



# Full wwPDB X-ray Structure Validation Report ⓘ

May 25, 2020 – 09:41 am BST

PDB ID : 6GPJ  
Title : Crystal structure of human GDP-D-mannose 4,6-dehydratase in complex with GDP-4F-Man  
Authors : Pfeiffer, M.; Krojer, T.; Johansson, C.; von Delft, F.; Bountra, C.; Arrow-smith, C.H.; Edwards, A.; Nidetzky, B.; Oppermann, U.; Structural Genomics Consortium (SGC)  
Deposited on : 2018-06-06  
Resolution : 1.94 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

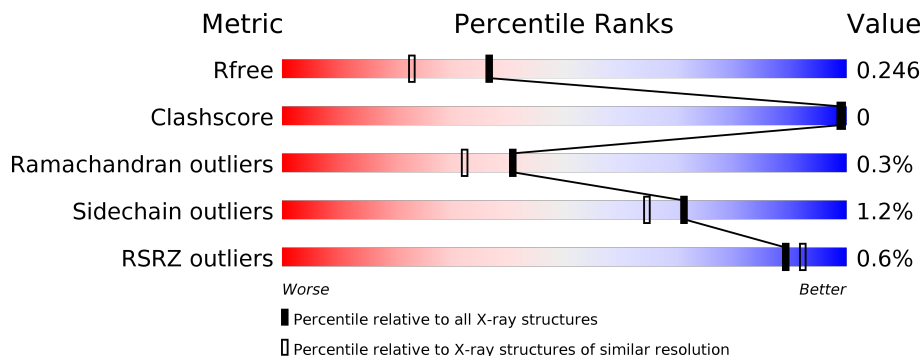
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 1.94 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	4310 (1.96-1.92)
Clashscore	141614	1023 (1.94-1.94)
Ramachandran outliers	138981	1007 (1.94-1.94)
Sidechain outliers	138945	1007 (1.94-1.94)
RSRZ outliers	127900	4250 (1.96-1.92)

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	352	 95%
1	B	352	 95%
1	C	352	 95%
1	D	352	 94%

## 2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 11972 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 GDP-mannose 4,6 dehydratase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	341	2703	1724	462	507	10	0	0	0
1	D	342	2726	1742	466	508	10	0	1	0
1	C	341	2714	1730	467	507	10	0	1	0
1	B	341	2711	1729	464	507	11	0	2	0

There are 8 discrepancies between the modelled and reference sequences:

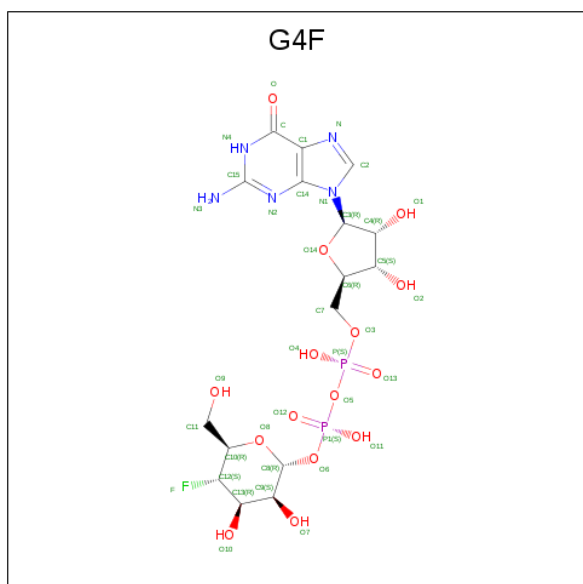
Chain	Residue	Modelled	Actual	Comment	Reference
A	21	SER	-	expression tag	UNP O60547
A	22	MET	-	expression tag	UNP O60547
D	21	SER	-	expression tag	UNP O60547
D	22	MET	-	expression tag	UNP O60547
C	21	SER	-	expression tag	UNP O60547
C	22	MET	-	expression tag	UNP O60547
B	21	SER	-	expression tag	UNP O60547
B	22	MET	-	expression tag	UNP O60547

- Molecule 2 is CITRIC ACID (three-letter code: CIT) (formula: C<sub>6</sub>H<sub>8</sub>O<sub>7</sub>).



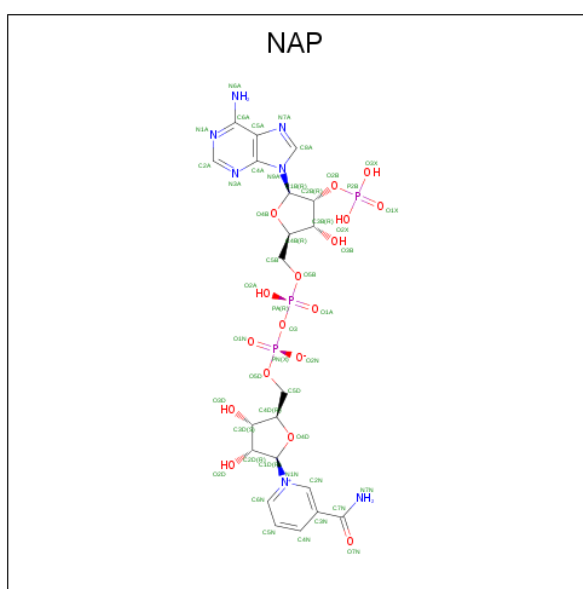
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf	
2	A	1	Total	C	O	0	0
			13	6	7		
2	B	1	Total	C	O	0	0
			13	6	7		

- Molecule 3 is [(2 {R},3 {S},4 {R},5 {R})-5-(2-azanyl-6-oxidanylidene-1 {H}-purin-9-yl)-3,4-bis(oxidanyl)oxolan-2-yl]methoxy-oxidanyl-phosphoryl [(2 {R},3 {S},4 {R},5 {S},6 {R})-5-fluoranyl-6-(hydroxymethyl)-3,4-bis(oxidanyl)oxan-2-yl] hydrogen phosphate (three-letter code: G4F) (formula: C<sub>16</sub>H<sub>24</sub>FN<sub>5</sub>O<sub>15</sub>P<sub>2</sub>).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	
3	A	1	Total	C	F	N	O	P	0	0
			39	16	1	5	15	2		
3	D	1	Total	C	F	N	O	P	0	0
			39	16	1	5	15	2		
3	C	1	Total	C	F	N	O	P	0	0
			39	16	1	5	15	2		
3	B	1	Total	C	F	N	O	P	0	0
			39	16	1	5	15	2		

- Molecule 4 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	
4	A	1	Total	C	N	O	P	0	0
			48	21	7	17	3		
4	D	1	Total	C	N	O	P	0	0
			48	21	7	17	3		
4	C	1	Total	C	N	O	P	0	0
			48	21	7	17	3		
4	B	1	Total	C	N	O	P	0	0
			48	21	7	17	3		

- Molecule 5 is 1,2-ETHANEDIOL (three-letter code: EDO) (formula: C<sub>2</sub>H<sub>6</sub>O<sub>2</sub>).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	D	1	Total C O 4 2 2	0	0
5	B	1	Total C O 4 2 2	0	0

- Molecule 6 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	A	187	Total O 187 187	0	0
6	D	173	Total O 173 173	0	0
6	C	163	Total O 163 163	0	0
6	B	213	Total O 213 213	0	0

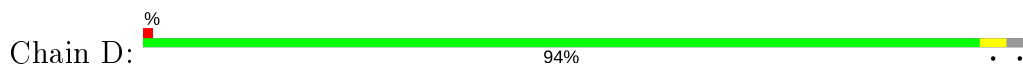
### 3 Residue-property plots [i](#)

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

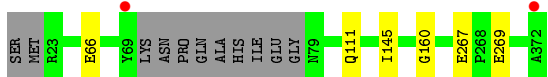
- Molecule 1: GDP-mannose 4,6 dehydratase



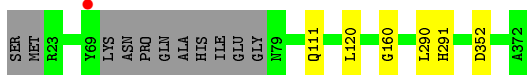
- Molecule 1: GDP-mannose 4,6 dehydratase



- Molecule 1: GDP-mannose 4,6 dehydratase



- Molecule 1: GDP-mannose 4,6 dehydratase



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	92.08Å 114.44Å 140.54Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	63.90 – 1.94 63.90 – 1.94	Depositor EDS
% Data completeness (in resolution range)	99.3 (63.90-1.94) 99.3 (63.90-1.94)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.70 (at 1.94Å)	Xtrriage
Refinement program	REFMAC 5.8.0158	Depositor
R, $R_{free}$	0.210 , 0.238 0.217 , 0.246	Depositor DCC
$R_{free}$ test set	5309 reflections (4.84%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	22.3	Xtrriage
Anisotropy	0.092	Xtrriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.33 , 41.9	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.33$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
$F_o, F_c$ correlation	0.95	EDS
Total number of atoms	11972	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	28.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 18.45% of the height of the origin peak. No significant pseudotranslation is detected.*

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

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



## 5 Model quality [i](#)

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

Bond lengths and bond angles in the following residue types are not validated in this section: NAP, EDO, G4F, CIT

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	0.57	0/2762	0.72	1/3744 (0.0%)
1	B	0.57	0/2777	0.69	0/3763
1	C	0.55	0/2774	0.70	0/3759
1	D	0.54	0/2786	0.70	0/3773
All	All	0.56	0/11099	0.71	1/15039 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	290	LEU	CB-CG-CD2	5.07	119.61	111.00

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	2703	0	2625	4	0
1	B	2711	0	2640	1	0
1	C	2714	0	2644	1	0
1	D	2726	0	2671	4	0
2	A	13	0	5	0	0
2	B	13	0	5	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	A	39	0	0	0	0
3	B	39	0	0	0	0
3	C	39	0	0	0	0
3	D	39	0	0	0	0
4	A	48	0	25	0	0
4	B	48	0	25	0	0
4	C	48	0	25	0	0
4	D	48	0	25	0	0
5	B	4	0	6	0	0
5	D	4	0	6	0	0
6	A	187	0	0	2	0
6	B	213	0	0	1	0
6	C	163	0	0	2	0
6	D	173	0	0	0	0
All	All	11972	0	10702	8	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 0.

All (8) 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:269:GLU:OE1	6:C:501:HOH:O	2.07	0.71
1:D:120:LEU:HD11	6:C:558:HOH:O	2.04	0.56
1:A:120:LEU:HD11	6:B:565:HOH:O	2.07	0.55
1:D:87:LEU:HD21	1:D:135[B]:LEU:HD11	1.92	0.52
6:A:522:HOH:O	1:B:120:LEU:HD21	2.11	0.50
1:A:90:SER:HB2	1:D:90:SER:HB2	1.99	0.45
1:A:91:THR:HG21	1:D:137:ASP:HB3	2.04	0.40
1:A:257:GLU:HB2	6:A:516:HOH:O	2.19	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	337/352 (96%)	331 (98%)	5 (2%)	1 (0%)	41	32
1	B	339/352 (96%)	335 (99%)	3 (1%)	1 (0%)	41	32
1	C	338/352 (96%)	332 (98%)	5 (2%)	1 (0%)	41	32
1	D	339/352 (96%)	333 (98%)	5 (2%)	1 (0%)	41	32
All	All	1353/1408 (96%)	1331 (98%)	18 (1%)	4 (0%)	41	32

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	D	160	GLY
1	A	160	GLY
1	B	160	GLY
1	C	160	GLY

### 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	286/304 (94%)	284 (99%)	2 (1%)	84	81
1	B	288/304 (95%)	284 (99%)	4 (1%)	67	58
1	C	288/304 (95%)	284 (99%)	4 (1%)	67	58
1	D	290/304 (95%)	286 (99%)	4 (1%)	67	58
All	All	1152/1216 (95%)	1138 (99%)	14 (1%)	71	64

All (14) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	111	GLN
1	A	290	LEU
1	D	66	GLU
1	D	111	GLN

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Mol	Chain	Res	Type
1	D	145	ILE
1	D	364	GLU
1	C	66	GLU
1	C	111	GLN
1	C	145	ILE
1	C	267	GLU
1	B	111	GLN
1	B	290	LEU
1	B	291	HIS
1	B	352	ASP

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

### 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 carbohydrates in this entry.

## 5.6 Ligand geometry [i](#)

12 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	G4F	B	403	-	35,42,42	0.98	3 (8%)	44,65,65	1.83	6 (13%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
3	G4F	C	401	-	35,42,42	1.00	2 (5%)	44,65,65	1.84	6 (13%)
3	G4F	D	402	-	35,42,42	1.08	2 (5%)	44,65,65	1.75	5 (11%)
3	G4F	A	402	-	35,42,42	1.06	3 (8%)	44,65,65	1.75	6 (13%)
4	NAP	B	404	-	45,52,52	1.12	3 (6%)	56,80,80	1.38	9 (16%)
2	CIT	A	401	-	3,12,12	0.51	0	3,17,17	2.65	1 (33%)
5	EDO	B	401	-	3,3,3	0.91	0	2,2,2	0.65	0
5	EDO	D	401	-	3,3,3	0.96	0	2,2,2	0.70	0
2	CIT	B	402	-	3,12,12	0.85	0	3,17,17	2.59	1 (33%)
4	NAP	C	402	-	45,52,52	0.91	1 (2%)	56,80,80	1.54	10 (17%)
4	NAP	D	403	-	45,52,52	1.05	4 (8%)	56,80,80	1.42	8 (14%)
4	NAP	A	403	-	45,52,52	0.79	0	56,80,80	1.18	7 (12%)

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	G4F	B	403	-	-	4/19/59/59	0/4/4/4
3	G4F	C	401	-	-	4/19/59/59	0/4/4/4
3	G4F	D	402	-	-	4/19/59/59	0/4/4/4
3	G4F	A	402	-	-	4/19/59/59	0/4/4/4
4	NAP	B	404	-	-	9/31/67/67	0/5/5/5
2	CIT	A	401	-	-	3/6/16/16	-
5	EDO	B	401	-	-	0/1/1/1	-
5	EDO	D	401	-	-	0/1/1/1	-
2	CIT	B	402	-	-	3/6/16/16	-
4	NAP	C	402	-	-	9/31/67/67	0/5/5/5
4	NAP	D	403	-	-	12/31/67/67	0/5/5/5
4	NAP	A	403	-	-	11/31/67/67	0/5/5/5

All (18) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	402	G4F	C-N4	3.90	1.39	1.33
3	D	402	G4F	C-N4	3.88	1.39	1.33
3	B	403	G4F	C-N4	3.65	1.39	1.33
3	C	401	G4F	C-N4	3.57	1.39	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	C	401	G4F	P1-O6	3.43	1.69	1.60
3	D	402	G4F	P1-O6	3.35	1.69	1.60
4	B	404	NAP	C5A-C4A	3.11	1.49	1.40
4	B	404	NAP	C2A-N3A	3.04	1.37	1.32
4	D	403	NAP	O4D-C1D	3.02	1.45	1.41
3	A	402	G4F	P1-O6	2.97	1.68	1.60
4	D	403	NAP	C2A-N3A	2.84	1.36	1.32
4	C	402	NAP	O4D-C1D	2.51	1.44	1.41
4	D	403	NAP	P2B-O2B	2.45	1.63	1.59
4	D	403	NAP	C5A-C4A	2.34	1.47	1.40
3	A	402	G4F	C2-N	-2.20	1.30	1.34
3	B	403	G4F	P1-O6	2.10	1.66	1.60
4	B	404	NAP	P2B-O2B	2.07	1.63	1.59
3	B	403	G4F	C2-N	-2.03	1.31	1.34

All (59) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	C	401	G4F	C1-C-N4	-8.04	112.44	123.43
3	B	403	G4F	C1-C-N4	-8.00	112.50	123.43
3	D	402	G4F	C1-C-N4	-7.97	112.53	123.43
3	A	402	G4F	C1-C-N4	-7.78	112.79	123.43
3	C	401	G4F	C-N4-C15	6.12	125.65	115.93
3	A	402	G4F	C-N4-C15	5.59	124.81	115.93
3	B	403	G4F	C-N4-C15	5.55	124.75	115.93
3	D	402	G4F	C-N4-C15	5.33	124.40	115.93
4	D	403	NAP	N3A-C2A-N1A	-4.81	121.16	128.68
4	C	402	NAP	N3A-C2A-N1A	-4.33	121.91	128.68
2	B	402	CIT	C3-C2-C1	-4.18	108.29	114.98
2	A	401	CIT	C3-C4-C5	-4.17	108.31	114.98
4	B	404	NAP	C3N-C7N-N7N	3.92	122.46	117.75
4	C	402	NAP	C6N-N1N-C2N	-3.81	118.50	121.97
4	B	404	NAP	N3A-C2A-N1A	-3.58	123.08	128.68
4	B	404	NAP	N6A-C6A-N1A	3.35	125.53	118.57
4	A	403	NAP	C3B-C2B-C1B	-3.15	96.96	102.89
4	D	403	NAP	C2A-N1A-C6A	3.14	124.12	118.75
4	B	404	NAP	O7N-C7N-N7N	-3.13	118.13	122.58
4	C	402	NAP	C3N-C7N-N7N	3.05	121.42	117.75
4	D	403	NAP	C3N-C7N-N7N	3.05	121.42	117.75
3	B	403	G4F	N2-C15-N4	-3.03	123.19	127.22
4	C	402	NAP	C5N-C4N-C3N	-3.02	116.77	120.34
3	C	401	G4F	N2-C15-N4	-2.98	123.24	127.22

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	402	G4F	N2-C15-N4	-2.98	123.25	127.22
4	D	403	NAP	O7N-C7N-C3N	-2.97	116.08	119.63
4	C	402	NAP	C2A-N1A-C6A	2.92	123.75	118.75
4	C	402	NAP	N6A-C6A-N1A	2.92	124.63	118.57
3	D	402	G4F	N2-C15-N4	-2.84	123.44	127.22
3	C	401	G4F	O5-P1-O6	-2.77	96.91	102.48
4	B	404	NAP	O3X-P2B-O2X	2.75	118.15	107.64
3	B	403	G4F	O8-C10-C12	-2.70	104.22	108.88
4	C	402	NAP	O2B-P2B-O1X	-2.69	98.99	109.39
3	C	401	G4F	C-C1-C14	-2.64	118.27	120.80
3	B	403	G4F	C-C1-C14	-2.61	118.31	120.80
4	A	403	NAP	N3A-C2A-N1A	-2.58	124.64	128.68
4	D	403	NAP	N6A-C6A-N1A	2.56	123.88	118.57
3	C	401	G4F	C15-N2-C14	-2.54	112.46	115.36
3	D	402	G4F	O5-P1-O6	-2.46	97.53	102.48
3	A	402	G4F	C15-N2-C14	-2.41	112.61	115.36
4	C	402	NAP	C1B-N9A-C4A	-2.38	122.47	126.64
3	A	402	G4F	C-C1-C14	-2.37	118.54	120.80
3	D	402	G4F	C-C1-C14	-2.33	118.57	120.80
4	A	403	NAP	C3D-C2D-C1D	-2.30	97.51	100.98
4	A	403	NAP	O3D-C3D-C4D	-2.30	104.40	111.05
3	B	403	G4F	O8-C8-O6	-2.29	108.38	111.36
4	D	403	NAP	C1B-N9A-C4A	-2.28	122.63	126.64
4	B	404	NAP	C5A-C6A-N6A	-2.26	116.91	120.35
4	A	403	NAP	C1B-N9A-C4A	-2.24	122.71	126.64
4	D	403	NAP	O2B-P2B-O1X	-2.21	100.86	109.39
4	D	403	NAP	O3D-C3D-C4D	-2.21	104.67	111.05
4	B	404	NAP	C2A-N1A-C6A	2.18	122.48	118.75
4	A	403	NAP	C2D-C3D-C4D	2.17	106.86	102.64
4	B	404	NAP	C3B-C2B-C1B	-2.17	98.81	102.89
4	B	404	NAP	O2A-PA-O1A	2.13	122.78	112.24
3	A	402	G4F	O5-P1-O6	-2.07	98.31	102.48
4	C	402	NAP	O4B-C1B-C2B	-2.06	103.01	106.59
4	A	403	NAP	PN-O3-PA	-2.02	125.89	132.83
4	C	402	NAP	O3D-C3D-C4D	-2.01	105.24	111.05

There are no chirality outliers.

All (63) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	B	403	G4F	C12-C10-C11-O9
3	C	401	G4F	C12-C10-C11-O9

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Mol	Chain	Res	Type	Atoms
3	D	402	G4F	C12-C10-C11-O9
3	A	402	G4F	P1-O5-P-O3
3	A	402	G4F	C12-C10-C11-O9
4	B	404	NAP	C2B-O2B-P2B-O1X
4	B	404	NAP	C2B-O2B-P2B-O3X
4	B	404	NAP	O4D-C1D-N1N-C2N
4	B	404	NAP	O4D-C1D-N1N-C6N
4	B	404	NAP	C2D-C1D-N1N-C2N
4	B	404	NAP	C2D-C1D-N1N-C6N
2	A	401	CIT	C1-C2-C3-C6
2	B	402	CIT	C2-C3-C4-C5
2	B	402	CIT	C6-C3-C4-C5
4	C	402	NAP	C2B-O2B-P2B-O1X
4	C	402	NAP	O4D-C1D-N1N-C2N
4	C	402	NAP	O4D-C1D-N1N-C6N
4	C	402	NAP	C2D-C1D-N1N-C2N
4	C	402	NAP	C2D-C1D-N1N-C6N
4	D	403	NAP	C2B-O2B-P2B-O3X
4	D	403	NAP	C5D-O5D-PN-O2N
4	D	403	NAP	O4D-C1D-N1N-C2N
4	D	403	NAP	O4D-C1D-N1N-C6N
4	D	403	NAP	C2D-C1D-N1N-C6N
4	A	403	NAP	C2B-O2B-P2B-O3X
4	A	403	NAP	O4D-C1D-N1N-C2N
4	A	403	NAP	O4D-C1D-N1N-C6N
4	A	403	NAP	C2D-C1D-N1N-C2N
4	A	403	NAP	C2D-C1D-N1N-C6N
3	B	403	G4F	O8-C10-C11-O9
2	A	401	CIT	C1-C2-C3-O7
3	C	401	G4F	O8-C10-C11-O9
3	A	402	G4F	O8-C10-C11-O9
3	D	402	G4F	O8-C10-C11-O9
2	B	402	CIT	O7-C3-C4-C5
2	A	401	CIT	C1-C2-C3-C4
4	B	404	NAP	PN-O3-PA-O1A
3	B	403	G4F	C8-O6-P1-O5
3	B	403	G4F	P1-O5-P-O3
3	C	401	G4F	P1-O5-P-O3
3	D	402	G4F	P1-O5-P-O3
4	D	403	NAP	C2B-O2B-P2B-O1X
4	D	403	NAP	C5D-O5D-PN-O3
4	A	403	NAP	C5D-O5D-PN-O3

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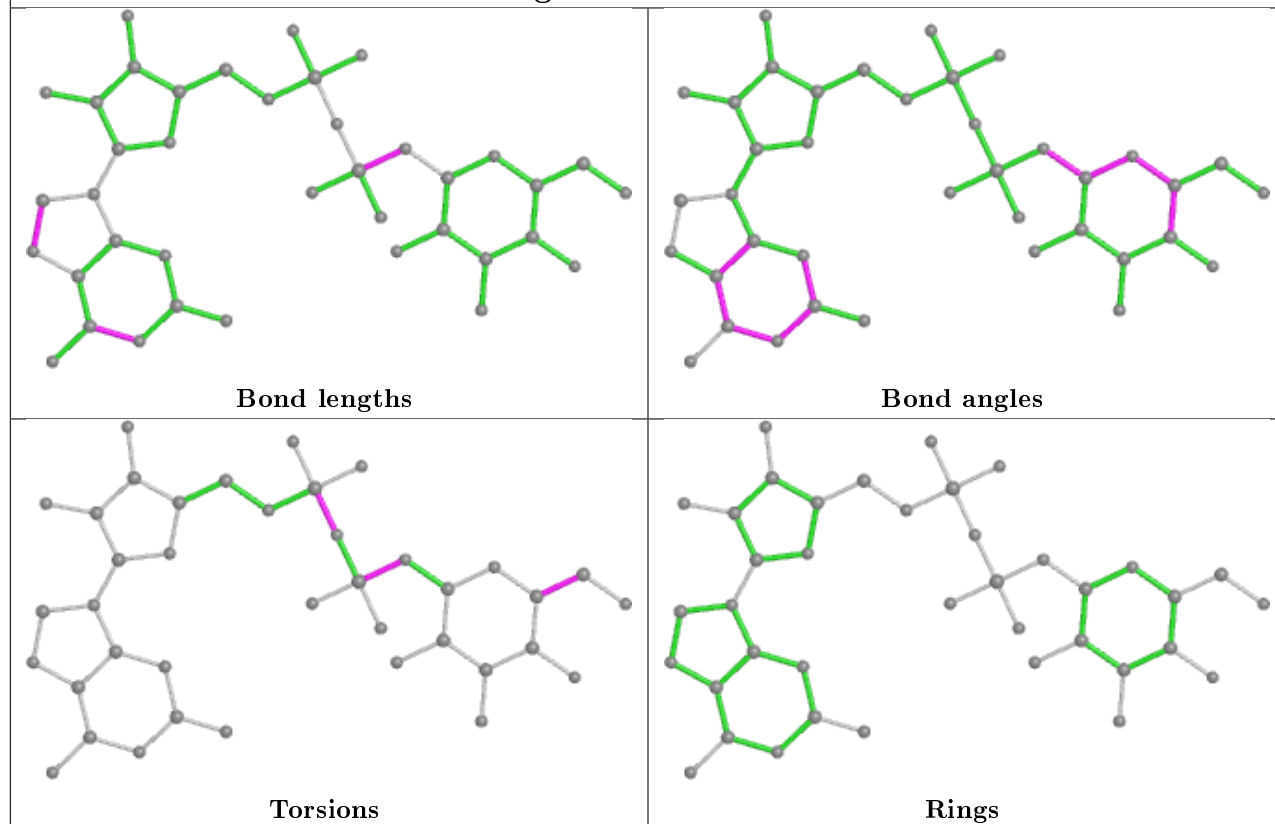
Mol	Chain	Res	Type	Atoms
4	C	402	NAP	PN-O3-PA-O1A
3	D	402	G4F	C8-O6-P1-O5
4	B	404	NAP	PN-O3-PA-O2A
4	C	402	NAP	PN-O3-PA-O2A
4	D	403	NAP	PN-O3-PA-O1A
4	A	403	NAP	PN-O3-PA-O1A
4	A	403	NAP	PN-O3-PA-O2A
4	D	403	NAP	PN-O3-PA-O2A
4	A	403	NAP	C2B-O2B-P2B-O1X
4	C	402	NAP	C5D-O5D-PN-O3
4	D	403	NAP	C2D-C1D-N1N-C2N
4	B	404	NAP	O4B-C4B-C5B-O5B
4	A	403	NAP	O4B-C4B-C5B-O5B
3	C	401	G4F	C8-O6-P1-O12
3	A	402	G4F	P-O5-P1-O12
4	D	403	NAP	C5D-O5D-PN-O1N
4	A	403	NAP	C5D-O5D-PN-O1N
4	C	402	NAP	O4B-C4B-C5B-O5B
4	D	403	NAP	O4B-C4B-C5B-O5B

There are no ring outliers.

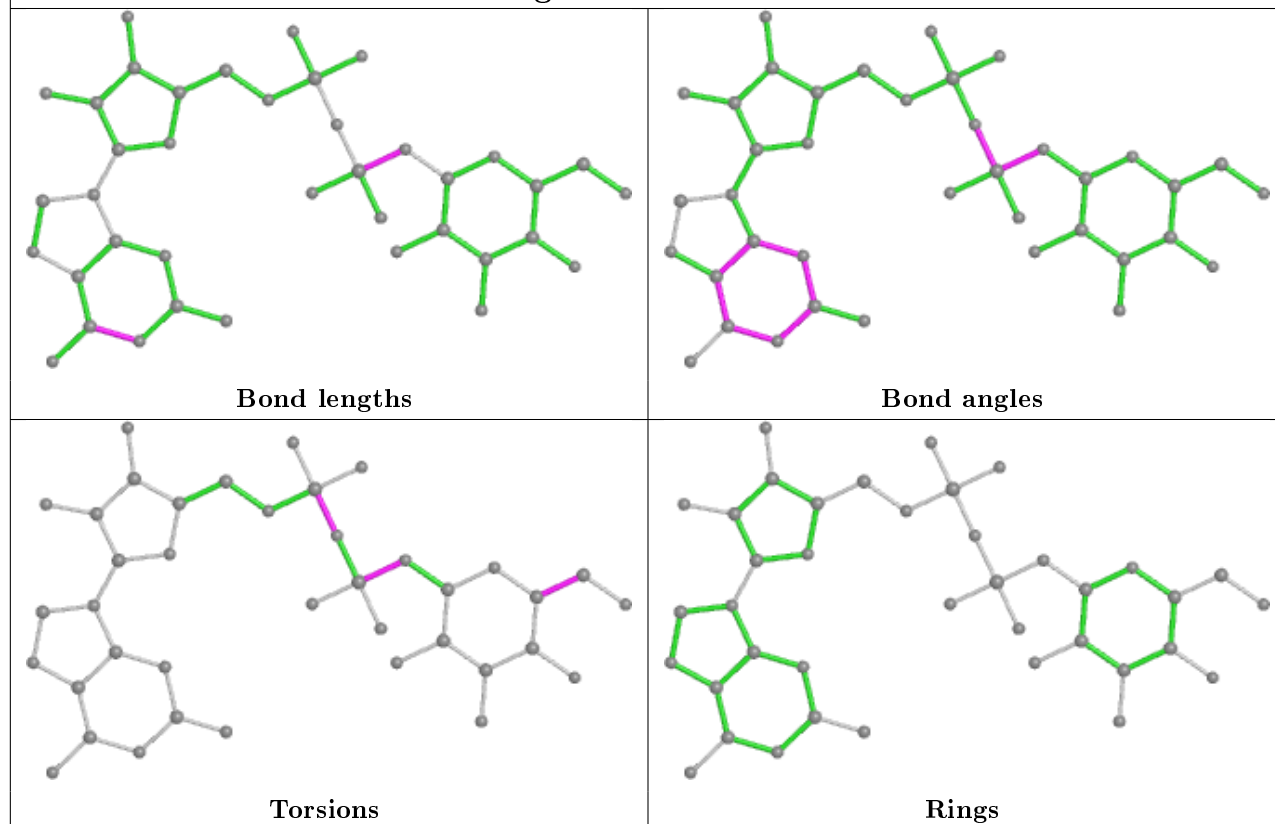
No monomer is involved in short contacts.

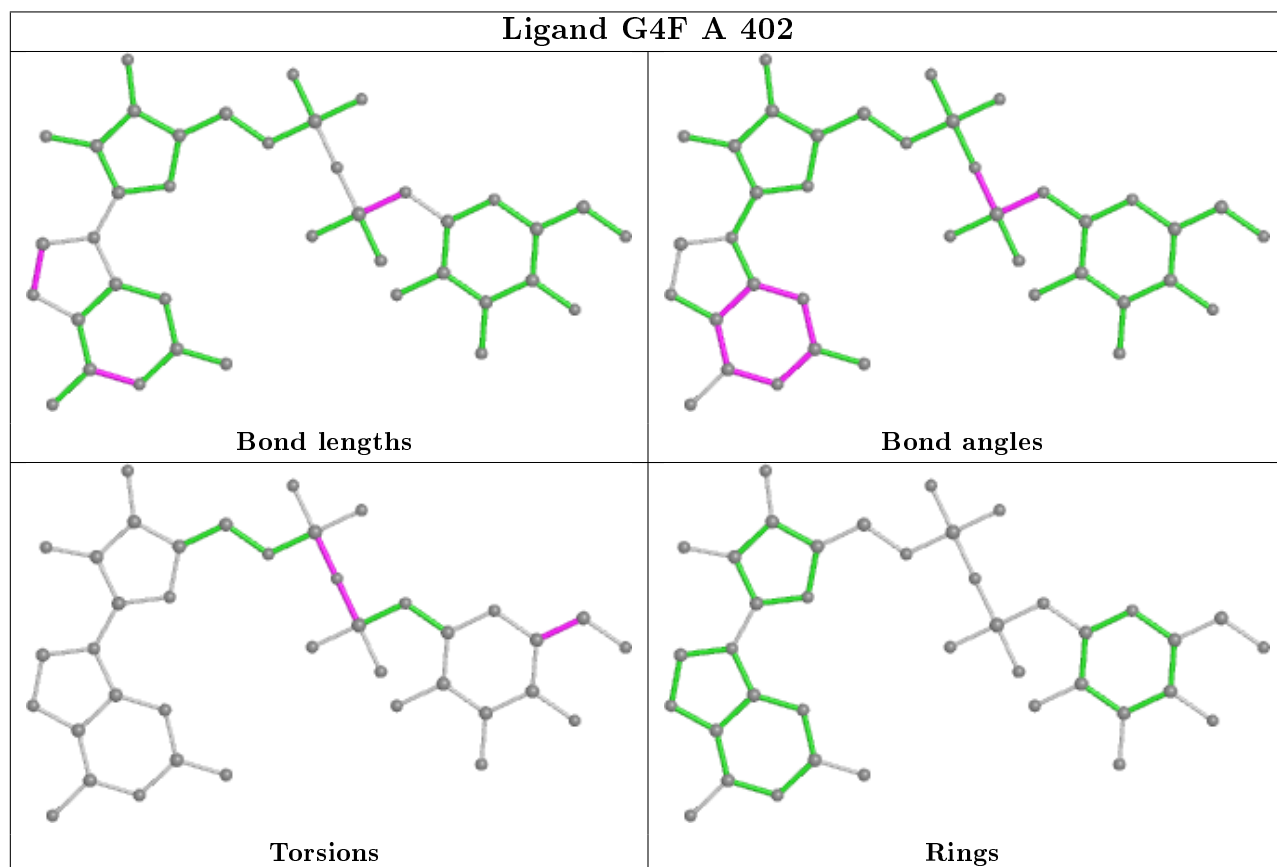
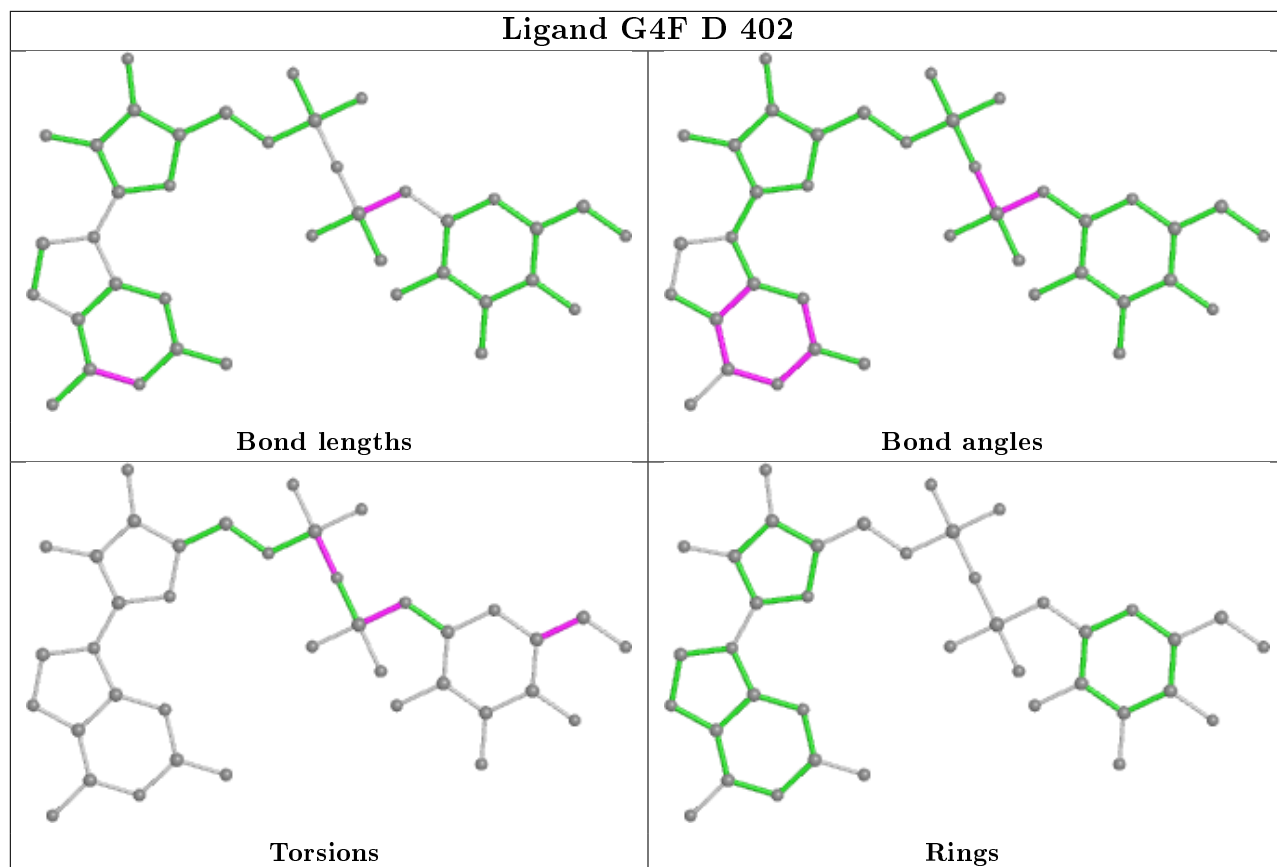
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

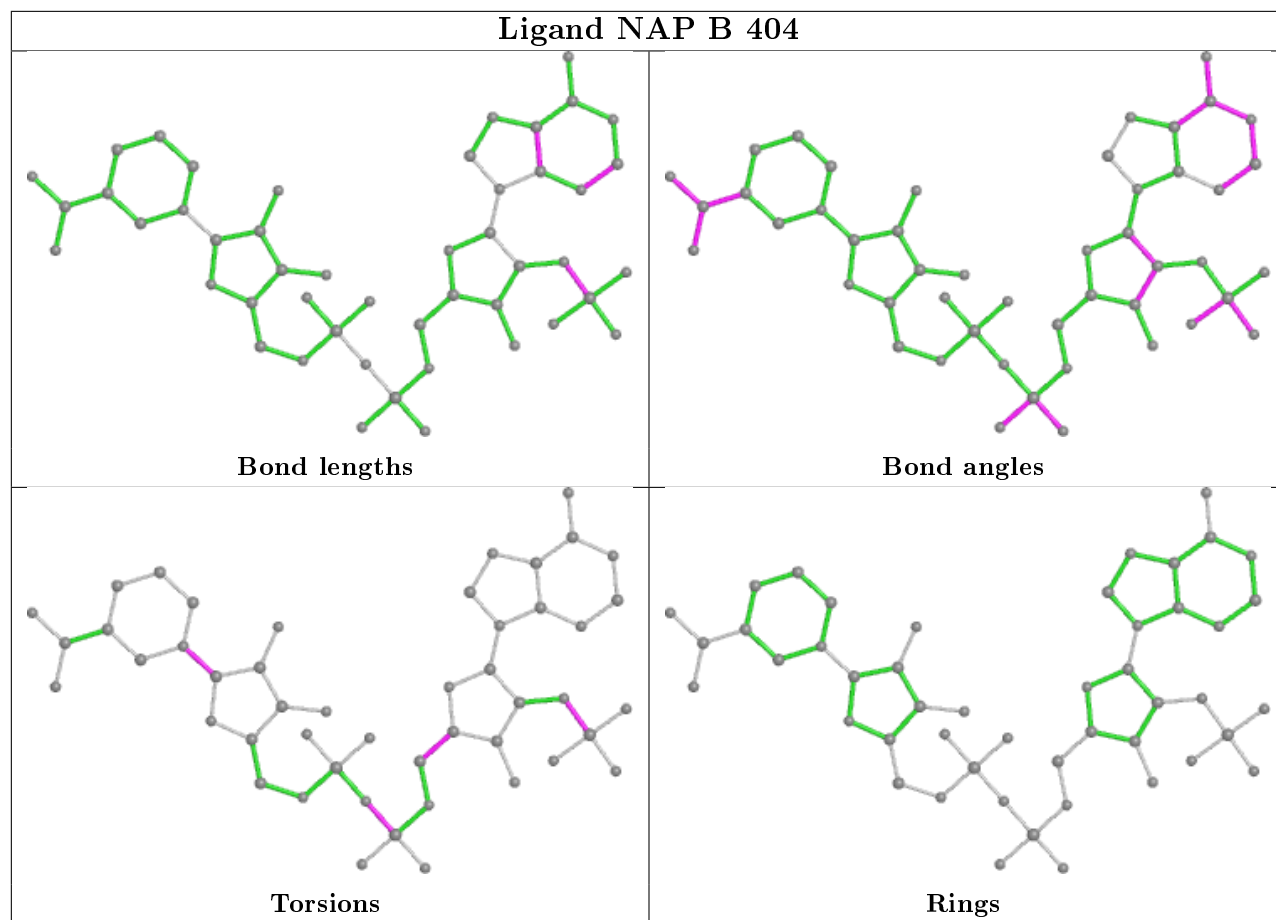
## Ligand G4F B 403

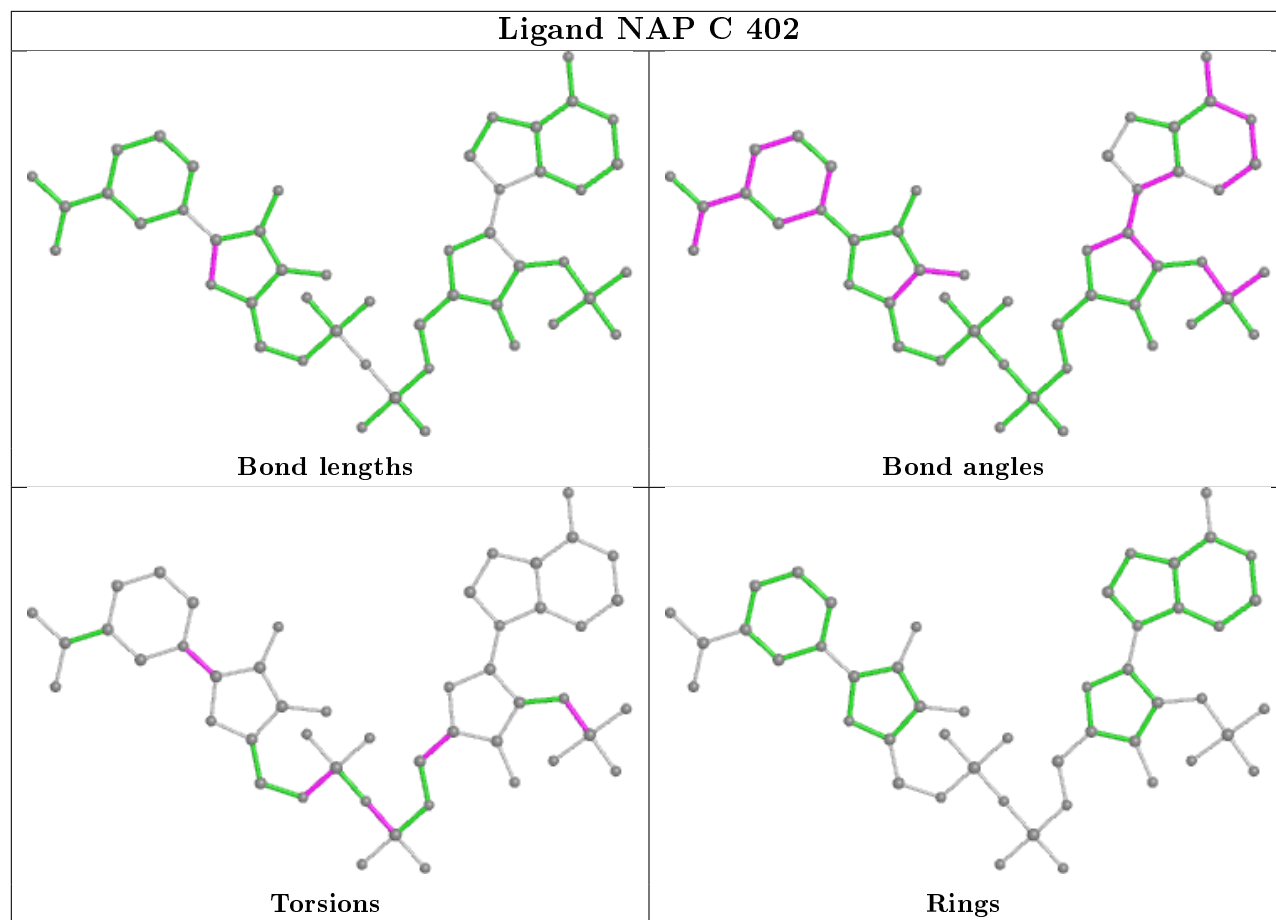


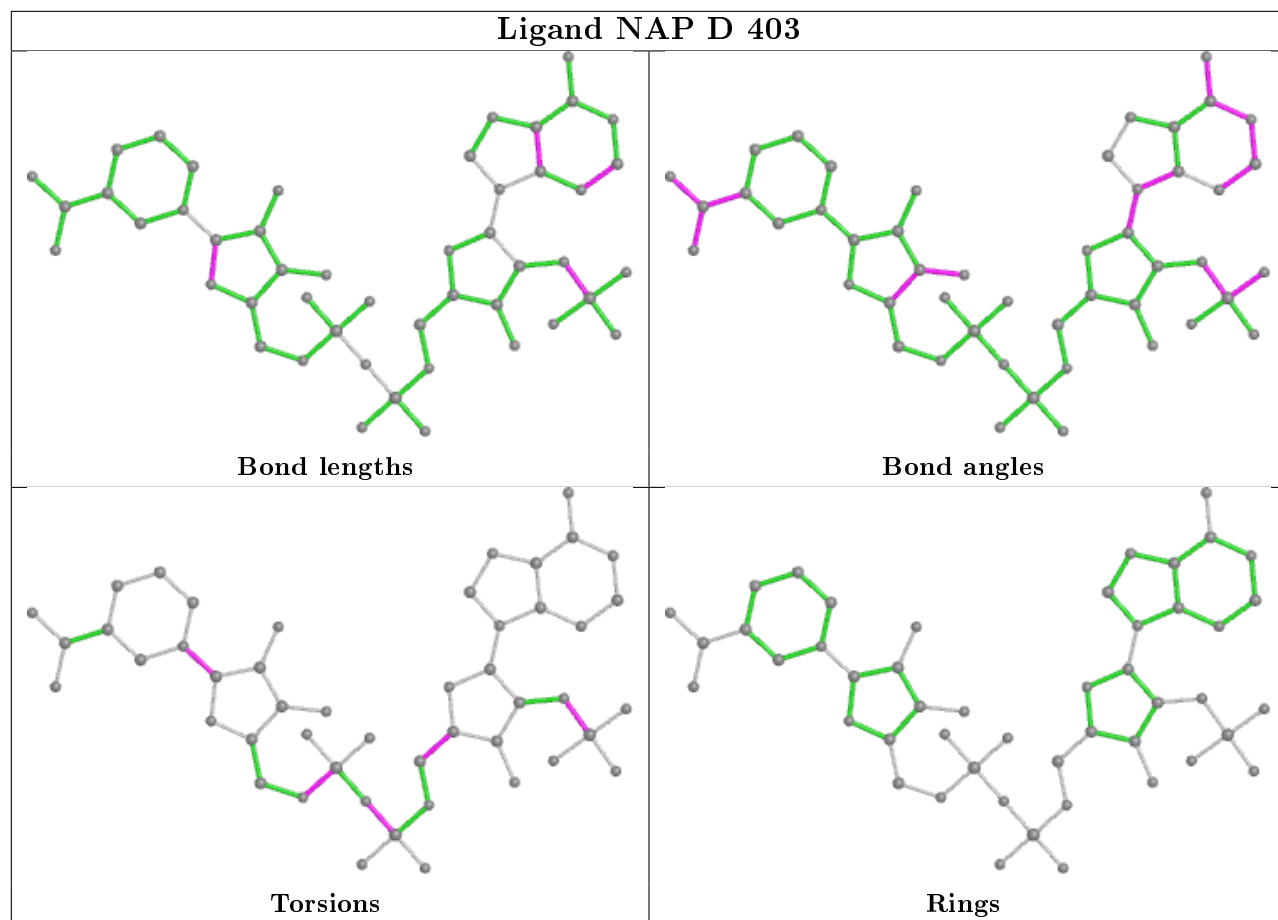
## Ligand G4F C 401

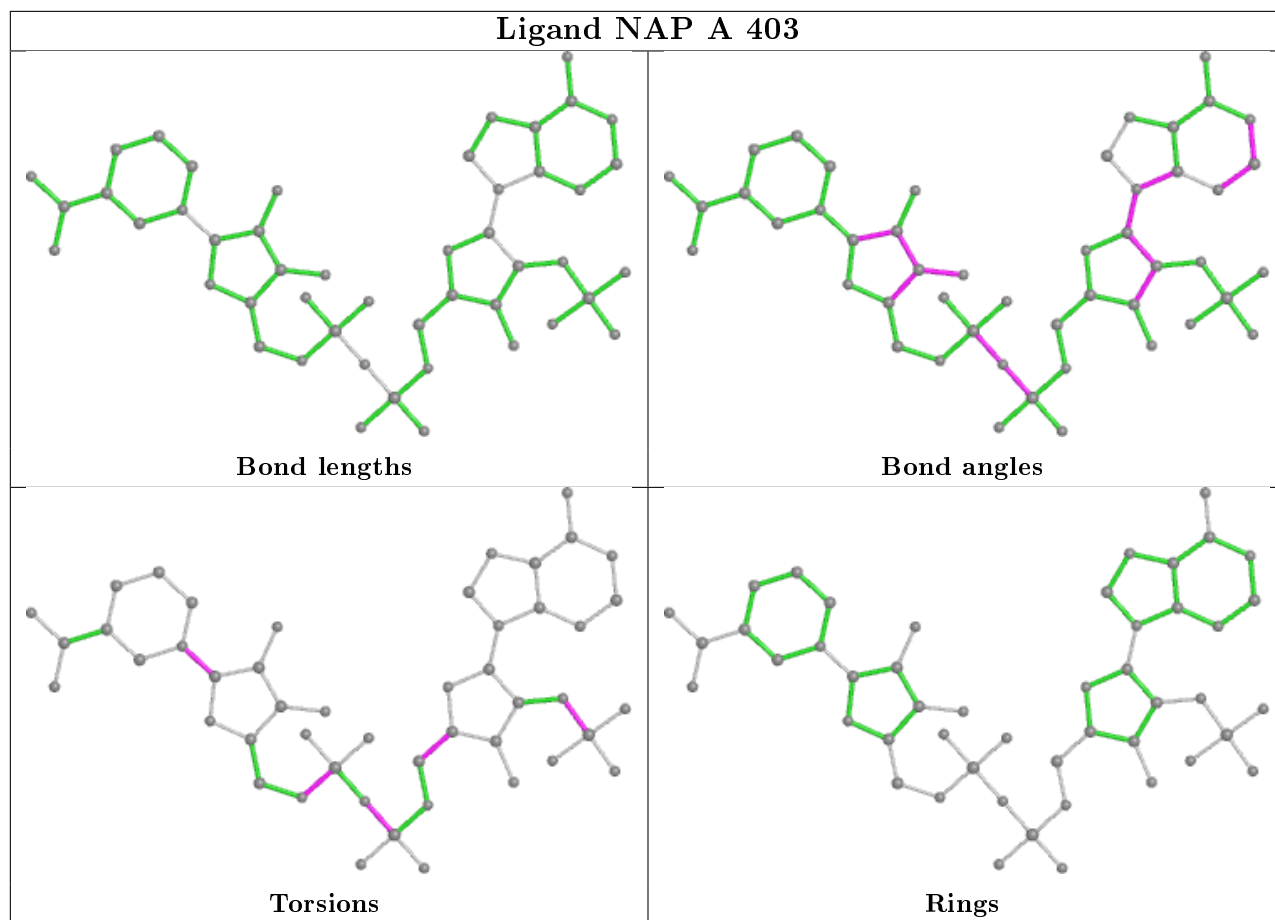












## 5.7 Other polymers [\(i\)](#)

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	341/352 (96%)	-0.10	2 (0%) 89   92	16, 25, 40, 68	0
1	B	341/352 (96%)	-0.17	1 (0%) 94   96	15, 24, 41, 63	0
1	C	341/352 (96%)	0.06	2 (0%) 89   92	18, 29, 49, 72	0
1	D	342/352 (97%)	-0.06	3 (0%) 84   87	16, 26, 43, 64	0
All	All	1365/1408 (96%)	-0.07	8 (0%) 89   92	15, 26, 45, 72	0

All (8) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	69	TYR	3.5
1	A	368	THR	3.3
1	D	69	TYR	3.2
1	C	372	ALA	3.0
1	A	69	TYR	2.9
1	D	22	MET	2.1
1	D	360	HIS	2.1
1	C	69	TYR	2.0

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

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

### 6.3 Carbohydrates [i](#)

There are no carbohydrates in this entry.



## 6.4 Ligands

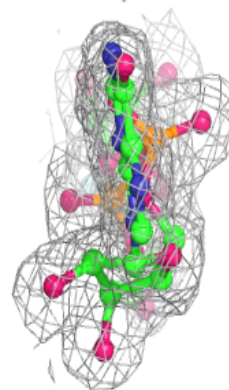
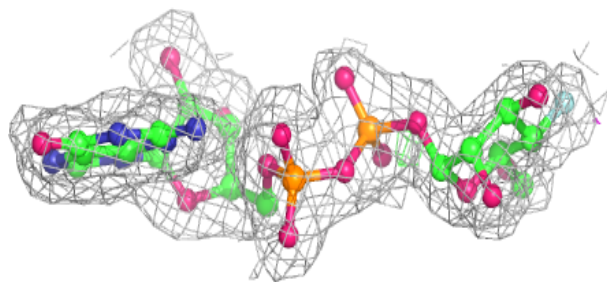
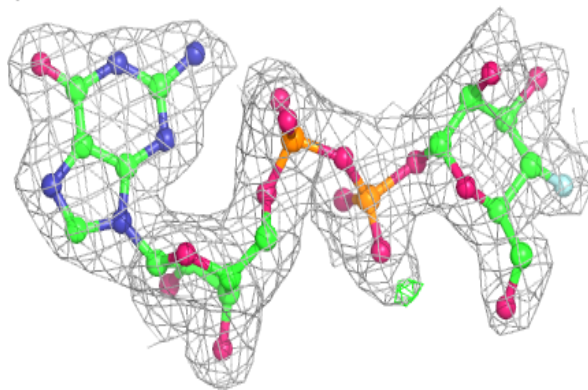
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled 'Q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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
5	EDO	D	401	4/4	0.65	0.19	35,38,40,41	0
5	EDO	B	401	4/4	0.77	0.25	32,38,40,41	0
2	CIT	A	401	13/13	0.82	0.24	36,51,60,65	0
2	CIT	B	402	13/13	0.83	0.18	38,49,65,69	0
3	G4F	C	401	39/39	0.96	0.09	22,27,34,38	0
3	G4F	D	402	39/39	0.97	0.09	18,22,31,39	0
3	G4F	A	402	39/39	0.97	0.08	17,20,28,38	0
3	G4F	B	403	39/39	0.97	0.08	16,18,26,30	0
4	NAP	C	402	48/48	0.97	0.09	18,22,24,25	0
4	NAP	D	403	48/48	0.97	0.08	17,19,21,23	0
4	NAP	B	404	48/48	0.98	0.09	15,18,20,22	0
4	NAP	A	403	48/48	0.98	0.07	15,18,20,20	0

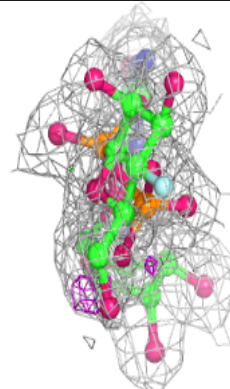
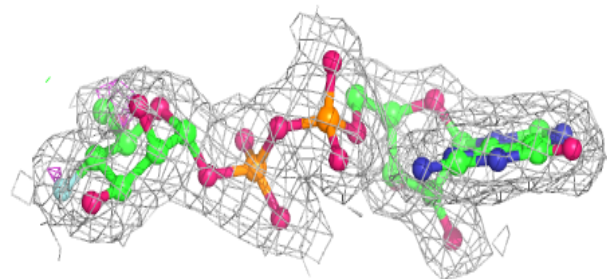
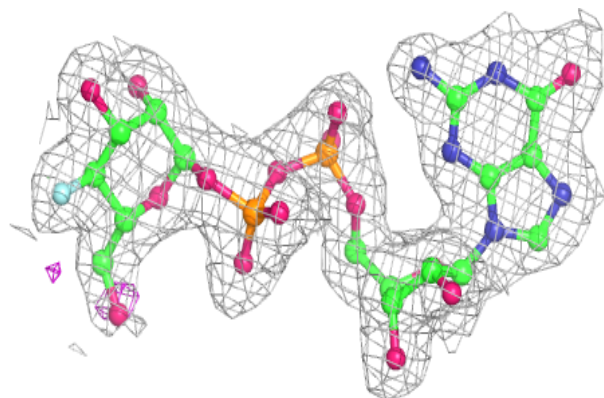
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

**Electron density around G4F C 401:**

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

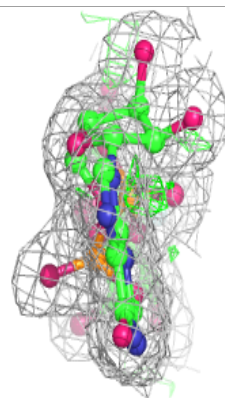
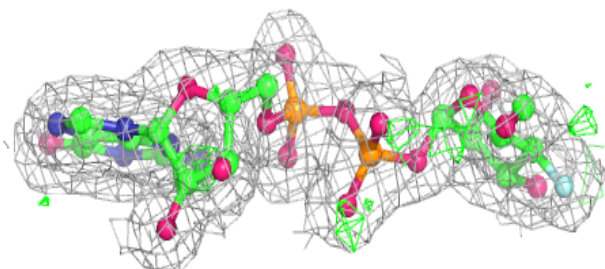
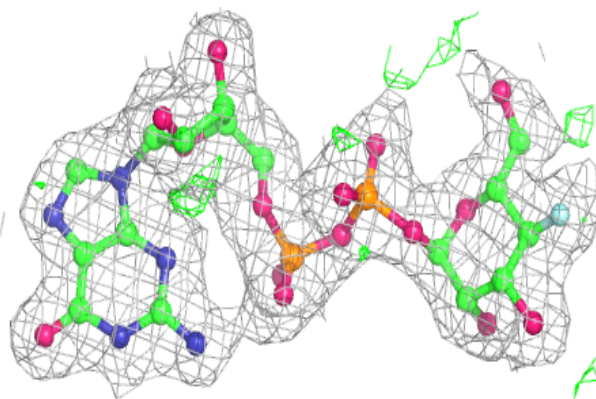
**Electron density around G4F D 402:**

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

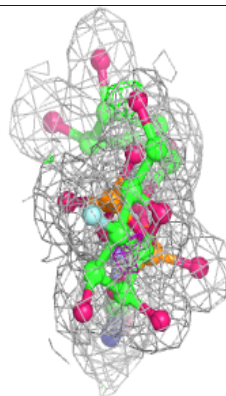
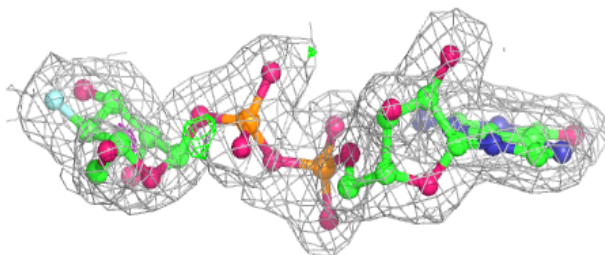
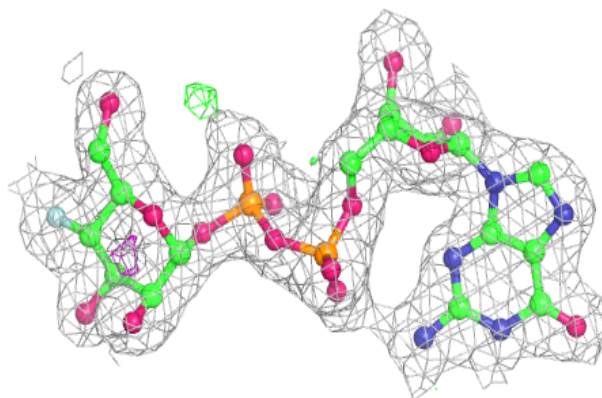


**Electron density around G4F A 402:**

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

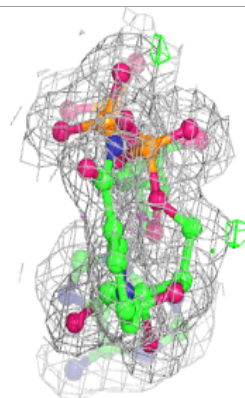
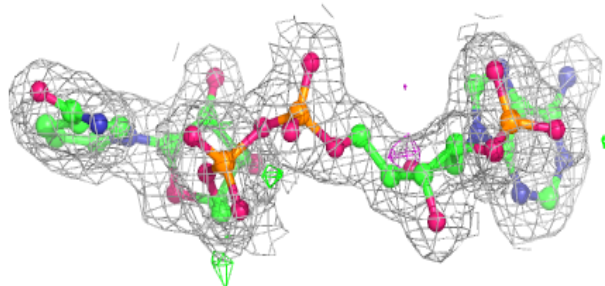
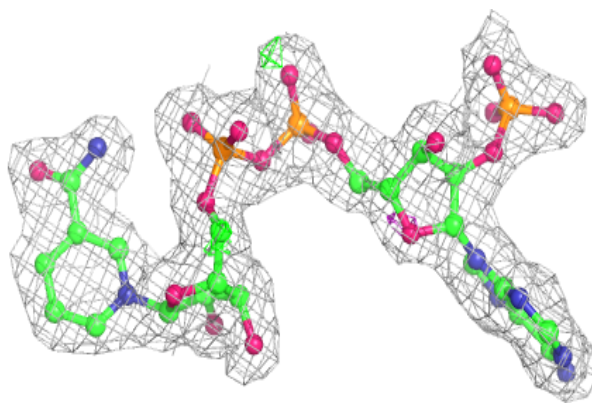
**Electron density around G4F B 403:**

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

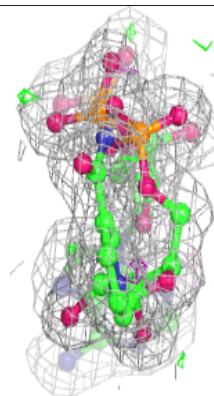
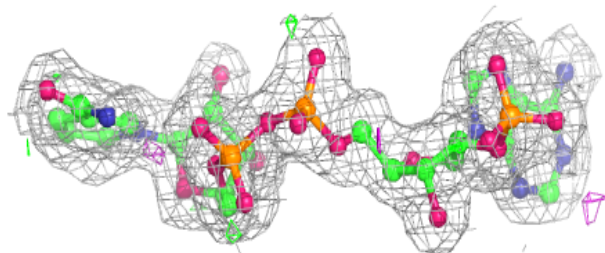
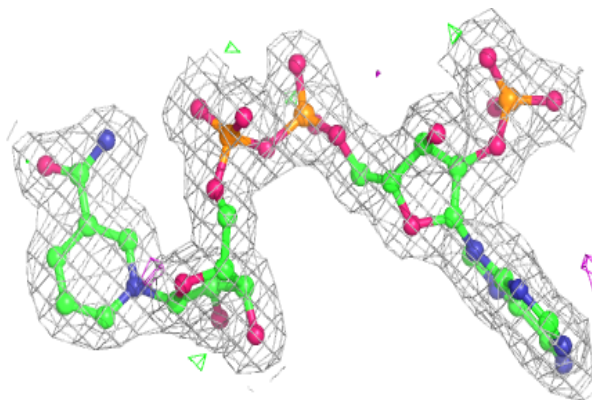


**Electron density around NAP C 402:**

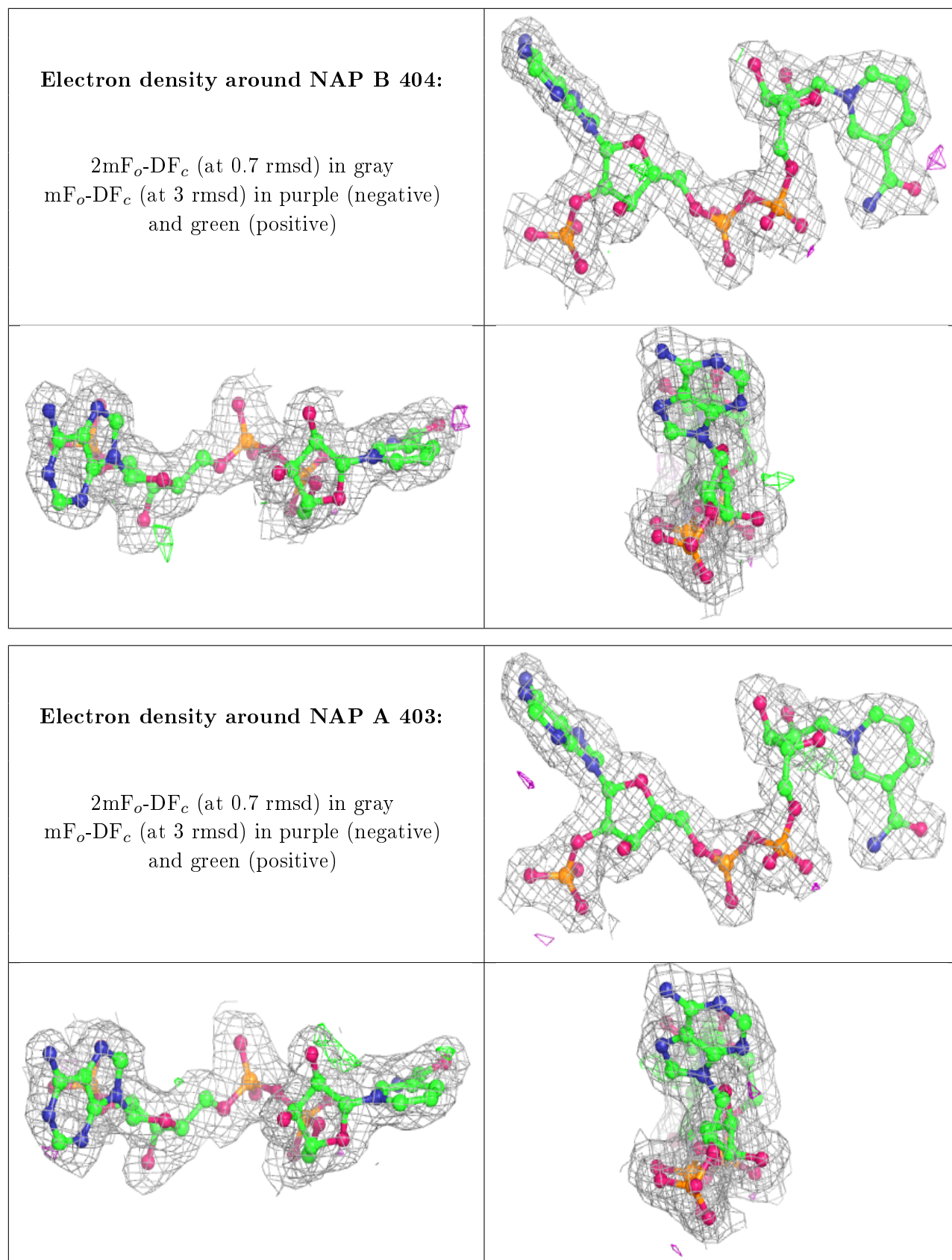
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)

**Electron density around NAP D 403:**

$2mF_o-DF_c$  (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.