



# wwPDB X-ray Structure Validation Summary Report ⓘ

Oct 5, 2024 – 01:35 PM EDT

PDB ID : 2AZN  
Title : X-RAY Structure of 2,5-diamino-6-ribosylamino-4(3h)-pyrimidinone 5-phosphate reductase  
Authors : Chatwell, L.; Bacher, A.; Huber, R.; Fischer, M.; Krojer, T.  
Deposited on : 2005-09-12  
Resolution : 2.70 Å(reported)

This is a wwPDB X-ray Structure Validation Summary Report for a publicly released PDB entry.

We welcome your comments at [validation@mail.wwpdb.org](mailto:validation@mail.wwpdb.org)

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

MolProbity	:	4.02b-467
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	1.20.1
EDS	:	3.0
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20231227.v01 (using entries in the PDB archive December 27th 2023)
CCP4	:	9.0.003 (Gargrove)
Density-Fitness	:	1.0.11
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.39

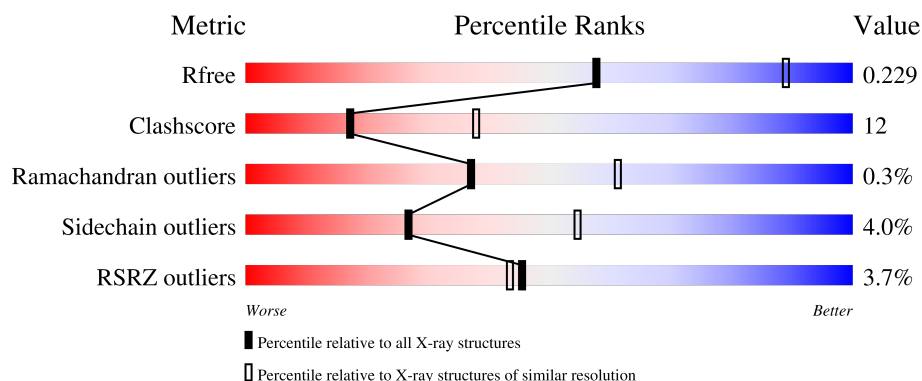
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.70 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))
$R_{free}$	164625	3333 (2.70-2.70)
Clashscore	180529	3684 (2.70-2.70)
Ramachandran outliers	177936	3633 (2.70-2.70)
Sidechain outliers	177891	3633 (2.70-2.70)
RSRZ outliers	164620	3333 (2.70-2.70)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions  $\leq 5\%$ . The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	219	<div> <div>3%</div> <div> <div></div> <div>74%</div> <div>24%</div> <div>.</div> </div> </div>
1	B	219	<div> <div>5%</div> <div> <div></div> <div>77%</div> <div>22%</div> <div>.</div> </div> </div>
1	C	219	<div> <div>2%</div> <div> <div></div> <div>76%</div> <div>22%</div> <div>.</div> </div> </div>
1	D	219	<div> <div>2%</div> <div> <div></div> <div>82%</div> <div>17%</div> <div>.</div> </div> </div>
1	E	219	<div> <div>4%</div> <div> <div></div> <div>78%</div> <div>21%</div> <div>.</div> </div> </div>

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Mol	Chain	Length	Quality of chain
1	F	219	 A horizontal bar chart showing the quality of chain 1. The bar is divided into three segments: a small red segment at the beginning labeled '5%', a large green segment in the middle labeled '75%', and a yellow segment at the end labeled '24%'. A small black dot is at the far right end of the bar.

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

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	MA5	B	1002	-	-	-	X

## 2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 11090 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 Putative 5-amino-6-(5-phosphoribosylamino)uracil reductase.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	219	Total	C	N	O	S	Se	26	0	0
			1710	1087	292	323	3	5			
1	B	219	Total	C	N	O	S	Se	35	0	0
			1710	1087	292	323	3	5			
1	C	219	Total	C	N	O	S	Se	25	0	0
			1710	1087	292	323	3	5			
1	D	219	Total	C	N	O	S	Se	25	0	0
			1710	1087	292	323	3	5			
1	E	219	Total	C	N	O	S	Se	29	0	0
			1710	1087	292	323	3	5			
1	F	219	Total	C	N	O	S	Se	29	0	0
			1710	1087	292	323	3	5			

There are 30 discrepancies between the modelled and reference sequences:

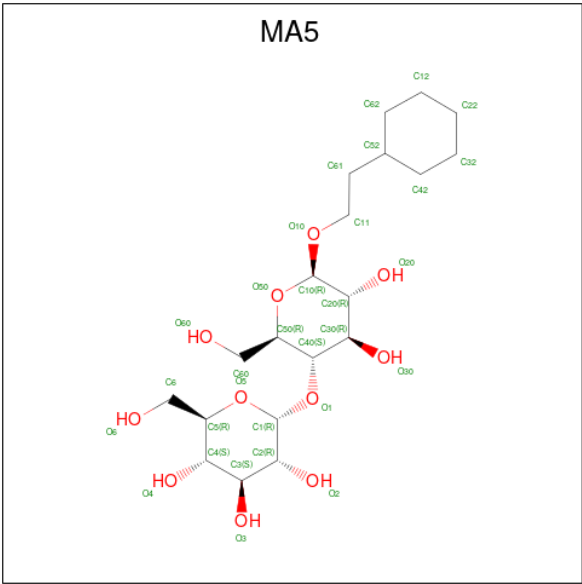
Chain	Residue	Modelled	Actual	Comment	Reference
A	17	MSE	MET	modified residue	UNP Q58085
A	52	MSE	MET	modified residue	UNP Q58085
A	122	MSE	MET	modified residue	UNP Q58085
A	140	MSE	MET	modified residue	UNP Q58085
A	163	MSE	MET	modified residue	UNP Q58085
B	17	MSE	MET	modified residue	UNP Q58085
B	52	MSE	MET	modified residue	UNP Q58085
B	122	MSE	MET	modified residue	UNP Q58085
B	140	MSE	MET	modified residue	UNP Q58085
B	163	MSE	MET	modified residue	UNP Q58085
C	17	MSE	MET	modified residue	UNP Q58085
C	52	MSE	MET	modified residue	UNP Q58085
C	122	MSE	MET	modified residue	UNP Q58085
C	140	MSE	MET	modified residue	UNP Q58085
C	163	MSE	MET	modified residue	UNP Q58085
D	17	MSE	MET	modified residue	UNP Q58085
D	52	MSE	MET	modified residue	UNP Q58085

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Chain	Residue	Modelled	Actual	Comment	Reference
D	122	MSE	MET	modified residue	UNP Q58085
D	140	MSE	MET	modified residue	UNP Q58085
D	163	MSE	MET	modified residue	UNP Q58085
E	17	MSE	MET	modified residue	UNP Q58085
E	52	MSE	MET	modified residue	UNP Q58085
E	122	MSE	MET	modified residue	UNP Q58085
E	140	MSE	MET	modified residue	UNP Q58085
E	163	MSE	MET	modified residue	UNP Q58085
F	17	MSE	MET	modified residue	UNP Q58085
F	52	MSE	MET	modified residue	UNP Q58085
F	122	MSE	MET	modified residue	UNP Q58085
F	140	MSE	MET	modified residue	UNP Q58085
F	163	MSE	MET	modified residue	UNP Q58085

- Molecule 2 is 2-(6-(2-CYCLOHEXYLETHOXY)-TETRAHYDRO-4,5-DIHYDROXY-2(HYDROXYMETHYL)-2H-PYRAN-3-YLOXY)-TETRAHYDRO-6(HYDROXYMETHYL)-2H-PY RAN-3,4,5-TRIOL (three-letter code: MA5) (formula: C<sub>20</sub>H<sub>36</sub>O<sub>11</sub>).



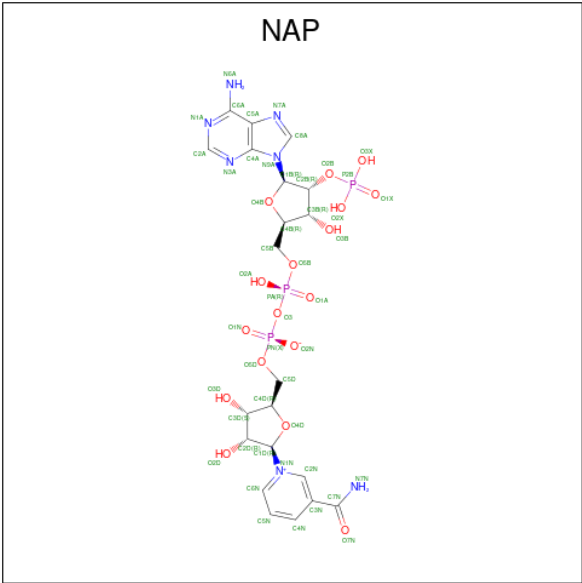
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total	C	O	15	0
			31	20	11		
2	B	1	Total	C	O	13	0
			31	20	11		
2	B	1	Total	C	O	12	0
			31	20	11		
2	C	1	Total	C	O	0	0
			31	20	11		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	C	1	Total	C	O	0	0
			31	20	11		
2	D	1	Total	C	O	15	0
			31	20	11		
2	F	1	Total	C	O	15	0
			31	20	11		
2	F	1	Total	C	O	7	0
			31	20	11		

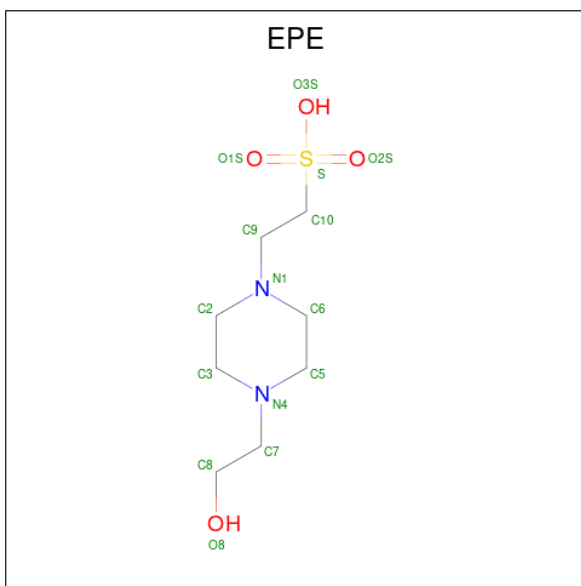
- Molecule 3 is NADP NICOTINAMIDE-ADENINE-DINUCLEOTIDE PHOSPHATE (three-letter code: NAP) (formula: C<sub>21</sub>H<sub>28</sub>N<sub>7</sub>O<sub>17</sub>P<sub>3</sub>).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	A	1	Total	C	N	O	P	0	0
			48	21	7	17	3		
3	B	1	Total	C	N	O	P	0	0
			48	21	7	17	3		
3	C	1	Total	C	N	O	P	0	0
			48	21	7	17	3		
3	D	1	Total	C	N	O	P	0	0
			48	21	7	17	3		
3	E	1	Total	C	N	O	P	0	0
			48	21	7	17	3		
3	F	1	Total	C	N	O	P	0	0
			48	21	7	17	3		

- Molecule 4 is 4-(2-HYDROXYETHYL)-1-PIPERAZINE ETHANESULFONIC ACID

(three-letter code: EPE) (formula: C<sub>8</sub>H<sub>18</sub>N<sub>2</sub>O<sub>4</sub>S).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
4	B	1	Total	C	N	O	S	0	0
			12	6	2	3	1		
4	F	1	Total	C	N	O	S	0	0
			12	6	2	3	1		

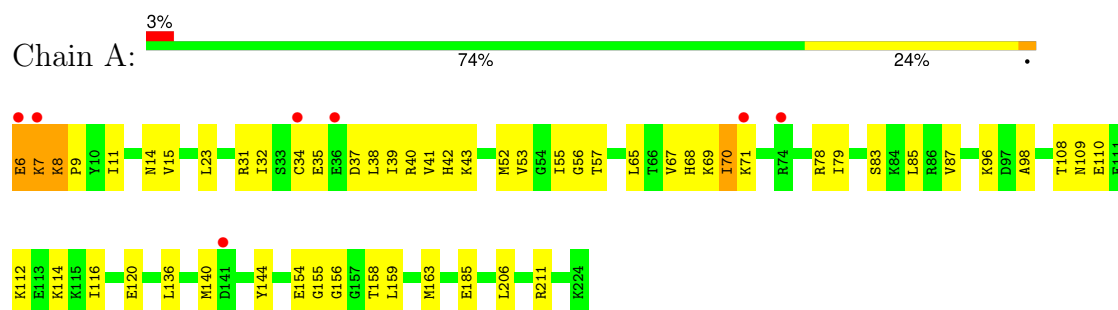
- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	37	Total	O	0	0
			37	37		
5	B	35	Total	O	0	0
			35	35		
5	C	50	Total	O	0	0
			50	50		
5	D	49	Total	O	0	0
			49	49		
5	E	56	Total	O	0	0
			56	56		
5	F	43	Total	O	0	0
			43	43		

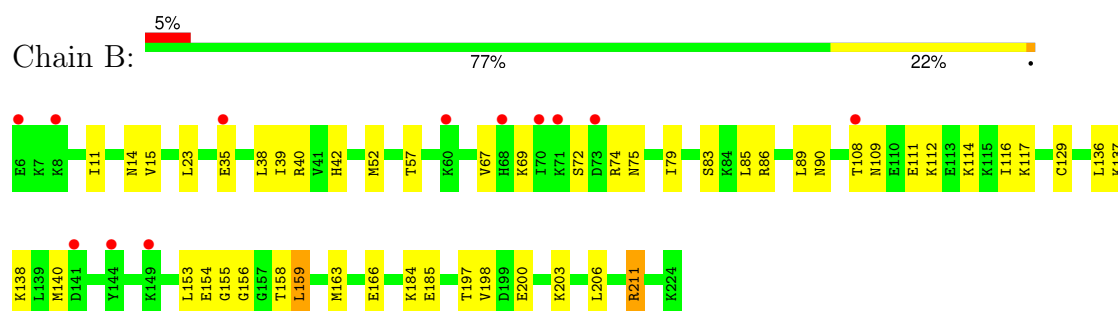
### 3 Residue-property plots [i](#)

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

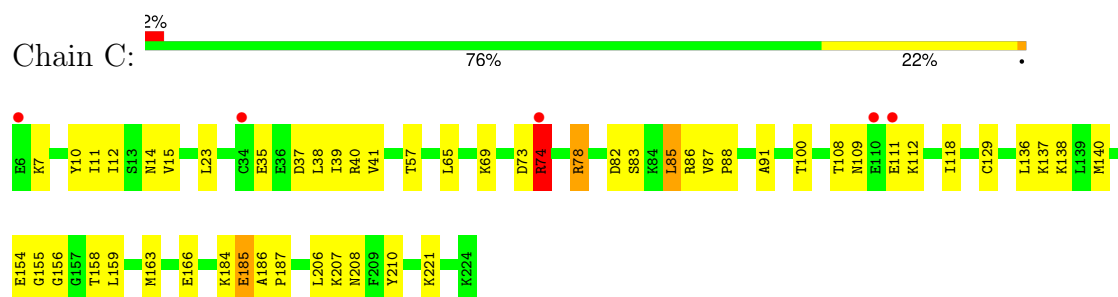
- Molecule 1: Putative 5-amino-6-(5-phosphoribosylamino)uracil reductase



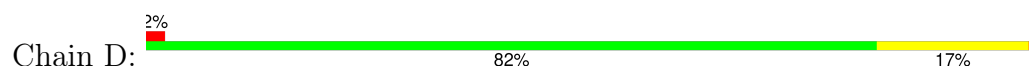
- Molecule 1: Putative 5-amino-6-(5-phosphoribosylamino)uracil reductase



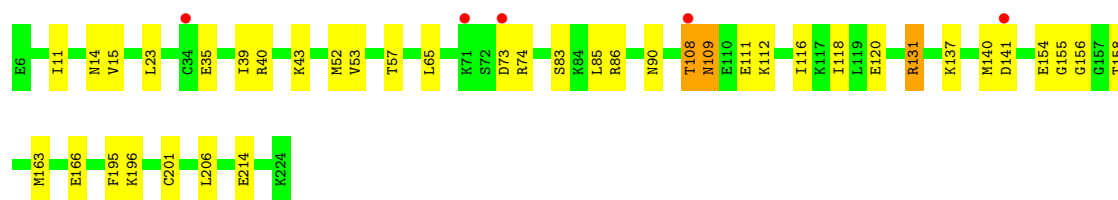
- Molecule 1: Putative 5-amino-6-(5-phosphoribosylamino)uracil reductase



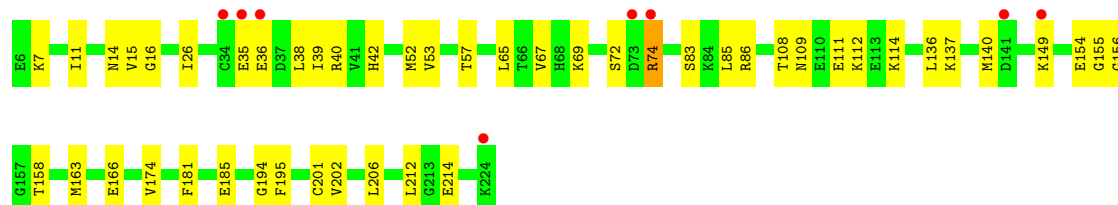
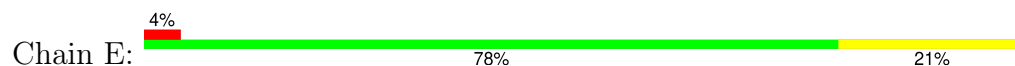
- Molecule 1: Putative 5-amino-6-(5-phosphoribosylamino)uracil reductase



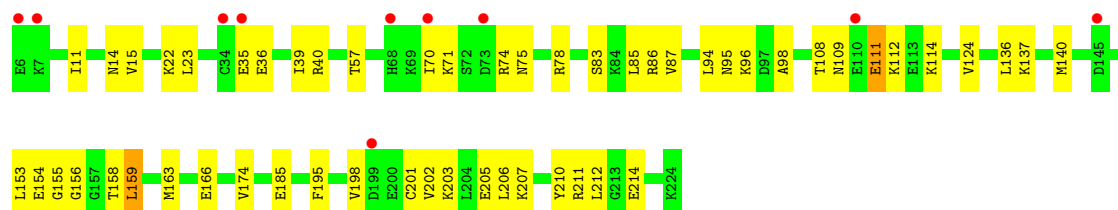
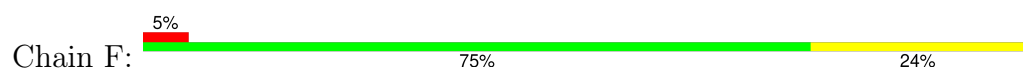




- Molecule 1: Putative 5-amino-6-(5-phosphoribosylamino)uracil reductase



- Molecule 1: Putative 5-amino-6-(5-phosphoribosylamino)uracil reductase



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 43 21 2	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	137.17Å 137.17Å 213.87Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	20.00 – 2.70 20.00 – 2.70	Depositor EDS
% Data completeness (in resolution range)	(Not available) (20.00-2.70) 99.4 (20.00-2.70)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.61 (at 2.51Å)	Xtriage
Refinement program	CNS	Depositor
R, $R_{free}$	0.230 , 0.253 0.209 , 0.229	Depositor DCC
$R_{free}$ test set	2786 reflections (4.94%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	55.8	Xtriage
Anisotropy	0.169	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.35 , 45.6	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.50$ , $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.94	EDS
Total number of atoms	11090	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	55.0	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 34.30 % 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 6.9778e-04. 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: EPE, MA5, 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	0.38	0/1724	0.67	0/2304
1	B	0.41	0/1724	0.67	0/2304
1	C	0.39	0/1724	0.67	0/2304
1	D	0.38	0/1724	0.67	0/2304
1	E	0.38	0/1724	0.66	0/2304
1	F	0.38	0/1724	0.68	0/2304
All	All	0.39	0/10344	0.67	0/13824

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

### 5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	1710	0	1801	52	0
1	B	1710	0	1801	44	0
1	C	1710	0	1801	45	0
1	D	1710	0	1801	36	0
1	E	1710	0	1801	43	0
1	F	1710	0	1801	43	0
2	A	31	0	36	5	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	B	62	0	72	6	0
2	C	62	0	72	12	0
2	D	31	0	36	4	0
2	F	62	0	72	3	0
3	A	48	0	25	13	0
3	B	48	0	25	7	0
3	C	48	0	25	8	0
3	D	48	0	25	8	0
3	E	48	0	25	6	0
3	F	48	0	25	6	0
4	B	12	0	13	4	0
4	F	12	0	13	5	0
5	A	37	0	0	2	0
5	B	35	0	0	2	0
5	C	50	0	0	7	0
5	D	49	0	0	3	0
5	E	56	0	0	6	0
5	F	43	0	0	6	0
All	All	11090	0	11270	268	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 12.

The worst 5 of 268 close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:78:ARG:HG2	5:C:2042:HOH:O	1.59	1.00
1:B:14:ASN:HD21	1:B:40:ARG:HH22	1.10	0.98
1:C:65:LEU:HB2	5:C:2042:HOH:O	1.63	0.96
1:F:111:GLU:HG2	4:F:3002:EPE:H61	1.46	0.96
1:C:14:ASN:HD21	1:C:40:ARG:HH22	1.13	0.96

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	217/219 (99%)	207 (95%)	9 (4%)	1 (0%)	25	49
1	B	217/219 (99%)	209 (96%)	8 (4%)	0	100	100
1	C	217/219 (99%)	207 (95%)	8 (4%)	2 (1%)	14	35
1	D	217/219 (99%)	209 (96%)	8 (4%)	0	100	100
1	E	217/219 (99%)	209 (96%)	8 (4%)	0	100	100
1	F	217/219 (99%)	208 (96%)	8 (4%)	1 (0%)	25	49
All	All	1302/1314 (99%)	1249 (96%)	49 (4%)	4 (0%)	37	61

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	7	LYS
1	A	7	LYS
1	C	74	ARG
1	F	70	ILE

### 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	191/187 (102%)	181 (95%)	10 (5%)	19	44
1	B	191/187 (102%)	183 (96%)	8 (4%)	25	53
1	C	191/187 (102%)	181 (95%)	10 (5%)	19	44
1	D	191/187 (102%)	185 (97%)	6 (3%)	35	64
1	E	191/187 (102%)	186 (97%)	5 (3%)	41	70
1	F	191/187 (102%)	184 (96%)	7 (4%)	29	58
All	All	1146/1122 (102%)	1100 (96%)	46 (4%)	27	55

5 of 46 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	D	85	LEU
1	E	85	LEU
1	D	108	THR
1	D	141	ASP
1	E	185	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 17 such sidechains are listed below:

Mol	Chain	Res	Type
1	F	14	ASN
1	F	109	ASN
1	C	109	ASN
1	D	14	ASN
1	D	27	ASN

### 5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

## 5.4 Non-standard residues in protein, DNA, RNA chains [i](#)

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

## 5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

## 5.6 Ligand geometry [i](#)

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
2	MA5	C	1003	-	33,33,33	0.61	1 (3%)	45,46,46	1.09	4 (8%)
2	MA5	A	1004	-	33,33,33	0.59	1 (3%)	45,46,46	0.90	1 (2%)
3	NAP	B	2002	-	46,52,52	1.44	8 (17%)	61,80,80	1.77	6 (9%)
3	NAP	C	2003	-	46,52,52	1.44	8 (17%)	61,80,80	1.72	5 (8%)
4	EPE	F	3002	-	12,12,15	1.52	1 (8%)	15,16,20	1.08	1 (6%)
2	MA5	D	1001	-	33,33,33	0.60	1 (3%)	45,46,46	0.88	3 (6%)
3	NAP	F	2006	-	46,52,52	1.42	6 (13%)	61,80,80	1.77	5 (8%)
3	NAP	A	2001	-	46,52,52	1.43	7 (15%)	61,80,80	1.91	7 (11%)
2	MA5	F	1005	-	33,33,33	0.62	1 (3%)	45,46,46	0.98	3 (6%)
2	MA5	B	1002	-	33,33,33	0.60	1 (3%)	45,46,46	0.84	1 (2%)
2	MA5	F	1008	-	33,33,33	0.60	1 (3%)	45,46,46	0.94	2 (4%)
3	NAP	D	2004	-	46,52,52	1.45	8 (17%)	61,80,80	1.78	6 (9%)
3	NAP	E	2005	-	46,52,52	1.44	8 (17%)	61,80,80	1.72	6 (9%)
4	EPE	B	3001	-	12,12,15	1.51	1 (8%)	15,16,20	1.10	1 (6%)
2	MA5	B	1007	-	33,33,33	0.60	1 (3%)	45,46,46	0.84	1 (2%)
2	MA5	C	1006	-	33,33,33	0.61	1 (3%)	45,46,46	0.84	1 (2%)

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
2	MA5	C	1003	-	-	4/14/62/62	0/3/3/3
2	MA5	A	1004	-	-	4/14/62/62	0/3/3/3
3	NAP	B	2002	-	-	3/31/67/67	0/5/5/5
3	NAP	C	2003	-	-	3/31/67/67	0/5/5/5
4	EPE	F	3002	-	-	2/6/14/19	1/1/1/1
2	MA5	D	1001	-	-	5/14/62/62	0/3/3/3
3	NAP	F	2006	-	-	5/31/67/67	0/5/5/5
3	NAP	A	2001	-	-	5/31/67/67	0/5/5/5
2	MA5	F	1005	-	-	4/14/62/62	0/3/3/3
2	MA5	B	1002	-	-	5/14/62/62	0/3/3/3
2	MA5	F	1008	-	-	5/14/62/62	0/3/3/3
3	NAP	D	2004	-	-	4/31/67/67	0/5/5/5
3	NAP	E	2005	-	-	3/31/67/67	0/5/5/5

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	EPE	B	3001	-	-	0/6/14/19	1/1/1/1
2	MA5	B	1007	-	-	5/14/62/62	0/3/3/3
2	MA5	C	1006	-	-	3/14/62/62	0/3/3/3

The worst 5 of 55 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	D	2004	NAP	C2N-N1N	5.33	1.40	1.35
3	C	2003	NAP	C2N-N1N	5.28	1.40	1.35
3	A	2001	NAP	C2N-N1N	5.28	1.40	1.35
3	E	2005	NAP	C2N-N1N	5.27	1.40	1.35
3	B	2002	NAP	C2N-N1N	5.27	1.40	1.35

The worst 5 of 53 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	F	2006	NAP	C4D-O4D-C1D	-8.72	101.94	109.92
3	B	2002	NAP	C4D-O4D-C1D	-8.60	102.05	109.92
3	A	2001	NAP	C4B-O4B-C1B	-8.52	102.12	109.92
3	C	2003	NAP	C4D-O4D-C1D	-8.44	102.19	109.92
3	D	2004	NAP	C4D-O4D-C1D	-8.26	102.36	109.92

There are no chirality outliers.

5 of 60 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	1004	MA5	O50-C10-O10-C11
2	B	1002	MA5	O50-C10-O10-C11
2	C	1003	MA5	O50-C10-O10-C11
2	C	1006	MA5	O50-C10-O10-C11
2	F	1005	MA5	O50-C10-O10-C11

All (2) ring outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	B	3001	EPE	C2-C3-C5-C6-N1-N4
4	F	3002	EPE	C2-C3-C5-C6-N1-N4

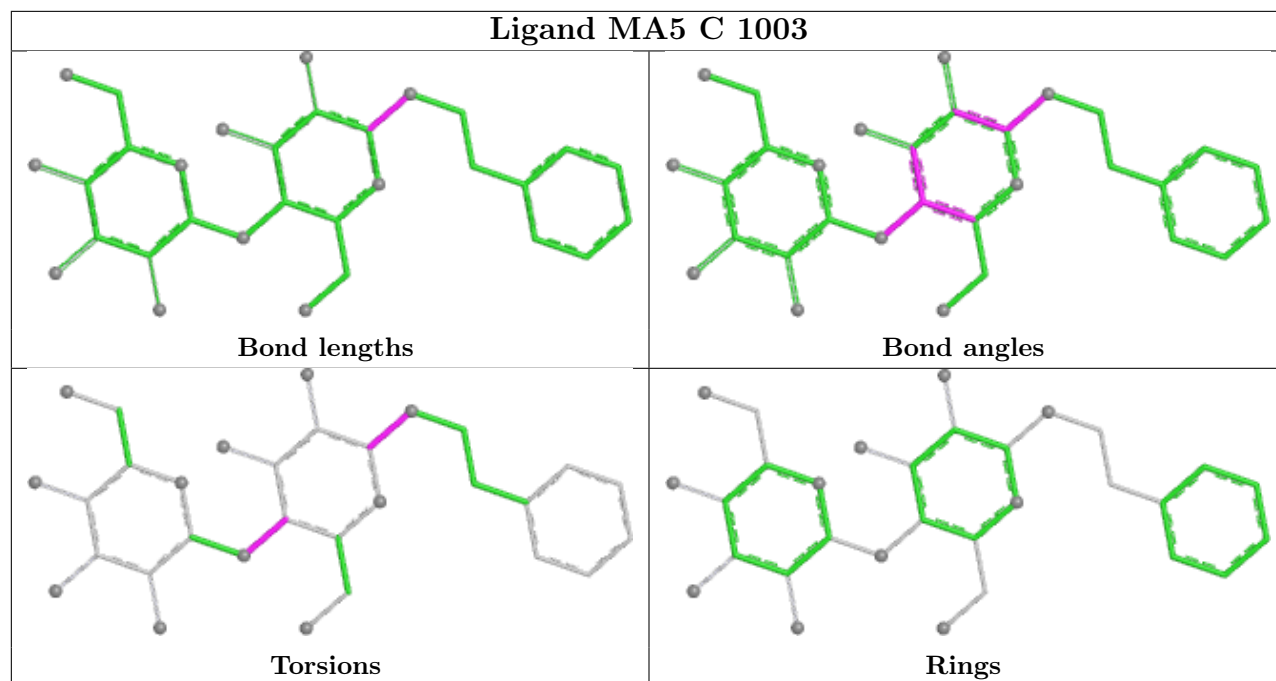
15 monomers are involved in 87 short contacts:



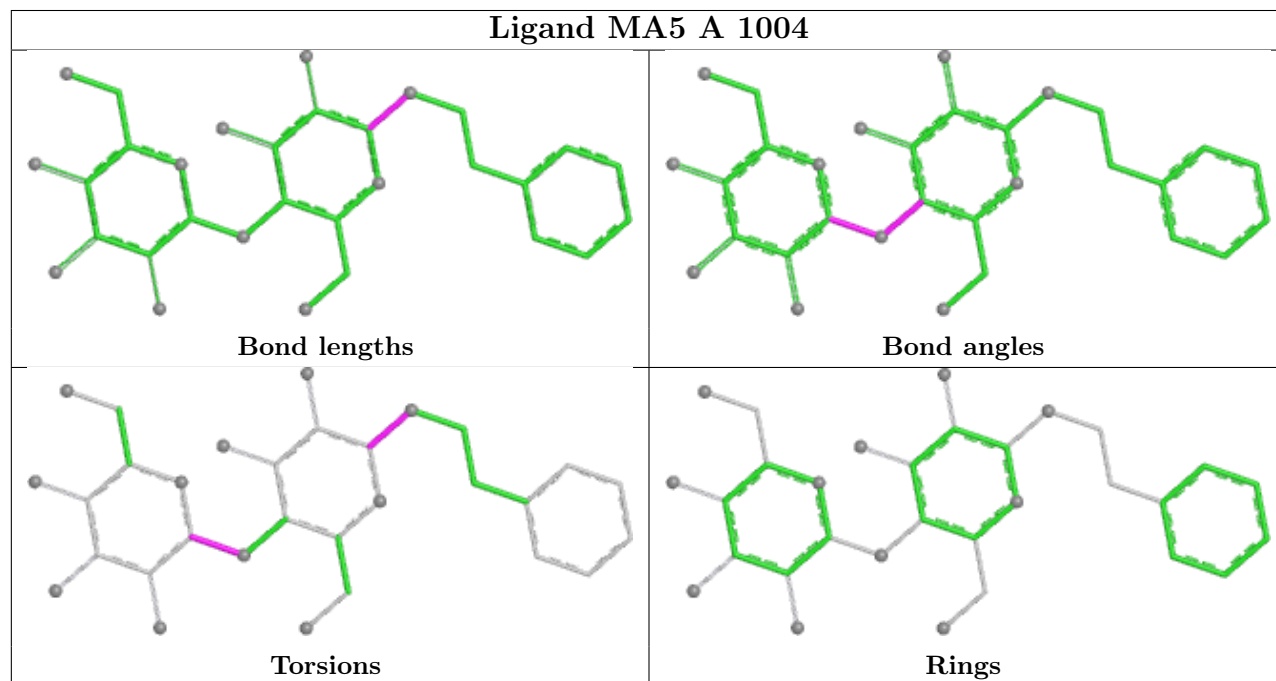
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	C	1003	MA5	4	0
2	A	1004	MA5	5	0
3	B	2002	NAP	7	0
3	C	2003	NAP	8	0
4	F	3002	EPE	5	0
2	D	1001	MA5	4	0
3	F	2006	NAP	6	0
3	A	2001	NAP	13	0
2	F	1005	MA5	3	0
2	B	1002	MA5	2	0
3	D	2004	NAP	8	0
3	E	2005	NAP	6	0
4	B	3001	EPE	4	0
2	B	1007	MA5	4	0
2	C	1006	MA5	8	0

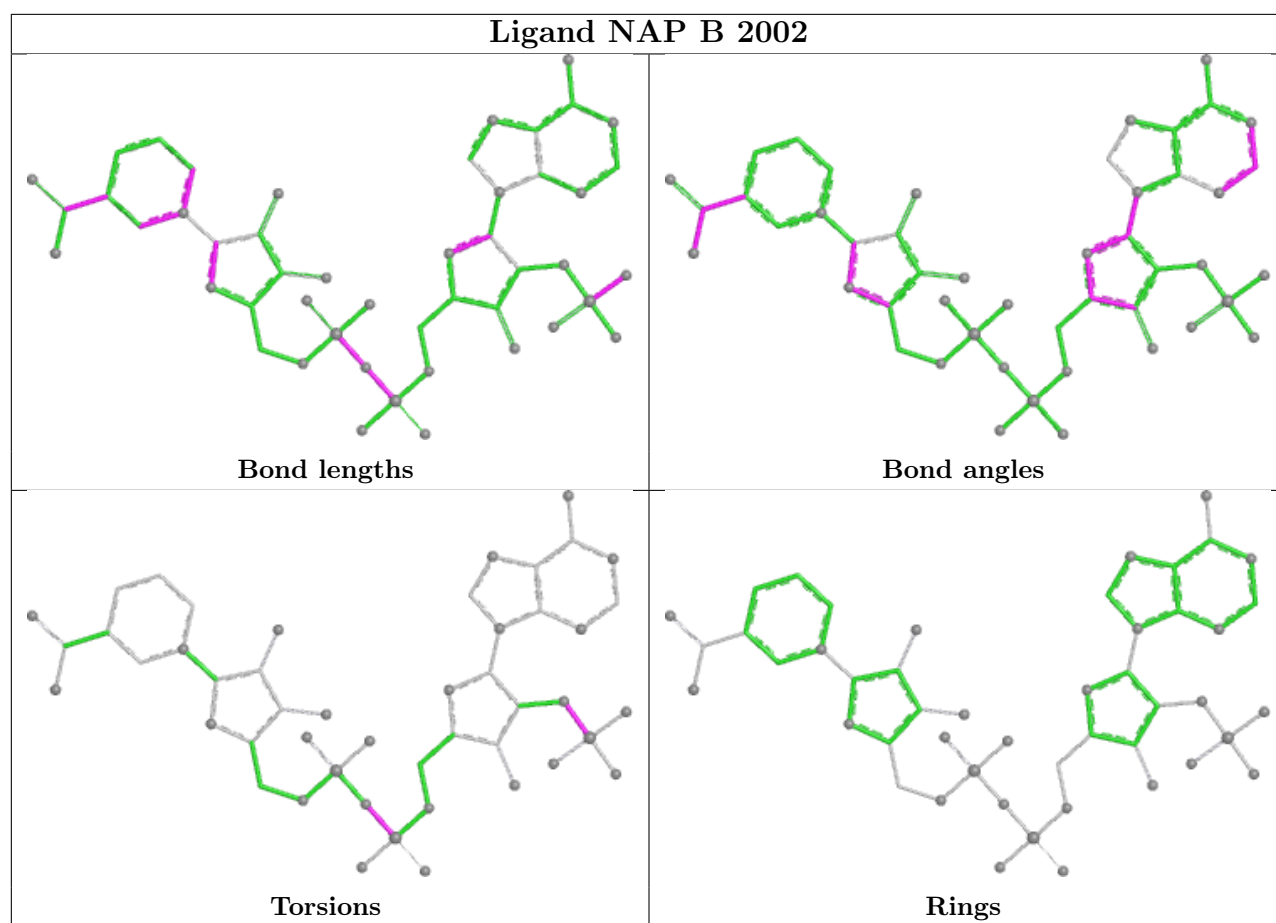
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

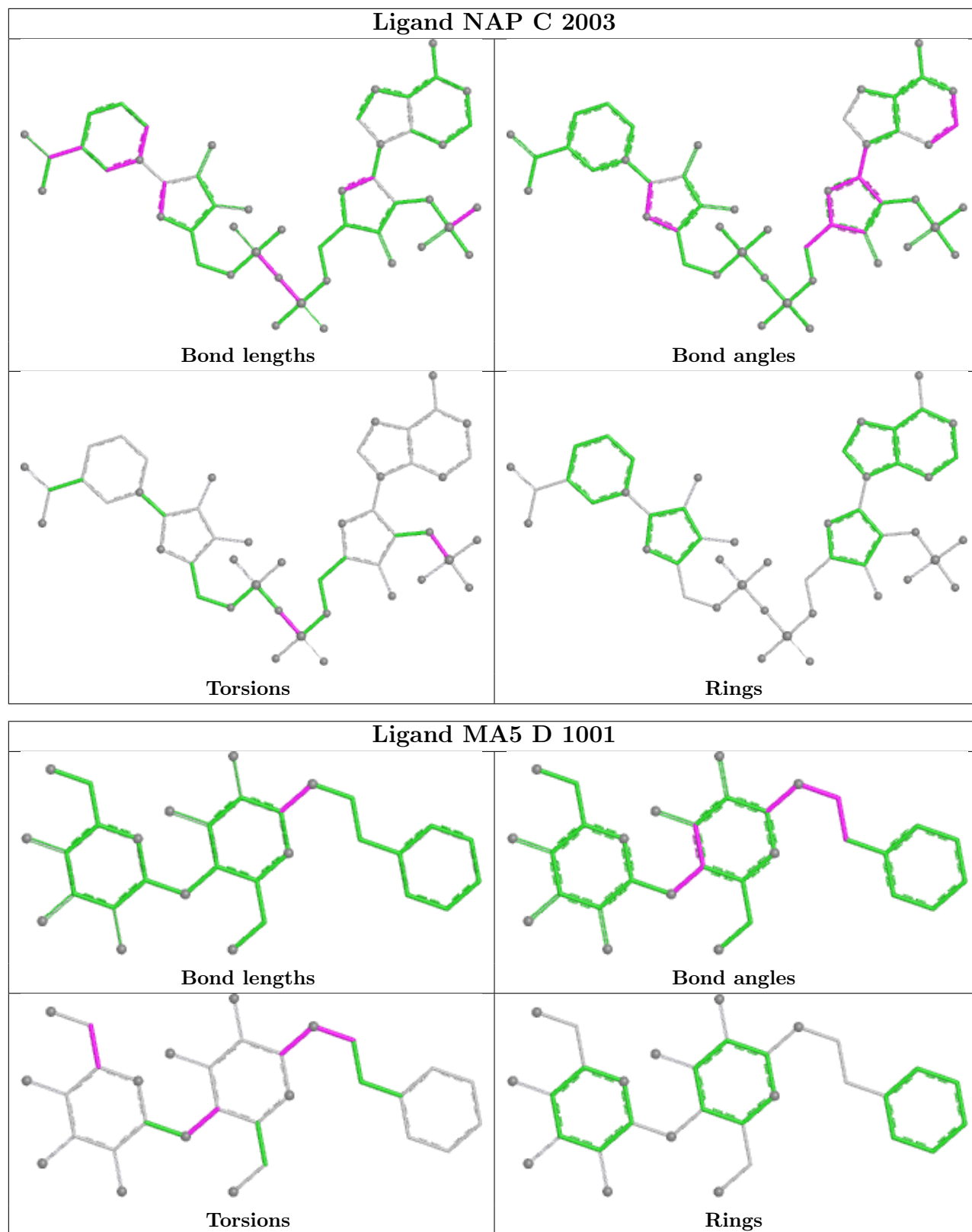
## Ligand MA5 C 1003

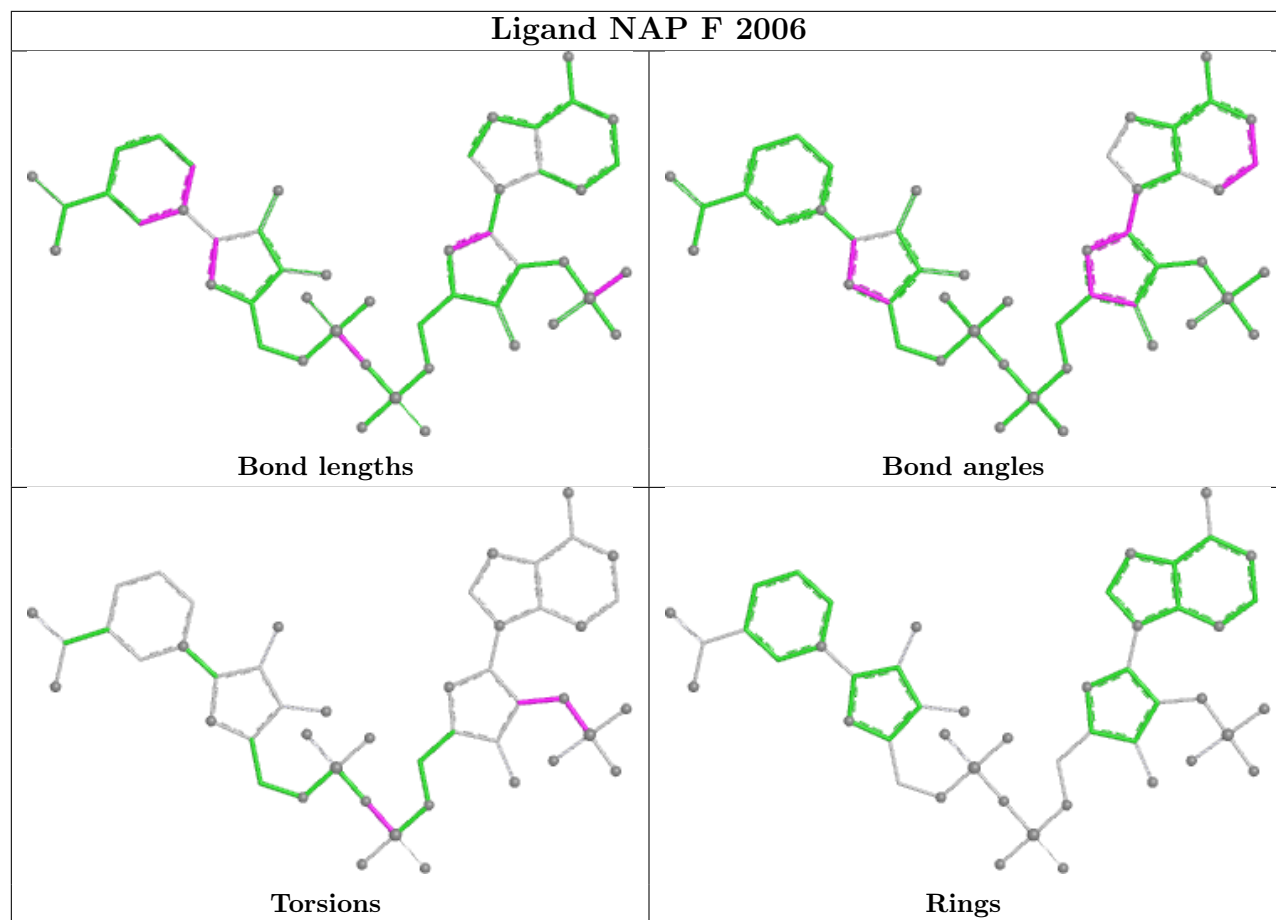


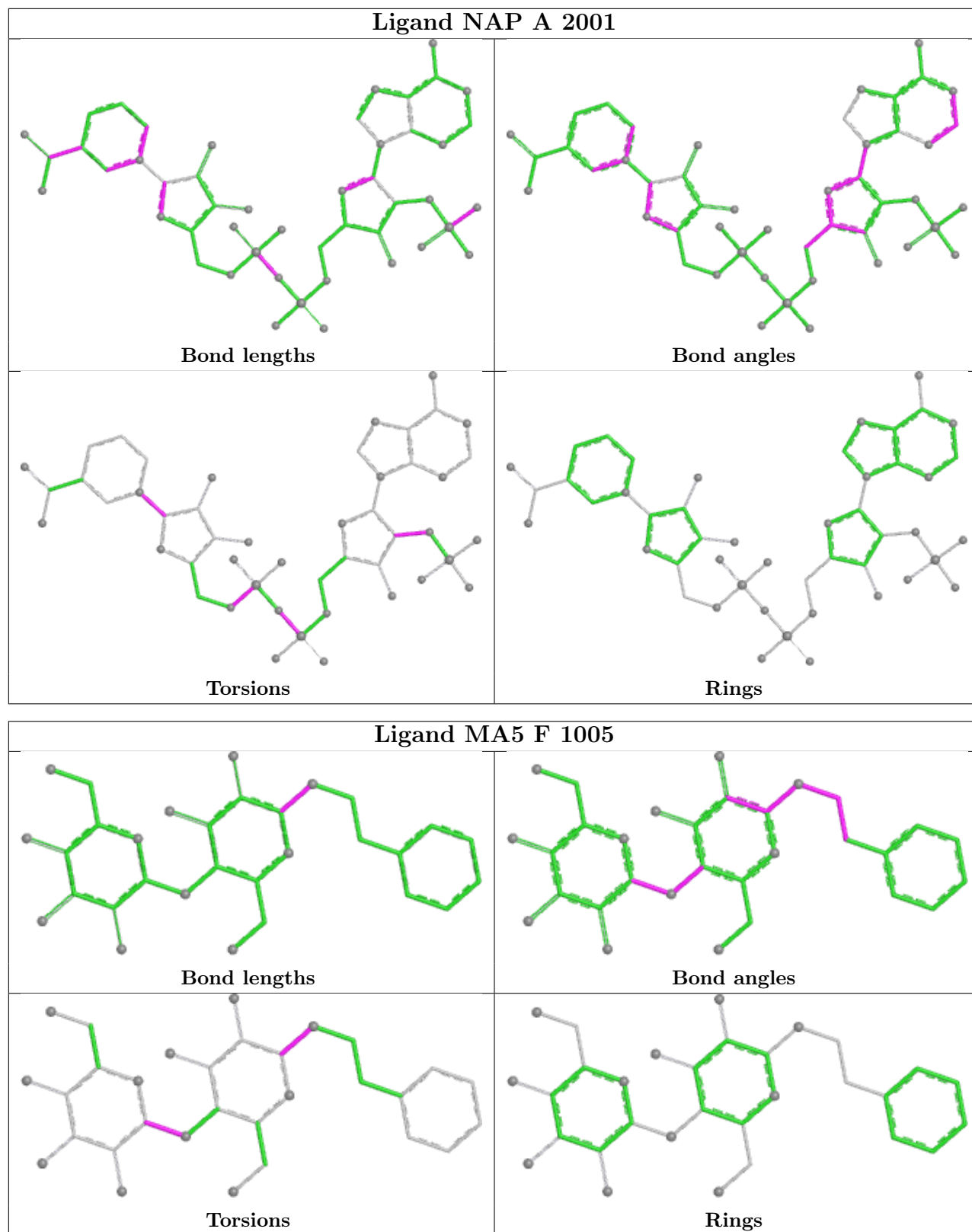
## Ligand MA5 A 1004

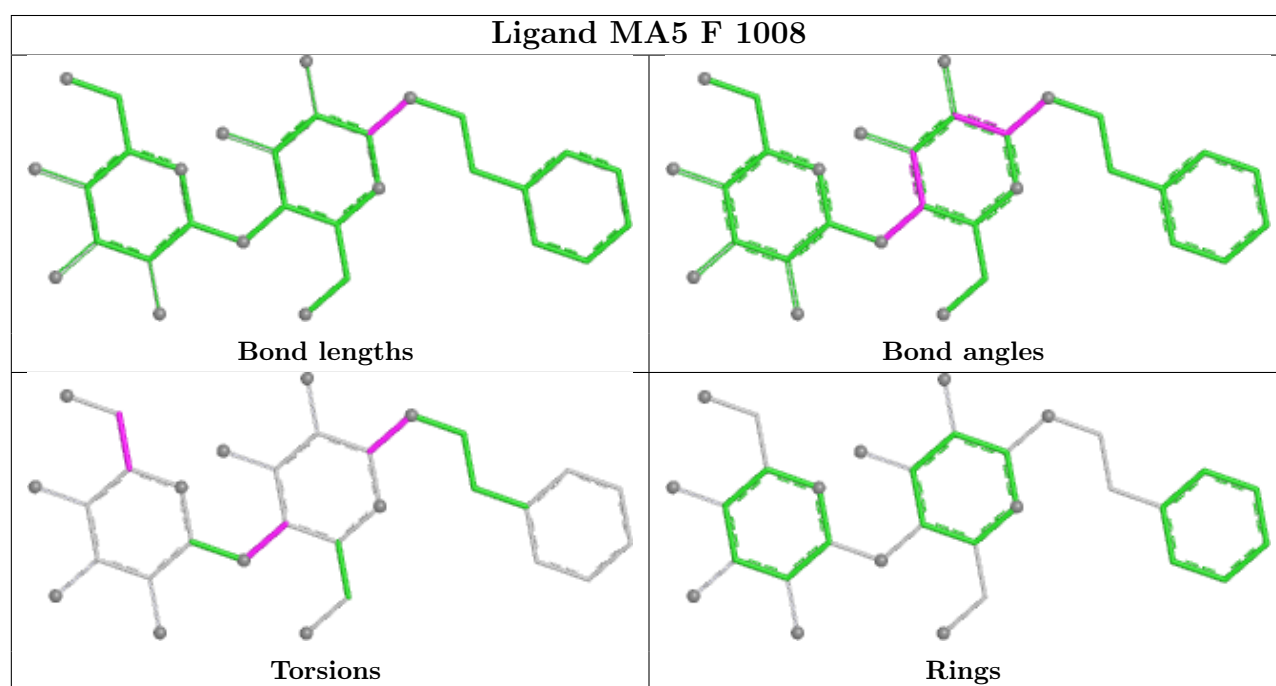
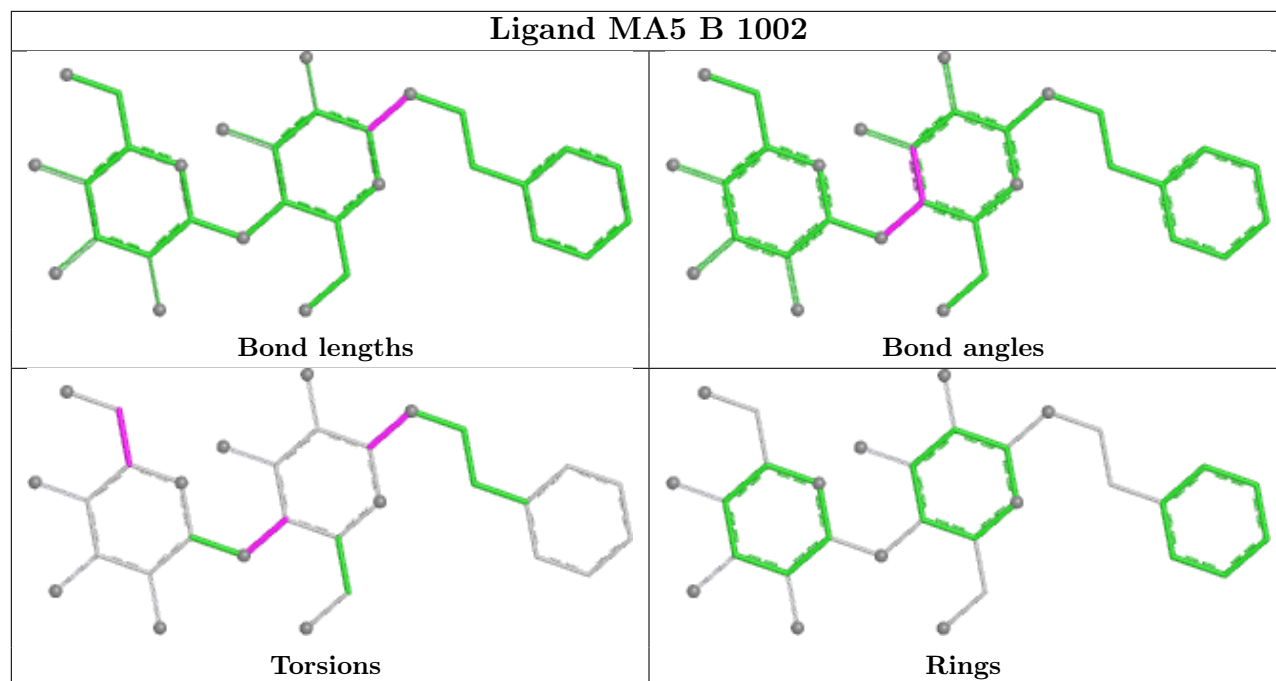


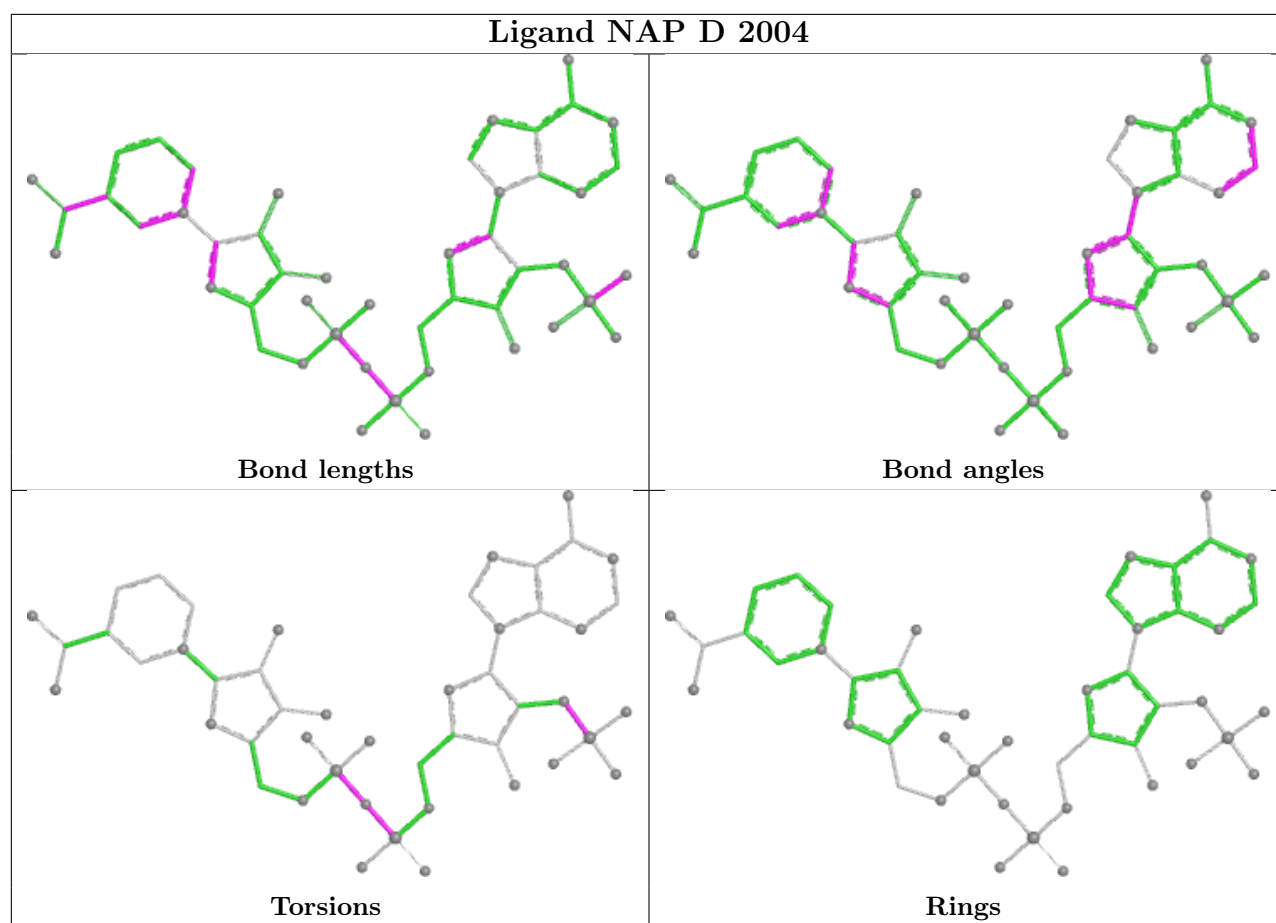




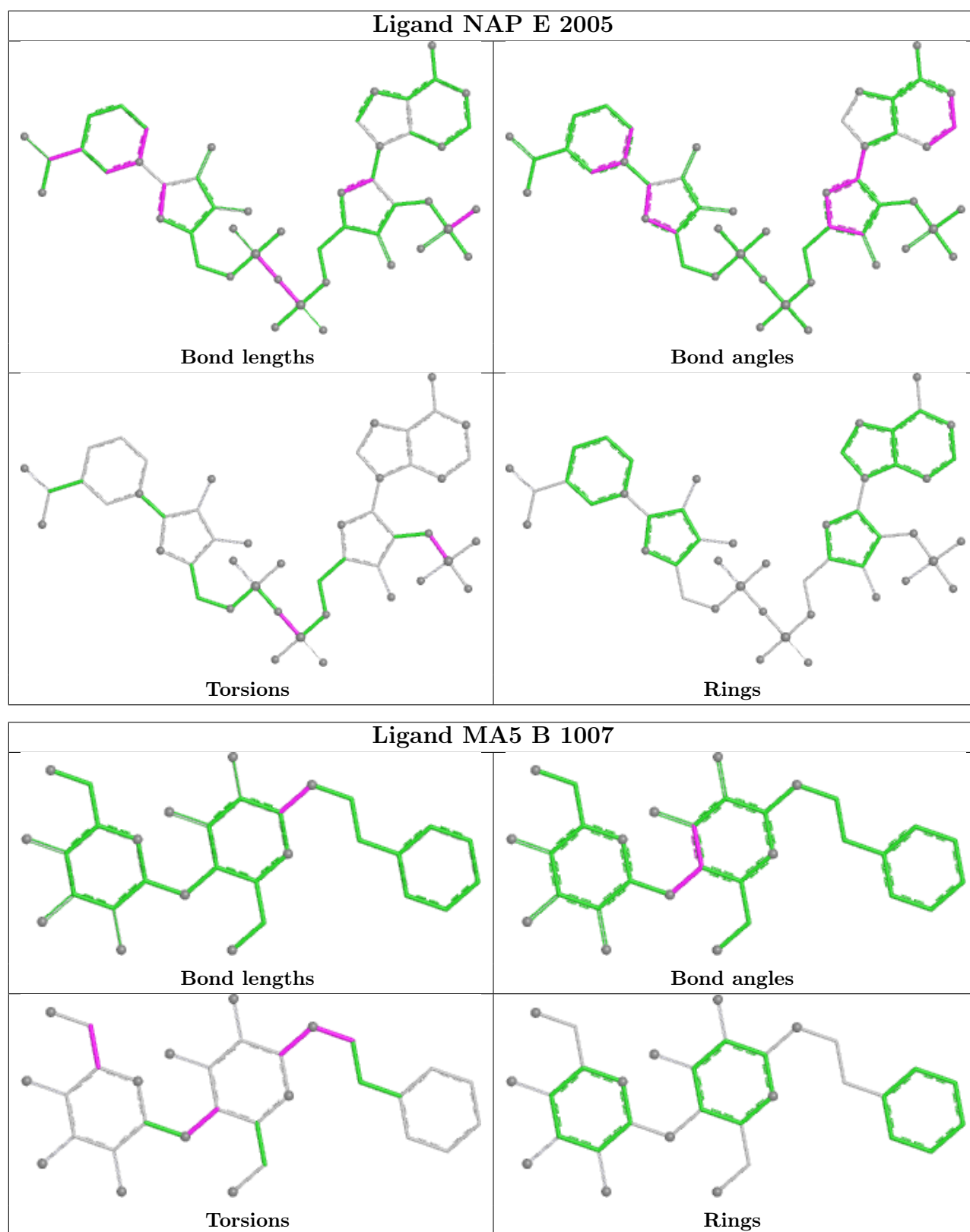


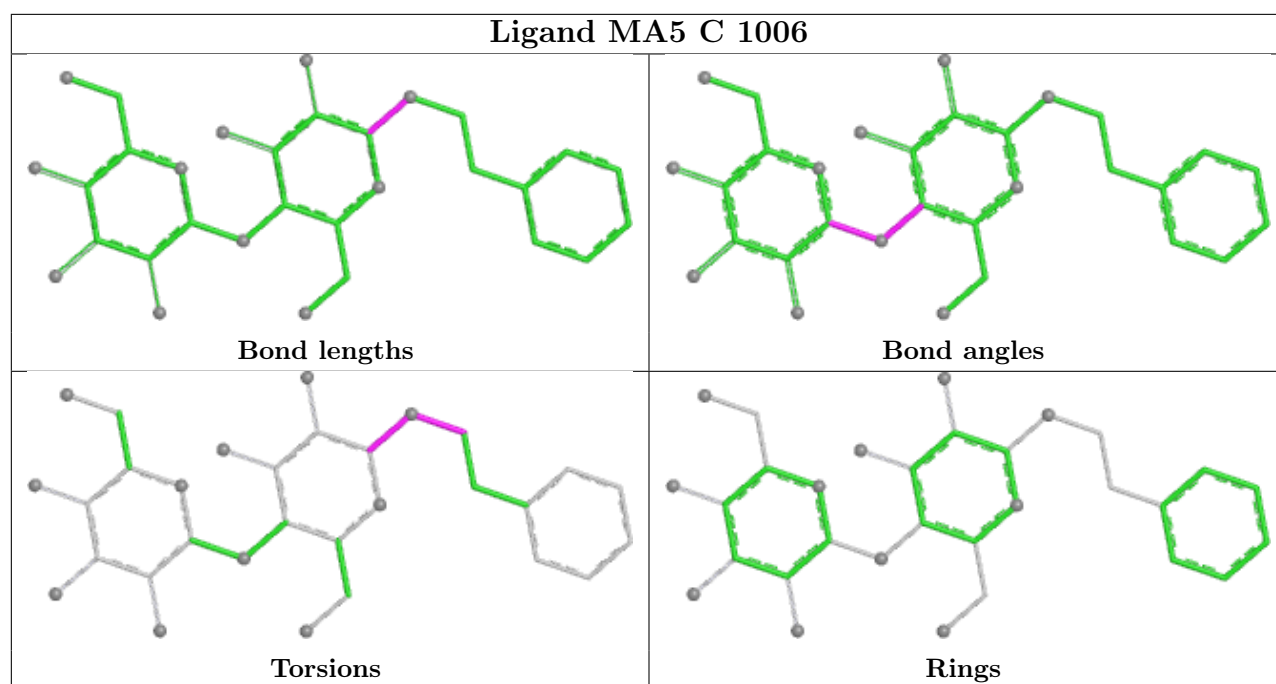












## 5.7 Other polymers [i](#)

There are no such residues in this entry.

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

There are no chain breaks in this entry.

## 6 Fit of model and data [i](#)

### 6.1 Protein, DNA and RNA chains [i](#)

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ > 2			OWAB(Å <sup>2</sup> )	Q < 0.9
1	A	214/219 (97%)	0.11	7 (3%)	49	47	28, 51, 76, 103	9 (4%)
1	B	214/219 (97%)	0.14	12 (5%)	31	29	32, 53, 73, 101	13 (6%)
1	C	214/219 (97%)	0.01	5 (2%)	61	60	32, 49, 70, 98	8 (3%)
1	D	214/219 (97%)	0.03	5 (2%)	61	60	31, 47, 70, 93	8 (3%)
1	E	214/219 (97%)	-0.05	8 (3%)	45	43	29, 48, 70, 88	9 (4%)
1	F	214/219 (97%)	0.03	10 (4%)	37	35	34, 51, 71, 101	9 (4%)
All	All	1284/1314 (97%)	0.04	47 (3%)	45	43	28, 50, 73, 103	56 (4%)

The worst 5 of 47 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	34	CYS	4.6
1	E	73	ASP	4.2
1	B	73	ASP	4.2
1	A	6	GLU	3.8
1	F	70	ILE	3.7

### 6.2 Non-standard residues in protein, DNA, RNA chains [i](#)

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

### 6.3 Carbohydrates [i](#)

There are no monosaccharides in this entry.

## 6.4 Ligands ⓘ

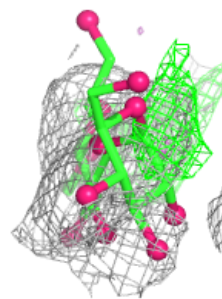
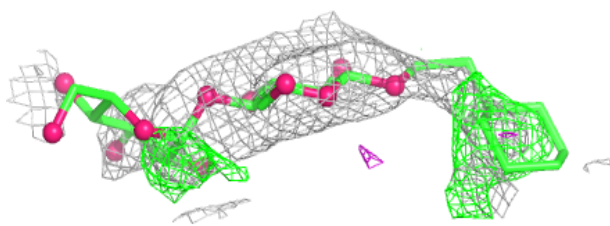
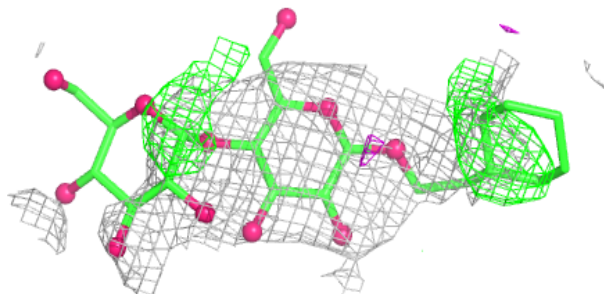
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 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
2	MA5	F	1005	31/31	0.39	0.26	107,109,110,111	15
2	MA5	A	1004	31/31	0.51	0.20	115,118,122,122	15
2	MA5	B	1002	31/31	0.61	0.41	105,107,108,108	13
4	EPE	F	3002	12/15	0.62	0.21	104,107,117,118	0
2	MA5	C	1003	31/31	0.70	0.21	68,77,81,83	0
2	MA5	D	1001	31/31	0.75	0.30	103,118,120,121	15
2	MA5	F	1008	31/31	0.76	0.25	71,91,95,95	7
2	MA5	B	1007	31/31	0.76	0.21	113,123,124,124	12
4	EPE	B	3001	12/15	0.78	0.20	104,104,105,105	0
2	MA5	C	1006	31/31	0.78	0.22	99,104,107,107	0
3	NAP	A	2001	48/48	0.81	0.18	79,88,103,103	0
3	NAP	D	2004	48/48	0.83	0.14	67,80,96,97	0
3	NAP	B	2002	48/48	0.86	0.16	72,77,104,104	0
3	NAP	F	2006	48/48	0.86	0.14	72,79,104,105	0
3	NAP	C	2003	48/48	0.87	0.13	56,64,87,88	0
3	NAP	E	2005	48/48	0.88	0.15	58,67,101,102	0

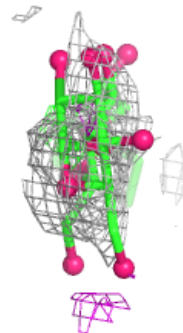
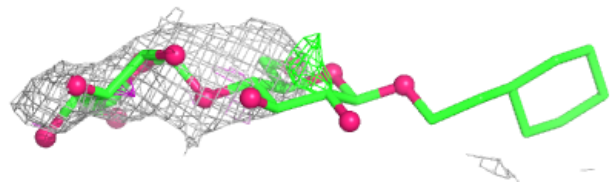
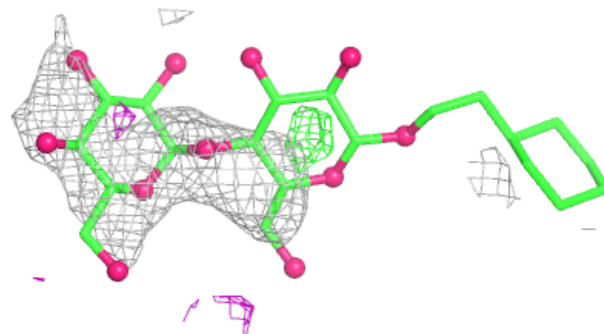
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

**Electron density around MA5 F 1005:**

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

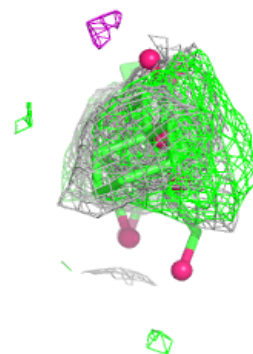
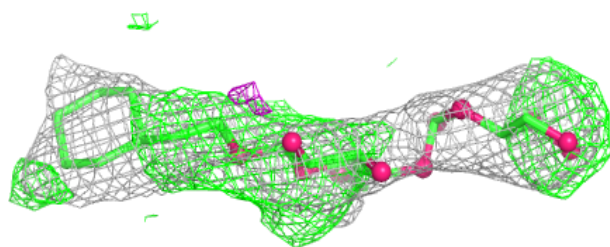
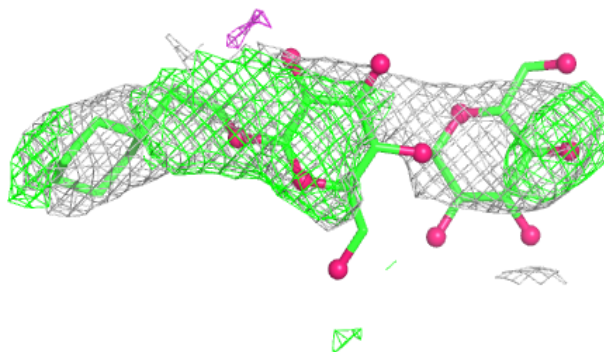
**Electron density around MA5 A 1004:**

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

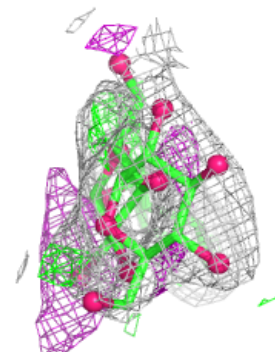
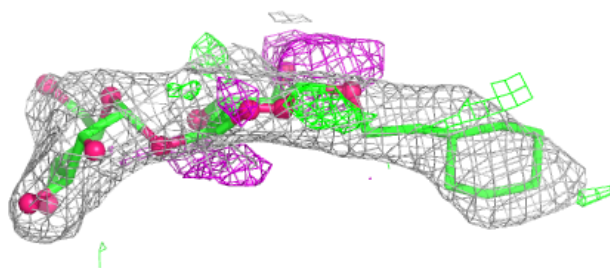
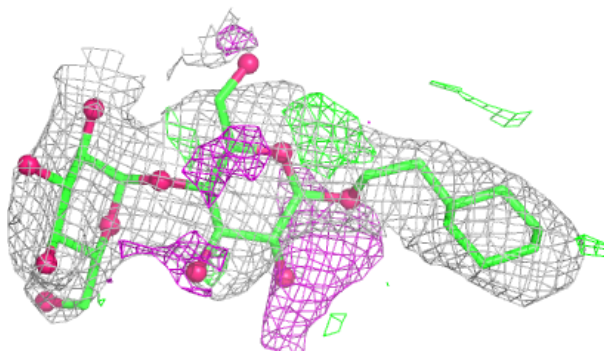


**Electron density around MA5 B 1002:**

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

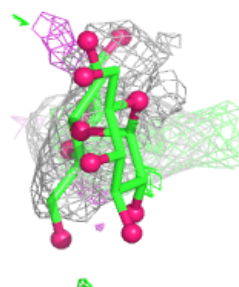
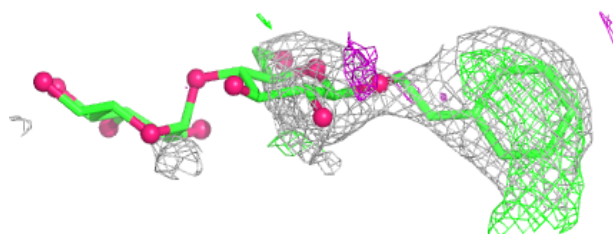
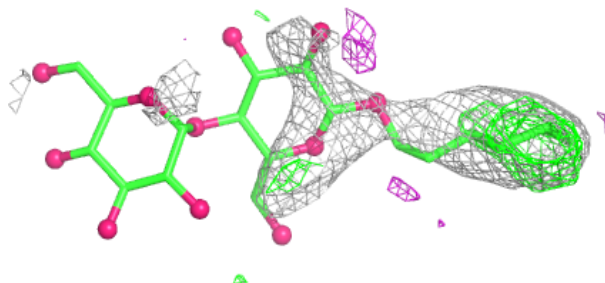
**Electron density around MA5 C 1003:**

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

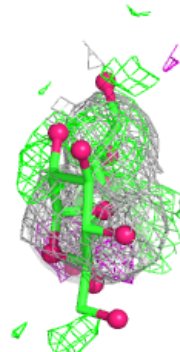
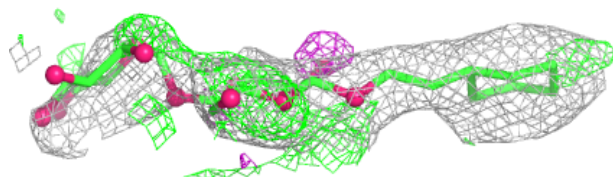
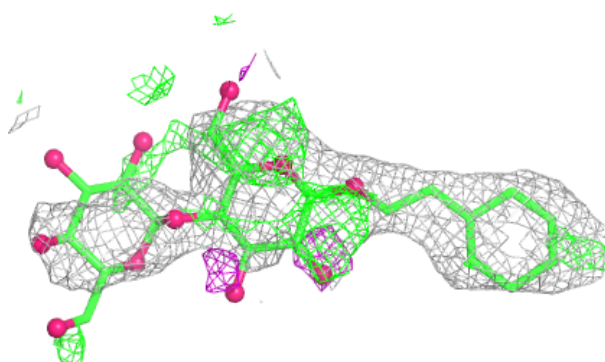


**Electron density around MA5 D 1001:**

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

**Electron density around MA5 F 1008:**

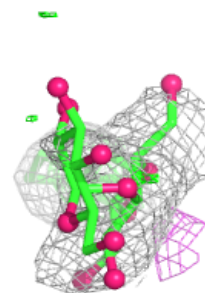
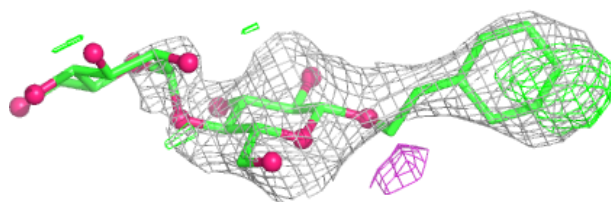
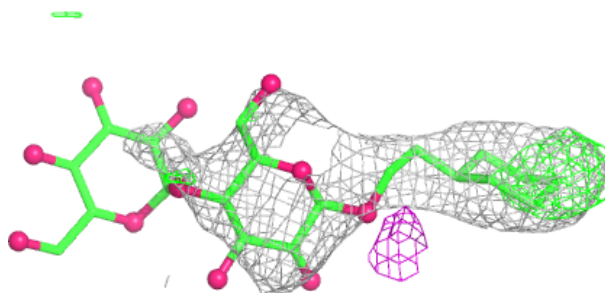
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and green (positive)



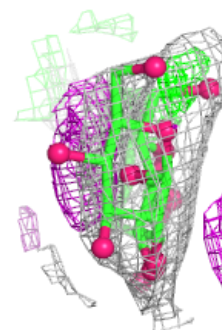
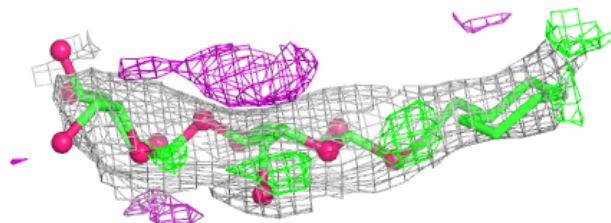
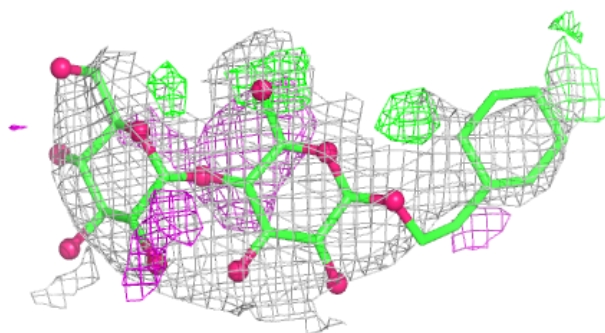


**Electron density around MA5 B 1007:**

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and green (positive)

**Electron density around MA5 C 1006:**

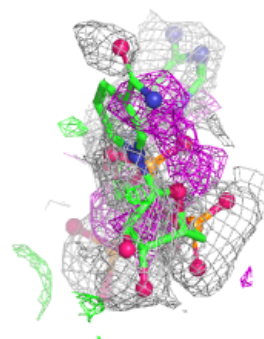
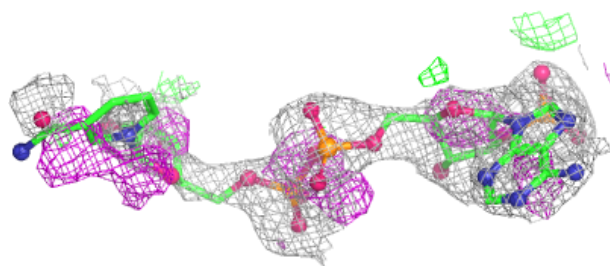
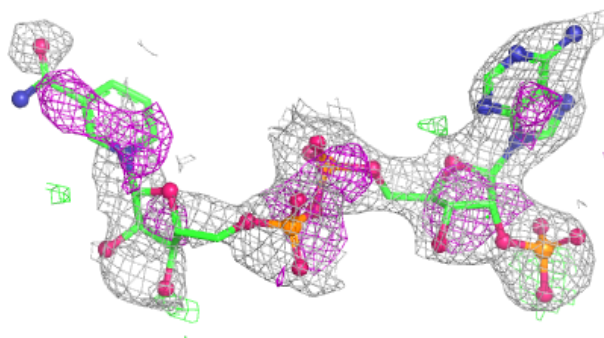
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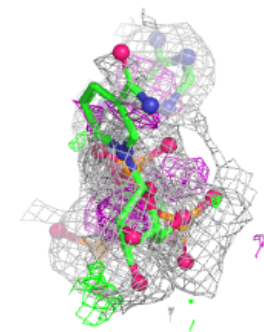
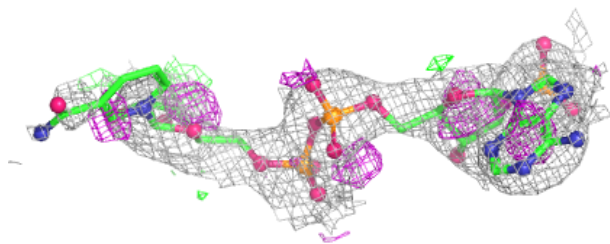
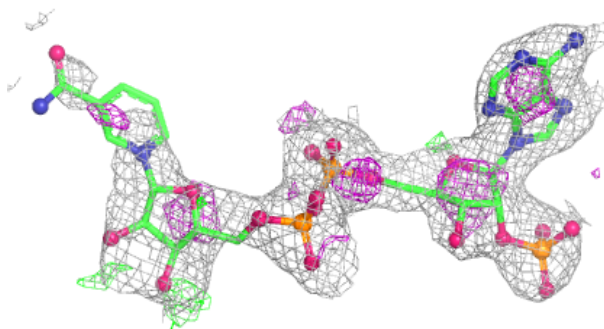


**Electron density around NAP A 2001:**

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and green (positive)

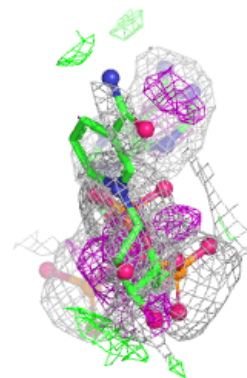
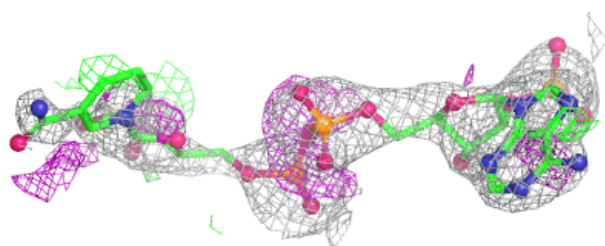
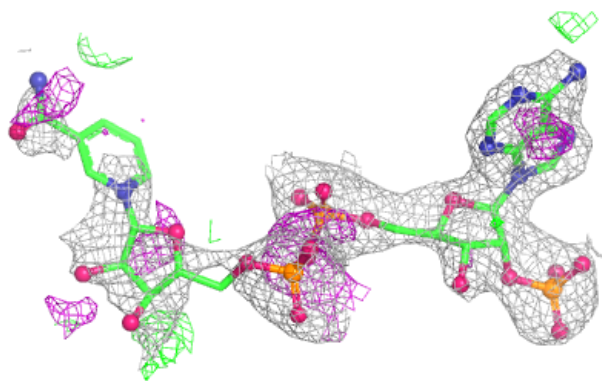
**Electron density around NAP D 2004:**

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and green (positive)

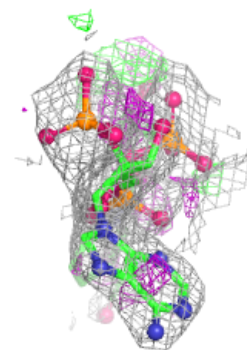
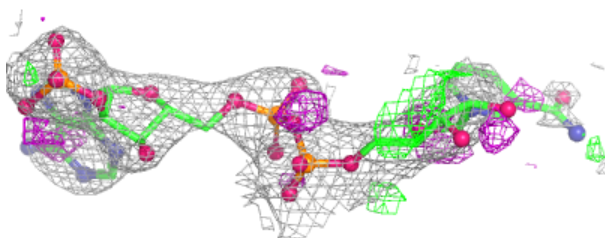
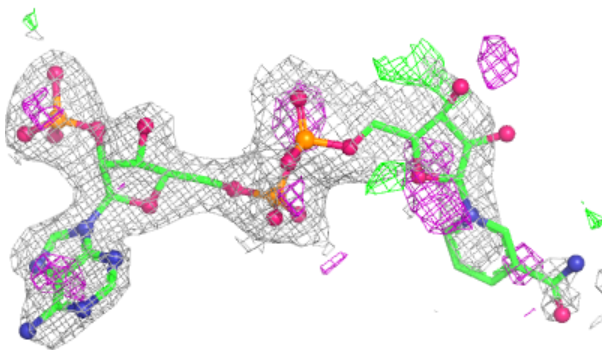


**Electron density around NAP B 2002:**

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

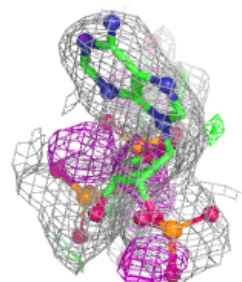
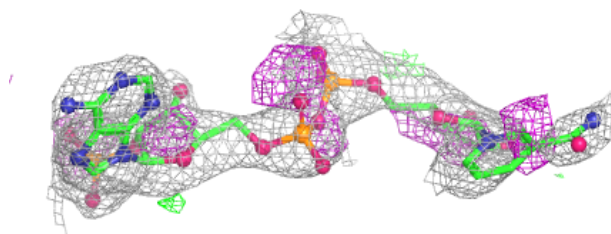
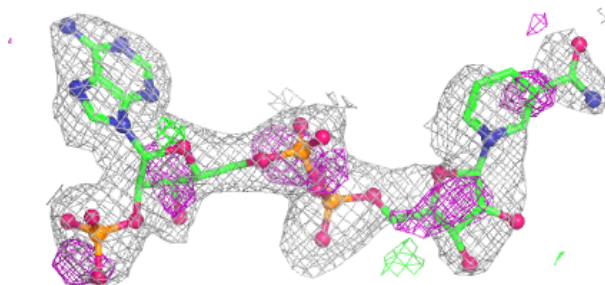
**Electron density around NAP F 2006:**

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

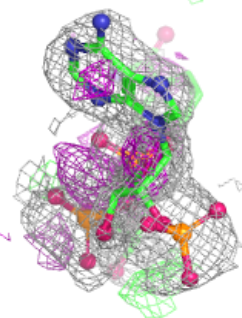
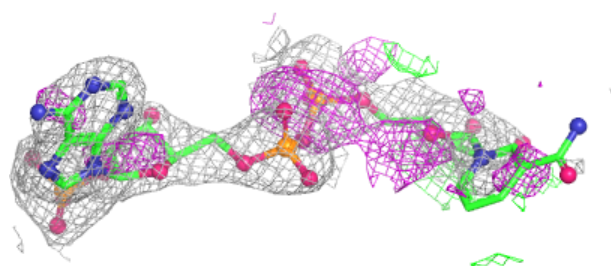
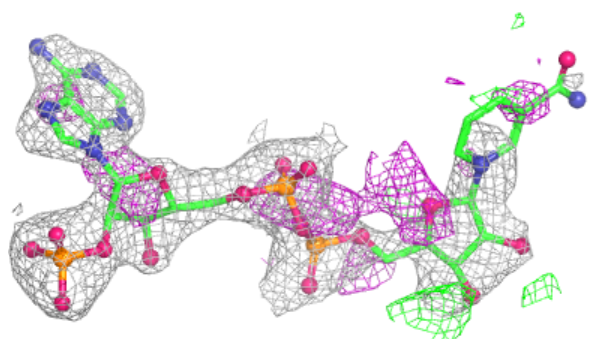


**Electron density around NAP C 2003:**

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

**Electron density around NAP E 2005:**

$2mF_o-DF_c$  (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.