



# Full wwPDB X-ray Structure Validation Report ⓘ

Jun 2, 2020 – 08:26 am BST

PDB ID : 5F2C  
Title : Thermostable aldehyde dehydrogenase from *Pyrobaculum* sp. 1860 crystallized in microgravity (complex with NADP+)  
Authors : Petrova, T.E.; Bezsudnova, E.Y.; Boyko, K.M.; Mardanov, A.V.; Gumerov, V.M.; Ravin, N.V.; Popov, V.O.  
Deposited on : 2015-12-01  
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](mailto:validation@mail.wwpdb.org)

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

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

MolProbity : 4.02b-467  
Mogul : 1.8.5 (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

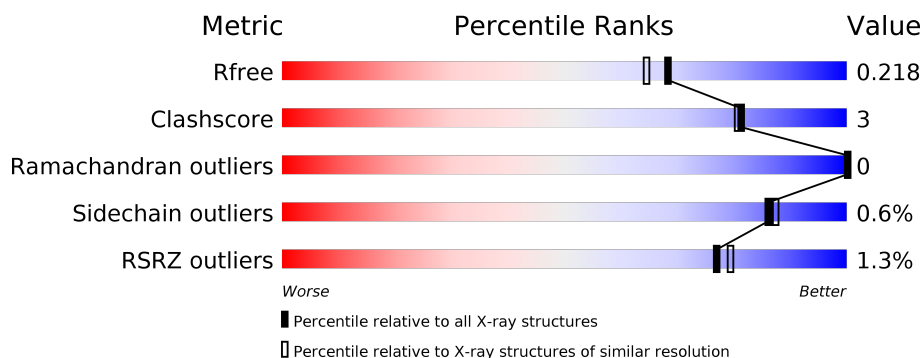
# 1 Overall quality at a glance

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  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions  $\leq 5\%$ . The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	491	<div> <div>92%</div> <div>7%</div> <div>•</div> </div>
1	B	491	<div> <div>91%</div> <div>7%</div> <div>•</div> </div>
1	C	491	<div> <div>93%</div> <div>6%</div> <div>•</div> </div>
1	D	491	<div> <div>93%</div> <div>5%</div> <div>•</div> </div>
1	E	491	<div> <div>93%</div> <div>6%</div> <div>•</div> </div>
1	F	491	<div> <div>94%</div> <div>6%</div> <div>•</div> </div>

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Mol	Chain	Length	Quality of chain
1	G	491	<div><div>%</div><div><div></div></div><div>90%</div><div>8%</div><div></div></div>
1	H	491	<div><div>%</div><div><div></div></div><div>95%</div><div>5%</div><div></div></div>

## 2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 34276 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 Aldehyde dehydrogenase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	488	Total	C	N	O	S	0	11	1
			3840	2448	671	708	13			
1	B	484	Total	C	N	O	S	0	14	0
			3837	2448	672	704	13			
1	C	490	Total	C	N	O	S	0	18	1
			3885	2476	677	718	14			
1	D	484	Total	C	N	O	S	0	11	1
			3793	2418	659	704	12			
1	E	485	Total	C	N	O	S	0	10	1
			3803	2426	668	696	13			
1	F	490	Total	C	N	O	S	0	9	1
			3843	2451	668	711	13			
1	G	484	Total	C	N	O	S	0	8	0
			3797	2421	664	699	13			
1	H	488	Total	C	N	O	S	0	19	1
			3892	2485	679	714	14			

- Molecule 2 is NADP NICOTINAMIDE-ADENINE-DINUCLEOTIDE PHOSPHATE (three-letter code: NAP) (formula: C<sub>21</sub>H<sub>28</sub>N<sub>7</sub>O<sub>17</sub>P<sub>3</sub>).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	N	O	P	0	1
			51	20	5	22	4		
2	B	1	Total	C	N	O	P	0	0
			39	15	5	16	3		
2	C	1	Total	C	N	O	P	0	1
			51	20	5	22	4		
2	D	1	Total	C	N	O	P	0	1
			51	20	5	22	4		
2	E	1	Total	C	N	O	P	0	1
			51	20	5	22	4		
2	F	1	Total	C	N	O	P	0	1
			51	20	5	22	4		
2	G	1	Total	C	N	O	P	0	1
			51	20	5	22	4		
2	H	1	Total	C	N	O	P	0	1
			51	20	5	22	4		

- Molecule 3 is GLYCEROL (three-letter code: GOL) (formula: C<sub>3</sub>H<sub>8</sub>O<sub>3</sub>).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	C	O	0	0
			6	3	3		

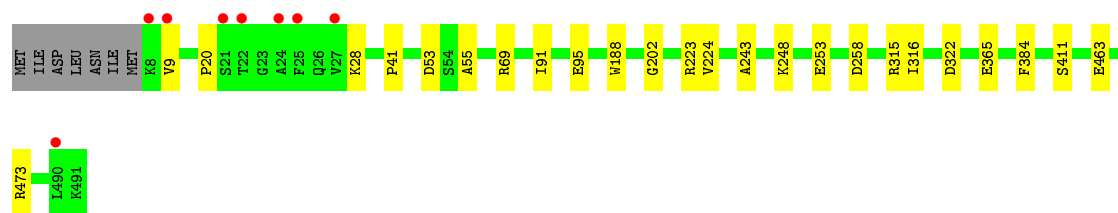
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	444	Total	O	0	2
			444	444		
4	B	404	Total	O	0	4
			404	404		
4	C	432	Total	O	0	6
			432	432		
4	D	364	Total	O	0	2
			364	364		
4	E	347	Total	O	0	5
			347	347		
4	F	396	Total	O	0	3
			396	396		
4	G	370	Total	O	0	2
			370	370		
4	H	427	Total	O	0	5
			427	427		

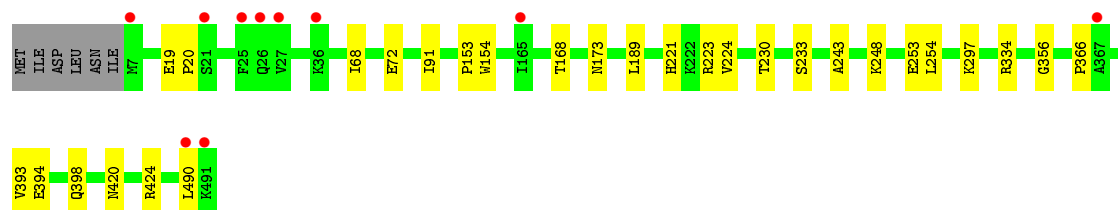
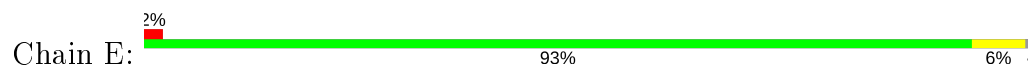


- Molecule 1: Aldehyde dehydrogenase

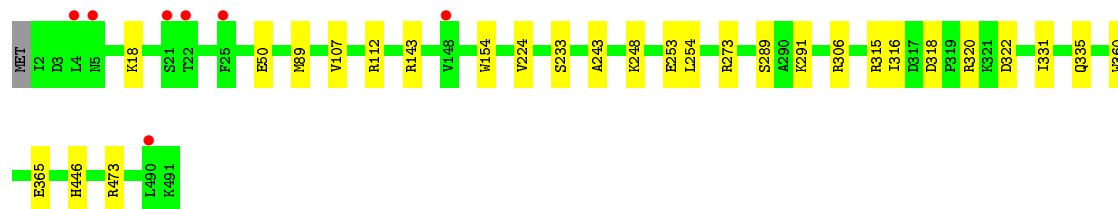




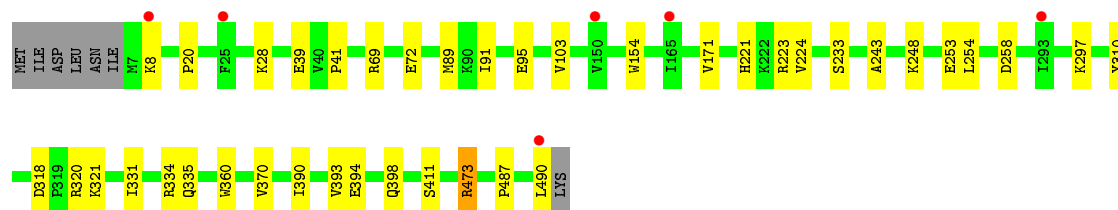
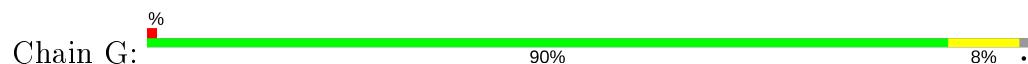
- Molecule 1: Aldehyde dehydrogenase



- Molecule 1: Aldehyde dehydrogenase



- Molecule 1: Aldehyde dehydrogenase



- Molecule 1: Aldehyde dehydrogenase





## 4 Data and refinement statistics

Property	Value	Source
Space group	P 2 <sub>1</sub> 2 <sub>1</sub> 2	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	185.36 Å   208.30 Å   163.81 Å 90.00°   90.00°   90.00°	Depositor
Resolution (Å)	29.14 – 1.90 29.63 – 1.90	Depositor EDS
% Data completeness (in resolution range)	87.6 (29.14-1.90) 87.6 (29.63-1.90)	Depositor EDS
$R_{merge}$	0.07	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.22 (at 1.89 Å)	Xtriage
Refinement program	PHENIX 1.8.4_1496	Depositor
R, $R_{free}$	0.184   ,   0.217 0.186   ,   0.218	Depositor DCC
$R_{free}$ test set	21766 reflections (5.01%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	25.0	Xtriage
Anisotropy	0.176	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.36   ,   48.1	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.52$ , $\langle L^2 \rangle = 0.35$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.97	EDS
Total number of atoms	34276	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	28.0	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 47.96 % 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 9.2060e-05. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

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

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

## 5 Model quality [i](#)

### 5.1 Standard geometry [i](#)

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

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	0.41	0/3949	0.55	1/5352 (0.0%)
1	B	0.39	0/3960	0.51	0/5364
1	C	0.79	2/3992 (0.1%)	0.57	4/5413 (0.1%)
1	D	0.39	0/3904	0.50	0/5296
1	E	0.36	0/3912	0.49	0/5302
1	F	0.39	0/3949	0.51	0/5354
1	G	0.37	0/3900	0.51	2/5286 (0.0%)
1	H	0.41	0/4014	0.52	0/5437
All	All	0.46	2/31580 (0.0%)	0.52	7/42804 (0.0%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	1

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	8[A]	LYS	CD-CE	30.47	2.27	1.51
1	C	8[B]	LYS	CD-CE	30.47	2.27	1.51

All (7) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	8[A]	LYS	CG-CD-CE	-7.89	88.23	111.90
1	C	8[B]	LYS	CG-CD-CE	-7.89	88.23	111.90
1	C	8[A]	LYS	CD-CE-NZ	7.71	129.44	111.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	8[B]	LYS	CD-CE-NZ	7.71	129.44	111.70
1	A	473	ARG	NE-CZ-NH2	-5.84	117.38	120.30
1	G	473[A]	ARG	NE-CZ-NH2	-5.01	117.80	120.30
1	G	473[B]	ARG	NE-CZ-NH2	-5.01	117.80	120.30

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	237[B]	ARG	Mainchain

## 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	3840	0	3838	24	0
1	B	3837	0	3861	28	0
1	C	3885	0	3857	18	0
1	D	3793	0	3768	17	0
1	E	3803	0	3804	20	0
1	F	3843	0	3847	16	0
1	G	3797	0	3796	27	0
1	H	3892	0	3911	16	0
2	A	51	0	12	4	0
2	B	39	0	17	0	0
2	C	51	0	12	3	0
2	D	51	0	12	2	0
2	E	51	0	12	7	0
2	F	51	0	12	2	0
2	G	51	0	12	5	0
2	H	51	0	12	3	0
3	A	6	0	8	0	0
4	A	444	0	0	0	0
4	B	404	0	0	3	0
4	C	432	0	0	1	0
4	D	364	0	0	4	0
4	E	347	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	F	396	0	0	2	0
4	G	370	0	0	3	0
4	H	427	0	0	2	0
All	All	34276	0	30791	162	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 3.

All (162) 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:E:334:ARG:NH1	2:E:500[B]:NAP:C1D	2.05	1.18
1:E:334:ARG:HH12	2:E:500[B]:NAP:C1D	1.63	1.03
1:C:269:ASP:OD1	1:C:306:ARG:NH1	2.07	0.88
1:C:26:GLN:OE1	1:C:42:ARG:NH1	2.15	0.78
1:E:334:ARG:NH1	2:E:500[B]:NAP:C2D	2.50	0.74
1:A:154:TRP:HE1	2:A:501[B]:NAP:H4D	1.53	0.73
1:D:20:PRO:HG3	1:D:41:PRO:HB3	1.72	0.71
1:A:297:LYS:HD3	1:A:394:GLU:HG2	1.74	0.69
1:G:20:PRO:HG3	1:G:41:PRO:HB3	1.76	0.67
1:B:305:GLU:OE1	1:B:306:ARG:NH1	2.28	0.66
1:C:154:TRP:HE1	2:C:500[B]:NAP:H4D	1.60	0.65
1:G:473[A]:ARG:NH2	1:H:426:ALA:O	2.29	0.65
1:G:69[A]:ARG:NH2	4:G:601:HOH:O	2.30	0.64
1:G:69[A]:ARG:NH1	1:G:72:GLU:OE2	2.31	0.64
1:A:315:ARG:NH2	1:A:322:ASP:OD2	2.28	0.62
1:D:316:ILE:HD12	1:D:365[A]:GLU:HG2	1.80	0.62
1:C:91:ILE:O	1:C:95:GLU:HB3	2.00	0.62
1:H:154:TRP:HE1	2:H:500[B]:NAP:H4D	1.65	0.61
1:E:334:ARG:HH11	2:E:500[B]:NAP:H2D	1.67	0.60
1:A:334:ARG:HE	2:A:501[B]:NAP:H2D	1.66	0.60
1:C:28:LYS:HE2	1:C:95:GLU:HG3	1.87	0.56
1:G:334:ARG:HH12	2:G:500[B]:NAP:H2D	1.70	0.56
1:E:334:ARG:NH1	2:E:500[B]:NAP:H2D	2.19	0.56
1:A:237[B]:ARG:HG2	1:B:247:LEU:HD21	1.87	0.55
1:H:316:ILE:HD12	1:H:365[B]:GLU:HG2	1.88	0.55
1:A:221:HIS:HE1	1:A:223:ARG:HG3	1.72	0.54
1:G:154:TRP:HE1	2:G:500[B]:NAP:H4D	1.72	0.54
1:H:223:ARG:HD3	4:H:949:HOH:O	2.08	0.53
1:G:370:VAL:HG12	1:G:390:ILE:HB	1.91	0.53
1:C:154:TRP:NE1	2:C:500[B]:NAP:H4D	2.25	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:315:ARG:NH1	4:D:605:HOH:O	2.42	0.52
1:A:154:TRP:NE1	2:A:501[B]:NAP:H4D	2.20	0.52
1:G:221:HIS:HE1	1:G:223:ARG:HG3	1.75	0.52
1:A:490:LEU:HD13	1:B:273:ARG:NH1	2.25	0.52
1:D:384:PHE:CE1	2:D:500[A]:NAP:H2D	2.45	0.52
1:F:233:SER:HA	1:F:254:LEU:HB3	1.91	0.52
1:G:91:ILE:O	1:G:95:GLU:HB3	2.09	0.52
1:C:243:ALA:HB1	1:C:248:LYS:HG3	1.92	0.52
1:G:490:LEU:HD13	1:H:273:ARG:NH1	2.25	0.52
1:G:473[A]:ARG:HD2	1:H:431:SER:O	2.10	0.52
1:E:393:VAL:HB	1:E:398[A]:GLN:HB3	1.91	0.52
1:H:352[B]:ARG:HG3	1:H:371:ASP:OD2	2.09	0.52
1:E:68:ILE:O	1:E:72[A]:GLU:HG3	2.09	0.51
1:E:221:HIS:HE1	1:E:223:ARG:HG3	1.76	0.51
1:F:143:ARG:NH1	4:F:608:HOH:O	2.43	0.51
1:E:233:SER:HA	1:E:254:LEU:HB3	1.92	0.50
1:E:297:LYS:HD3	1:E:394:GLU:HG2	1.93	0.50
1:B:45[A]:ARG:NH2	4:B:604:HOH:O	2.44	0.50
1:C:370:VAL:HG12	1:C:390:ILE:HB	1.94	0.50
1:C:69[A]:ARG:NH2	4:C:607:HOH:O	2.44	0.49
1:H:154:TRP:NE1	2:H:500[B]:NAP:H4D	2.27	0.49
1:B:27:VAL:HG11	1:B:36:LYS:HD2	1.94	0.49
1:C:221:HIS:HE1	1:C:223:ARG:HG3	1.78	0.49
1:B:221:HIS:HE1	1:B:223:ARG:HG3	1.77	0.49
1:G:310:TYR:CE1	1:H:490:LEU:HD11	2.48	0.49
1:A:258:ASP:OD2	1:A:411:SER:HB3	2.13	0.49
1:F:289:SER:HB3	1:F:291:LYS:HE3	1.94	0.49
1:F:243:ALA:HB1	1:F:248:LYS:HG3	1.94	0.49
1:D:28:LYS:HE2	1:D:95:GLU:HG3	1.94	0.48
1:G:318:ASP:OD1	1:G:320:ARG:HD3	2.13	0.48
1:A:243:ALA:HB1	1:A:248:LYS:HG3	1.95	0.48
1:B:243:ALA:HB1	1:B:248:LYS:HG3	1.95	0.48
1:G:243:ALA:HB1	1:G:248:LYS:HG3	1.96	0.47
1:D:315:ARG:NH2	1:D:322:ASP:OD2	2.41	0.47
1:G:154:TRP:NE1	2:G:500[B]:NAP:H4D	2.30	0.47
1:B:318:ASP:HB3	1:B:321:LYS:HG3	1.97	0.46
1:G:224:VAL:O	1:G:248:LYS:HE3	2.16	0.46
1:D:9:VAL:HB	1:D:188:TRP:CG	2.51	0.46
1:G:89:MET:HE3	1:G:103:VAL:HG23	1.97	0.46
1:B:45[A]:ARG:HH22	1:B:216:GLU:HG2	1.81	0.46
1:B:487:PRO:HG2	1:B:490:LEU:HD22	1.98	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:490:LEU:HD13	1:F:273:ARG:NH1	2.30	0.46
1:G:8:LYS:HE3	1:G:39:GLU:OE2	2.17	0.45
1:F:318:ASP:OD1	1:F:320:ARG:HD3	2.16	0.45
1:A:101:ARG:HG2	1:B:485:PRO:HB2	1.98	0.45
1:B:28:LYS:HD3	1:B:28:LYS:HA	1.65	0.45
1:G:487:PRO:HD2	1:G:490:LEU:HD12	1.98	0.45
1:D:243:ALA:HB1	1:D:248:LYS:HG3	1.98	0.45
1:G:297:LYS:NZ	1:G:394:GLU:O	2.48	0.45
1:B:306:ARG:HA	1:B:306:ARG:HD3	1.79	0.45
1:F:331:ILE:HG22	1:F:335:GLN:HG3	1.99	0.45
1:B:127[A]:ARG:NH2	4:B:603:HOH:O	2.42	0.45
1:C:393:VAL:HB	1:C:398:GLN:HB3	1.99	0.45
1:B:9:VAL:HG22	1:B:188:TRP:CD2	2.52	0.44
1:F:360:TRP:HZ3	1:F:365[B]:GLU:HG3	1.82	0.44
1:H:243:ALA:HB1	1:H:248:LYS:HG3	1.99	0.44
1:A:221:HIS:CE1	1:A:223:ARG:HG3	2.52	0.44
1:G:393:VAL:HB	1:G:398:GLN:HB3	1.98	0.44
1:D:258:ASP:OD2	1:D:411:SER:HB3	2.18	0.44
1:F:316:ILE:HD12	1:F:365[B]:GLU:HG2	2.00	0.44
1:A:356:GLY:HA3	1:A:366:PRO:O	2.18	0.44
1:H:258:ASP:OD2	1:H:411:SER:HB3	2.18	0.44
1:B:8:LYS:HD2	1:B:39:GLU:HB2	2.00	0.44
1:F:154:TRP:HE1	2:F:500[B]:NAP:H4D	1.82	0.44
1:H:20:PRO:HD3	1:H:41:PRO:HB3	1.99	0.44
1:E:153:PRO:HD3	1:E:230:THR:HB	1.99	0.44
1:E:19:GLU:HB2	1:E:20:PRO:HD2	1.99	0.44
1:E:356:GLY:HA3	1:E:366:PRO:O	2.18	0.44
1:E:420:ASN:HB3	1:E:424[B]:ARG:NH1	2.32	0.44
1:F:315:ARG:NH2	1:F:322:ASP:OD1	2.33	0.44
1:D:53:ASP:OD1	1:D:223:ARG:NH2	2.51	0.44
1:A:448:PRO:HB3	1:A:464:TRP:CG	2.53	0.43
1:G:258:ASP:OD2	1:G:411:SER:HB3	2.18	0.43
1:B:233[A]:SER:HA	1:B:254:LEU:HB3	1.99	0.43
1:D:365[B]:GLU:HG2	4:D:805:HOH:O	2.18	0.43
1:E:91:ILE:HG13	1:E:189:LEU:HD11	2.00	0.43
1:B:233[B]:SER:HA	1:B:254:LEU:HB3	2.00	0.43
1:D:91:ILE:O	1:D:95:GLU:HB3	2.18	0.43
1:G:28:LYS:HE2	1:G:95:GLU:HG3	2.00	0.43
1:F:89:MET:HG3	1:F:107:VAL:HG21	1.99	0.43
1:G:233:SER:HA	1:G:254:LEU:HB3	2.00	0.43
1:A:28:LYS:HE2	1:A:95:GLU:HG3	1.99	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:154:TRP:HE1	2:E:500[B]:NAP:H4D	1.84	0.43
1:A:69:ARG:HH11	1:A:72[A]:GLU:HB3	1.83	0.43
1:C:317:ASP:OD2	1:C:321:LYS:HE3	2.18	0.43
1:D:463[A]:GLU:OE2	4:D:601:HOH:O	2.21	0.43
1:B:8:LYS:HE2	4:B:929:HOH:O	2.19	0.42
1:E:224:VAL:O	1:E:248:LYS:HE3	2.19	0.42
1:H:360:TRP:HZ3	1:H:365[B]:GLU:HG3	1.84	0.42
1:G:223:ARG:HD3	4:G:902:HOH:O	2.19	0.42
1:C:224:VAL:O	1:C:248:LYS:HE3	2.18	0.42
1:A:355:ILE:HG13	1:A:356:GLY:N	2.35	0.42
1:C:306:ARG:HD3	1:C:306:ARG:HA	1.87	0.42
2:G:500[A]:NAP:H52N	4:G:713:HOH:O	2.19	0.42
1:B:89:MET:HG3	1:B:107:VAL:HG21	1.99	0.42
1:A:306:ARG:HA	1:A:306:ARG:HD3	1.78	0.42
1:G:318:ASP:HB3	1:G:321:LYS:HG3	2.02	0.42
1:C:283:GLN:HG3	1:C:327:LEU:HD22	2.00	0.42
1:A:273:ARG:HH12	1:B:490:LEU:HG	1.85	0.42
1:D:20:PRO:CG	1:D:41:PRO:HB3	2.46	0.42
1:F:365[A]:GLU:HG2	4:F:721:HOH:O	2.19	0.42
1:A:237[B]:ARG:HG2	1:B:247:LEU:CD2	2.48	0.41
1:F:112:ARG:NH2	1:H:69[B]:ARG:HH12	2.18	0.41
1:H:331:ILE:HG22	1:H:335:GLN:HG3	2.02	0.41
1:E:243:ALA:HB1	1:E:248:LYS:HG3	2.01	0.41
1:F:18:LYS:NZ	1:F:50:GLU:OE2	2.45	0.41
1:D:55:ALA:HA	1:D:202:GLY:O	2.20	0.41
1:B:29:THR:HG22	1:B:36:LYS:HD3	2.02	0.41
1:E:168:THR:HG22	1:E:173:ASN:HB2	2.01	0.41
1:A:420:ASN:HB3	1:A:424[B]:ARG:NH1	2.34	0.41
1:A:490:LEU:HD11	1:B:310:TYR:CE1	2.55	0.41
1:B:68:ILE:O	1:B:72[A]:GLU:HG3	2.20	0.41
1:C:153:PRO:HD3	1:C:230:THR:HB	2.02	0.41
1:C:356:GLY:HA3	1:C:366:PRO:O	2.20	0.41
1:F:224:VAL:O	1:F:248:LYS:HE3	2.21	0.41
1:A:153:PRO:HD3	1:A:230:THR:HB	2.03	0.41
1:C:331:ILE:HG22	1:C:335:GLN:HG3	2.03	0.41
1:G:331:ILE:HG22	1:G:335:GLN:HG3	2.03	0.41
1:B:153:PRO:HD3	1:B:230:THR:HB	2.03	0.41
1:H:398[B]:GLN:HG3	4:H:864:HOH:O	2.19	0.41
1:A:89:MET:HG3	1:A:107:VAL:HG21	2.03	0.40
1:D:224:VAL:O	1:D:248:LYS:HE3	2.21	0.40
1:D:69:ARG:NH2	4:D:619:HOH:O	2.55	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:91:ILE:O	1:B:95:GLU:HB3	2.22	0.40
1:B:490:LEU:HD12	1:B:490:LEU:HA	1.90	0.40

There are no symmetry-related clashes.

## 5.3 Torsion angles [i](#)

### 5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	496/491 (101%)	484 (98%)	12 (2%)	0	100	100
1	B	495/491 (101%)	483 (98%)	12 (2%)	0	100	100
1	C	503/491 (102%)	491 (98%)	12 (2%)	0	100	100
1	D	492/491 (100%)	480 (98%)	12 (2%)	0	100	100
1	E	492/491 (100%)	478 (97%)	14 (3%)	0	100	100
1	F	496/491 (101%)	482 (97%)	14 (3%)	0	100	100
1	G	489/491 (100%)	474 (97%)	15 (3%)	0	100	100
1	H	503/491 (102%)	491 (98%)	12 (2%)	0	100	100
All	All	3966/3928 (101%)	3863 (97%)	103 (3%)	0	100	100

There are no Ramachandran outliers to report.

### 5.3.2 Protein sidechains [i](#)

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

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



Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	408/408 (100%)	406 (100%)	2 (0%)	88	89
1	B	408/408 (100%)	406 (100%)	2 (0%)	88	89
1	C	411/408 (101%)	409 (100%)	2 (0%)	88	89
1	D	401/408 (98%)	399 (100%)	2 (0%)	88	89
1	E	400/408 (98%)	399 (100%)	1 (0%)	92	93
1	F	408/408 (100%)	404 (99%)	4 (1%)	76	76
1	G	401/408 (98%)	398 (99%)	3 (1%)	84	84
1	H	416/408 (102%)	410 (99%)	6 (1%)	67	65
All	All	3253/3264 (100%)	3231 (99%)	22 (1%)	86	84

All (22) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	171	VAL
1	A	253[B]	GLU
1	B	253[B]	GLU
1	B	490	LEU
1	C	253[B]	GLU
1	C	360	TRP
1	D	253[B]	GLU
1	D	473	ARG
1	E	253[B]	GLU
1	F	253[B]	GLU
1	F	306	ARG
1	F	446	HIS
1	F	473	ARG
1	G	171	VAL
1	G	253[B]	GLU
1	G	360	TRP
1	H	5[A]	ASN
1	H	5[B]	ASN
1	H	69[A]	ARG
1	H	69[B]	ARG
1	H	253[B]	GLU
1	H	473	ARG

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

### 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 ⓘ

16 ligands are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with  $|Z| > 2$  is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z  > 2$	Counts	RMSZ	$\# Z  > 2$
3	GOL	A	502	-	5,5,5	0.29	0	5,5,5	0.78	0
2	NAP	C	500[A]	-	36,42,52	1.97	10 (27%)	43,65,80	1.63	6 (13%)
2	NAP	D	500[B]	-	36,42,52	1.88	9 (25%)	43,65,80	1.60	7 (16%)
2	NAP	B	500	-	36,42,52	1.92	9 (25%)	43,65,80	1.65	7 (16%)
2	NAP	H	500[A]	-	36,42,52	1.98	8 (22%)	43,65,80	1.55	6 (13%)
2	NAP	F	500[B]	-	36,42,52	1.86	9 (25%)	43,65,80	1.58	7 (16%)
2	NAP	E	500[B]	-	36,42,52	1.86	9 (25%)	43,65,80	1.55	7 (16%)
2	NAP	A	501[B]	-	36,42,52	1.92	10 (27%)	43,65,80	1.44	8 (18%)
2	NAP	G	500[B]	-	36,42,52	1.92	8 (22%)	43,65,80	1.49	6 (13%)
2	NAP	H	500[B]	-	36,42,52	1.89	9 (25%)	43,65,80	1.47	6 (13%)
2	NAP	E	500[A]	-	36,42,52	1.98	10 (27%)	43,65,80	1.71	8 (18%)
2	NAP	C	500[B]	-	36,42,52	1.90	9 (25%)	43,65,80	1.54	5 (11%)
2	NAP	F	500[A]	-	36,42,52	1.95	9 (25%)	43,65,80	1.54	6 (13%)
2	NAP	A	501[A]	-	36,42,52	1.99	10 (27%)	43,65,80	1.59	9 (20%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
2	NAP	D	500[A]	-	36,42,52	1.86	8 (22%)	43,65,80	1.52	6 (13%)
2	NAP	G	500[A]	-	36,42,52	1.92	8 (22%)	43,65,80	1.49	7 (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	GOL	A	502	-	-	0/4/4/4	-
2	NAP	C	500[A]	-	-	3/23/56/67	0/4/4/5
2	NAP	D	500[B]	-	-	6/23/56/67	0/4/4/5
2	NAP	B	500	-	-	3/23/56/67	0/4/4/5
2	NAP	H	500[A]	-	-	3/23/56/67	0/4/4/5
2	NAP	F	500[B]	-	-	4/23/56/67	0/4/4/5
2	NAP	E	500[B]	-	-	3/23/56/67	0/4/4/5
2	NAP	A	501[B]	-	-	4/23/56/67	0/4/4/5
2	NAP	G	500[B]	-	-	4/23/56/67	0/4/4/5
2	NAP	H	500[B]	-	-	3/23/56/67	0/4/4/5
2	NAP	E	500[A]	-	-	4/23/56/67	0/4/4/5
2	NAP	C	500[B]	-	-	3/23/56/67	0/4/4/5
2	NAP	F	500[A]	-	-	3/23/56/67	0/4/4/5
2	NAP	A	501[A]	-	-	2/23/56/67	0/4/4/5
2	NAP	D	500[A]	-	-	5/23/56/67	0/4/4/5
2	NAP	G	500[A]	-	-	3/23/56/67	0/4/4/5

All (135) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	H	500[A]	NAP	C2D-C3D	-5.42	1.44	1.53
2	A	501[A]	NAP	C2D-C3D	-5.19	1.45	1.53
2	E	500[A]	NAP	C2D-C3D	-5.14	1.45	1.53
2	B	500	NAP	C3B-C2B	-5.12	1.41	1.52
2	F	500[A]	NAP	C2D-C3D	-5.06	1.45	1.53
2	C	500[A]	NAP	C2D-C3D	-5.06	1.45	1.53
2	C	500[A]	NAP	C3B-C2B	-5.04	1.41	1.52
2	C	500[B]	NAP	C3B-C2B	-5.04	1.41	1.52
2	A	501[B]	NAP	C3B-C2B	-5.01	1.41	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	501[A]	NAP	C3B-C2B	-5.01	1.41	1.52
2	G	500[B]	NAP	C3B-C2B	-4.98	1.41	1.52
2	G	500[A]	NAP	C3B-C2B	-4.98	1.41	1.52
2	F	500[A]	NAP	C3B-C2B	-4.95	1.41	1.52
2	F	500[B]	NAP	C3B-C2B	-4.95	1.41	1.52
2	E	500[A]	NAP	C3B-C2B	-4.90	1.42	1.52
2	E	500[B]	NAP	C3B-C2B	-4.90	1.42	1.52
2	H	500[B]	NAP	C3B-C2B	-4.88	1.42	1.52
2	H	500[A]	NAP	C3B-C2B	-4.88	1.42	1.52
2	D	500[B]	NAP	C3B-C2B	-4.76	1.42	1.52
2	D	500[A]	NAP	C3B-C2B	-4.76	1.42	1.52
2	G	500[A]	NAP	C2D-C3D	-4.67	1.46	1.53
2	D	500[B]	NAP	C2D-C3D	-4.60	1.46	1.53
2	D	500[A]	NAP	C2D-C3D	-4.56	1.46	1.53
2	G	500[B]	NAP	C2D-C3D	-4.52	1.46	1.53
2	A	501[B]	NAP	C2D-C3D	-4.52	1.46	1.53
2	B	500	NAP	C2D-C3D	-4.50	1.46	1.53
2	G	500[B]	NAP	C6A-N6A	4.33	1.49	1.34
2	G	500[A]	NAP	C6A-N6A	4.33	1.49	1.34
2	E	500[A]	NAP	C6A-N6A	4.27	1.49	1.34
2	E	500[B]	NAP	C6A-N6A	4.27	1.49	1.34
2	A	501[B]	NAP	C6A-N6A	4.26	1.49	1.34
2	A	501[A]	NAP	C6A-N6A	4.26	1.49	1.34
2	C	500[A]	NAP	C6A-N6A	4.25	1.49	1.34
2	C	500[B]	NAP	C6A-N6A	4.25	1.49	1.34
2	H	500[B]	NAP	C2D-C3D	-4.24	1.46	1.53
2	C	500[B]	NAP	C2D-C3D	-4.23	1.46	1.53
2	F	500[A]	NAP	C6A-N6A	4.19	1.49	1.34
2	F	500[B]	NAP	C6A-N6A	4.19	1.49	1.34
2	H	500[B]	NAP	C6A-N6A	4.15	1.49	1.34
2	H	500[A]	NAP	C6A-N6A	4.15	1.49	1.34
2	B	500	NAP	C6A-N6A	4.15	1.49	1.34
2	D	500[B]	NAP	C6A-N6A	4.12	1.49	1.34
2	D	500[A]	NAP	C6A-N6A	4.12	1.49	1.34
2	F	500[B]	NAP	C2D-C3D	-3.99	1.47	1.53
2	E	500[B]	NAP	C2D-C3D	-3.98	1.47	1.53
2	A	501[A]	NAP	O3D-C3D	-3.58	1.34	1.43
2	H	500[A]	NAP	O3D-C3D	-3.57	1.34	1.43
2	E	500[A]	NAP	O3D-C3D	-3.54	1.34	1.43
2	C	500[A]	NAP	O3D-C3D	-3.51	1.34	1.43
2	G	500[B]	NAP	O3D-C3D	-3.44	1.34	1.43
2	D	500[B]	NAP	O3D-C3D	-3.40	1.35	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	501[B]	NAP	O3D-C3D	-3.39	1.35	1.43
2	H	500[B]	NAP	O3D-C3D	-3.33	1.35	1.43
2	G	500[A]	NAP	O3D-C3D	-3.31	1.35	1.43
2	F	500[A]	NAP	O3D-C3D	-3.29	1.35	1.43
2	C	500[B]	NAP	O3D-C3D	-3.29	1.35	1.43
2	E	500[B]	NAP	O3D-C3D	-3.21	1.35	1.43
2	F	500[B]	NAP	O3D-C3D	-3.18	1.35	1.43
2	D	500[A]	NAP	O3D-C3D	-3.13	1.35	1.43
2	B	500	NAP	O3D-C3D	-3.04	1.35	1.43
2	H	500[B]	NAP	C5D-C4D	-3.02	1.42	1.51
2	C	500[B]	NAP	C5D-C4D	-2.93	1.42	1.51
2	F	500[B]	NAP	C5D-C4D	-2.93	1.42	1.51
2	G	500[B]	NAP	C5D-C4D	-2.92	1.42	1.51
2	E	500[B]	NAP	C5D-C4D	-2.90	1.42	1.51
2	E	500[A]	NAP	O2D-C2D	-2.85	1.37	1.43
2	H	500[A]	NAP	O2D-C2D	-2.84	1.37	1.43
2	A	501[B]	NAP	C5D-C4D	-2.83	1.42	1.51
2	H	500[A]	NAP	C5D-C4D	-2.81	1.42	1.51
2	E	500[A]	NAP	C5D-C4D	-2.78	1.42	1.51
2	C	500[A]	NAP	O2D-C2D	-2.76	1.37	1.43
2	D	500[B]	NAP	C5D-C4D	-2.76	1.43	1.51
2	E	500[B]	NAP	C3D-C4D	-2.76	1.45	1.53
2	F	500[B]	NAP	C3D-C4D	-2.76	1.45	1.53
2	C	500[A]	NAP	C5D-C4D	-2.73	1.43	1.51
2	A	501[A]	NAP	C5D-C4D	-2.73	1.43	1.51
2	F	500[A]	NAP	C5D-C4D	-2.73	1.43	1.51
2	G	500[A]	NAP	O2D-C2D	-2.72	1.37	1.43
2	A	501[A]	NAP	C3D-C4D	-2.71	1.46	1.53
2	G	500[A]	NAP	C5D-C4D	-2.71	1.43	1.51
2	B	500	NAP	C5D-C4D	-2.70	1.43	1.51
2	C	500[B]	NAP	C3D-C4D	-2.67	1.46	1.53
2	A	501[A]	NAP	O2D-C2D	-2.65	1.37	1.43
2	B	500	NAP	O2D-C2D	-2.64	1.37	1.43
2	H	500[A]	NAP	C3D-C4D	-2.64	1.46	1.53
2	E	500[A]	NAP	C3D-C4D	-2.64	1.46	1.53
2	C	500[B]	NAP	O2D-C2D	-2.64	1.37	1.43
2	H	500[B]	NAP	O2D-C2D	-2.63	1.37	1.43
2	F	500[A]	NAP	O2D-C2D	-2.59	1.37	1.43
2	F	500[A]	NAP	C3D-C4D	-2.59	1.46	1.53
2	H	500[B]	NAP	C3D-C4D	-2.58	1.46	1.53
2	C	500[A]	NAP	C3D-C4D	-2.57	1.46	1.53
2	A	501[B]	NAP	O2D-C2D	-2.54	1.38	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	500[A]	NAP	O2D-C2D	-2.54	1.38	1.43
2	G	500[B]	NAP	C3D-C4D	-2.53	1.46	1.53
2	G	500[B]	NAP	O2D-C2D	-2.50	1.38	1.43
2	G	500[A]	NAP	C3D-C4D	-2.49	1.46	1.53
2	D	500[B]	NAP	C3D-C4D	-2.47	1.46	1.53
2	B	500	NAP	C3D-C4D	-2.47	1.46	1.53
2	A	501[B]	NAP	C3D-C4D	-2.45	1.46	1.53
2	D	500[B]	NAP	O2D-C2D	-2.42	1.38	1.43
2	D	500[A]	NAP	C5D-C4D	-2.40	1.44	1.51
2	F	500[B]	NAP	O2D-C2D	-2.39	1.38	1.43
2	E	500[B]	NAP	O2D-C2D	-2.39	1.38	1.43
2	B	500	NAP	O4B-C4B	-2.32	1.39	1.45
2	H	500[B]	NAP	O4B-C4B	-2.27	1.39	1.45
2	H	500[A]	NAP	O4B-C4B	-2.27	1.39	1.45
2	E	500[A]	NAP	O4B-C4B	-2.15	1.40	1.45
2	E	500[B]	NAP	O4B-C4B	-2.15	1.40	1.45
2	C	500[A]	NAP	O4B-C4B	-2.14	1.40	1.45
2	C	500[B]	NAP	O4B-C4B	-2.14	1.40	1.45
2	D	500[B]	NAP	C3B-C4B	-2.13	1.47	1.53
2	D	500[A]	NAP	C3B-C4B	-2.13	1.47	1.53
2	E	500[A]	NAP	O5D-C5D	-2.11	1.36	1.44
2	A	501[B]	NAP	C3B-C4B	-2.09	1.47	1.53
2	A	501[A]	NAP	C3B-C4B	-2.09	1.47	1.53
2	D	500[B]	NAP	O4B-C4B	-2.08	1.40	1.45
2	D	500[A]	NAP	O4B-C4B	-2.08	1.40	1.45
2	A	501[B]	NAP	O4B-C4B	-2.08	1.40	1.45
2	A	501[A]	NAP	O4B-C4B	-2.08	1.40	1.45
2	F	500[A]	NAP	C3B-C4B	-2.06	1.47	1.53
2	F	500[B]	NAP	C3B-C4B	-2.06	1.47	1.53
2	F	500[A]	NAP	O4B-C4B	-2.06	1.40	1.45
2	F	500[B]	NAP	O4B-C4B	-2.06	1.40	1.45
2	E	500[A]	NAP	C3B-C4B	-2.04	1.47	1.53
2	E	500[B]	NAP	C3B-C4B	-2.04	1.47	1.53
2	A	501[B]	NAP	P2B-O2X	-2.04	1.47	1.54
2	A	501[A]	NAP	P2B-O2X	-2.04	1.47	1.54
2	C	500[A]	NAP	P2B-O2X	-2.04	1.47	1.54
2	C	500[B]	NAP	P2B-O2X	-2.04	1.47	1.54
2	G	500[B]	NAP	C3B-C4B	-2.03	1.47	1.53
2	G	500[A]	NAP	C3B-C4B	-2.03	1.47	1.53
2	H	500[B]	NAP	O4D-C1D	-2.02	1.39	1.43
2	B	500	NAP	P2B-O2X	-2.01	1.47	1.54
2	C	500[A]	NAP	O5D-C5D	-2.01	1.37	1.44

All (101) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	500	NAP	C1B-N9A-C4A	-6.78	114.72	126.64
2	F	500[A]	NAP	C1B-N9A-C4A	-6.44	115.32	126.64
2	F	500[B]	NAP	C1B-N9A-C4A	-6.44	115.32	126.64
2	C	500[A]	NAP	C1B-N9A-C4A	-6.38	115.43	126.64
2	C	500[B]	NAP	C1B-N9A-C4A	-6.38	115.43	126.64
2	D	500[B]	NAP	C1B-N9A-C4A	-6.08	115.96	126.64
2	D	500[A]	NAP	C1B-N9A-C4A	-6.08	115.96	126.64
2	E	500[A]	NAP	C1B-N9A-C4A	-5.99	116.11	126.64
2	E	500[B]	NAP	C1B-N9A-C4A	-5.99	116.11	126.64
2	G	500[B]	NAP	C1B-N9A-C4A	-5.43	117.10	126.64
2	G	500[A]	NAP	C1B-N9A-C4A	-5.43	117.10	126.64
2	H	500[B]	NAP	C1B-N9A-C4A	-5.39	117.17	126.64
2	H	500[A]	NAP	C1B-N9A-C4A	-5.39	117.17	126.64
2	A	501[B]	NAP	C1B-N9A-C4A	-4.67	118.44	126.64
2	A	501[A]	NAP	C1B-N9A-C4A	-4.67	118.44	126.64
2	E	500[A]	NAP	O2D-C2D-C3D	-4.36	103.00	111.27
2	H	500[A]	NAP	O2D-C2D-C3D	-4.28	103.15	111.27
2	A	501[A]	NAP	O2D-C2D-C3D	-4.23	103.25	111.27
2	F	500[A]	NAP	N3A-C2A-N1A	-4.06	122.34	128.68
2	F	500[B]	NAP	N3A-C2A-N1A	-4.06	122.34	128.68
2	B	500	NAP	N3A-C2A-N1A	-4.01	122.41	128.68
2	E	500[A]	NAP	N3A-C2A-N1A	-3.85	122.66	128.68
2	E	500[B]	NAP	N3A-C2A-N1A	-3.85	122.66	128.68
2	D	500[B]	NAP	N3A-C2A-N1A	-3.82	122.71	128.68
2	D	500[A]	NAP	N3A-C2A-N1A	-3.82	122.71	128.68
2	C	500[A]	NAP	N3A-C2A-N1A	-3.78	122.77	128.68
2	C	500[B]	NAP	N3A-C2A-N1A	-3.78	122.77	128.68
2	H	500[B]	NAP	N3A-C2A-N1A	-3.66	122.96	128.68
2	H	500[A]	NAP	N3A-C2A-N1A	-3.66	122.96	128.68
2	A	501[B]	NAP	N3A-C2A-N1A	-3.54	123.15	128.68
2	A	501[A]	NAP	N3A-C2A-N1A	-3.54	123.15	128.68
2	G	500[B]	NAP	N3A-C2A-N1A	-3.50	123.20	128.68
2	G	500[A]	NAP	N3A-C2A-N1A	-3.50	123.20	128.68
2	G	500[A]	NAP	PN-O3-PA	-3.48	120.89	132.83
2	C	500[A]	NAP	PN-O3-PA	-3.46	120.96	132.83
2	D	500[B]	NAP	C1D-C2D-C3D	3.38	106.77	101.63
2	H	500[B]	NAP	C1D-O4D-C4D	-3.37	100.31	108.16
2	E	500[A]	NAP	C1D-C2D-C3D	3.34	106.72	101.63
2	C	500[A]	NAP	O2D-C2D-C3D	-3.31	105.00	111.27
2	B	500	NAP	O4D-C4D-C3D	-3.28	101.80	104.70
2	A	501[B]	NAP	C1D-O4D-C4D	-3.11	100.91	108.16
2	C	500[B]	NAP	C1D-O4D-C4D	-3.00	101.15	108.16

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	G	500[B]	NAP	O4B-C1B-C2B	-2.98	101.42	106.59
2	G	500[A]	NAP	O4B-C1B-C2B	-2.98	101.42	106.59
2	F	500[B]	NAP	PN-O3-PA	-2.93	122.76	132.83
2	E	500[A]	NAP	PN-O3-PA	-2.90	122.87	132.83
2	E	500[B]	NAP	PN-O3-PA	-2.84	123.08	132.83
2	E	500[B]	NAP	C1D-C2D-C3D	2.82	105.92	101.63
2	A	501[B]	NAP	O4B-C1B-C2B	-2.82	101.70	106.59
2	A	501[A]	NAP	O4B-C1B-C2B	-2.82	101.70	106.59
2	F	500[B]	NAP	C1D-C2D-C3D	2.81	105.91	101.63
2	G	500[B]	NAP	C1D-C2D-C3D	2.80	105.90	101.63
2	H	500[A]	NAP	O5D-C5D-C4D	2.78	118.54	108.99
2	D	500[A]	NAP	O5D-C5D-C4D	2.75	118.45	108.99
2	A	501[A]	NAP	C1D-C2D-C3D	2.75	105.81	101.63
2	C	500[B]	NAP	PN-O3-PA	-2.71	123.51	132.83
2	G	500[B]	NAP	PN-O3-PA	-2.70	123.57	132.83
2	F	500[A]	NAP	O2D-C2D-C3D	-2.68	106.19	111.27
2	D	500[B]	NAP	O4D-C4D-C3D	2.68	107.07	104.70
2	G	500[B]	NAP	C1D-O4D-C4D	-2.67	101.92	108.16
2	C	500[A]	NAP	C1D-C2D-C3D	2.66	105.68	101.63
2	A	501[A]	NAP	PN-O3-PA	-2.65	123.72	132.83
2	F	500[A]	NAP	O5D-C5D-C4D	2.65	118.10	108.99
2	A	501[A]	NAP	O5D-C5D-C4D	2.63	118.04	108.99
2	F	500[B]	NAP	O5D-C5D-C4D	2.63	118.03	108.99
2	E	500[B]	NAP	O5D-C5D-C4D	2.62	118.01	108.99
2	C	500[B]	NAP	C1D-C2D-C3D	2.61	105.60	101.63
2	D	500[B]	NAP	PN-O3-PA	-2.59	123.94	132.83
2	D	500[A]	NAP	C1D-C2D-C3D	2.58	105.55	101.63
2	A	501[B]	NAP	PN-O3-PA	-2.57	124.00	132.83
2	A	501[A]	NAP	O4D-C4D-C3D	-2.54	102.46	104.70
2	B	500	NAP	C1D-C2D-C3D	2.50	105.43	101.63
2	H	500[A]	NAP	C1D-C2D-C3D	2.47	105.39	101.63
2	G	500[A]	NAP	O2D-C2D-C3D	-2.45	106.62	111.27
2	E	500[A]	NAP	O5D-C5D-C4D	2.45	117.42	108.99
2	H	500[B]	NAP	PN-O3-PA	-2.43	124.48	132.83
2	F	500[A]	NAP	PN-O3-PA	-2.43	124.49	132.83
2	B	500	NAP	O5D-C5D-C4D	2.42	117.32	108.99
2	H	500[B]	NAP	C1D-C2D-C3D	2.42	105.31	101.63
2	B	500	NAP	PN-O3-PA	-2.40	124.58	132.83
2	C	500[A]	NAP	O5D-C5D-C4D	2.40	117.24	108.99
2	B	500	NAP	C1D-O4D-C4D	-2.39	102.58	108.16
2	G	500[A]	NAP	C1D-C2D-C3D	2.38	105.26	101.63
2	G	500[A]	NAP	O5D-C5D-C4D	2.37	117.16	108.99

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	500[A]	NAP	O3D-C3D-C2D	-2.26	106.59	112.04
2	E	500[A]	NAP	O3D-C3D-C2D	-2.26	106.59	112.04
2	A	501[B]	NAP	O5D-C5D-C4D	2.23	116.68	108.99
2	H	500[B]	NAP	O4B-C1B-C2B	-2.23	102.72	106.59
2	H	500[A]	NAP	O4B-C1B-C2B	-2.23	102.72	106.59
2	E	500[B]	NAP	C5D-C4D-C3D	-2.21	106.90	115.18
2	F	500[B]	NAP	C5D-C4D-C3D	-2.20	106.92	115.18
2	A	501[B]	NAP	C1D-C2D-C3D	2.19	104.97	101.63
2	D	500[B]	NAP	O4B-C1B-C2B	-2.10	102.94	106.59
2	D	500[A]	NAP	O4B-C1B-C2B	-2.10	102.94	106.59
2	A	501[B]	NAP	C4A-C5A-N7A	-2.06	107.25	109.40
2	A	501[A]	NAP	C4A-C5A-N7A	-2.06	107.25	109.40
2	E	500[A]	NAP	O4B-C1B-C2B	-2.05	103.03	106.59
2	E	500[B]	NAP	O4B-C1B-C2B	-2.05	103.03	106.59
2	D	500[B]	NAP	O2D-C2D-C3D	-2.05	107.39	111.27
2	F	500[A]	NAP	O4B-C1B-C2B	-2.01	103.11	106.59
2	F	500[B]	NAP	O4B-C1B-C2B	-2.01	103.11	106.59

There are no chirality outliers.

All (53) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	D	500[B]	NAP	C5D-O5D-PN-O1N
2	G	500[B]	NAP	O4D-C4D-C5D-O5D
2	D	500[B]	NAP	O4D-C4D-C5D-O5D
2	D	500[B]	NAP	C3D-C4D-C5D-O5D
2	H	500[B]	NAP	O4D-C4D-C5D-O5D
2	H	500[B]	NAP	C3D-C4D-C5D-O5D
2	A	501[B]	NAP	O4D-C4D-C5D-O5D
2	A	501[B]	NAP	C3D-C4D-C5D-O5D
2	G	500[B]	NAP	C3D-C4D-C5D-O5D
2	F	500[B]	NAP	O4D-C4D-C5D-O5D
2	E	500[B]	NAP	O4D-C4D-C5D-O5D
2	C	500[B]	NAP	O4D-C4D-C5D-O5D
2	C	500[B]	NAP	C3D-C4D-C5D-O5D
2	F	500[B]	NAP	C3D-C4D-C5D-O5D
2	E	500[B]	NAP	C3D-C4D-C5D-O5D
2	E	500[A]	NAP	C3D-C4D-C5D-O5D
2	D	500[A]	NAP	C3D-C4D-C5D-O5D
2	D	500[A]	NAP	O4D-C4D-C5D-O5D
2	C	500[A]	NAP	PN-O3-PA-O5B
2	D	500[B]	NAP	PN-O3-PA-O5B

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Mol	Chain	Res	Type	Atoms
2	F	500[B]	NAP	PN-O3-PA-O5B
2	D	500[A]	NAP	PN-O3-PA-O5B
2	D	500[A]	NAP	C4D-C5D-O5D-PN
2	C	500[A]	NAP	C4D-C5D-O5D-PN
2	G	500[A]	NAP	C4D-C5D-O5D-PN
2	E	500[A]	NAP	O4D-C4D-C5D-O5D
2	H	500[A]	NAP	C4D-C5D-O5D-PN
2	B	500	NAP	C4D-C5D-O5D-PN
2	F	500[A]	NAP	C4D-C5D-O5D-PN
2	E	500[A]	NAP	C4D-C5D-O5D-PN
2	A	501[B]	NAP	C4D-C5D-O5D-PN
2	A	501[A]	NAP	C4D-C5D-O5D-PN
2	F	500[A]	NAP	PN-O3-PA-O5B
2	H	500[A]	NAP	PN-O3-PA-O5B
2	B	500	NAP	C3D-C4D-C5D-O5D
2	D	500[B]	NAP	C5D-O5D-PN-O3
2	G	500[B]	NAP	C2B-O2B-P2B-O2X
2	G	500[A]	NAP	C2B-O2B-P2B-O2X
2	C	500[A]	NAP	C5B-O5B-PA-O1A
2	D	500[B]	NAP	C5B-O5B-PA-O1A
2	H	500[B]	NAP	C5B-O5B-PA-O1A
2	B	500	NAP	C5B-O5B-PA-O1A
2	F	500[A]	NAP	C5B-O5B-PA-O1A
2	H	500[A]	NAP	C5B-O5B-PA-O1A
2	A	501[B]	NAP	C5B-O5B-PA-O1A
2	G	500[B]	NAP	C5B-O5B-PA-O1A
2	F	500[B]	NAP	C5B-O5B-PA-O1A
2	E	500[A]	NAP	C5B-O5B-PA-O1A
2	A	501[A]	NAP	C5B-O5B-PA-O1A
2	E	500[B]	NAP	C5B-O5B-PA-O1A
2	C	500[B]	NAP	C5B-O5B-PA-O1A
2	D	500[A]	NAP	C5B-O5B-PA-O1A
2	G	500[A]	NAP	C5B-O5B-PA-O1A

There are no ring outliers.

9 monomers are involved in 26 short contacts:

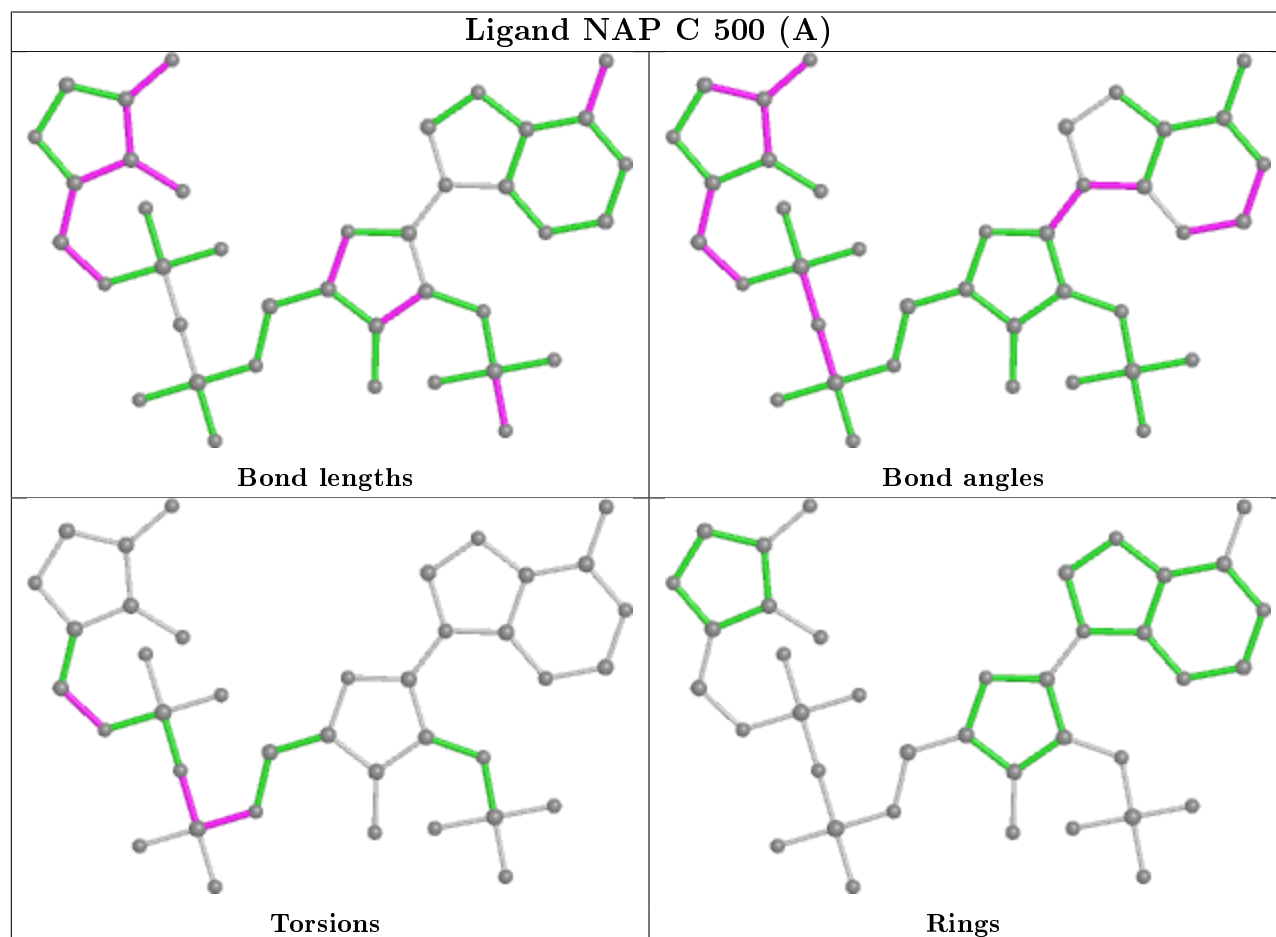
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	D	500[B]	NAP	1	0
2	F	500[B]	NAP	2	0
2	E	500[B]	NAP	7	0
2	A	501[B]	NAP	4	0

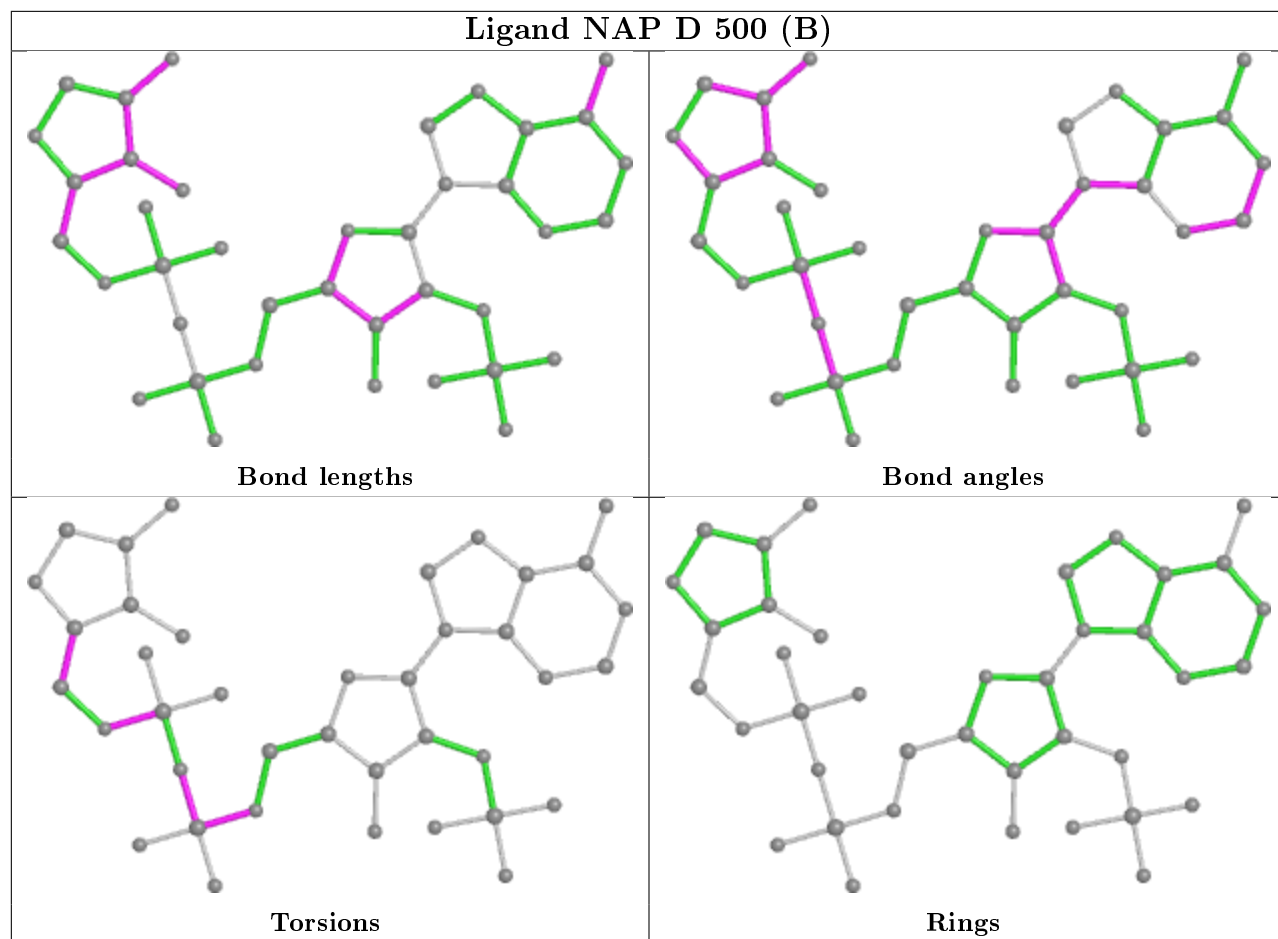
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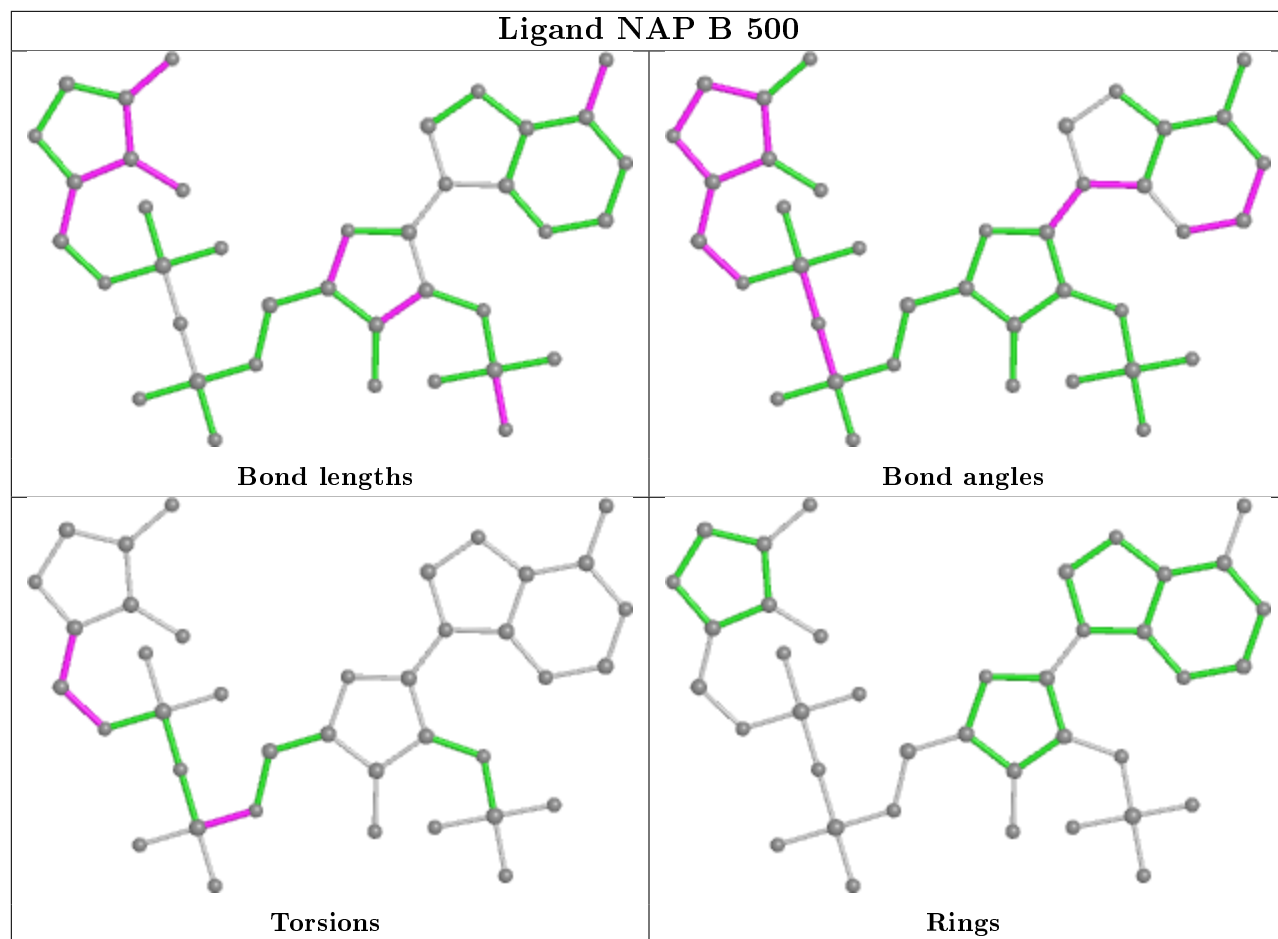
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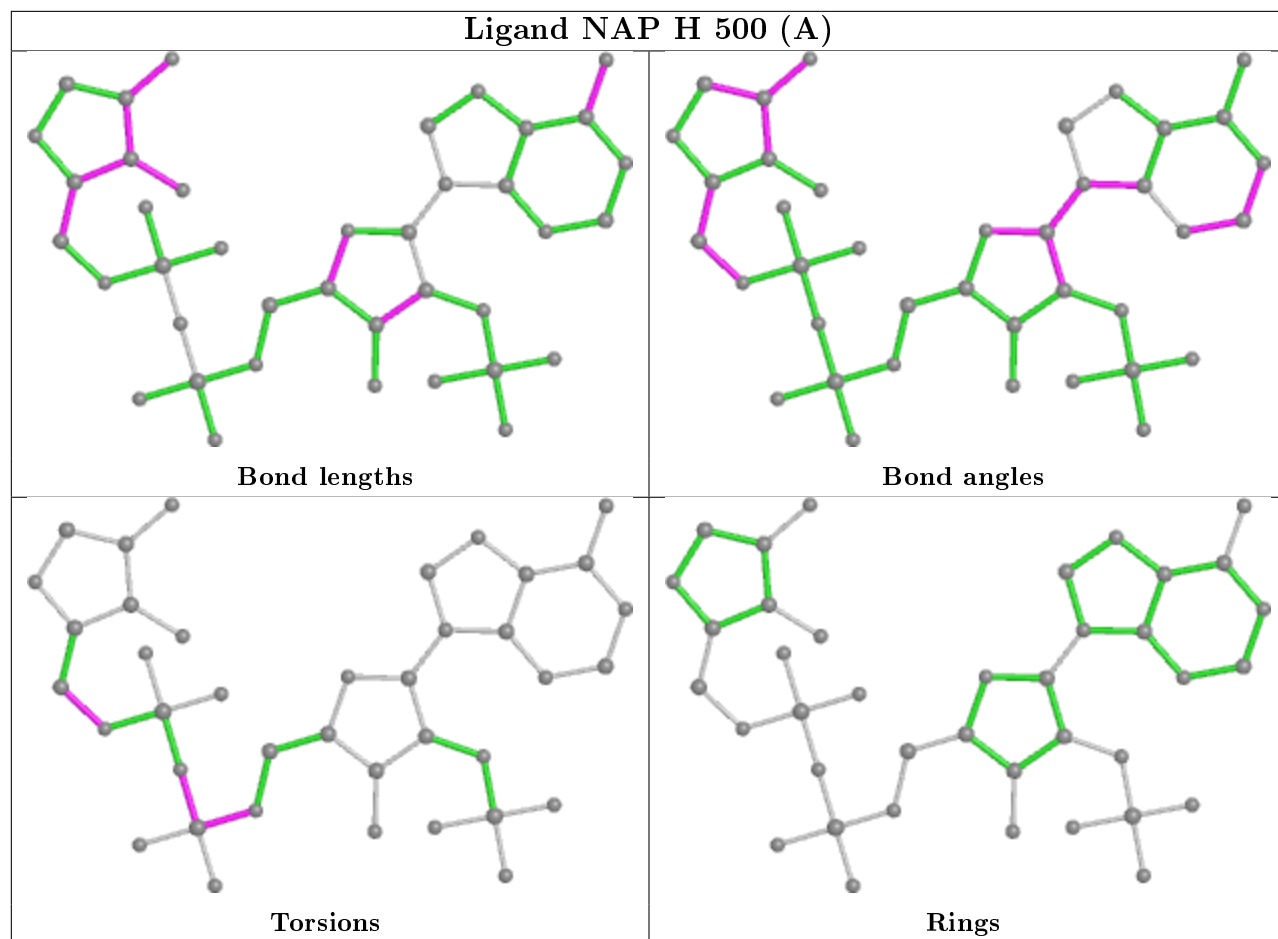
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	G	500[B]	NAP	4	0
2	H	500[B]	NAP	3	0
2	C	500[B]	NAP	3	0
2	D	500[A]	NAP	1	0
2	G	500[A]	NAP	1	0

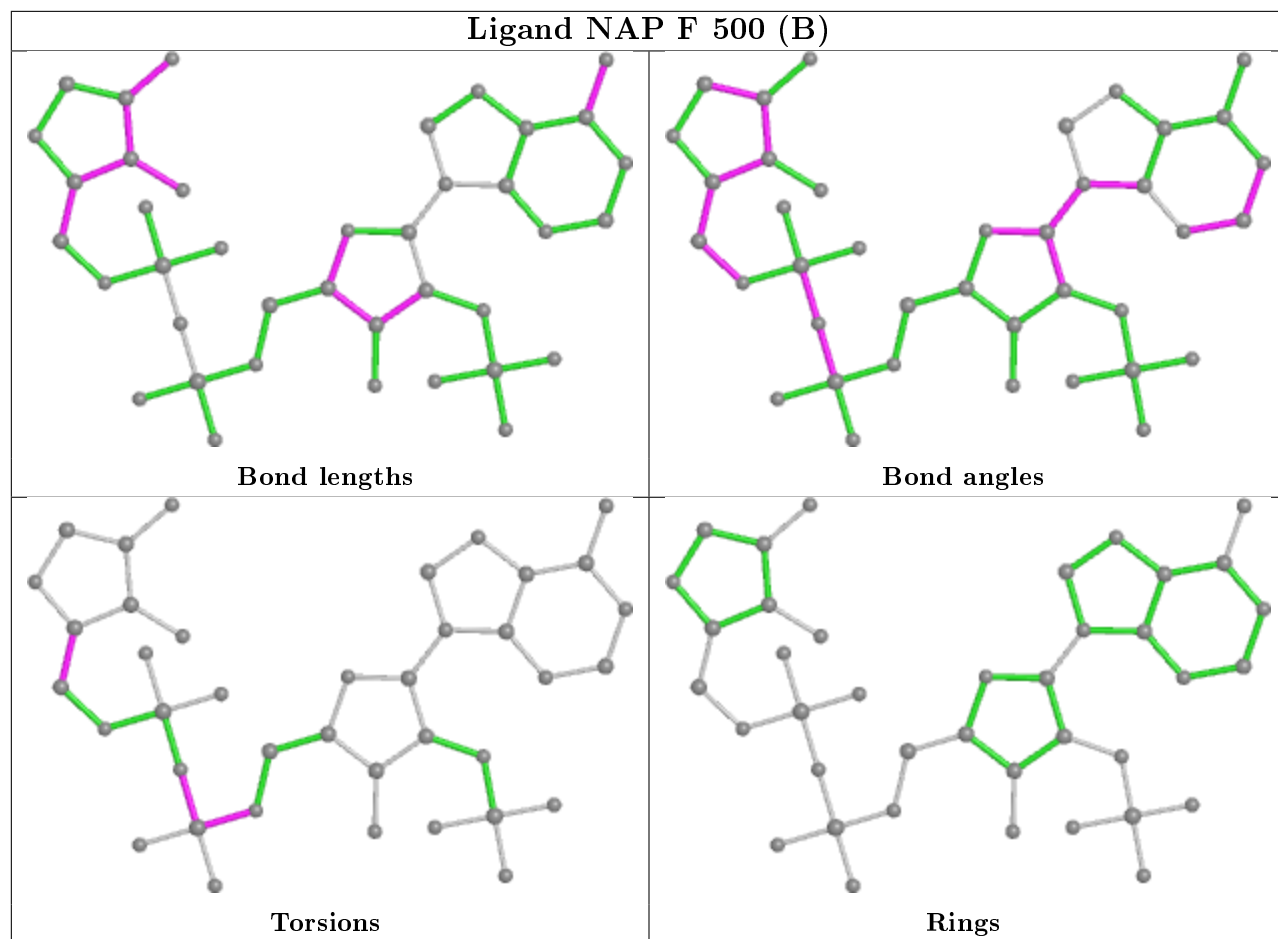
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

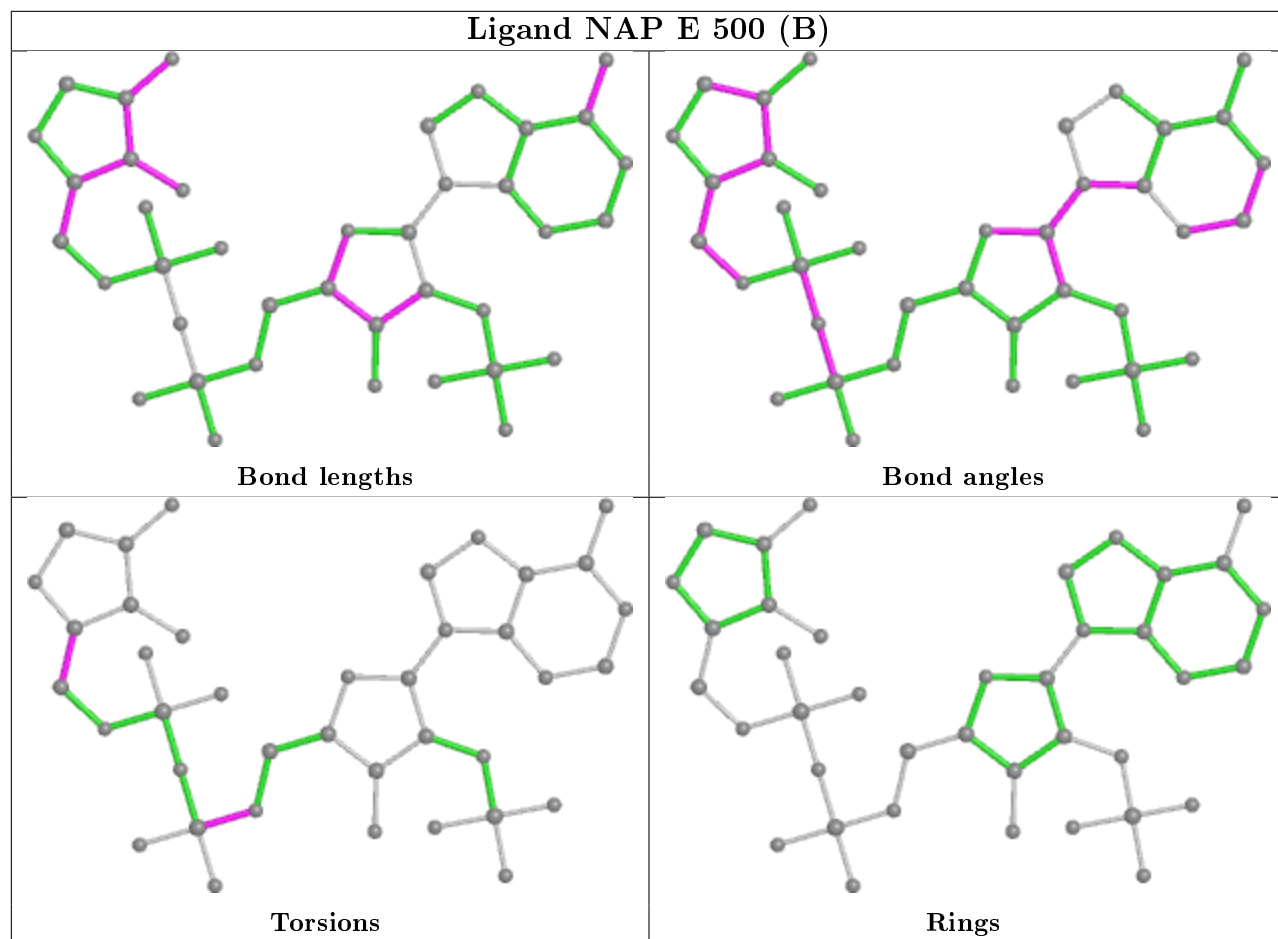




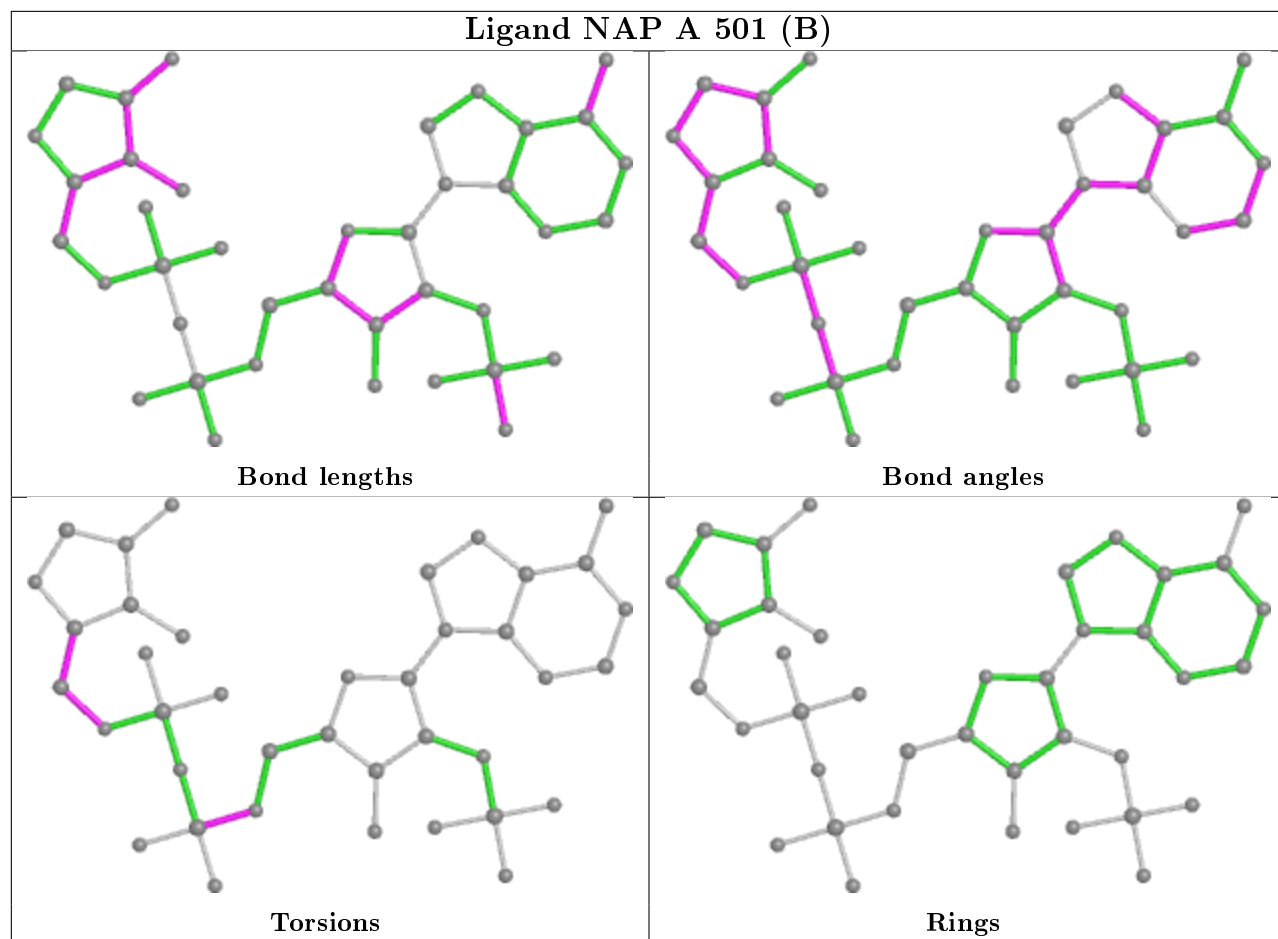


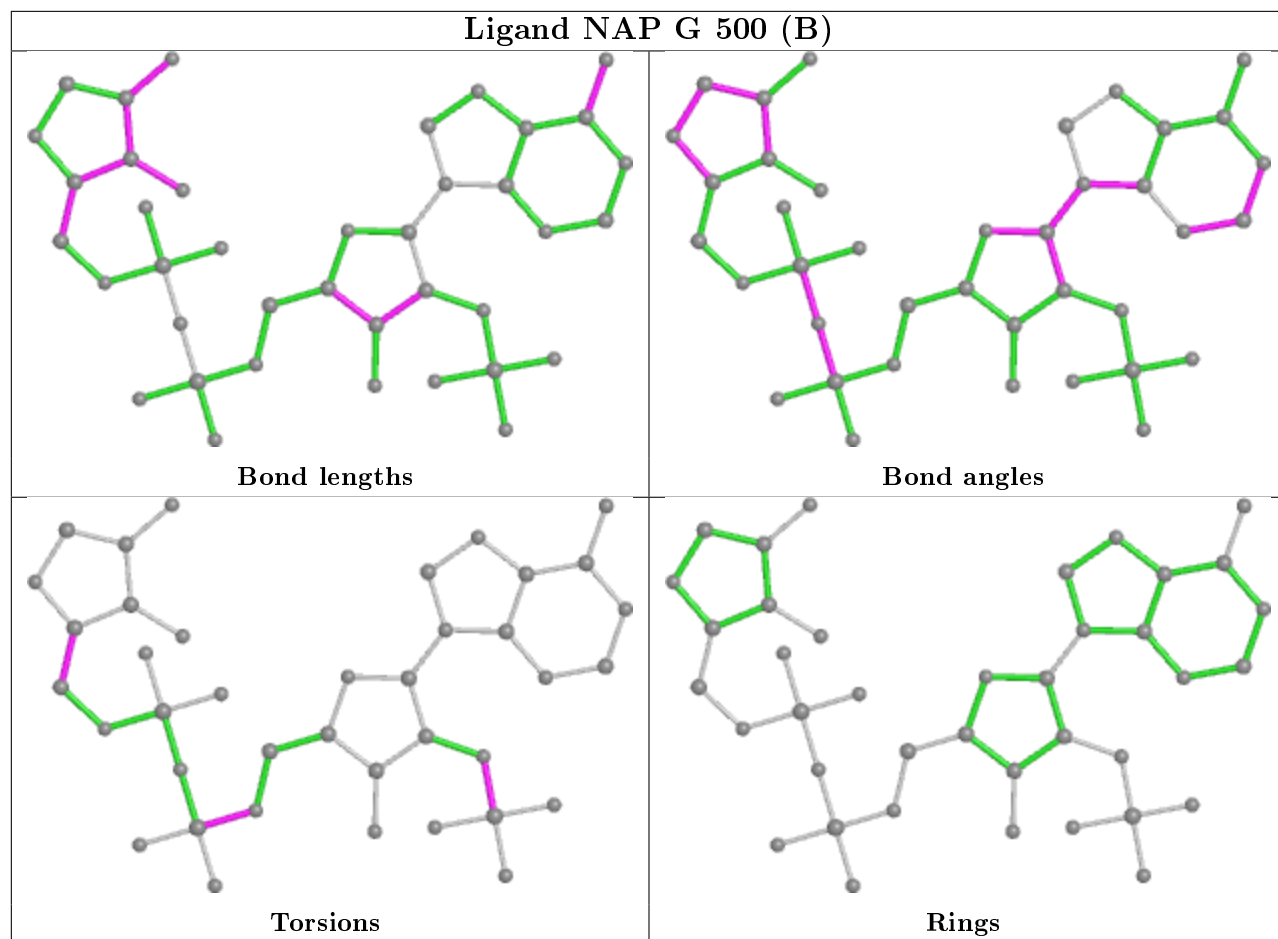


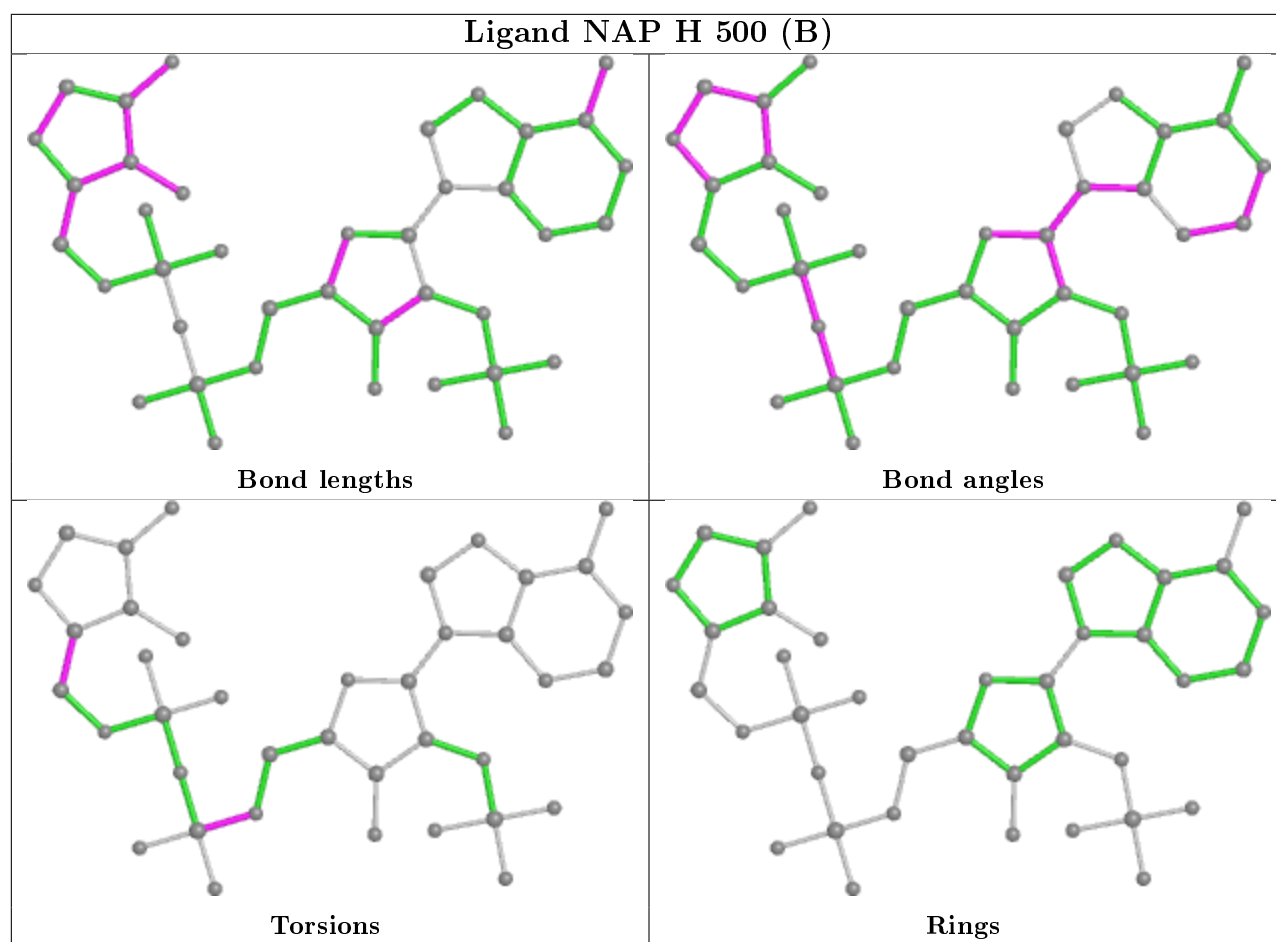


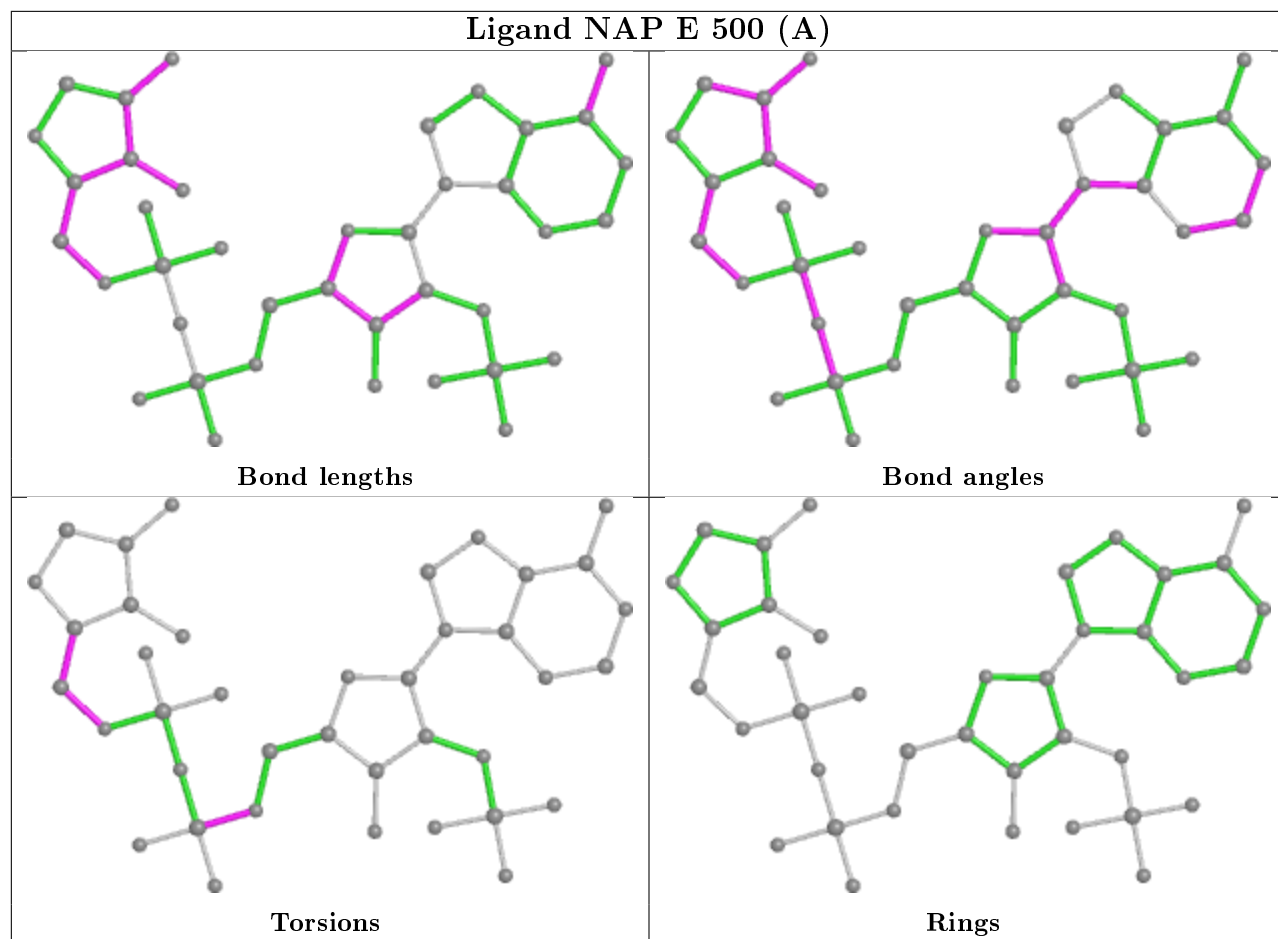


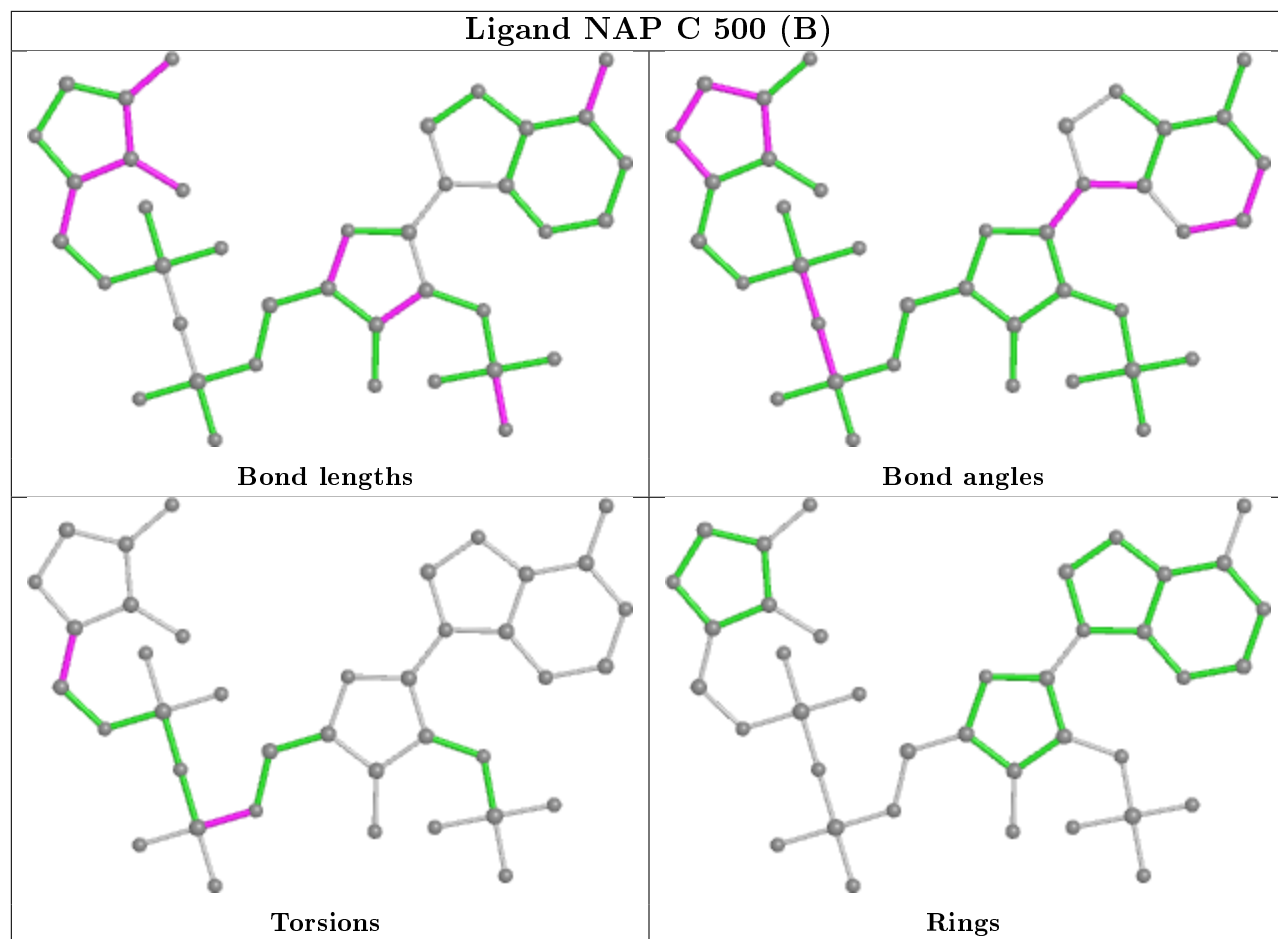


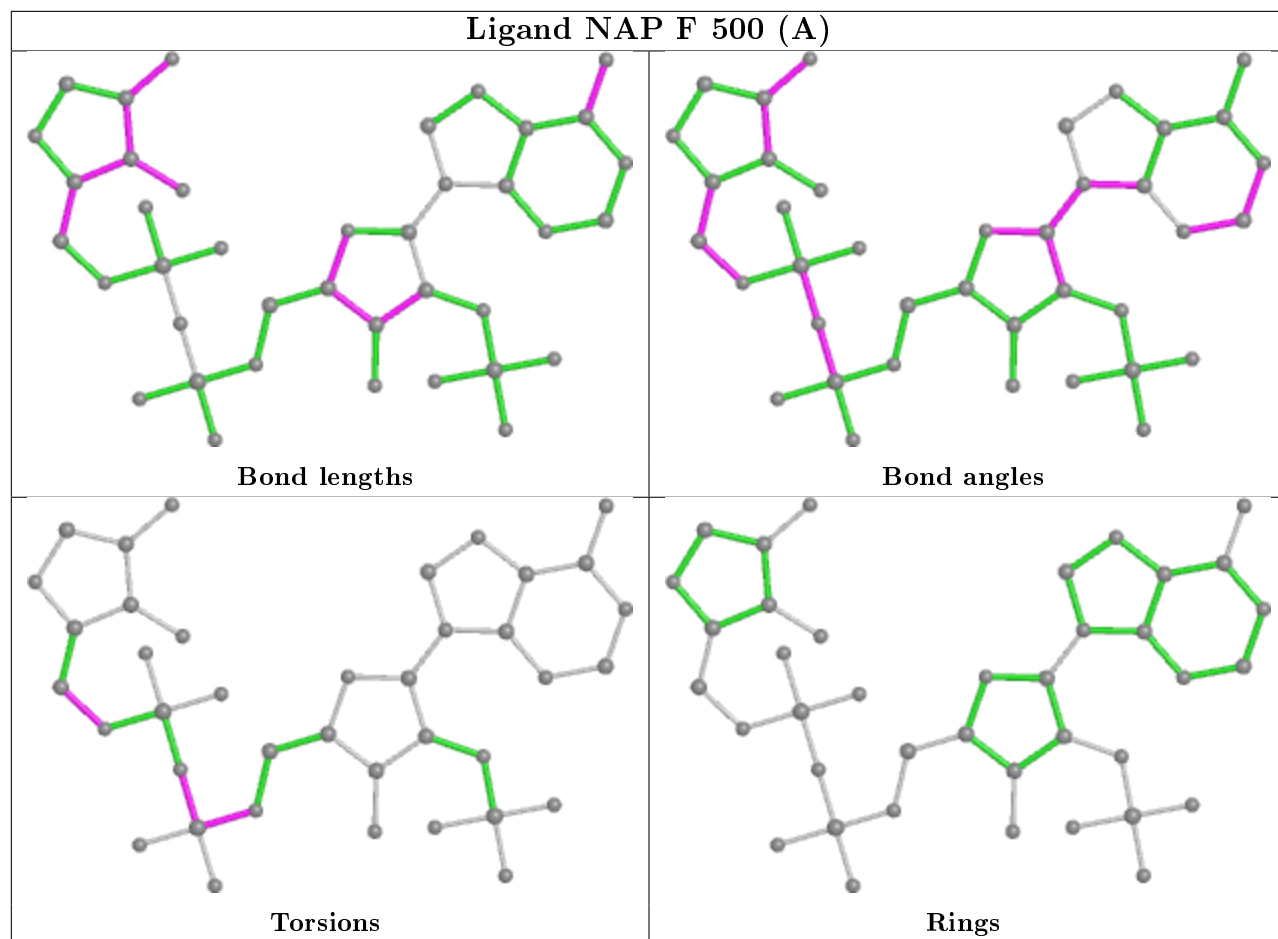


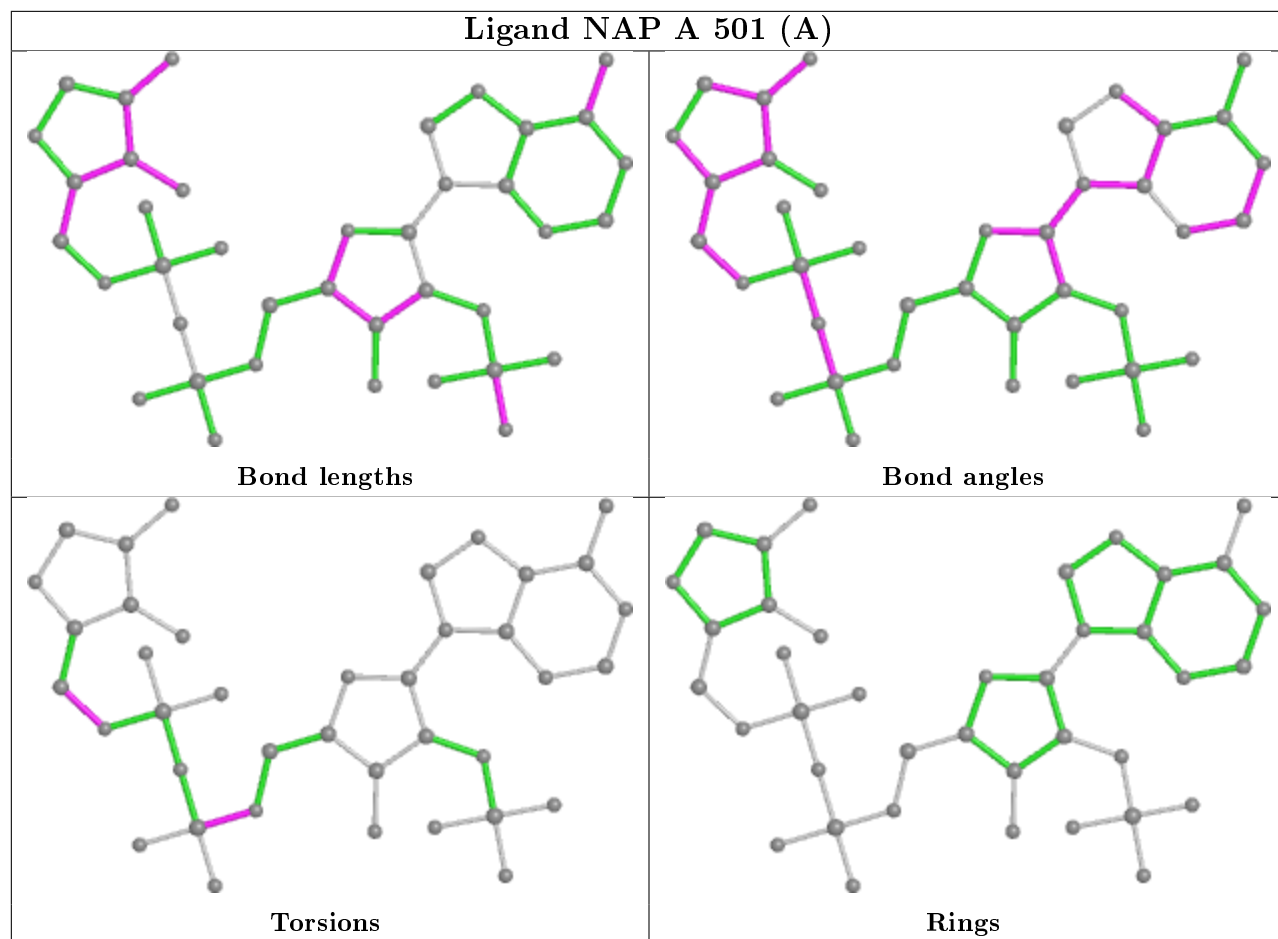


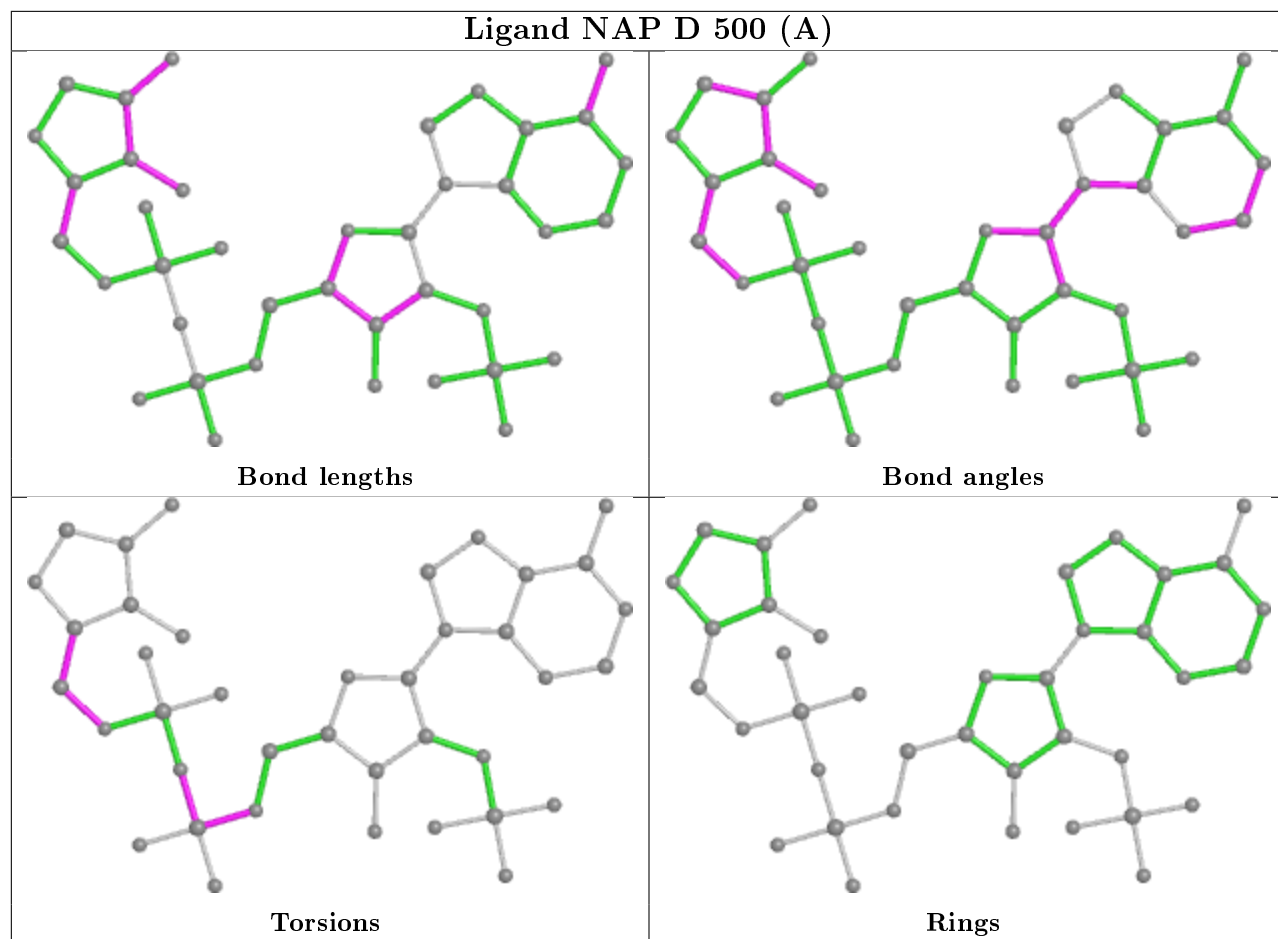




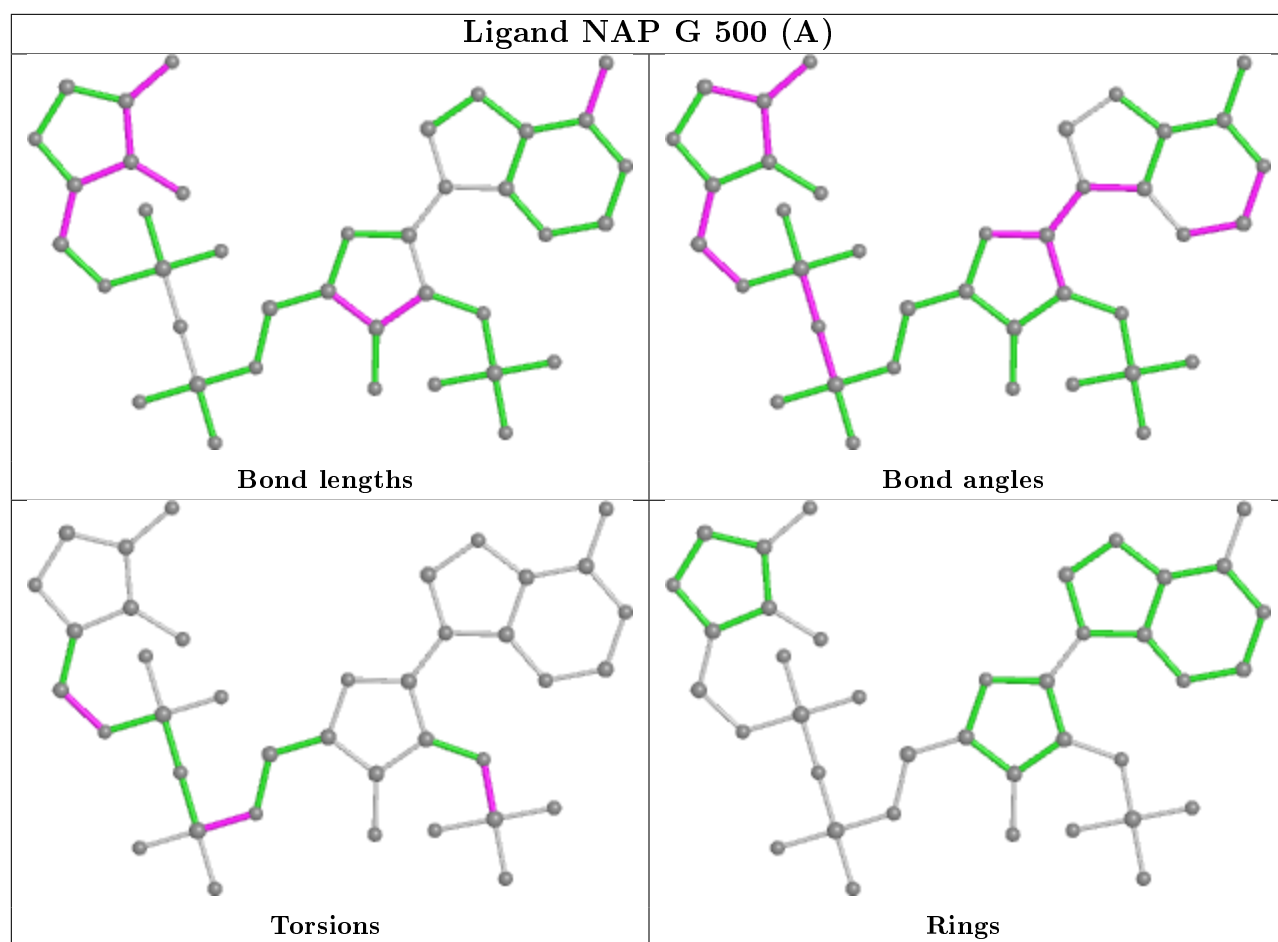












## 5.7 Other polymers [i](#)

There are no such residues in this entry.

## 5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

## 6 Fit of model and data ⓘ

### 6.1 Protein, DNA and RNA chains ⓘ

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å <sup>2</sup> )	Q<0.9
1	A	488/491 (99%)	-0.26	4 (0%) 86 87	16, 24, 39, 62	1 (0%)
1	B	484/491 (98%)	-0.27	4 (0%) 86 87	16, 25, 43, 63	1 (0%)
1	C	490/491 (99%)	-0.27	6 (1%) 79 81	16, 25, 39, 62	3 (0%)
1	D	484/491 (98%)	-0.22	8 (1%) 70 72	16, 27, 46, 57	1 (0%)
1	E	485/491 (98%)	-0.13	10 (2%) 63 66	17, 29, 49, 73	1 (0%)
1	F	490/491 (99%)	-0.29	7 (1%) 75 77	17, 26, 42, 57	1 (0%)
1	G	484/491 (98%)	-0.24	6 (1%) 79 81	16, 28, 43, 54	1 (0%)
1	H	488/491 (99%)	-0.30	4 (0%) 86 87	16, 23, 39, 67	2 (0%)
All	All	3893/3928 (99%)	-0.25	49 (1%) 77 79	16, 26, 43, 73	11 (0%)

All (49) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	F	25	PHE	4.4
1	H	490	LEU	4.2
1	C	490	LEU	4.0
1	D	25	PHE	3.9
1	C	25	PHE	3.9
1	E	27	VAL	3.9
1	B	25	PHE	3.8
1	G	490	LEU	3.8
1	E	7	MET	3.8
1	B	490	LEU	3.7
1	G	25	PHE	3.6
1	F	490	LEU	3.6
1	C	491	LYS	3.6
1	C	2[A]	ILE	3.5
1	D	27	VAL	3.4
1	E	25	PHE	3.3

*Continued on next page...*

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Mol	Chain	Res	Type	RSRZ
1	D	490	LEU	3.3
1	A	490	LEU	2.9
1	A	25	PHE	2.9
1	H	4[A]	LEU	2.9
1	D	21	SER	2.8
1	B	7	MET	2.8
1	E	490	LEU	2.7
1	D	22	THR	2.7
1	H	6[A]	ILE	2.7
1	F	4	LEU	2.6
1	D	8	LYS	2.5
1	A	5	ASN	2.5
1	D	24	ALA	2.5
1	F	22	THR	2.5
1	A	491	LYS	2.4
1	G	165	ILE	2.4
1	C	489	ALA	2.4
1	E	26	GLN	2.4
1	E	491	LYS	2.3
1	F	21	SER	2.3
1	H	25	PHE	2.3
1	E	165	ILE	2.3
1	G	293	ILE	2.3
1	F	5	ASN	2.2
1	F	148	VAL	2.2
1	E	367	ALA	2.1
1	E	36	LYS	2.1
1	B	22	THR	2.1
1	G	150	VAL	2.1
1	C	134	GLU	2.1
1	D	9	VAL	2.0
1	G	8	LYS	2.0
1	E	21	SER	2.0

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

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

## 6.3 Carbohydrates ⓘ

There are no carbohydrates in this entry.

## 6.4 Ligands ⓘ

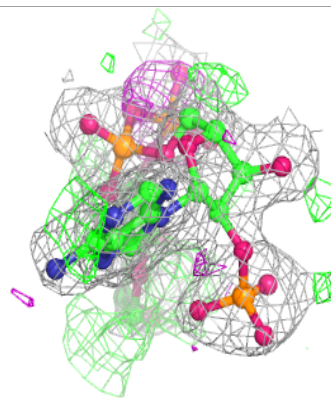
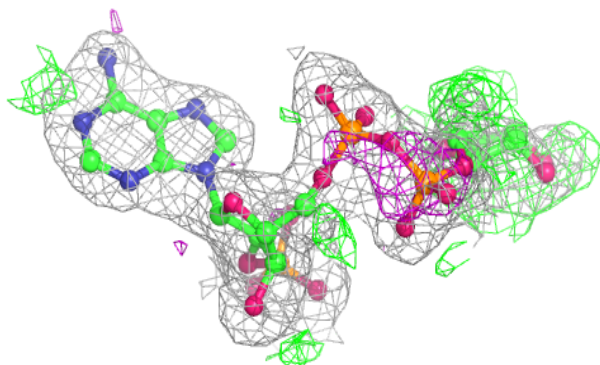
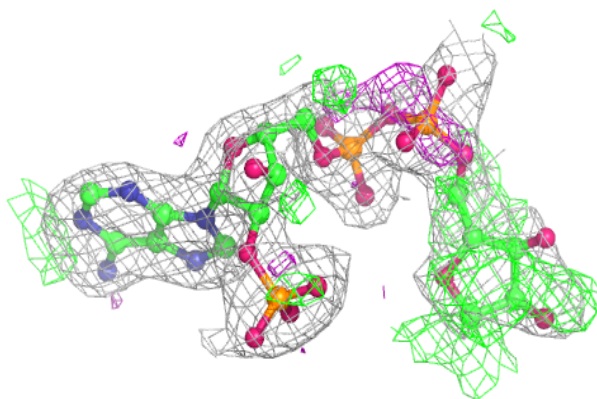
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled 'Q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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å <sup>2</sup> )	Q<0.9
3	GOL	A	502	6/6	0.88	0.20	32,34,36,38	6
2	NAP	D	500[B]	39/48	0.92	0.15	30,37,43,49	12
2	NAP	E	500[A]	39/48	0.92	0.14	34,40,50,54	12
2	NAP	E	500[B]	39/48	0.92	0.14	31,40,48,54	12
2	NAP	D	500[A]	39/48	0.92	0.15	26,35,41,49	12
2	NAP	H	500[A]	39/48	0.94	0.13	21,29,36,38	12
2	NAP	A	501[B]	39/48	0.94	0.16	23,32,38,39	12
2	NAP	G	500[B]	39/48	0.94	0.13	28,35,42,44	12
2	NAP	F	500[B]	39/48	0.94	0.14	29,33,39,44	12
2	NAP	C	500[A]	39/48	0.94	0.14	24,30,38,41	12
2	NAP	A	501[A]	39/48	0.94	0.16	23,31,35,38	12
2	NAP	H	500[B]	39/48	0.94	0.13	24,30,38,39	12
2	NAP	C	500[B]	39/48	0.94	0.14	24,31,38,41	12
2	NAP	F	500[A]	39/48	0.94	0.14	26,32,38,39	12
2	NAP	G	500[A]	39/48	0.94	0.13	28,33,42,44	12
2	NAP	B	500	39/48	0.95	0.11	23,28,36,46	39

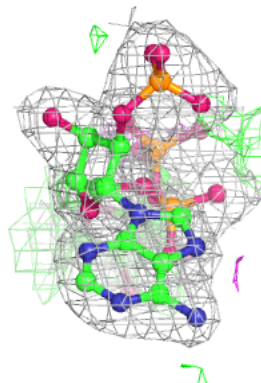
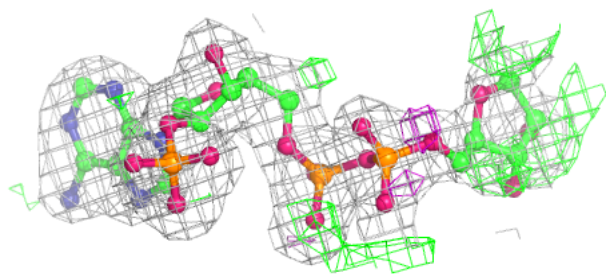
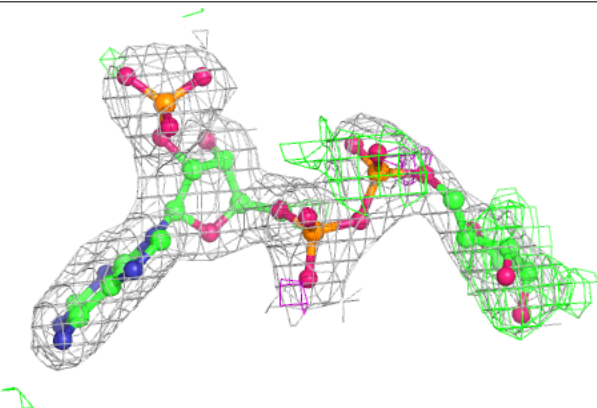
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

**Electron density around NAP D 500 (B):**

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

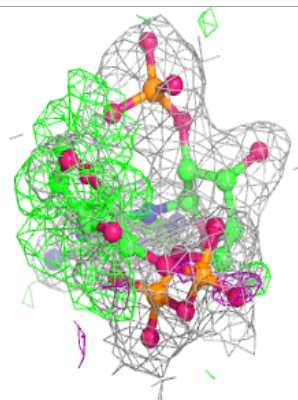
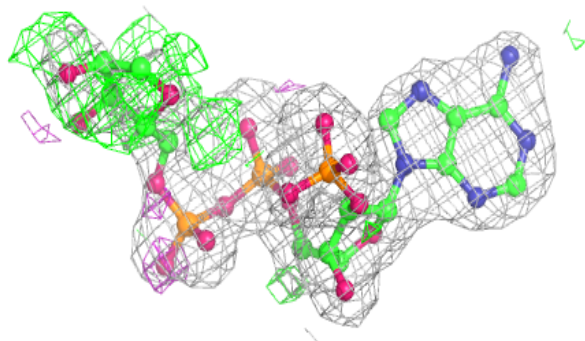
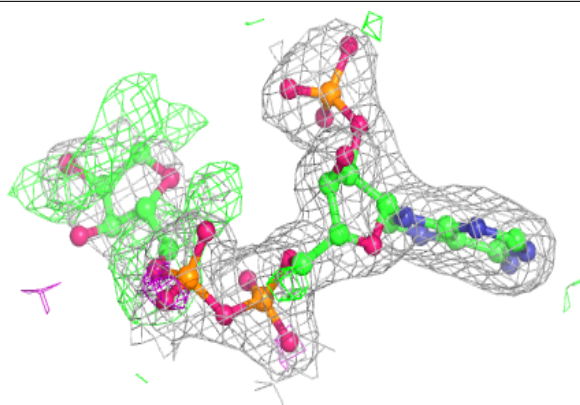
**Electron density around NAP E 500 (A):**

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

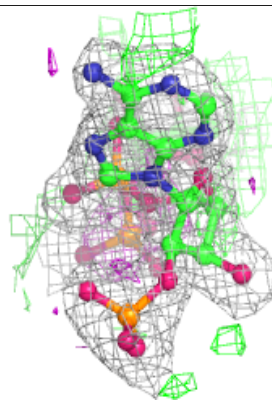
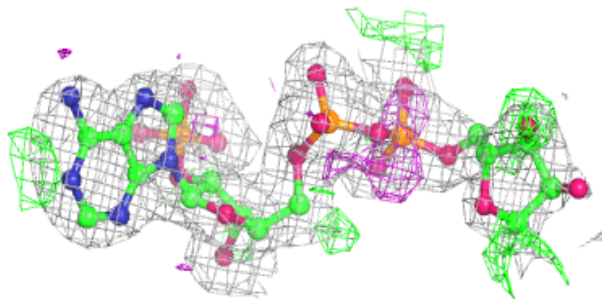
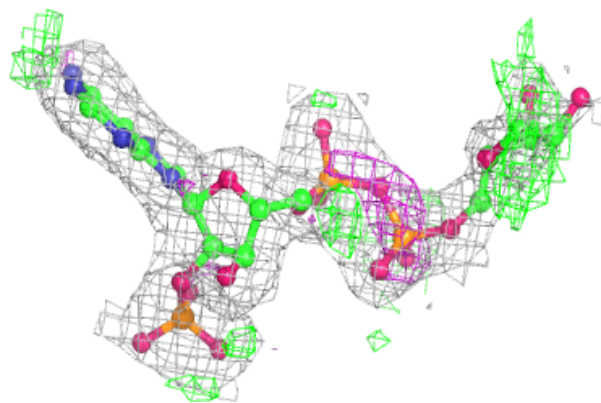


**Electron density around NAP E 500 (B):**

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

**Electron density around NAP D 500 (A):**

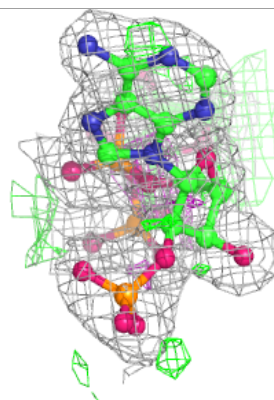
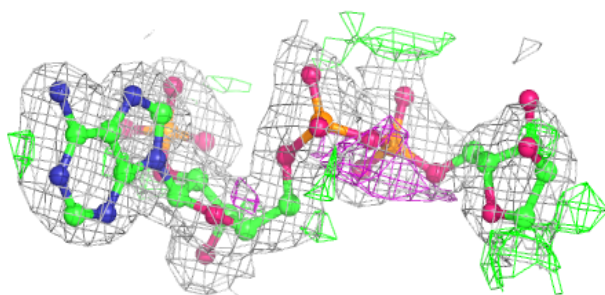
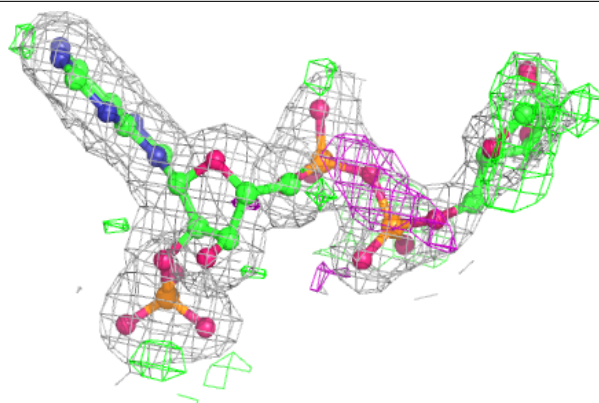
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



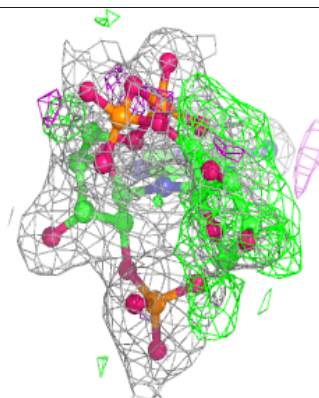
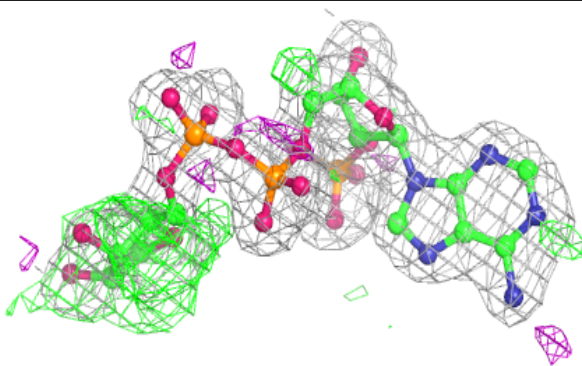
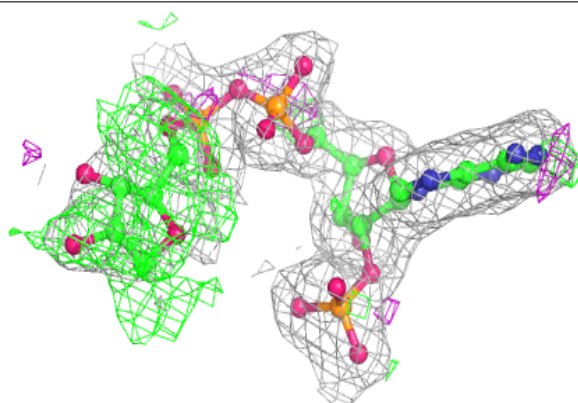


**Electron density around NAP H 500 (A):**

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

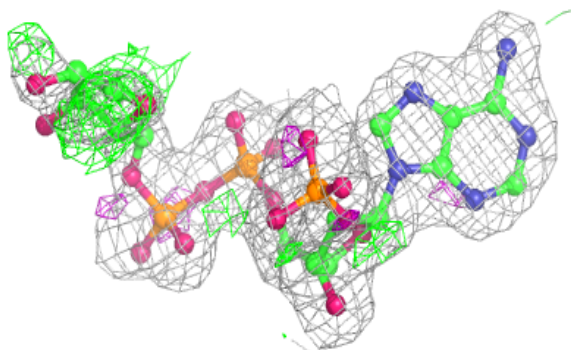
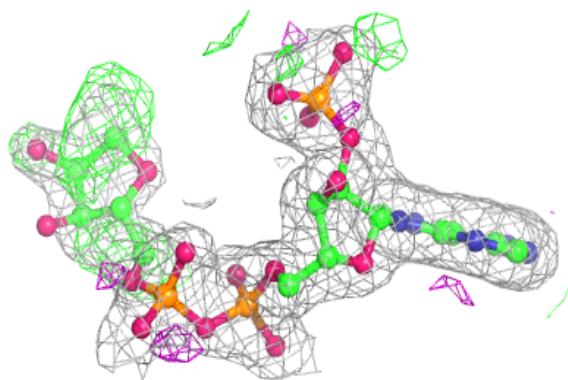
**Electron density around NAP A 501 (B):**

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and green (positive)

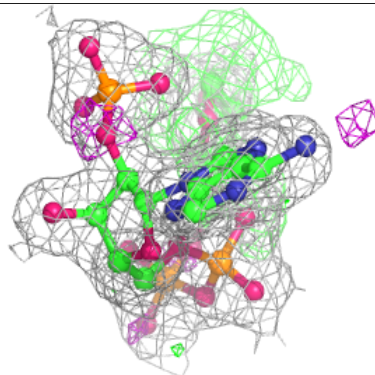
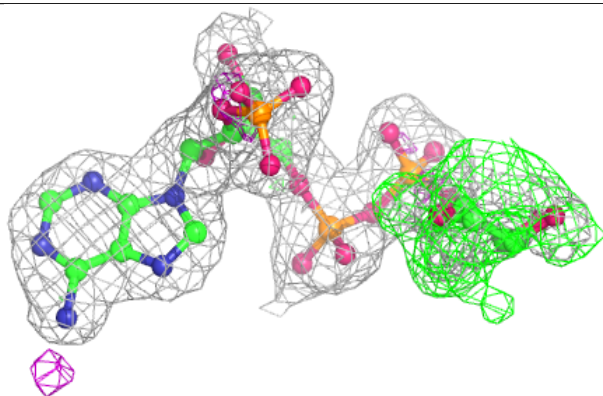
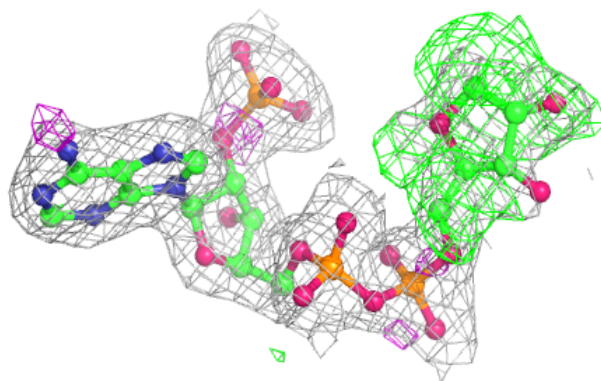


**Electron density around NAP G 500 (B):**

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

**Electron density around NAP F 500 (B):**

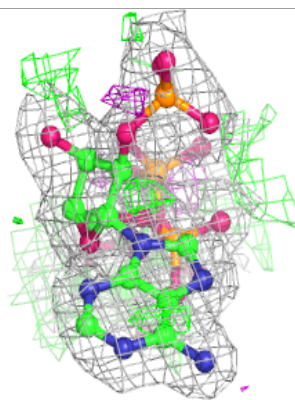
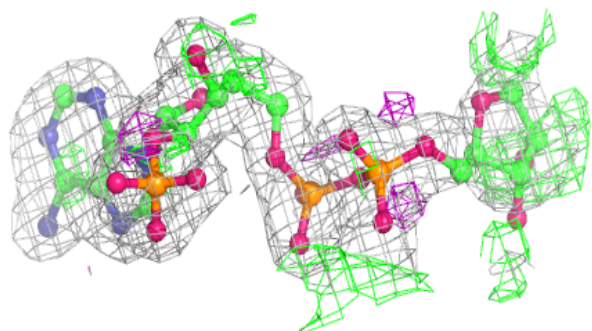
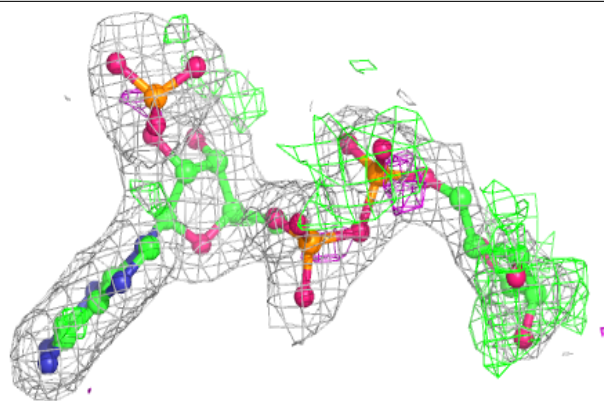
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



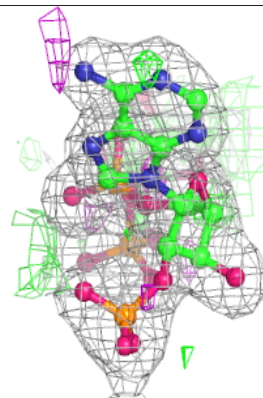
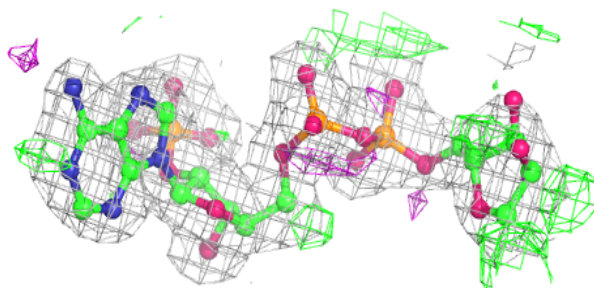
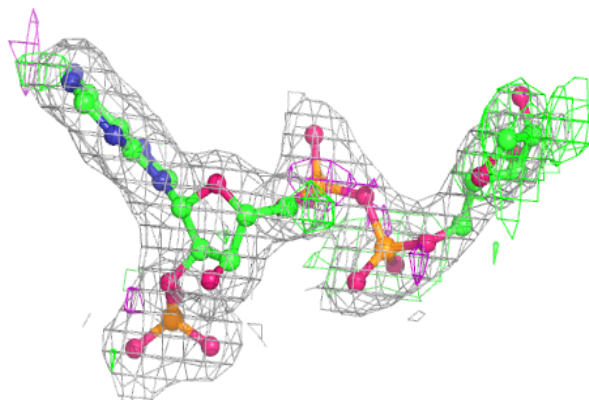


**Electron density around NAP C 500 (A):**

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

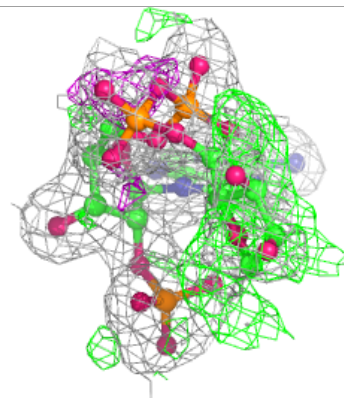
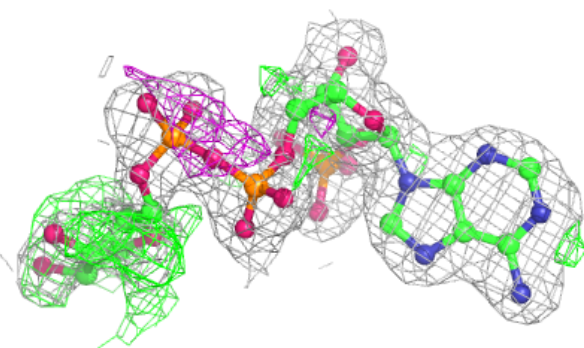
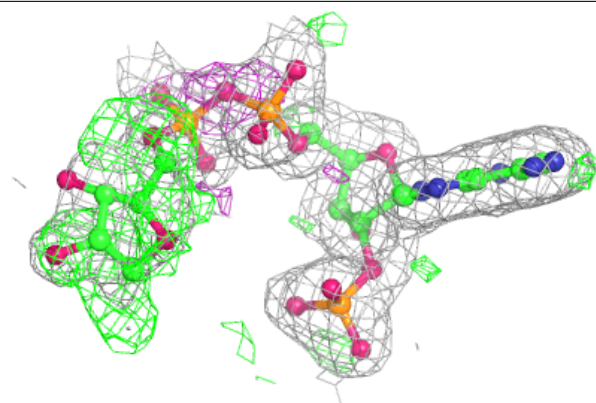
**Electron density around NAP A 501 (A):**

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

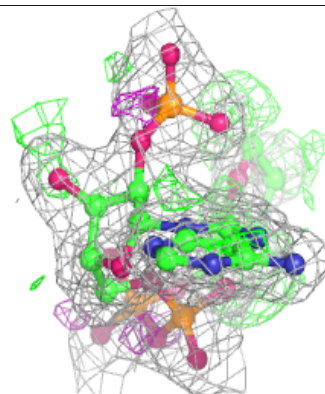
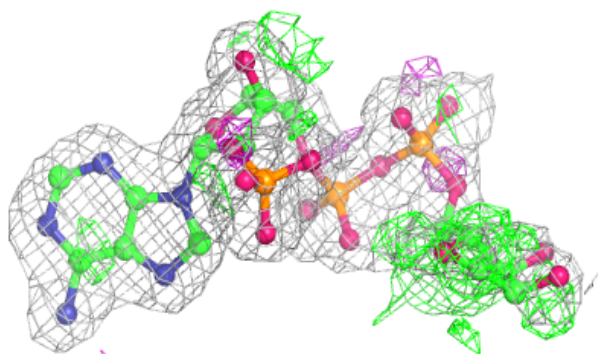
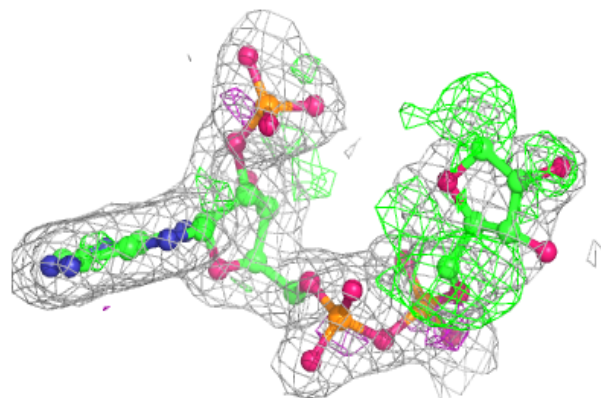


**Electron density around NAP H 500 (B):**

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

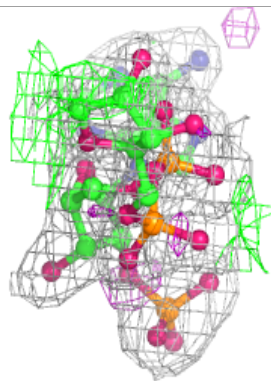
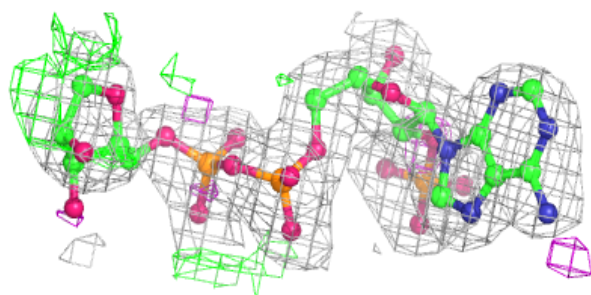
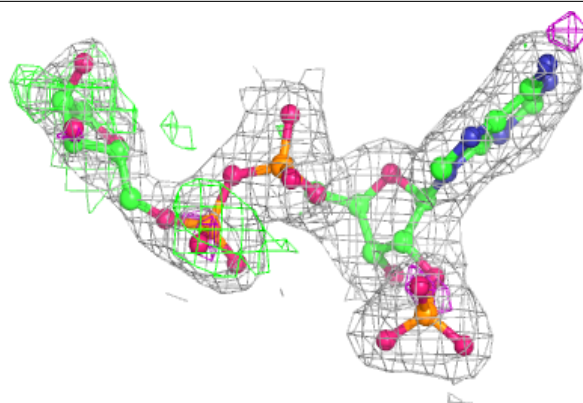
**Electron density around NAP C 500 (B):**

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

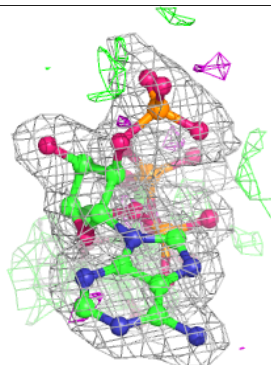
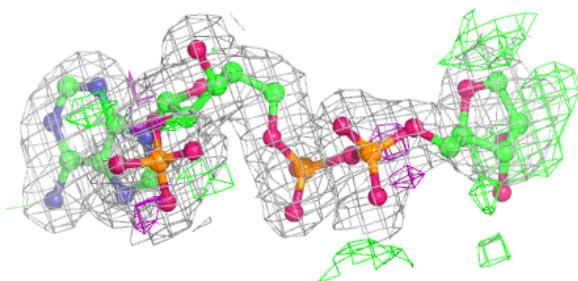
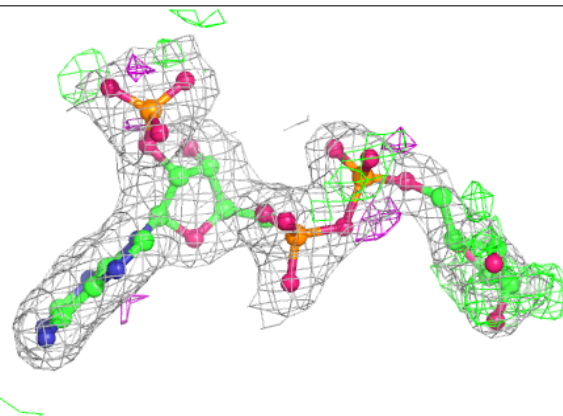


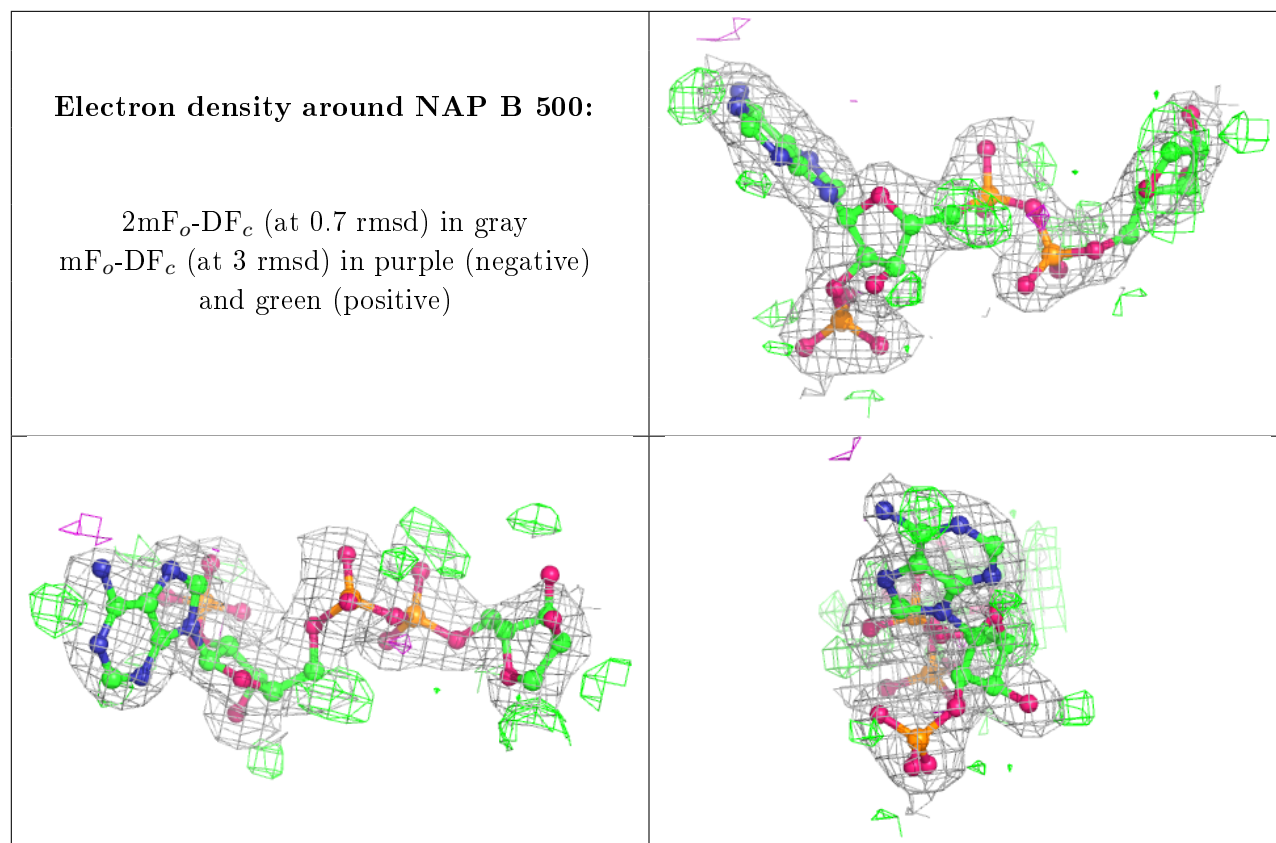
**Electron density around NAP F 500 (A):**

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

**Electron density around NAP G 500 (A):**

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





## 6.5 Other polymers ⓘ

There are no such residues in this entry.