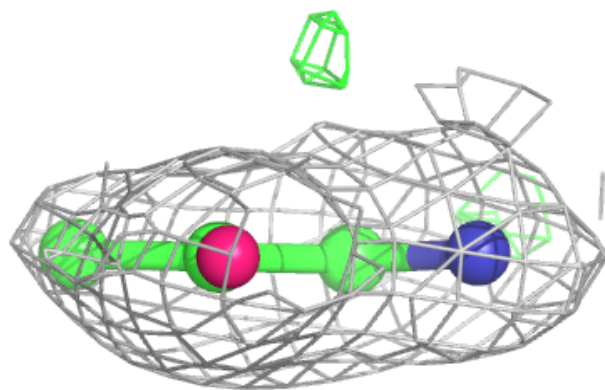
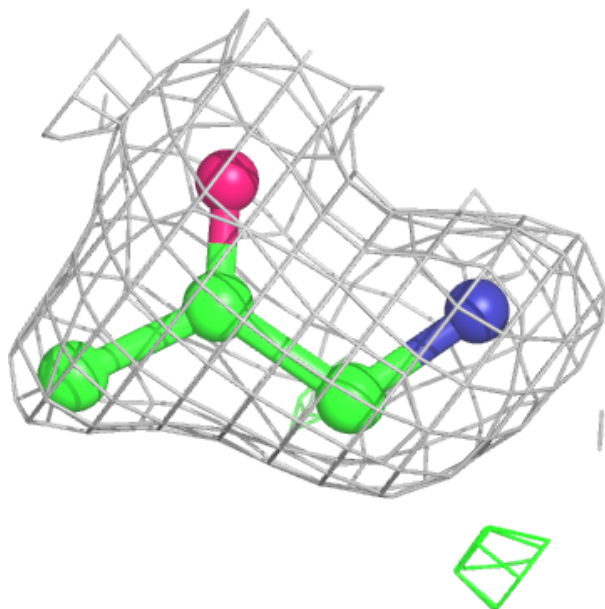
**Electron density around NAP K 301:**

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



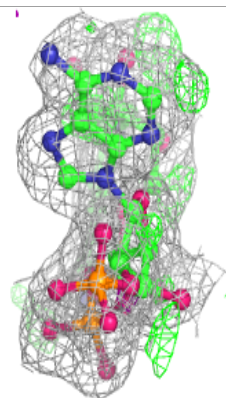
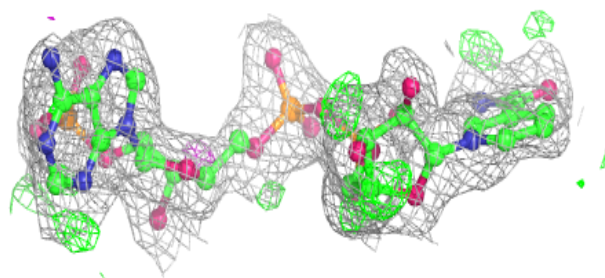
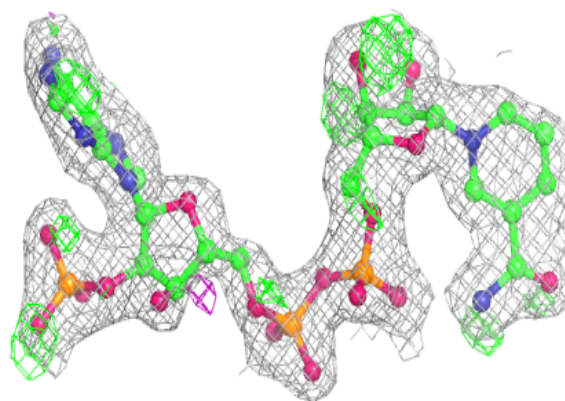
Electron density around F3V F 302:

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and green (positive)

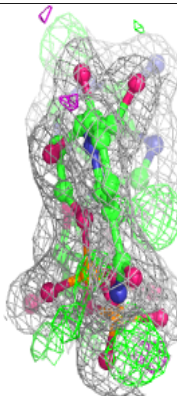
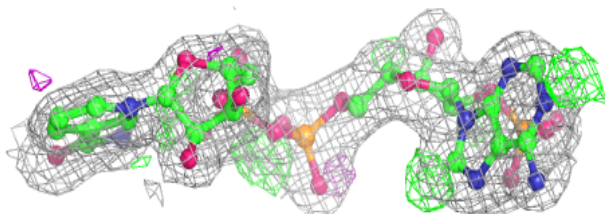
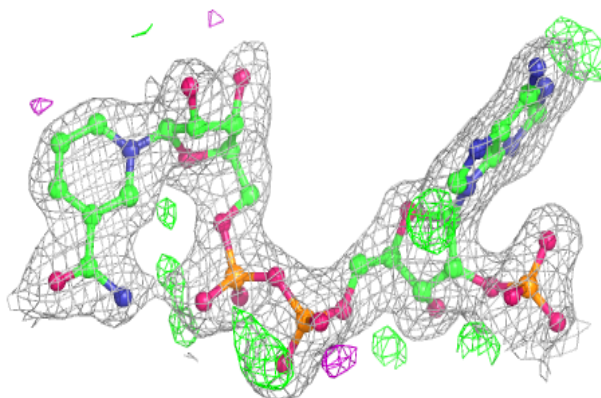


Electron density around NAP N 301:

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and green (positive)

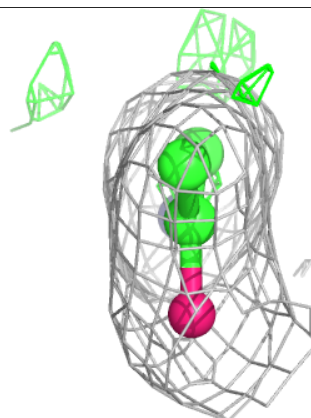
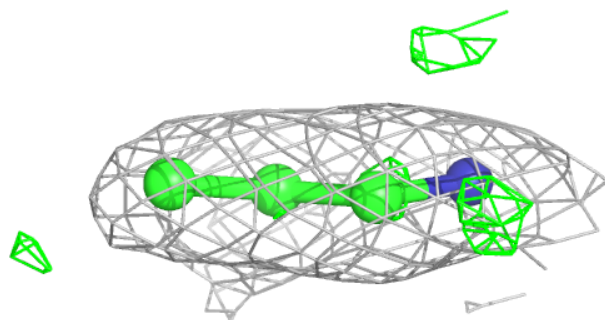
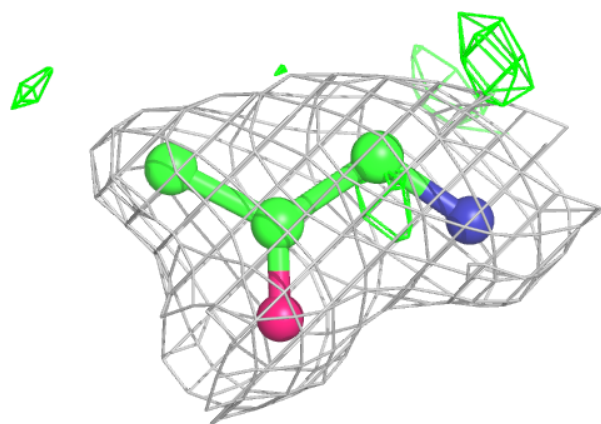
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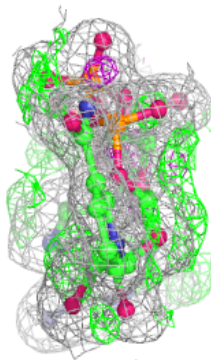
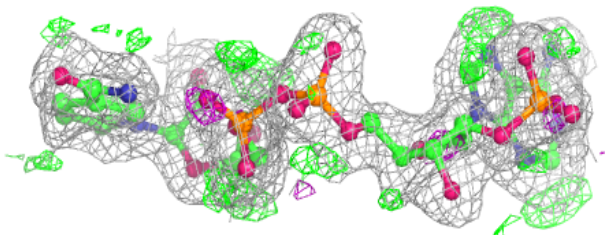
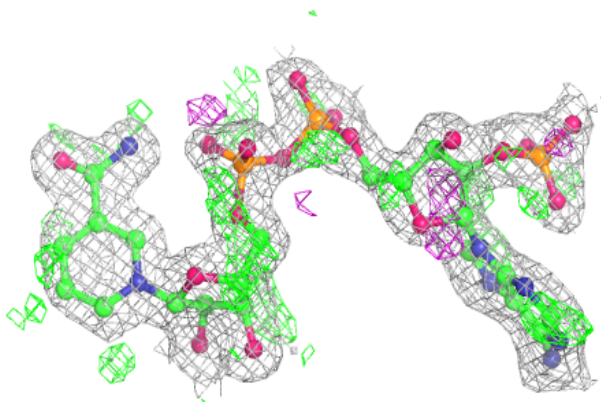


Electron density around F3V C 302:

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

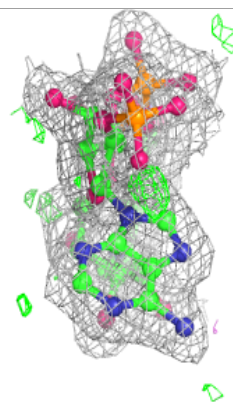
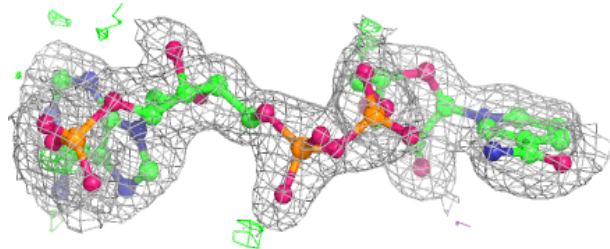
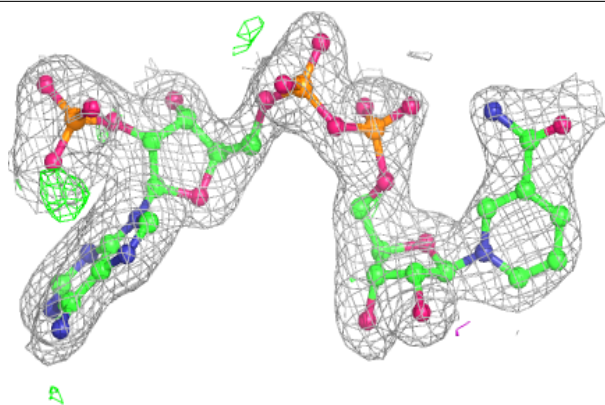
**Electron density around NAP E 301:**

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



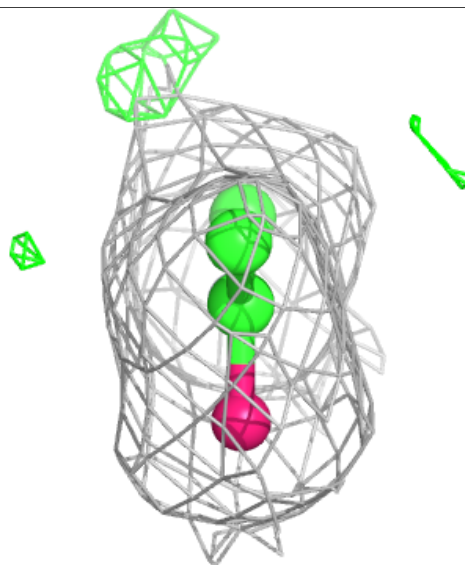
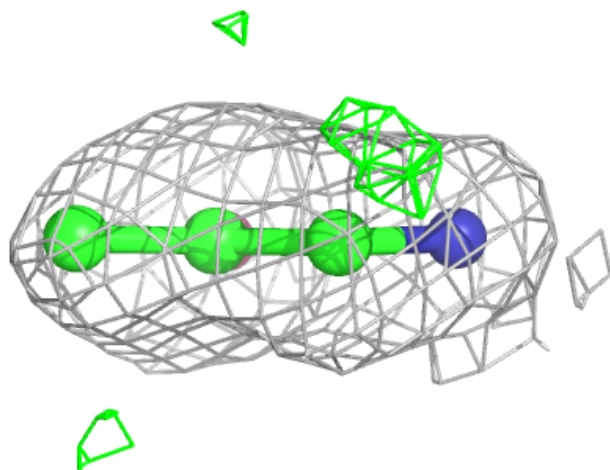
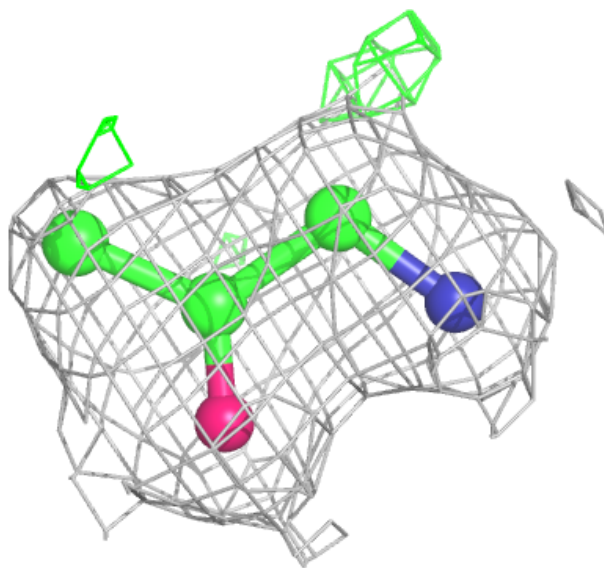
Electron density around NAP L 301:

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and green (positive)



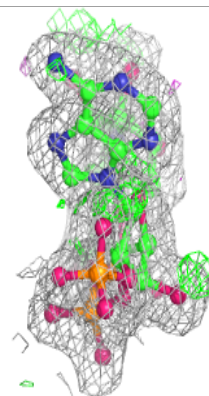
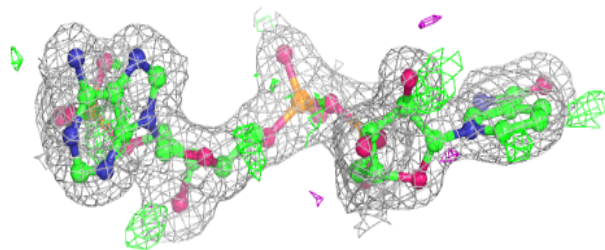
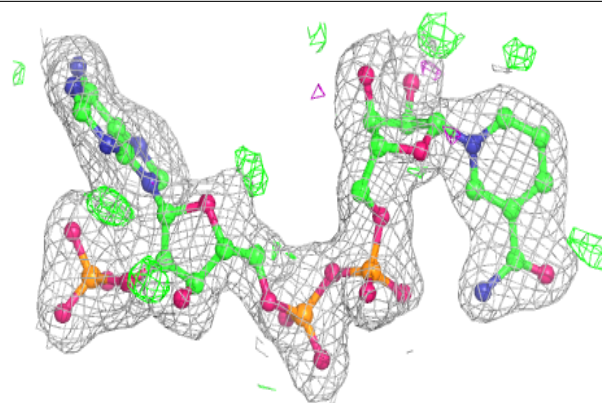
Electron density around F3V K 302:

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



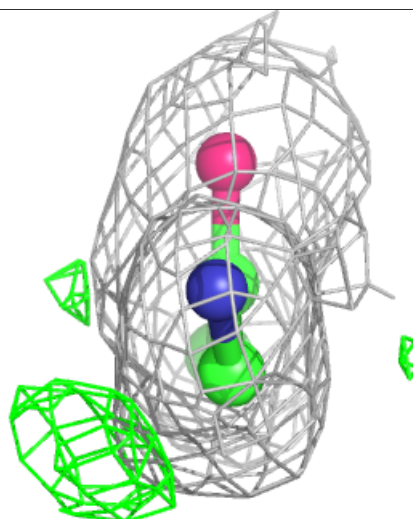
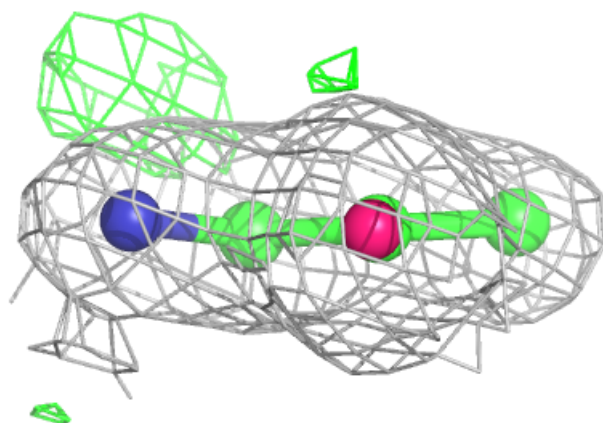
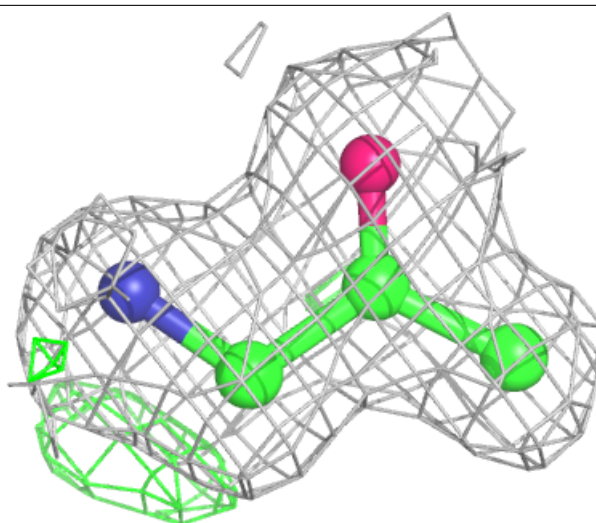
Electron density around NAP F 301:

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



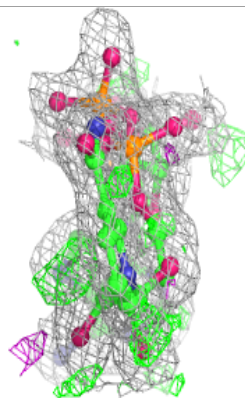
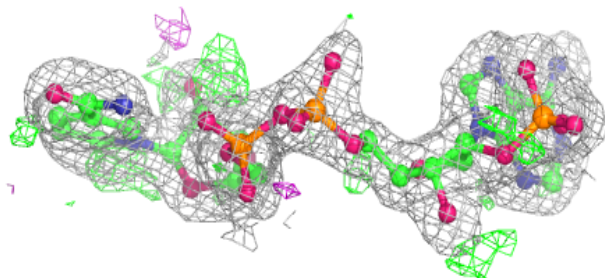
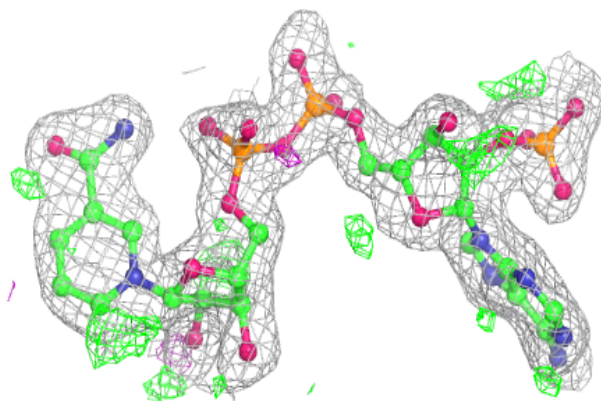
Electron density around F3V D 302:

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

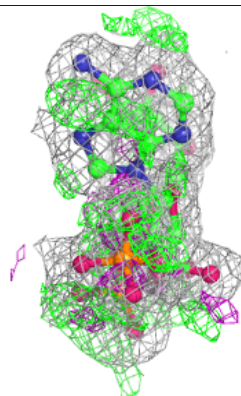
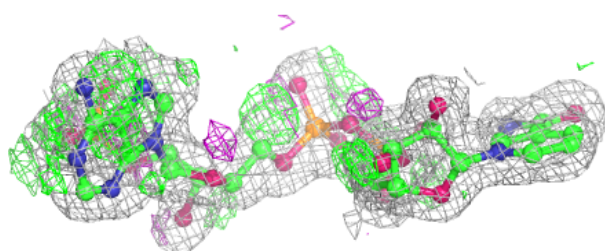
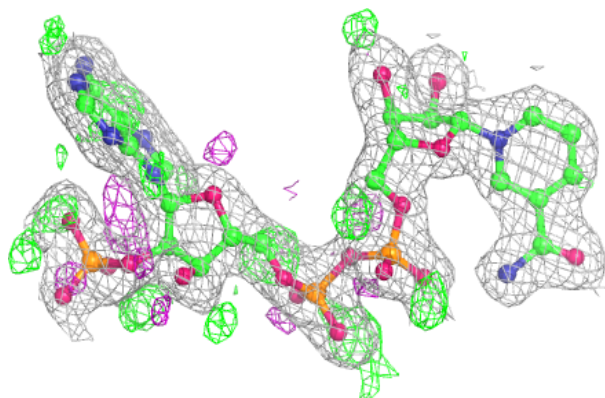


Electron density around NAP A 301:

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

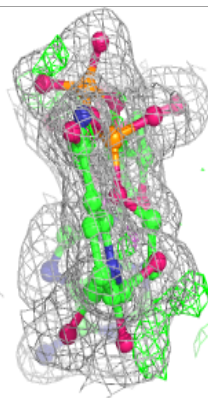
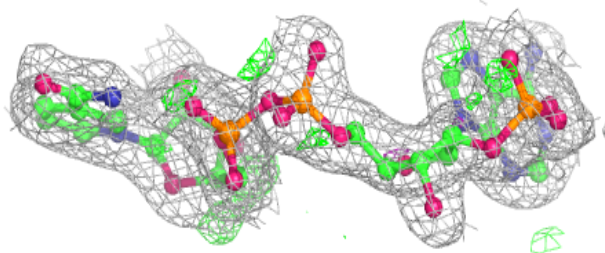
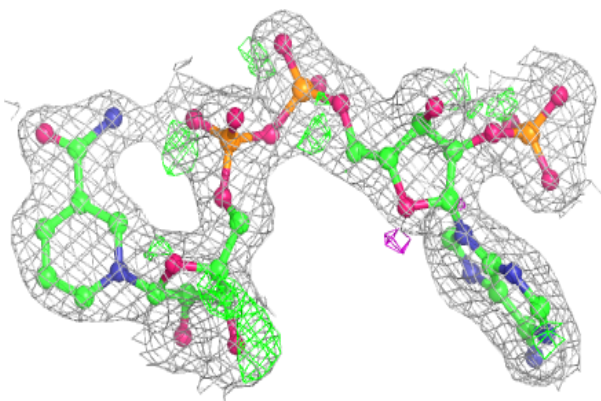
**Electron density around NAP D 301:**

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



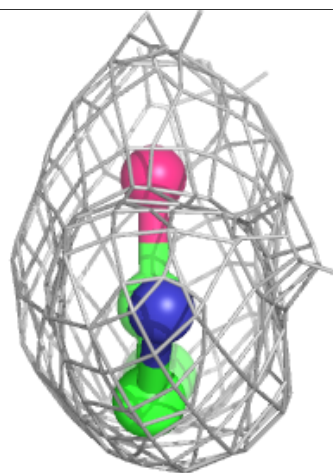
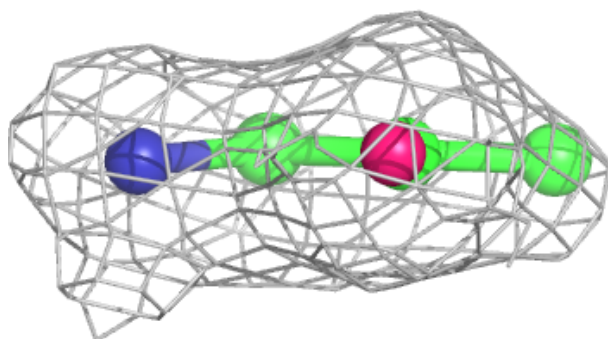
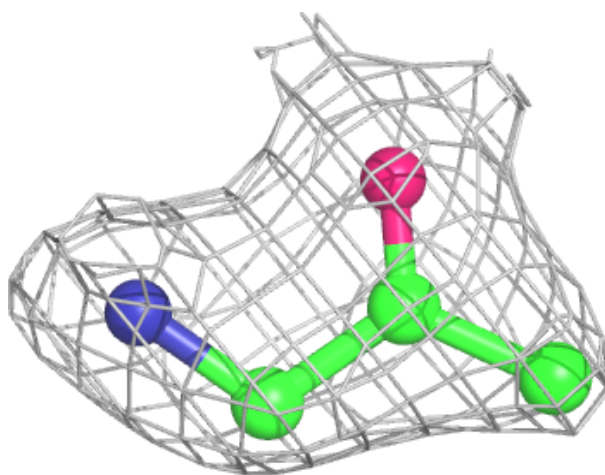
Electron density around NAP J 301:

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



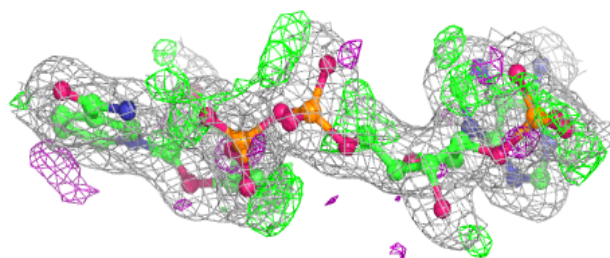
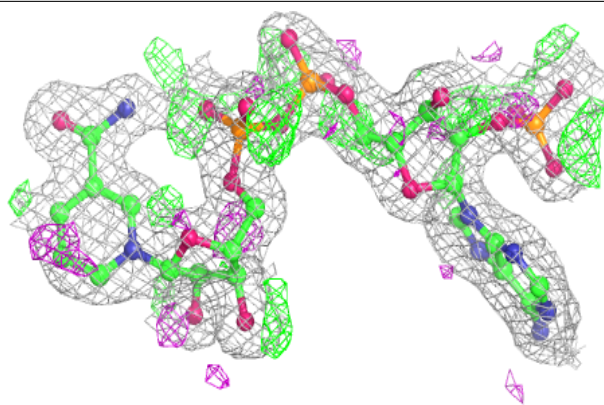
Electron density around F3V L 302:

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

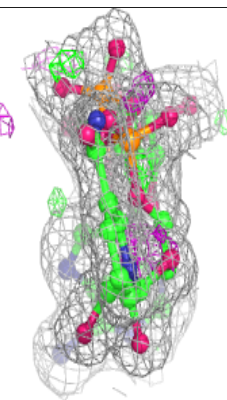
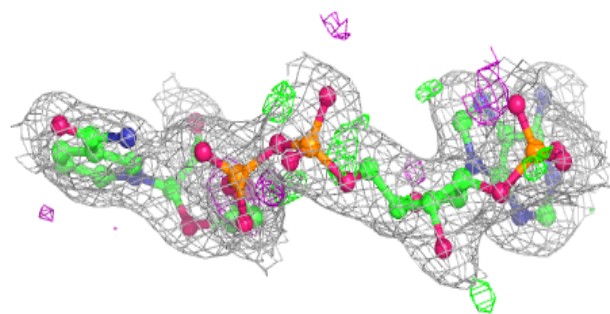
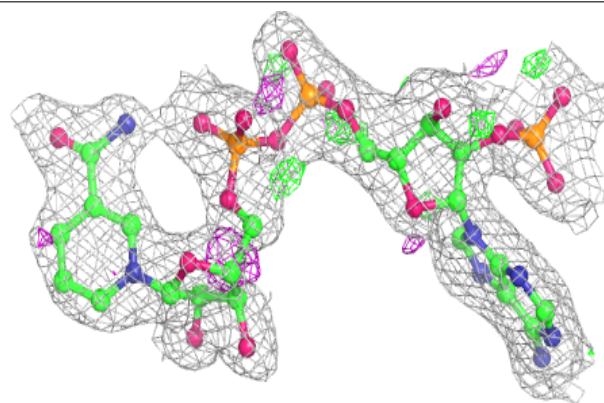


Electron density around NAP H 301:

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

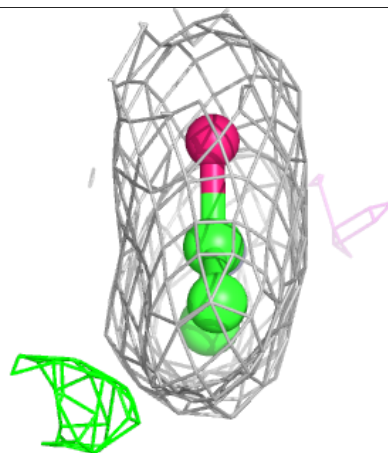
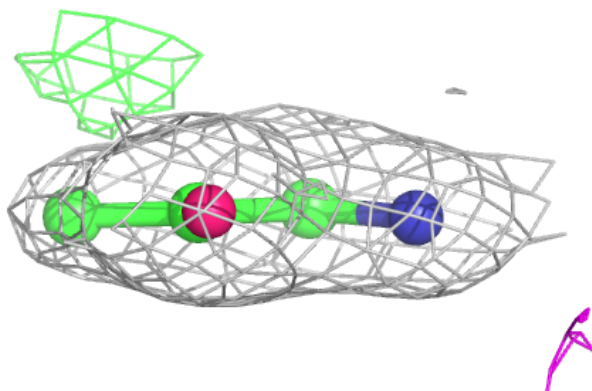
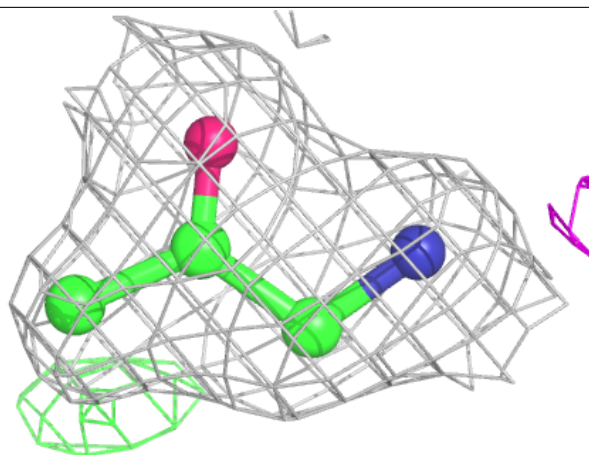
**Electron density around NAP O 301:**

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



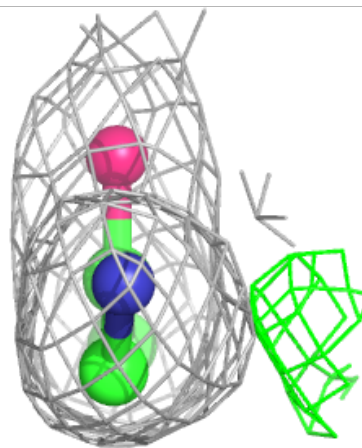
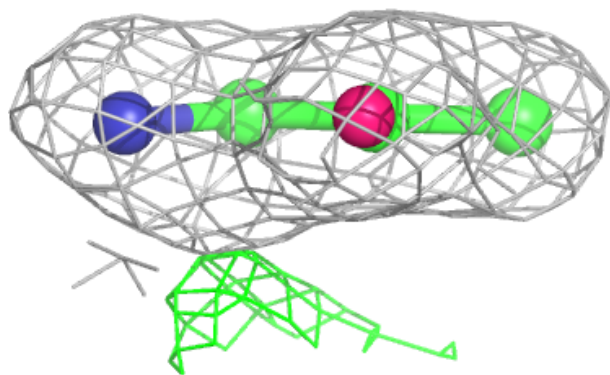
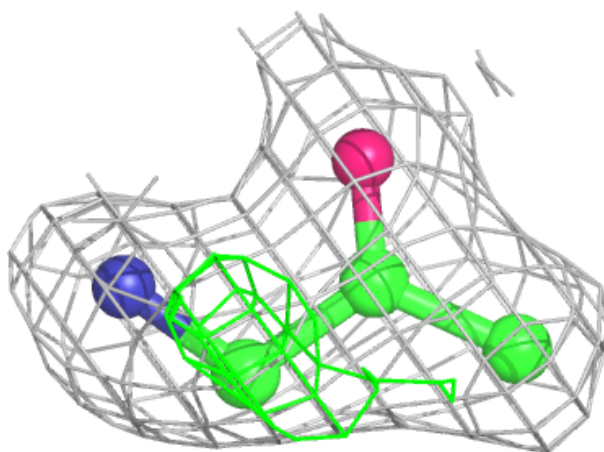
Electron density around F3V H 302:

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



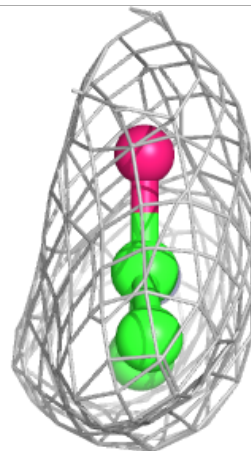
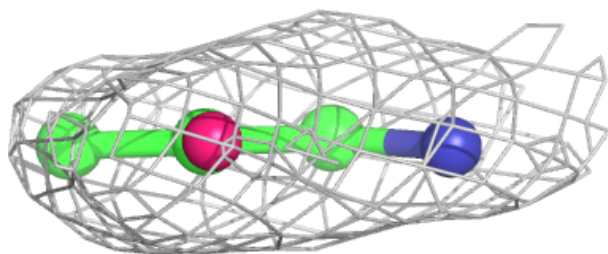
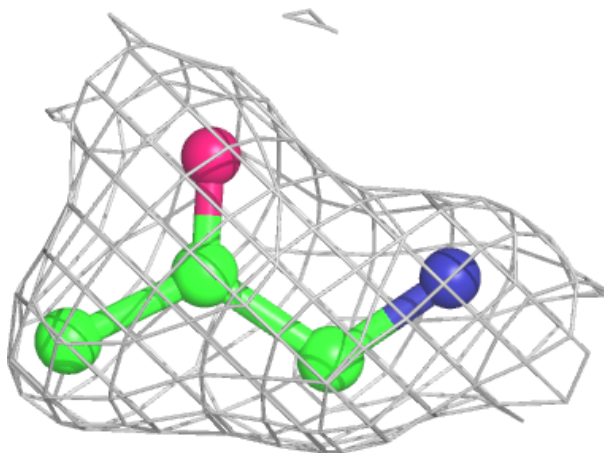
Electron density around F3V A 302:

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



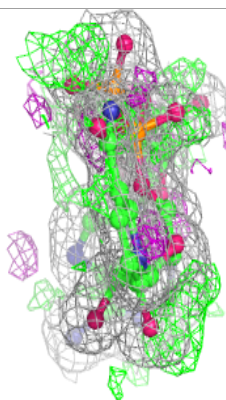
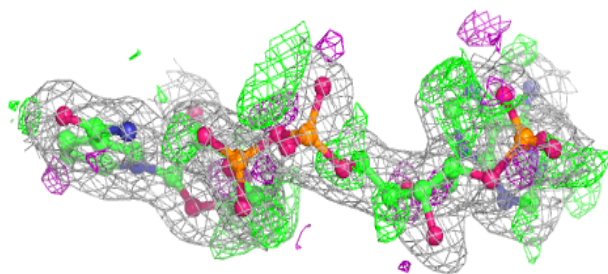
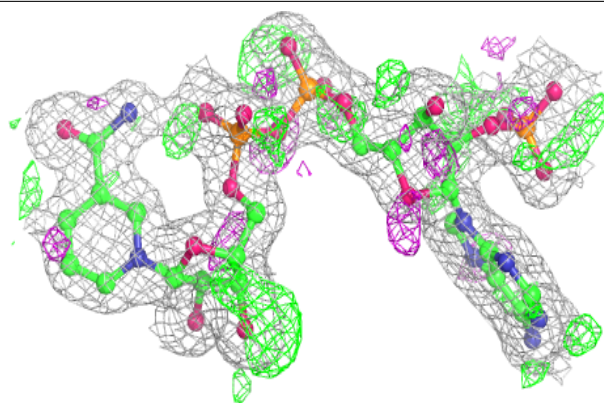
Electron density around F3V J 302:

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



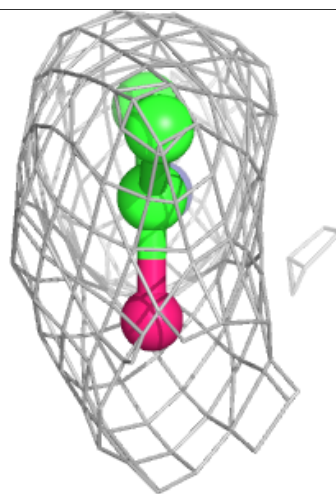
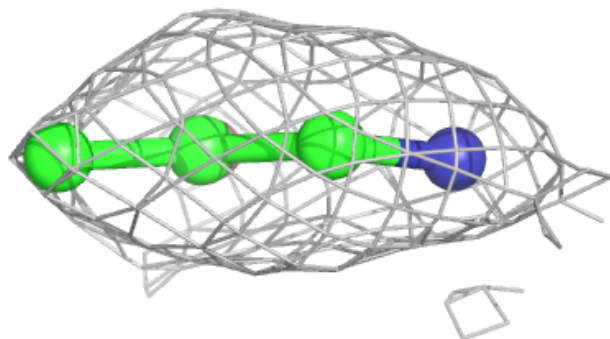
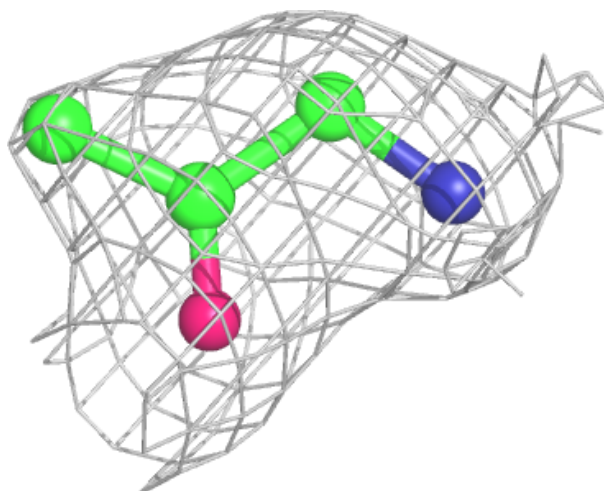
Electron density around NAP C 301:

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



Electron density around F3V O 302:

$2mF_o-DF_c$ (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.