



wwPDB X-ray Structure Validation Summary Report ⓘ

Dec 9, 2023 – 11:06 am GMT

PDB ID : 2J3N
Title : X-ray structure of human thioredoxin reductase 1
Authors : Fritz-Wolf, K.; Urig, S.; Becker, K.
Deposited on : 2006-08-22
Resolution : 2.80 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

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>.

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

MolProbity : 4.02b-467
Mogul : 1.8.4, CSD as541be (2020)
Xtriage (Phenix) : 1.13
EDS : 2.36
buster-report : 1.1.7 (2018)
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac : 5.8.0158
CCP4 : 7.0.044 (Gargrove)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.36

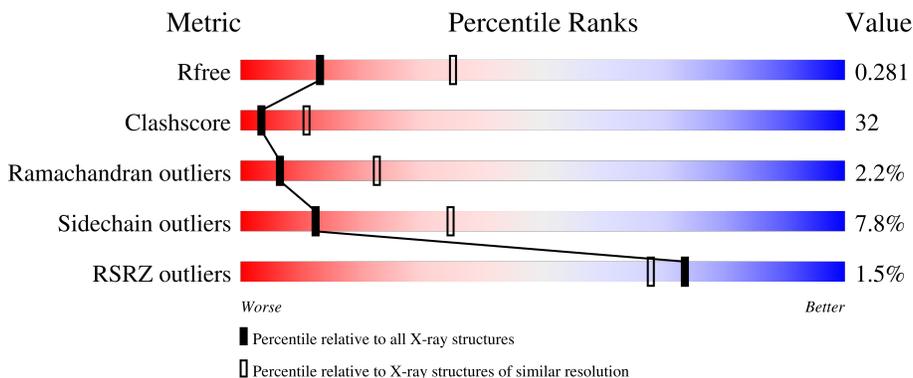
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.80 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	3140 (2.80-2.80)
Clashscore	141614	3569 (2.80-2.80)
Ramachandran outliers	138981	3498 (2.80-2.80)
Sidechain outliers	138945	3500 (2.80-2.80)
RSRZ outliers	127900	3078 (2.80-2.80)

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 ≥ 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	519	
1	B	519	
1	C	519	
1	D	519	
1	E	519	

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Mol	Chain	Length	Quality of chain
1	F	519	 <p>%</p> <p>48% 40% 6% 6%</p>

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

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
3	NAP	A	601	X	-	-	-
3	NAP	B	601	X	-	-	-
3	NAP	C	601	X	-	-	-

2 Entry composition [i](#)

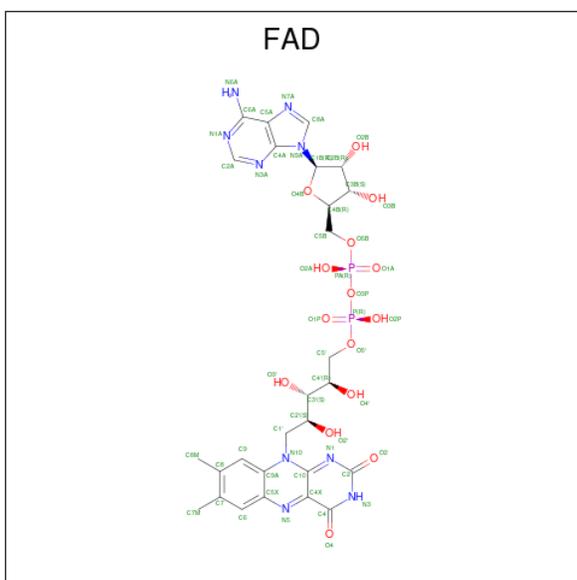
There are 5 unique types of molecules in this entry. The entry contains 23294 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 THIOREDOXIN REDUCTASE 1.

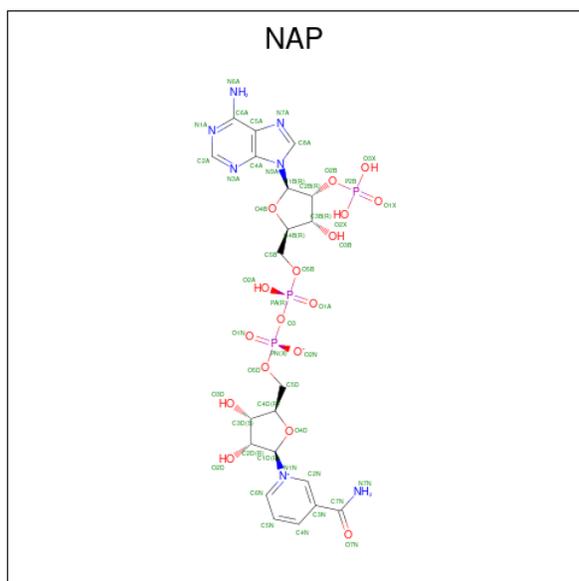
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	487	Total 3756	C 2387	N 642	O 708	S 19	0	0	1
1	B	487	Total 3760	C 2390	N 643	O 708	S 19	0	0	1
1	C	490	Total 3776	C 2397	N 645	O 713	S 21	0	0	0
1	D	491	Total 3785	C 2403	N 647	O 714	S 21	0	0	0
1	E	490	Total 3776	C 2397	N 645	O 713	S 21	0	0	0
1	F	486	Total 3751	C 2385	N 641	O 706	S 19	0	0	1

- Molecule 2 is FLAVIN-ADENINE DINUCLEOTIDE (three-letter code: FAD) (formula: $C_{27}H_{33}N_9O_{15}P_2$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	
2	A	1	Total	C	N	O	P	0	0
			53	27	9	15	2		
2	B	1	Total	C	N	O	P	0	0
			53	27	9	15	2		
2	C	1	Total	C	N	O	P	0	0
			53	27	9	15	2		
2	D	1	Total	C	N	O	P	0	0
			53	27	9	15	2		
2	E	1	Total	C	N	O	P	0	0
			53	27	9	15	2		
2	F	1	Total	C	N	O	P	0	0
			53	27	9	15	2		

- Molecule 3 is NADP NICOTINAMIDE-ADENINE-DINUCLEOTIDE PHOSPHATE (three-letter code: NAP) (formula: C₂₁H₂₈N₇O₁₇P₃).



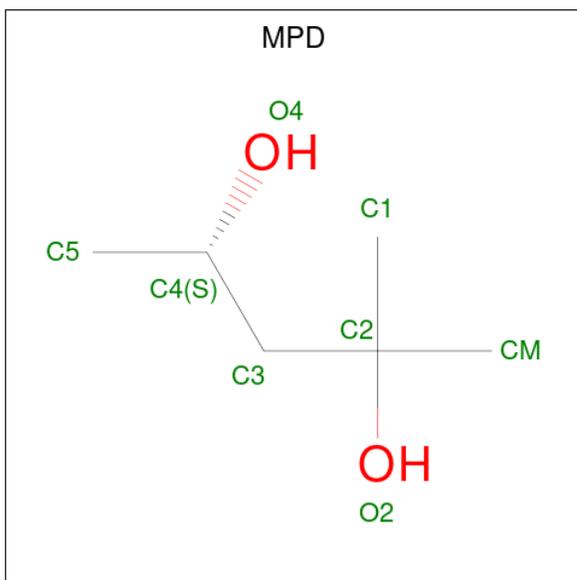
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	
3	A	1	Total	C	N	O	P	0	0
			48	21	7	17	3		
3	B	1	Total	C	N	O	P	0	0
			48	21	7	17	3		
3	C	1	Total	C	N	O	P	0	0
			48	21	7	17	3		
3	D	1	Total	C	N	O	P	0	0
			48	21	7	17	3		
3	E	1	Total	C	N	O	P	0	0
			48	21	7	17	3		

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

- Molecule 4 is (4S)-2-METHYL-2,4-PENTANEDIOL (three-letter code: MPD) (formula: C₆H₁₄O₂).



Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
4	A	1	8	2	0	0
4	B	1	8	2	0	0
4	B	1	8	2	0	0
4	D	1	8	2	0	0
4	F	1	8	2	0	0

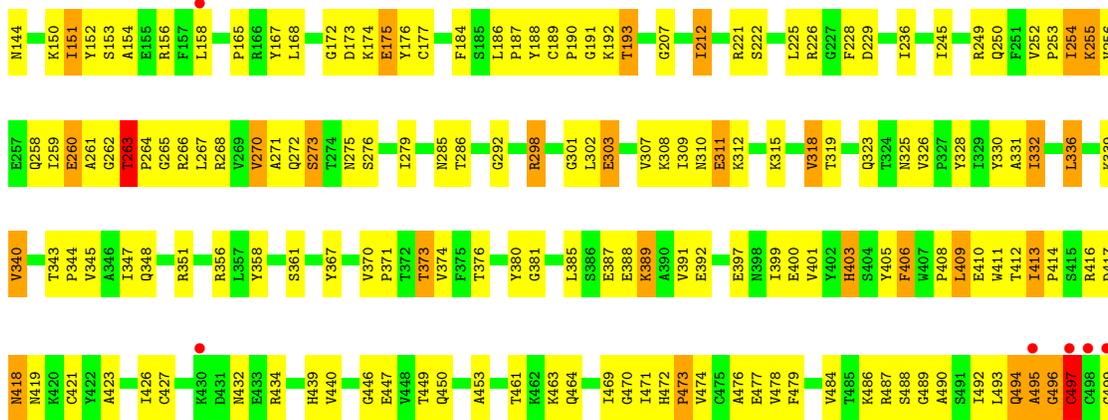
- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
5	A	9	9	9	0	0
5	B	9	9	9	0	0
5	C	7	7	7	0	0

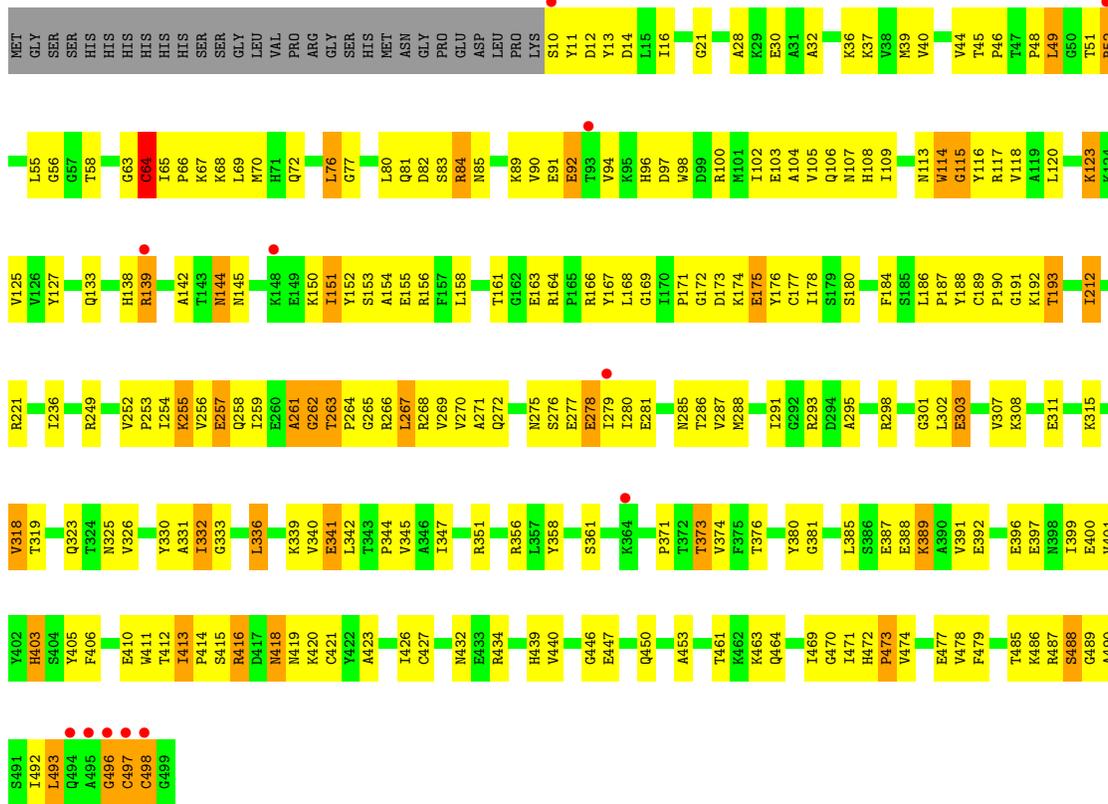
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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	D	8	Total O 8 8	0	0
5	E	4	Total O 4 4	0	0
5	F	7	Total O 7 7	0	0

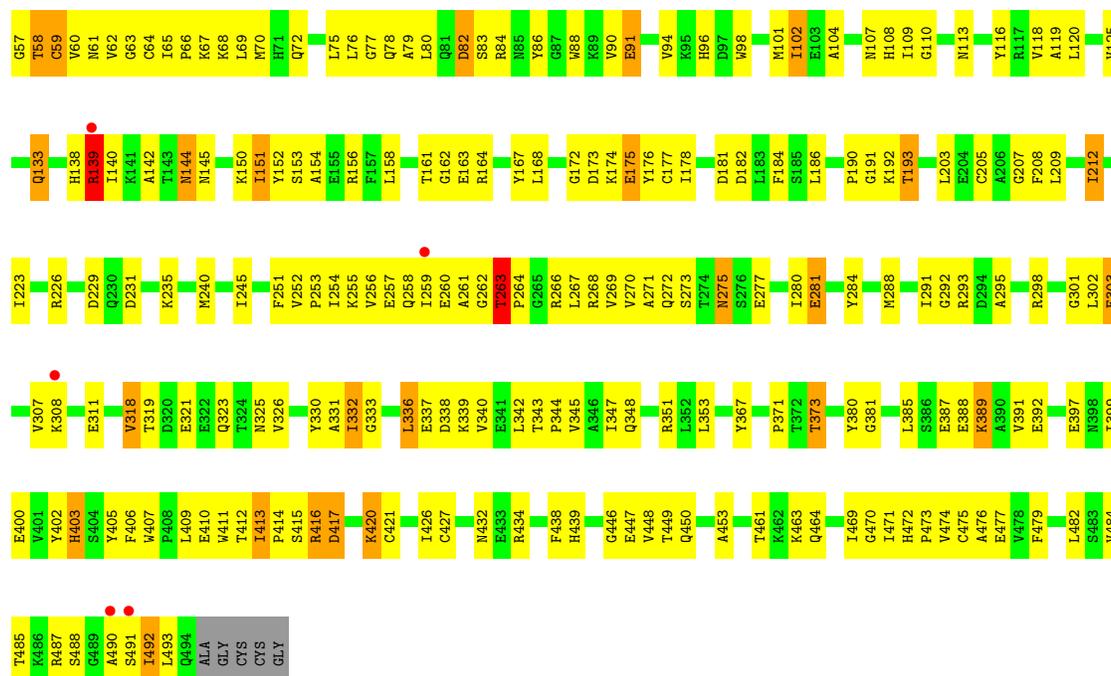


• Molecule 1: THIOREDOXIN REDUCTASE 1



• Molecule 1: THIOREDOXIN REDUCTASE 1





4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	144.63Å 90.64Å 166.60Å 90.00° 112.46° 90.00°	Depositor
Resolution (Å)	15.00 – 2.80 19.99 – 2.80	Depositor EDS
% Data completeness (in resolution range)	92.8 (15.00-2.80) 99.5 (19.99-2.80)	Depositor EDS
R_{merge}	0.10	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.02 (at 2.79Å)	Xtrriage
Refinement program	CNS 1.1	Depositor
R, R_{free}	0.249 , 0.287 0.246 , 0.281	Depositor DCC
R_{free} test set	4885 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å ²)	57.1	Xtrriage
Anisotropy	0.259	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 65.9	EDS
L-test for twinning ²	$\langle L \rangle = 0.46$, $\langle L^2 \rangle = 0.28$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
F_o, F_c correlation	0.91	EDS
Total number of atoms	23294	wwPDB-VP
Average B, all atoms (Å ²)	55.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.84% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

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

5 Model quality [i](#)

5.1 Standard geometry [i](#)

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

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
1	A	0.44	0/3830	0.66	1/5187 (0.0%)
1	B	0.44	0/3834	0.66	1/5191 (0.0%)
1	C	0.43	0/3850	0.66	1/5211 (0.0%)
1	D	0.44	0/3859	0.79	4/5222 (0.1%)
1	E	0.41	0/3850	0.64	1/5211 (0.0%)
1	F	0.41	0/3825	0.65	2/5179 (0.0%)
All	All	0.43	0/23048	0.68	10/31201 (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	B	0	1

There are no bond length outliers.

The worst 5 of 10 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	139	ARG	NE-CZ-NH2	21.20	130.90	120.30
1	D	139	ARG	NE-CZ-NH1	-20.89	109.86	120.30
1	D	139	ARG	CD-NE-CZ	10.58	138.41	123.60
1	C	263	THR	C-N-CD	6.38	141.81	128.40
1	D	263	THR	C-N-CD	6.08	141.17	128.40

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	B	13	TYR	Sidechain

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	3756	0	3764	247	0
1	B	3760	0	3772	261	0
1	C	3776	0	3780	273	0
1	D	3785	0	3793	254	0
1	E	3776	0	3778	325	0
1	F	3751	0	3764	279	0
2	A	53	0	31	4	0
2	B	53	0	31	1	0
2	C	53	0	31	0	0
2	D	53	0	31	5	0
2	E	53	0	31	4	0
2	F	53	0	31	10	0
3	A	48	0	24	1	0
3	B	48	0	24	6	0
3	C	48	0	24	1	0
3	D	48	0	25	4	0
3	E	48	0	25	1	0
3	F	48	0	25	1	0
4	A	8	0	14	2	0
4	B	16	0	28	5	0
4	D	8	0	14	3	0
4	F	8	0	14	5	0
5	A	9	0	0	2	0
5	B	9	0	0	3	0
5	C	7	0	0	1	0
5	D	8	0	0	3	0
5	E	4	0	0	2	0
5	F	7	0	0	2	0
All	All	23294	0	23054	1495	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 32.

The worst 5 of 1495 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:F:46:PRO:HG3	1:F:52:ARG:HE	1.15	1.10
1:E:80:LEU:HD23	1:F:80:LEU:HD23	1.34	1.10
1:B:199:SER:HB3	3:B:601:NAP:H52A	1.37	1.05
1:D:418:ASN:HD21	1:D:495:ALA:HB2	1.19	1.05
1:A:199:SER:HB3	3:A:601:NAP:H52A	1.39	1.04

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	485/519 (93%)	426 (88%)	51 (10%)	8 (2%)	9	31
1	B	485/519 (93%)	419 (86%)	60 (12%)	6 (1%)	13	39
1	C	488/519 (94%)	425 (87%)	51 (10%)	12 (2%)	5	19
1	D	489/519 (94%)	424 (87%)	51 (10%)	14 (3%)	4	15
1	E	488/519 (94%)	421 (86%)	54 (11%)	13 (3%)	5	17
1	F	484/519 (93%)	417 (86%)	55 (11%)	12 (2%)	5	19
All	All	2919/3114 (94%)	2532 (87%)	322 (11%)	65 (2%)	6	22

5 of 65 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	489	GLY
1	B	263	THR
1	C	263	THR
1	C	276	SER
1	C	278	GLU

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	399/426 (94%)	370 (93%)	29 (7%)	14	38
1	B	400/426 (94%)	372 (93%)	28 (7%)	15	40
1	C	401/426 (94%)	362 (90%)	39 (10%)	8	24
1	D	402/426 (94%)	371 (92%)	31 (8%)	13	35
1	E	401/426 (94%)	370 (92%)	31 (8%)	13	35
1	F	399/426 (94%)	370 (93%)	29 (7%)	14	38
All	All	2402/2556 (94%)	2215 (92%)	187 (8%)	12	35

5 of 187 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	D	303	GLU
1	E	267	LEU
1	D	340	VAL
1	E	64	CYS
1	E	389	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 91 such sidechains are listed below:

Mol	Chain	Res	Type
1	D	348	GLN
1	E	325	ASN
1	D	432	ASN
1	E	129	ASN
1	E	439	HIS

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no monosaccharides in this entry.

5.6 Ligand geometry [i](#)

17 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	FAD	B	600	-	53,58,58	1.60	9 (16%)	68,89,89	1.29	8 (11%)
3	NAP	D	601	-	45,52,52	1.91	9 (20%)	56,80,80	1.25	4 (7%)
4	MPD	F	700	-	7,7,7	0.38	0	9,10,10	0.42	0
2	FAD	D	600	-	53,58,58	1.96	10 (18%)	68,89,89	1.25	7 (10%)
2	FAD	F	600	-	53,58,58	1.59	9 (16%)	68,89,89	1.24	5 (7%)
4	MPD	D	700	-	7,7,7	0.32	0	9,10,10	0.24	0
3	NAP	C	601	-	45,52,52	1.71	8 (17%)	56,80,80	2.93	10 (17%)
2	FAD	C	600	-	53,58,58	1.68	8 (15%)	68,89,89	1.19	6 (8%)
3	NAP	F	601	-	45,52,52	1.50	6 (13%)	56,80,80	1.28	4 (7%)
3	NAP	E	601	-	45,52,52	1.56	7 (15%)	56,80,80	1.26	8 (14%)
4	MPD	B	701	-	7,7,7	0.35	0	9,10,10	0.32	0
3	NAP	B	601	-	45,52,52	1.60	8 (17%)	56,80,80	2.72	10 (17%)
4	MPD	A	701	-	7,7,7	0.31	0	9,10,10	0.41	0
4	MPD	B	700	-	7,7,7	0.32	0	9,10,10	0.42	0
2	FAD	A	600	-	53,58,58	1.69	7 (13%)	68,89,89	1.24	6 (8%)
2	FAD	E	600	-	53,58,58	1.64	9 (16%)	68,89,89	1.18	5 (7%)
3	NAP	A	601	-	45,52,52	1.74	8 (17%)	56,80,80	2.98	10 (17%)

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	FAD	B	600	-	-	6/30/50/50	0/6/6/6
3	NAP	D	601	-	-	11/31/67/67	0/5/5/5
4	MPD	F	700	-	-	0/5/5/5	-
2	FAD	D	600	-	-	6/30/50/50	0/6/6/6
2	FAD	F	600	-	-	6/30/50/50	0/6/6/6
4	MPD	D	700	-	-	0/5/5/5	-
3	NAP	C	601	-	1/1/12/12	12/31/67/67	0/5/5/5
2	FAD	C	600	-	-	6/30/50/50	0/6/6/6
3	NAP	F	601	-	-	14/31/67/67	0/5/5/5
3	NAP	E	601	-	-	9/31/67/67	0/5/5/5
4	MPD	B	701	-	-	0/5/5/5	-
3	NAP	B	601	-	1/1/12/12	6/31/67/67	0/5/5/5
4	MPD	A	701	-	-	0/5/5/5	-
4	MPD	B	700	-	-	0/5/5/5	-
2	FAD	A	600	-	-	6/30/50/50	0/6/6/6
2	FAD	E	600	-	-	6/30/50/50	0/6/6/6
3	NAP	A	601	-	1/1/12/12	5/31/67/67	0/5/5/5

The worst 5 of 98 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	600	FAD	O4B-C1B	6.86	1.50	1.41
2	D	600	FAD	C4X-N5	6.65	1.43	1.30
2	C	600	FAD	C4X-N5	6.10	1.42	1.30
3	A	601	NAP	O4B-C4B	5.97	1.58	1.45
3	D	601	NAP	O4B-C1B	5.94	1.49	1.41

The worst 5 of 83 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	601	NAP	C5B-C4B-C3B	15.14	171.93	115.18
3	B	601	NAP	C5B-C4B-C3B	14.49	169.49	115.18
3	C	601	NAP	C5B-C4B-C3B	14.35	168.96	115.18
3	A	601	NAP	O4B-C4B-C5B	-8.62	81.03	109.37
3	B	601	NAP	O4B-C4B-C5B	-7.88	83.43	109.37

All (3) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
3	A	601	NAP	C4B
3	B	601	NAP	C4B
3	C	601	NAP	C4B

5 of 93 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	600	FAD	C5B-O5B-PA-O2A
2	B	600	FAD	C5B-O5B-PA-O2A
2	B	600	FAD	O4B-C4B-C5B-O5B
2	C	600	FAD	C5B-O5B-PA-O2A
2	C	600	FAD	C4B-C5B-O5B-PA

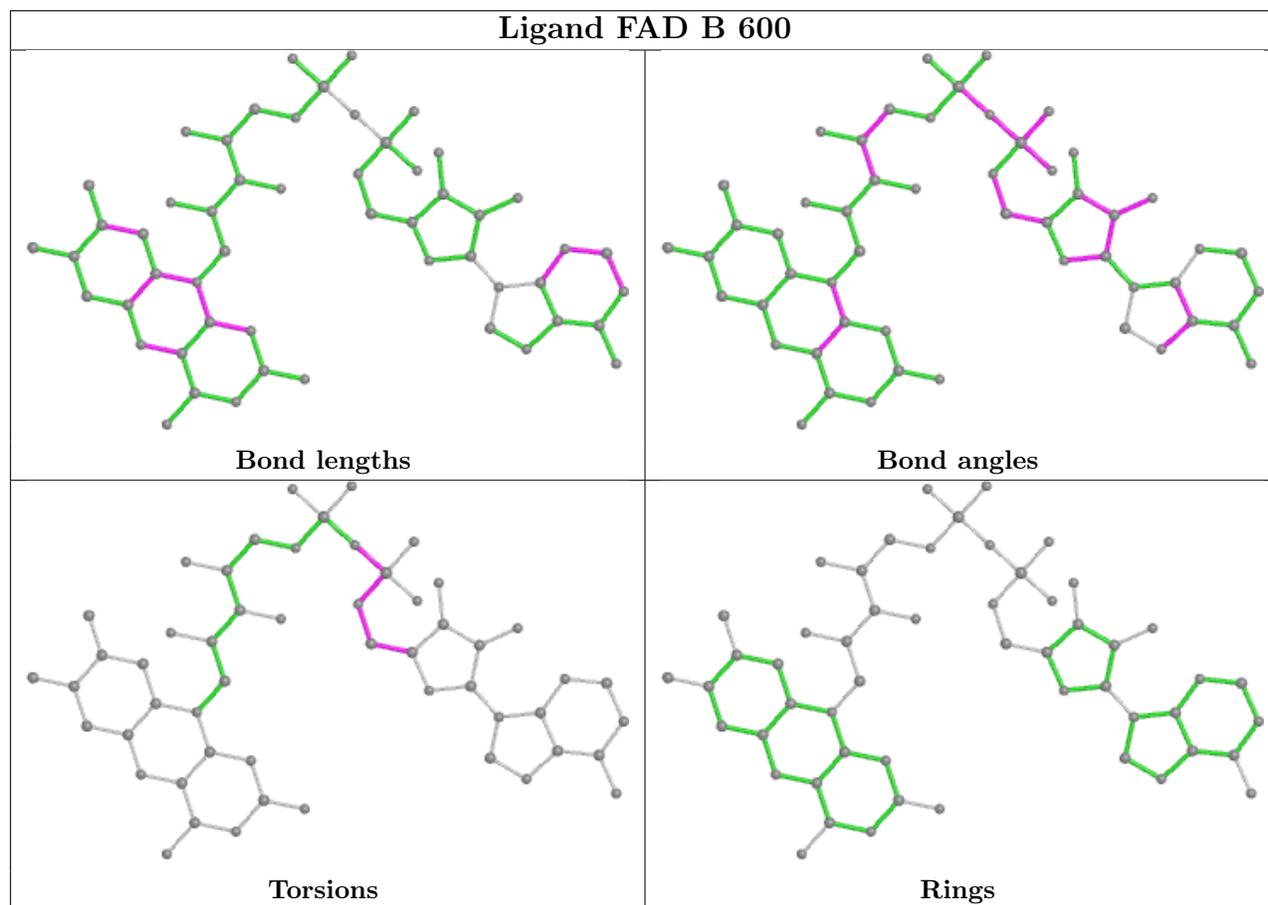
There are no ring outliers.

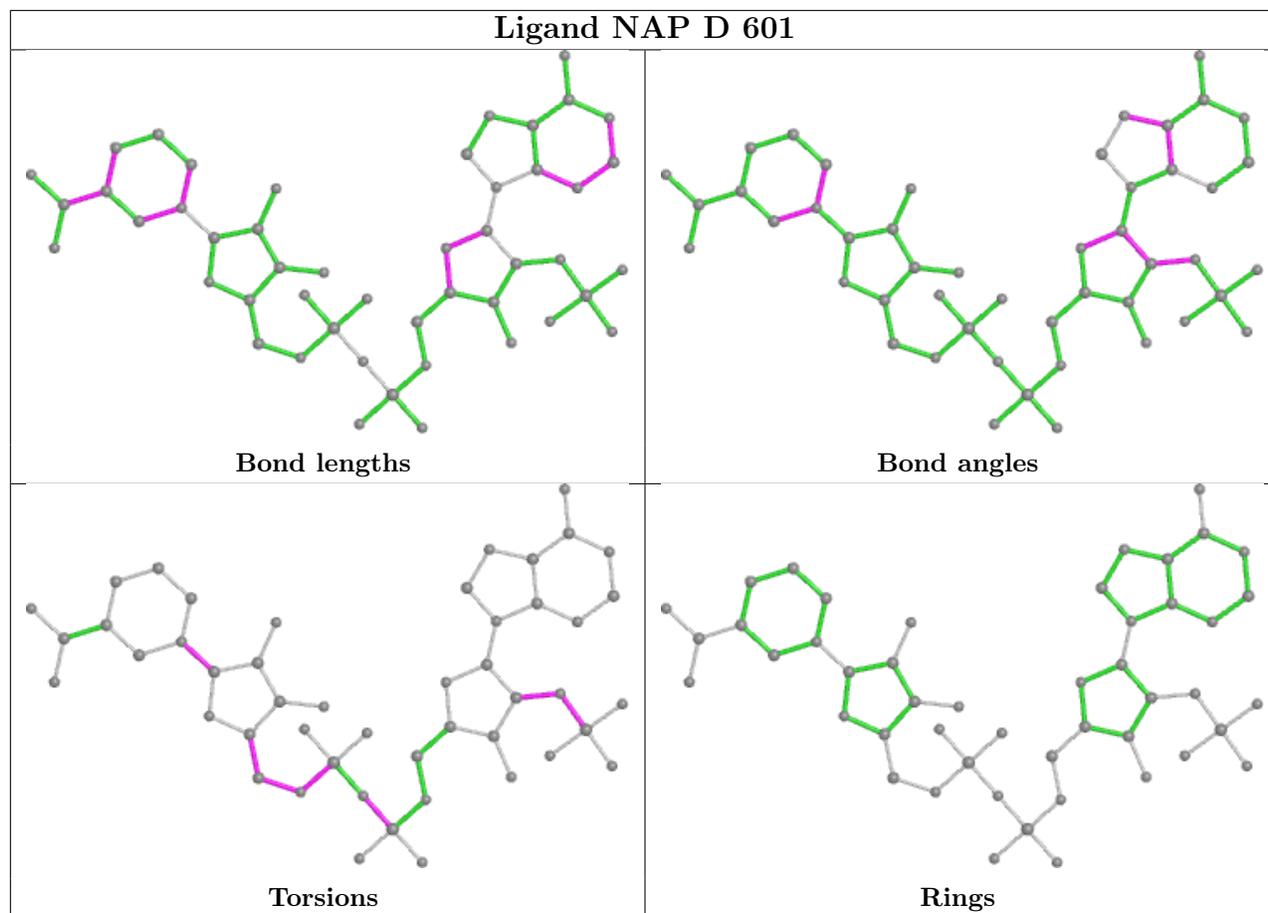
16 monomers are involved in 53 short contacts:

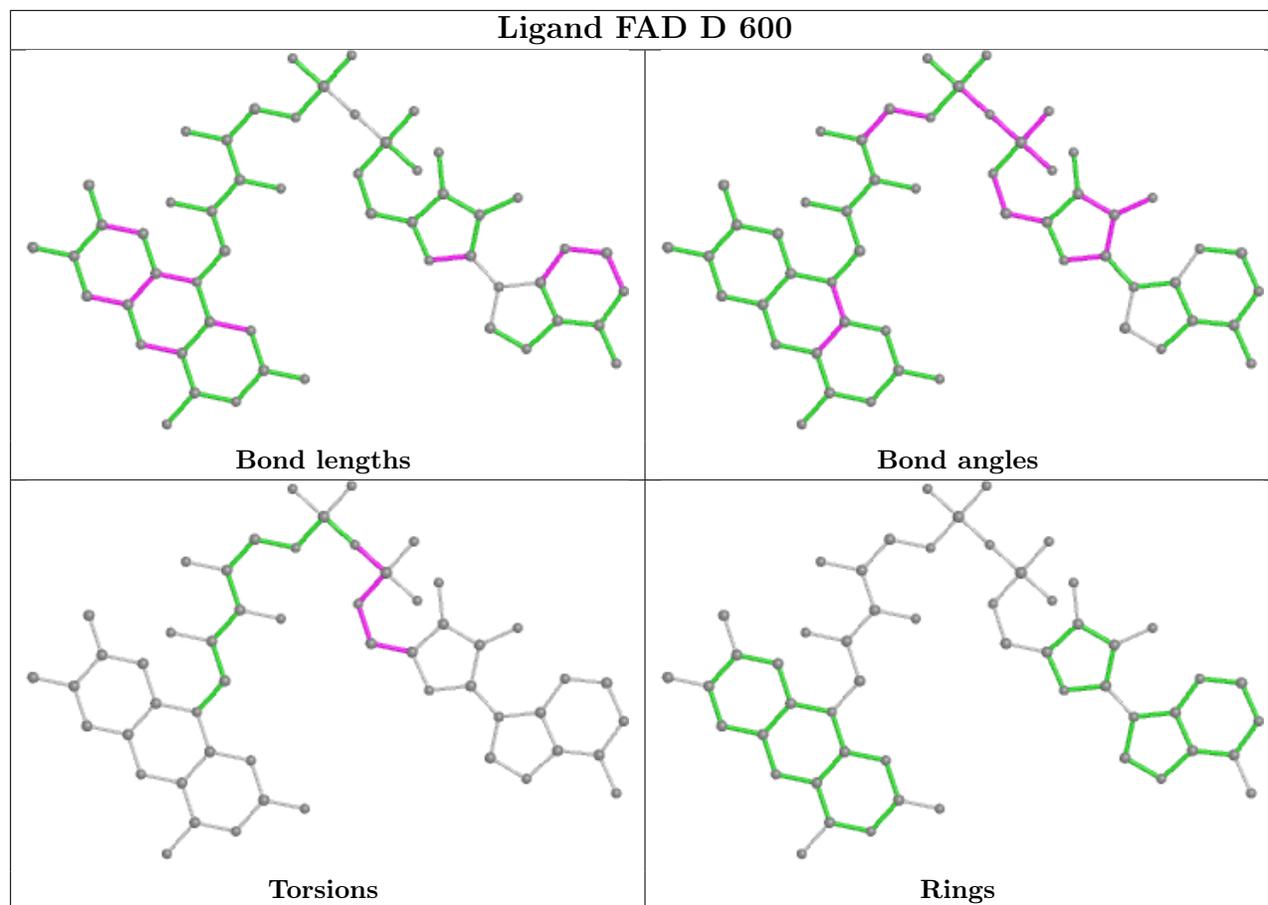
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	600	FAD	1	0
3	D	601	NAP	4	0
4	F	700	MPD	5	0
2	D	600	FAD	5	0
2	F	600	FAD	10	0
4	D	700	MPD	3	0
3	C	601	NAP	1	0
3	F	601	NAP	1	0
3	E	601	NAP	1	0
4	B	701	MPD	3	0
3	B	601	NAP	6	0
4	A	701	MPD	2	0
4	B	700	MPD	2	0
2	A	600	FAD	4	0
2	E	600	FAD	4	0
3	A	601	NAP	1	0

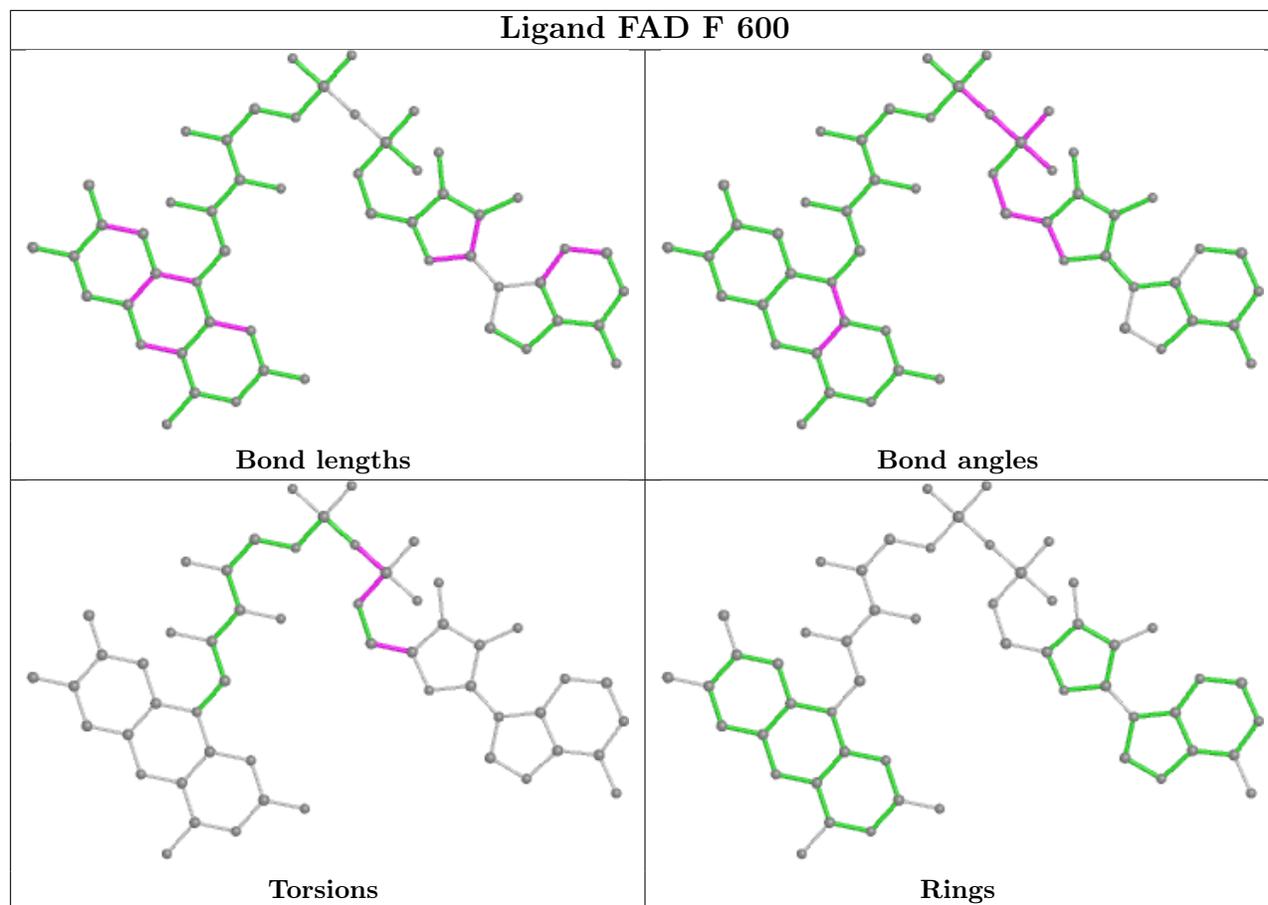
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

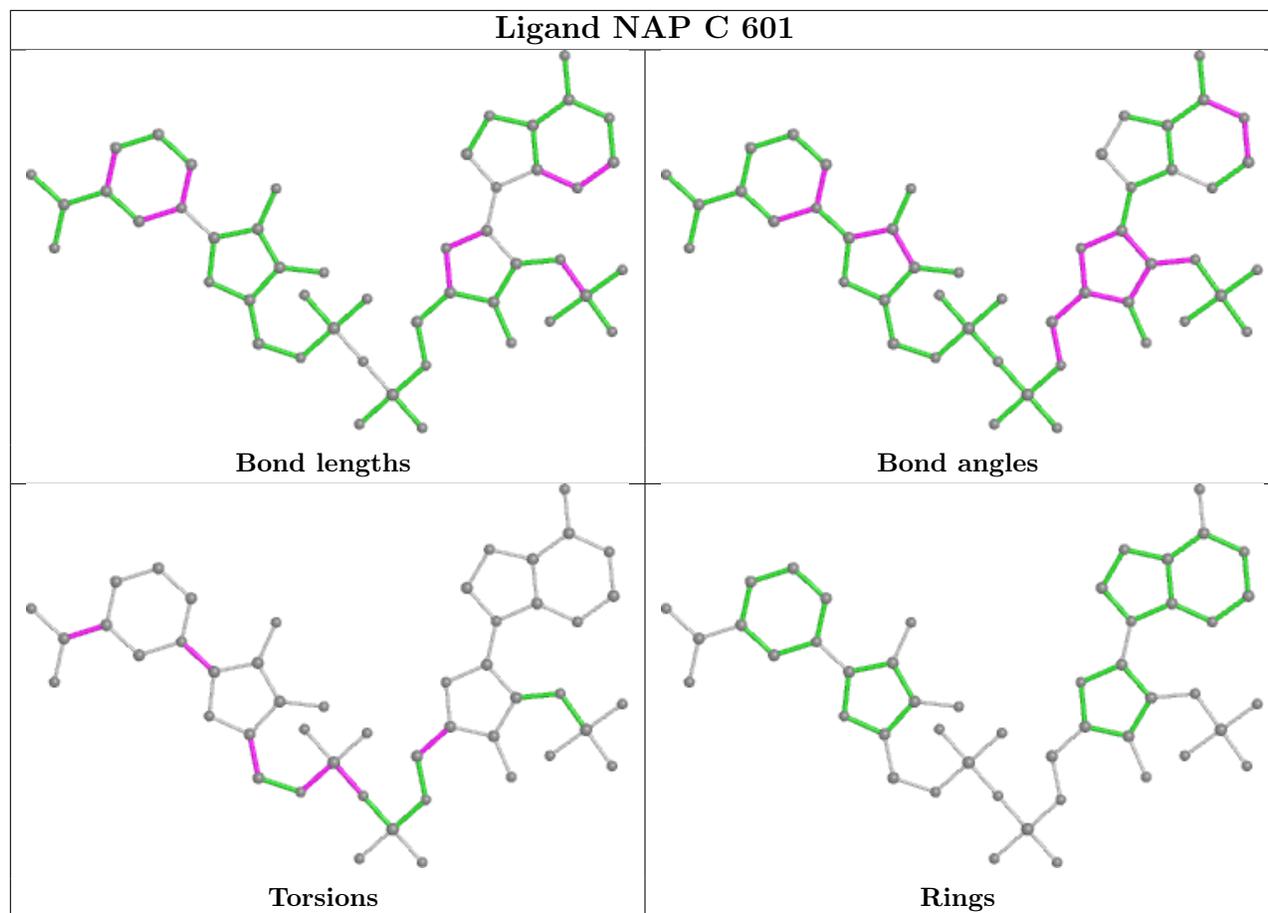
any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

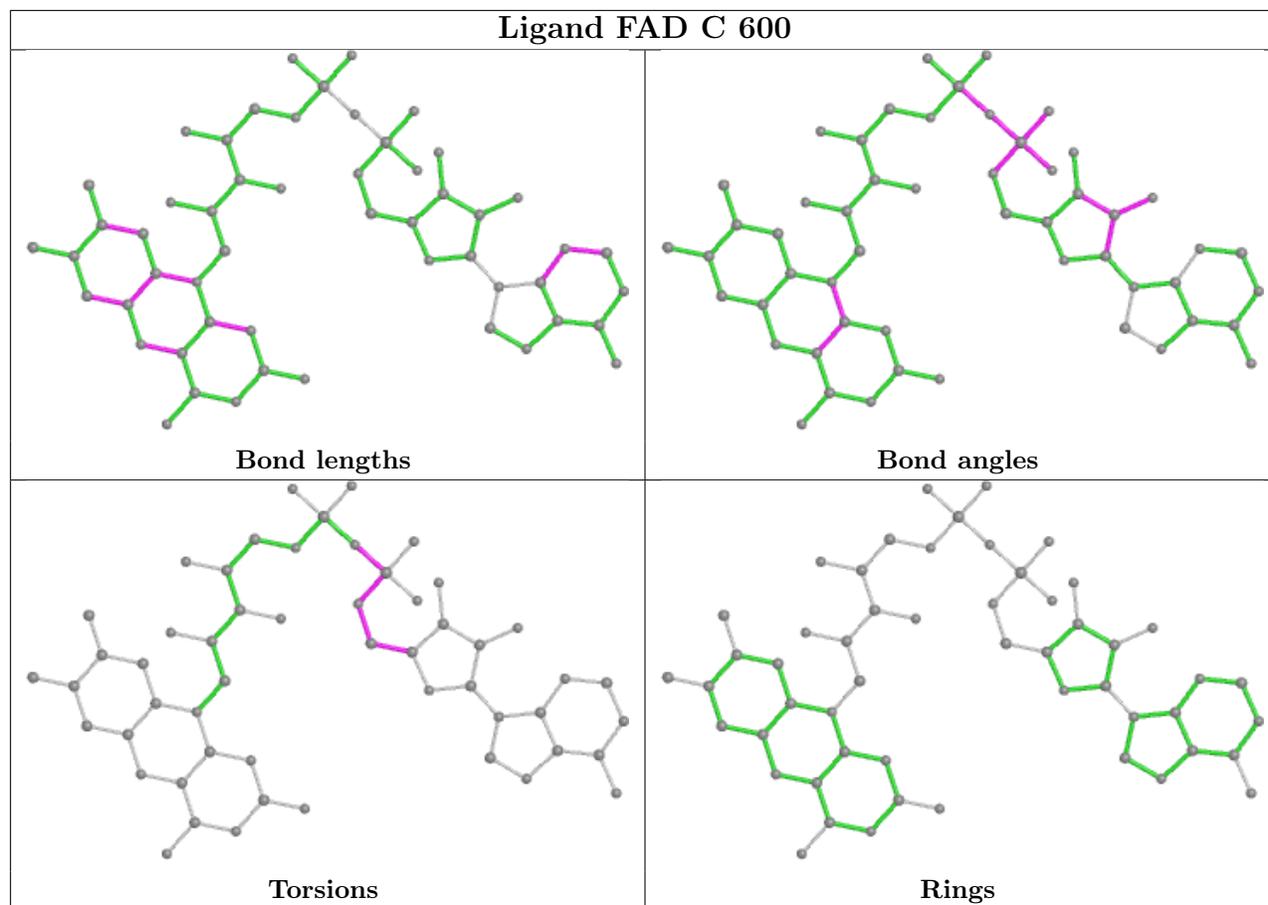


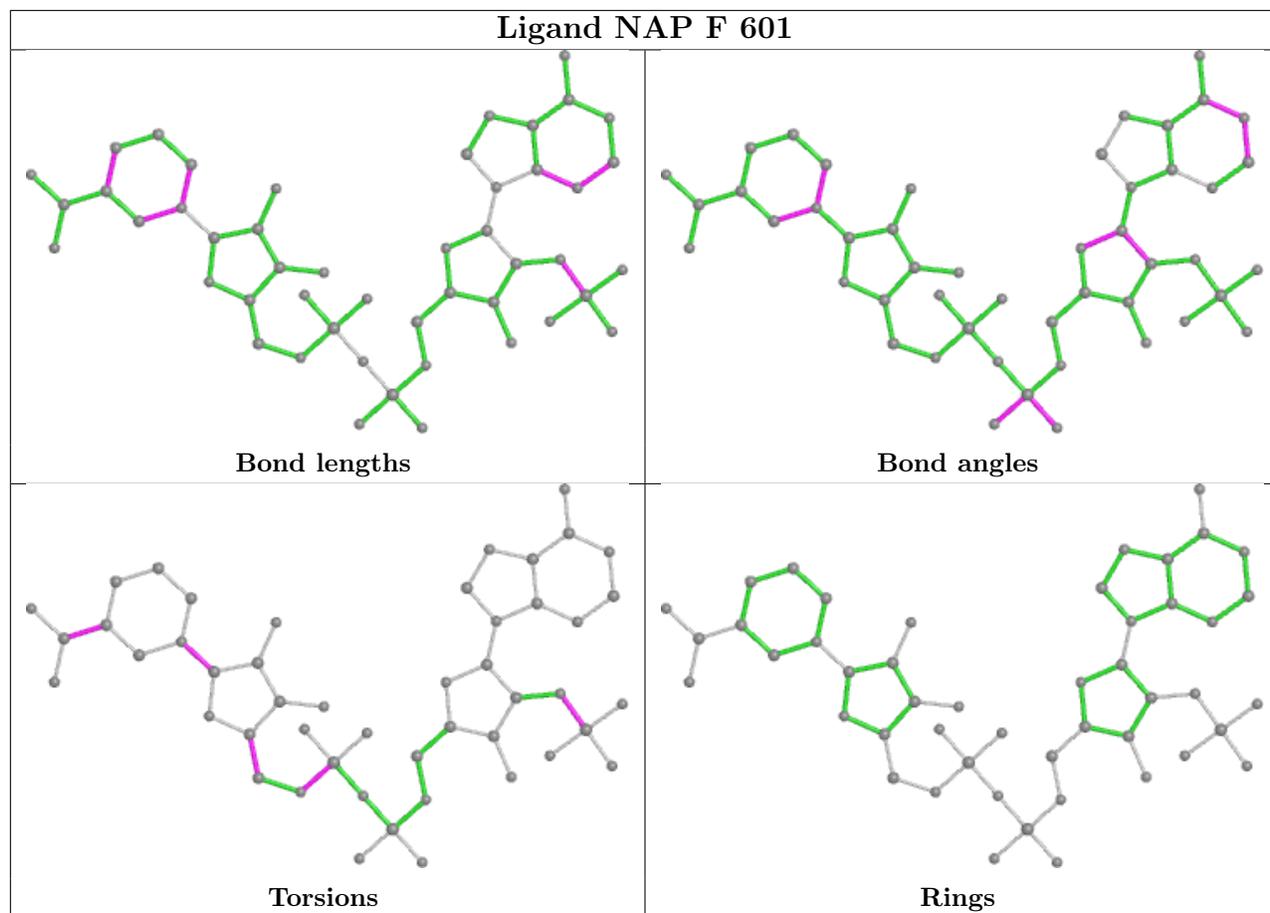


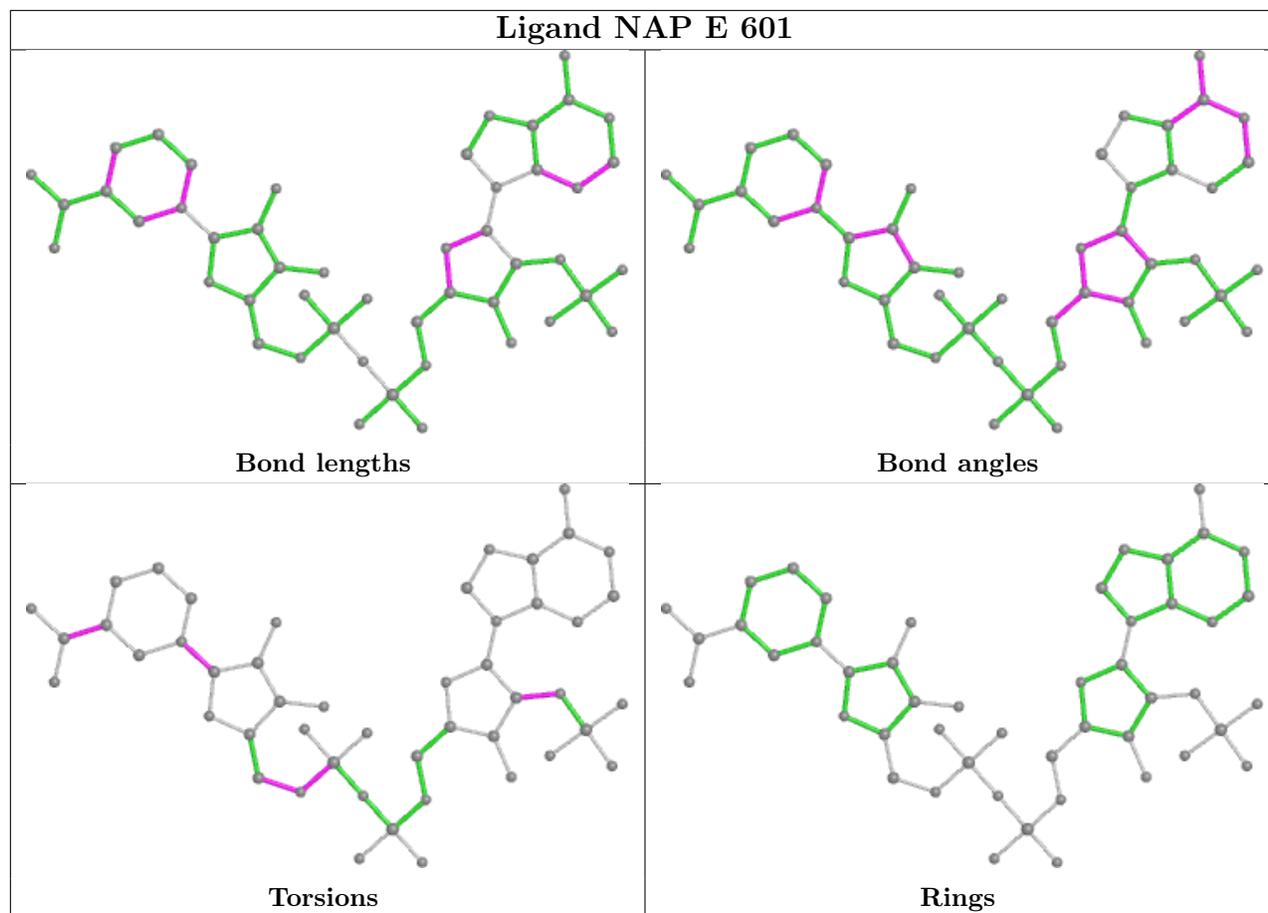


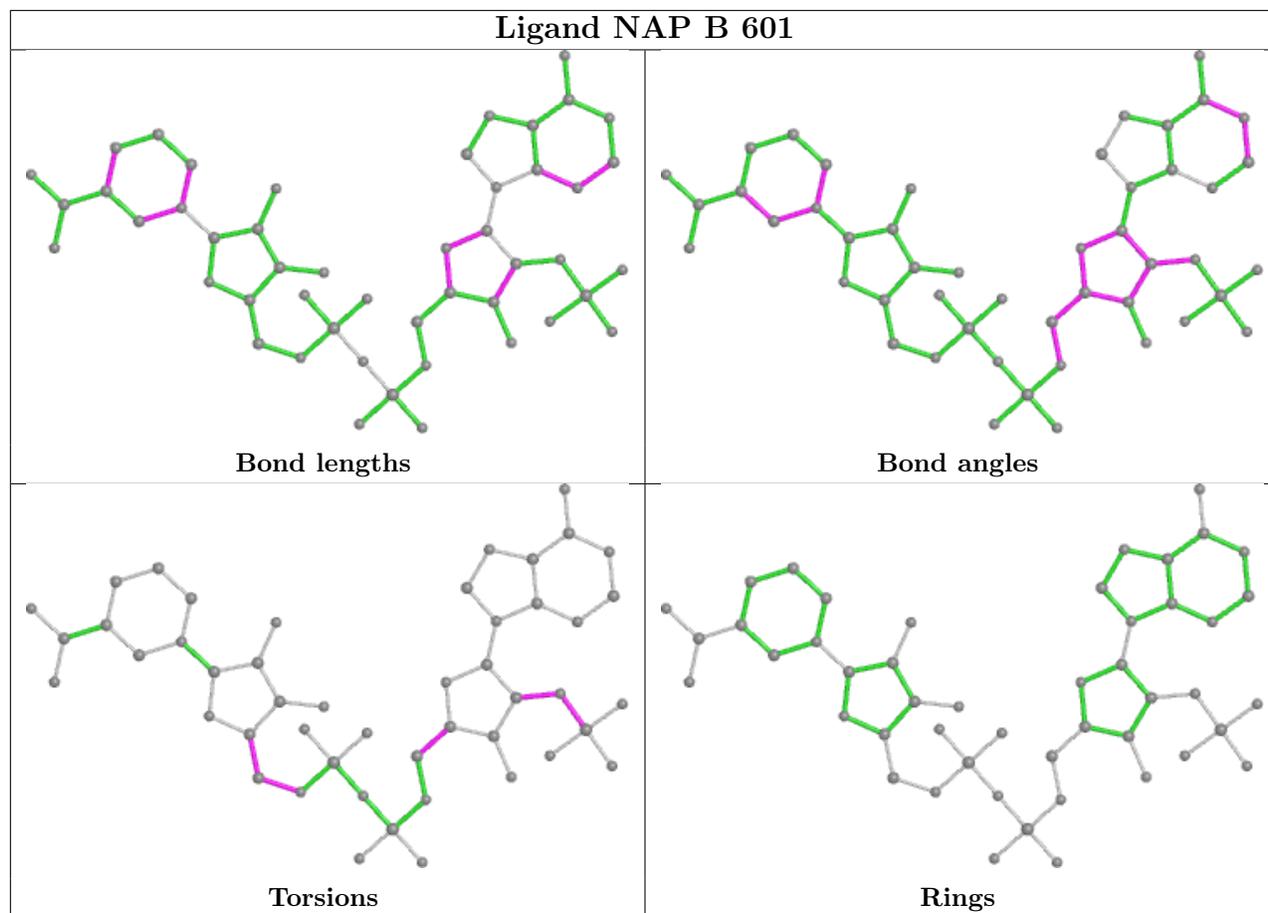


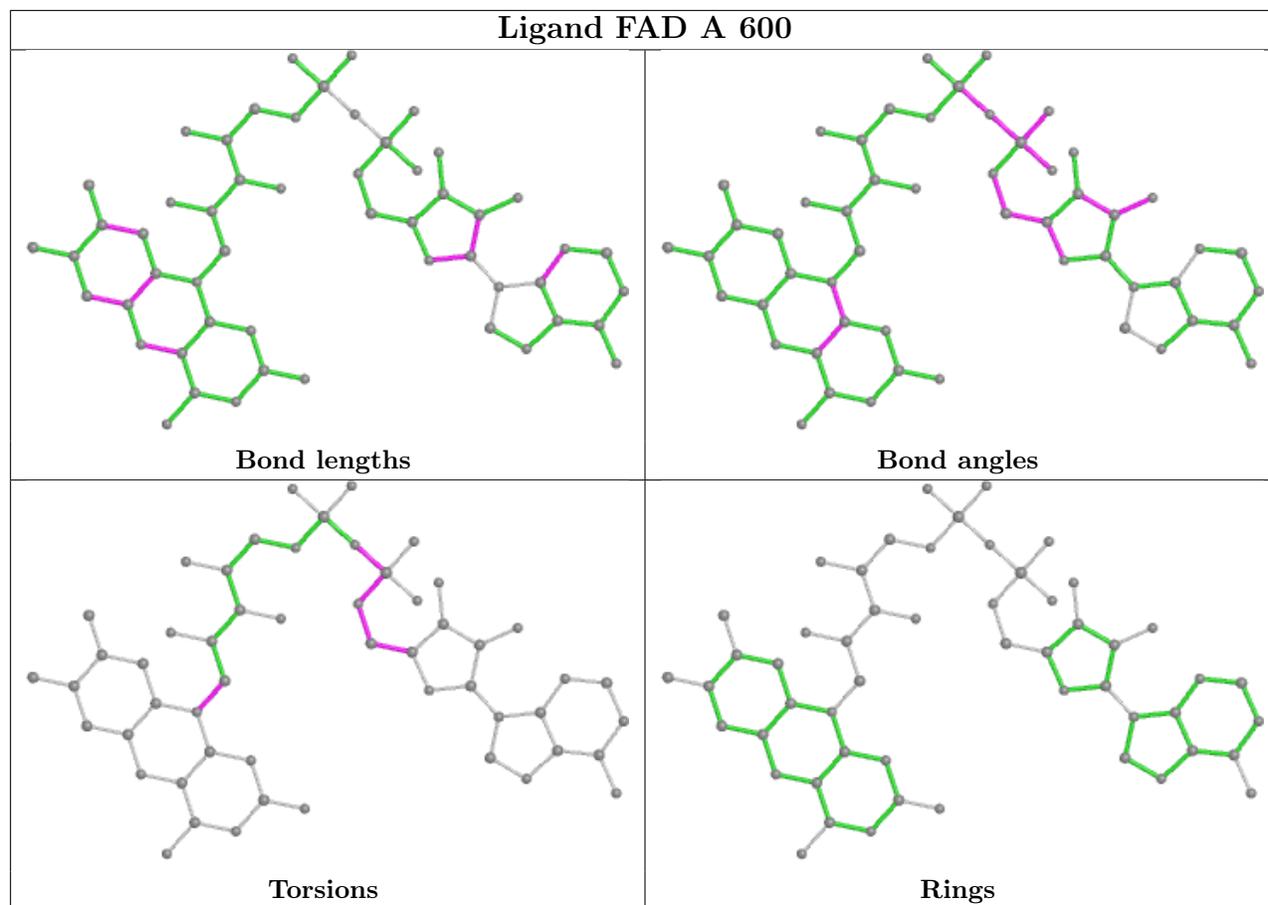


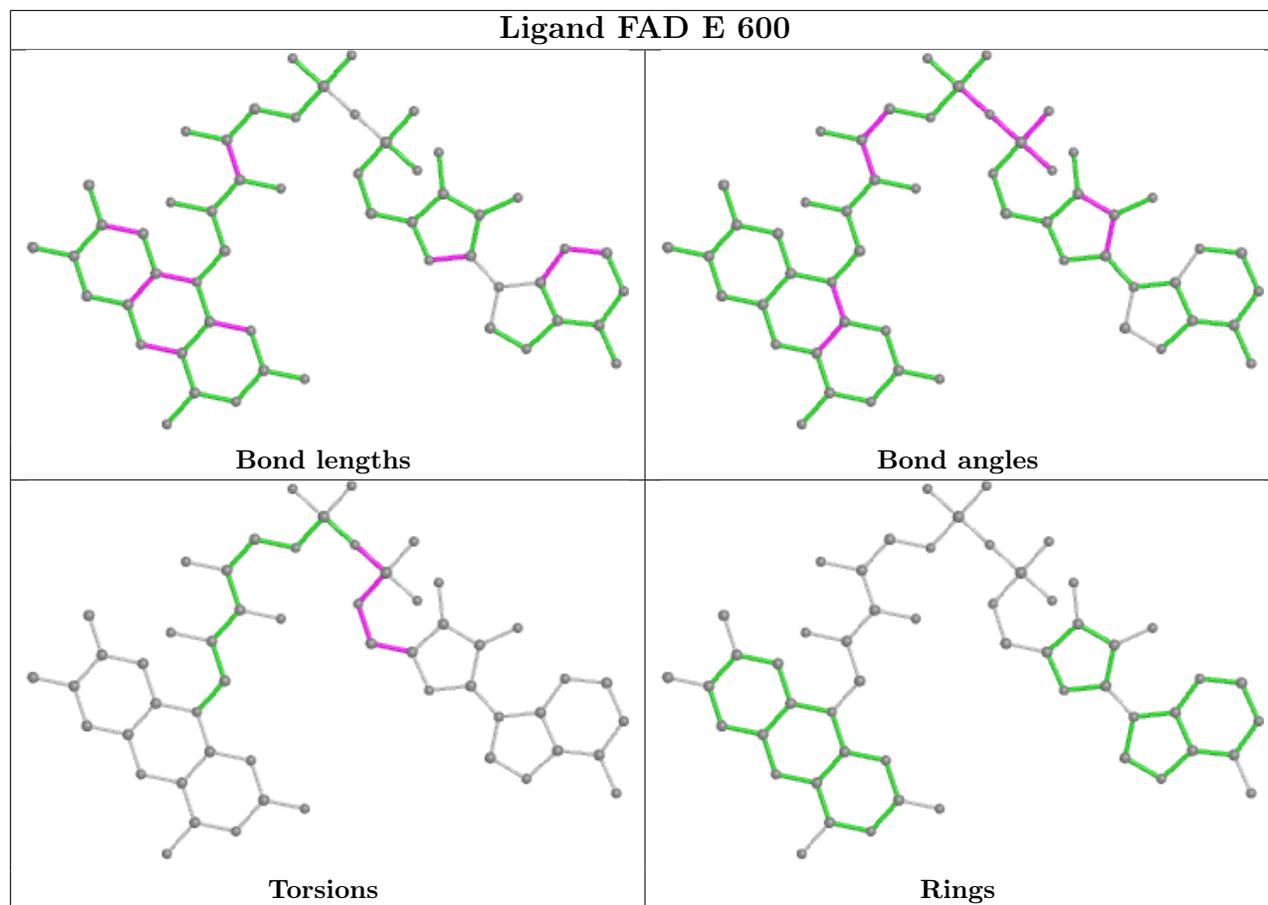


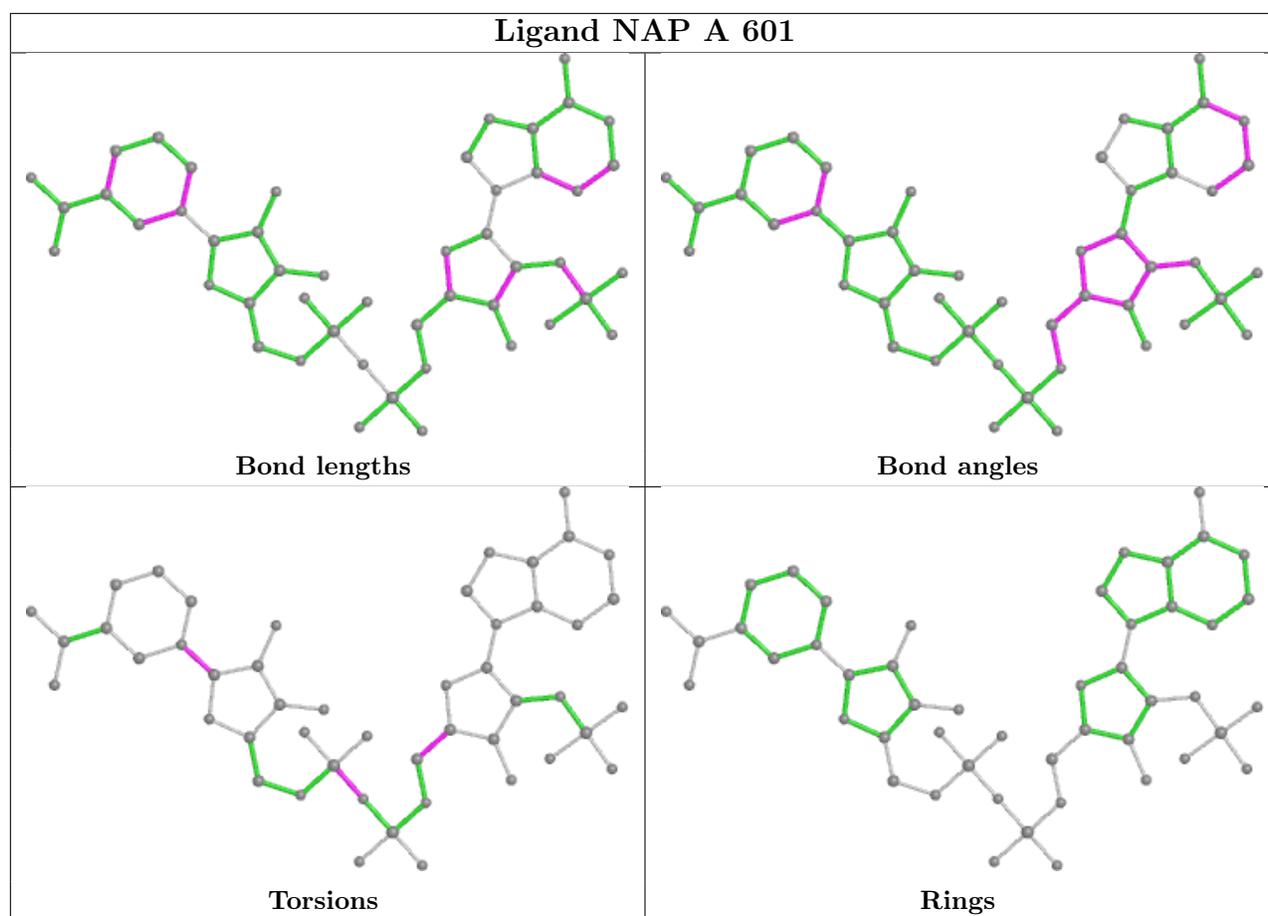












5.7 Other polymers [\(i\)](#)

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 [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, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q < 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	487/519 (93%)	-0.19	2 (0%) 92 91	25, 51, 70, 83	0
1	B	487/519 (93%)	-0.22	4 (0%) 86 81	26, 51, 69, 93	0
1	C	490/519 (94%)	-0.10	10 (2%) 65 56	31, 55, 75, 102	0
1	D	491/519 (94%)	-0.15	8 (1%) 72 66	26, 52, 73, 107	0
1	E	490/519 (94%)	-0.01	12 (2%) 59 49	32, 59, 82, 105	0
1	F	486/519 (93%)	-0.09	7 (1%) 75 70	29, 57, 77, 91	0
All	All	2931/3114 (94%)	-0.13	43 (1%) 73 68	25, 54, 75, 107	0

The worst 5 of 43 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	499	GLY	4.6
1	B	495	ALA	4.1
1	E	496	GLY	3.9
1	E	498	CYS	3.9
1	C	498	CYS	3.8

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

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

6.3 Carbohydrates [i](#)

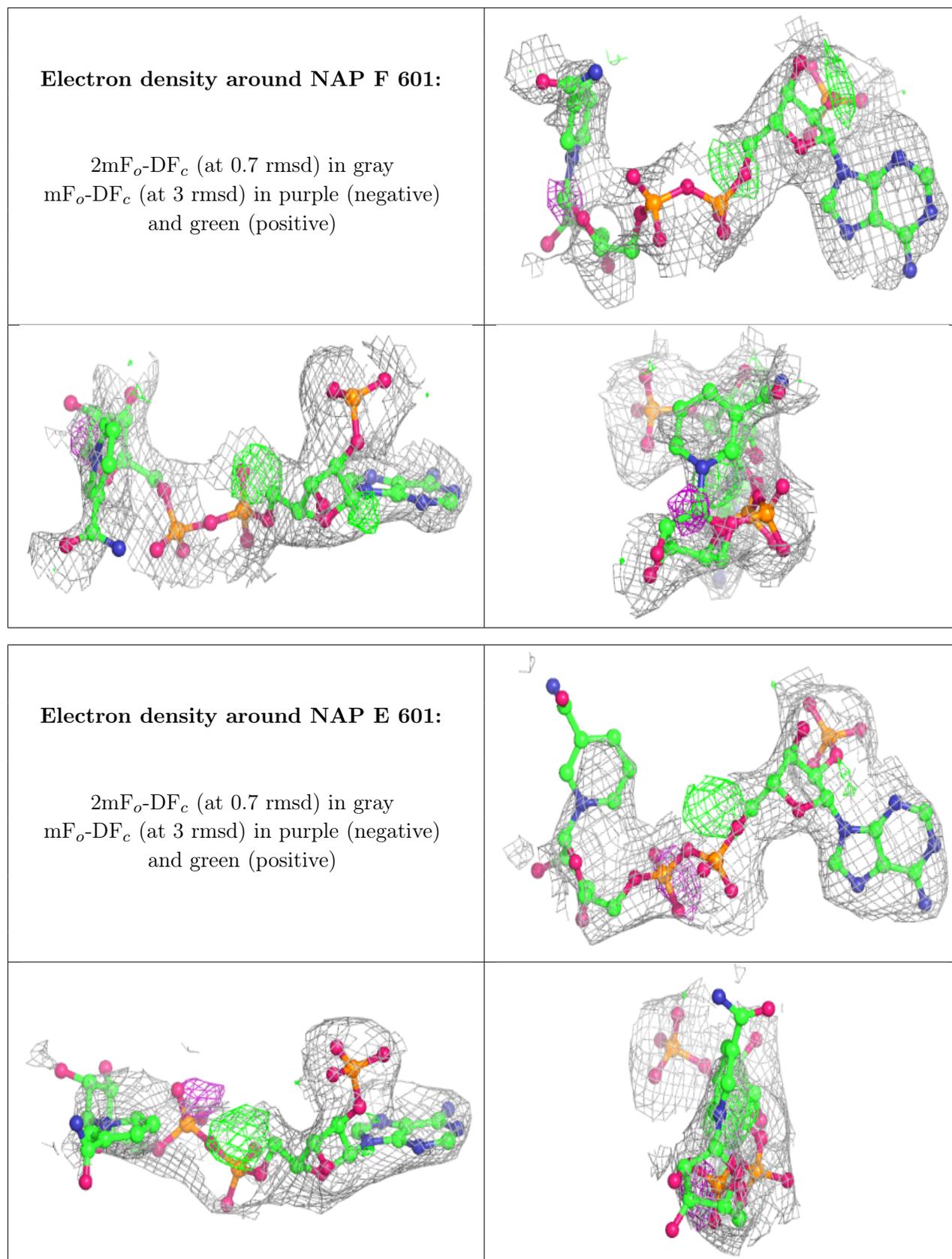
There are no monosaccharides in this entry.

6.4 Ligands

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

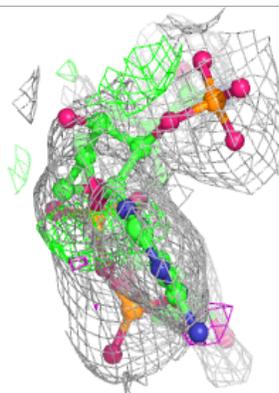
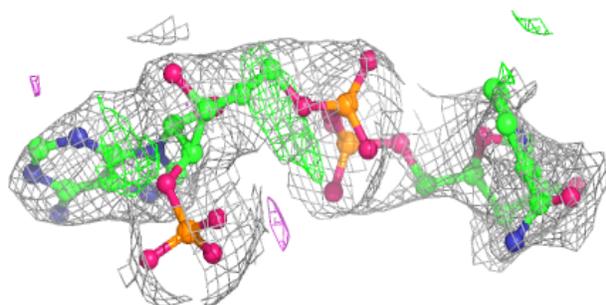
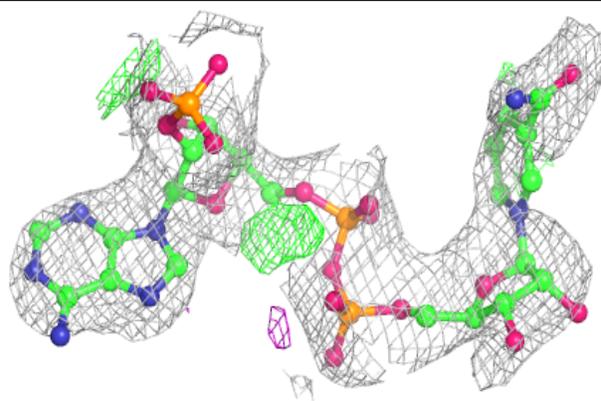
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
3	NAP	F	601	48/48	0.81	0.21	83,108,119,120	0
3	NAP	E	601	48/48	0.84	0.25	73,104,121,121	0
4	MPD	B	701	8/8	0.85	0.29	58,60,61,62	0
4	MPD	A	701	8/8	0.86	0.41	76,78,79,79	0
3	NAP	C	601	48/48	0.87	0.22	80,95,101,102	0
3	NAP	B	601	48/48	0.88	0.21	63,86,104,105	0
3	NAP	D	601	48/48	0.89	0.20	26,68,87,87	0
3	NAP	A	601	48/48	0.90	0.20	68,86,102,104	0
4	MPD	D	700	8/8	0.92	0.20	39,41,43,43	0
2	FAD	D	600	53/53	0.94	0.16	25,49,70,70	0
4	MPD	B	700	8/8	0.94	0.18	34,38,39,44	0
2	FAD	E	600	53/53	0.94	0.20	54,59,83,84	0
2	FAD	F	600	53/53	0.94	0.21	52,60,62,64	0
4	MPD	F	700	8/8	0.94	0.17	34,35,37,37	0
2	FAD	B	600	53/53	0.95	0.16	35,45,50,52	0
2	FAD	A	600	53/53	0.96	0.15	25,35,44,47	0
2	FAD	C	600	53/53	0.96	0.15	20,40,61,62	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.

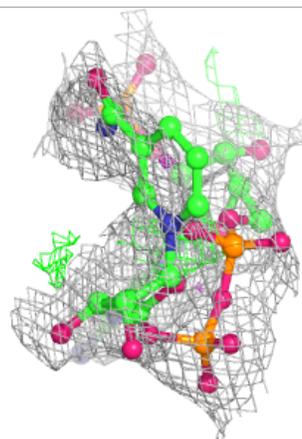
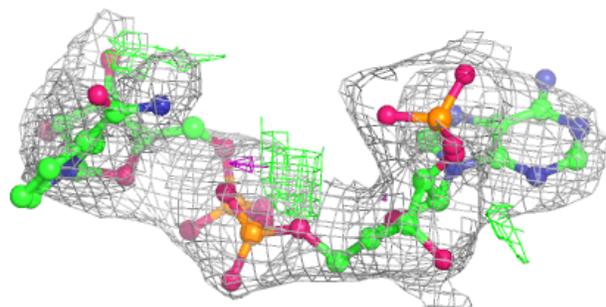
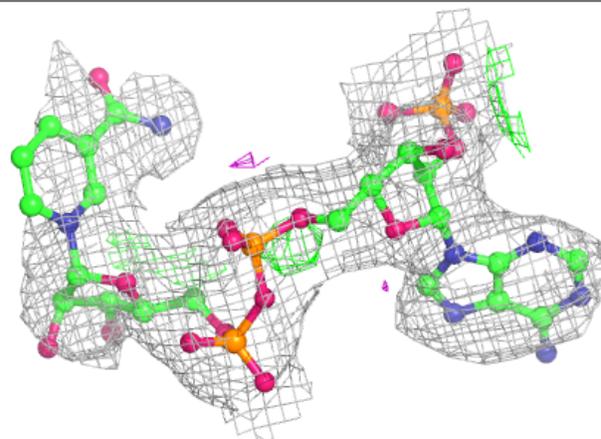


Electron density around NAP C 601:

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

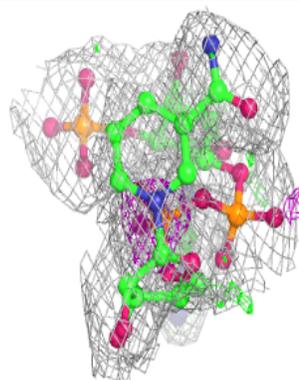
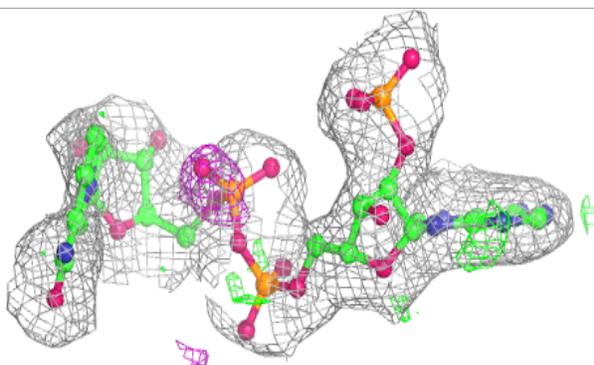
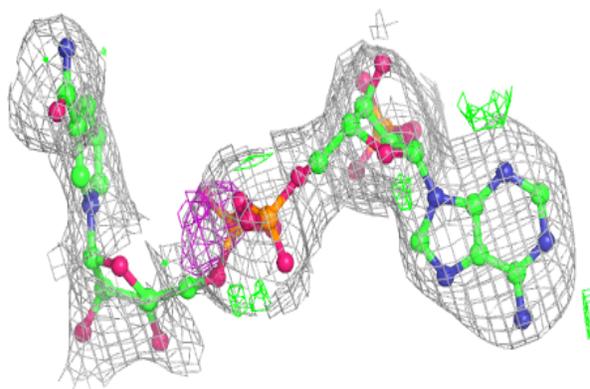
**Electron density around NAP B 601:**

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

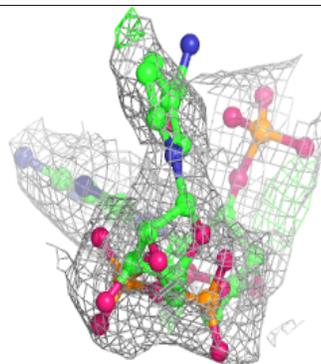
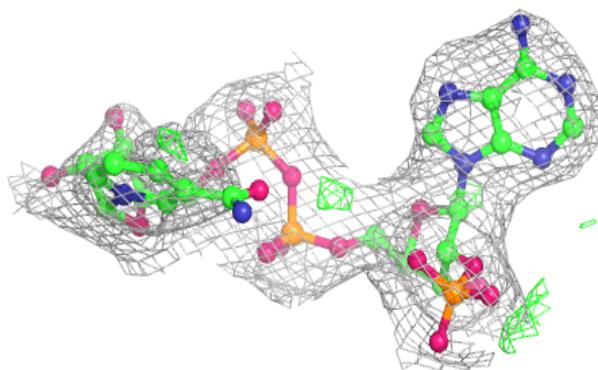
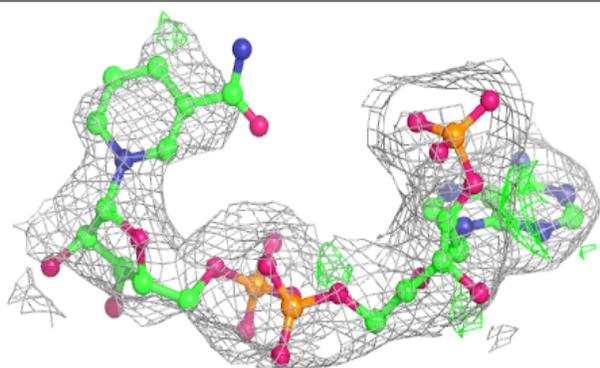


Electron density around NAP D 601:

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

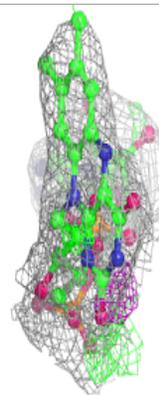
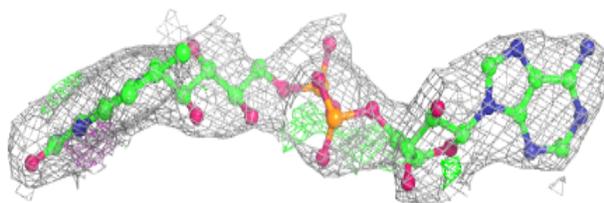
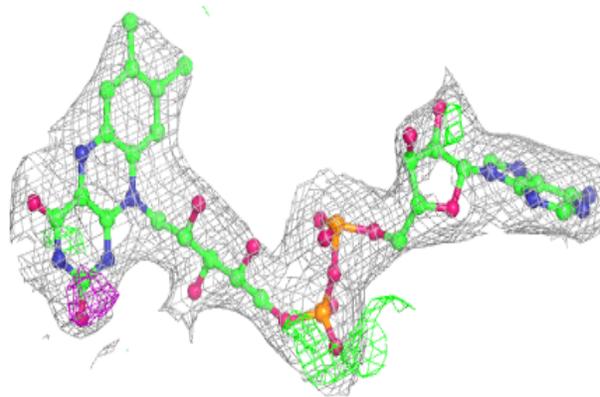
**Electron density around NAP A 601:**

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

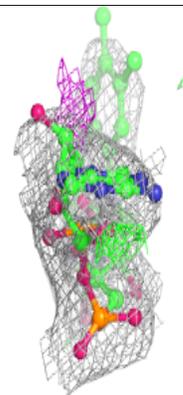
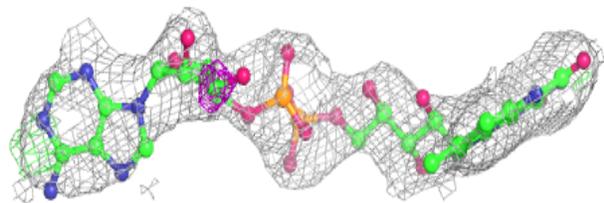
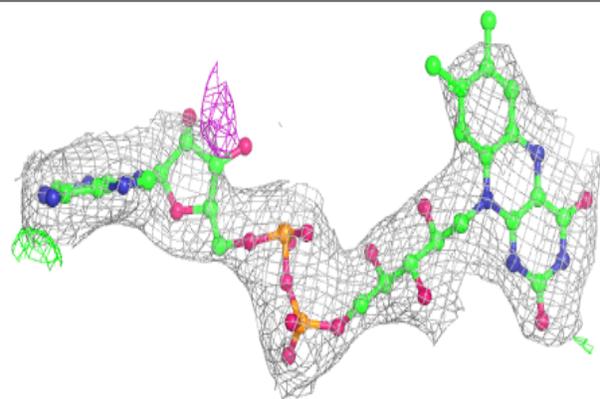


Electron density around FAD D 600:

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

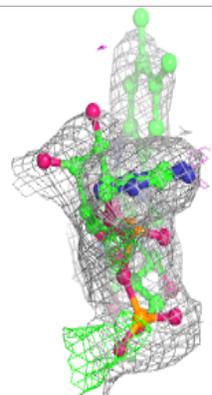
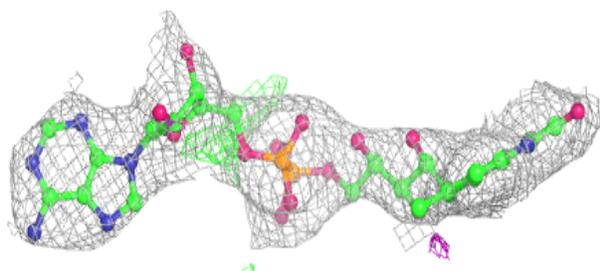
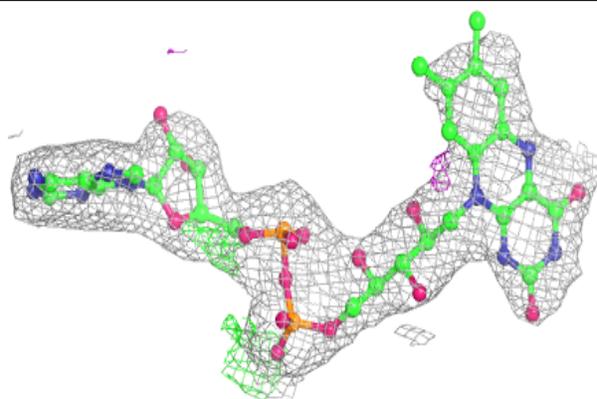
**Electron density around FAD E 600:**

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

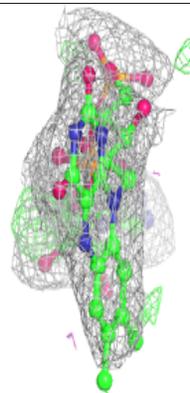
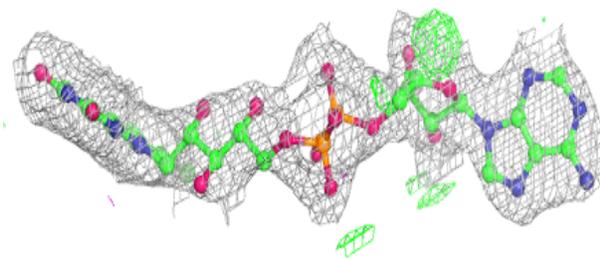
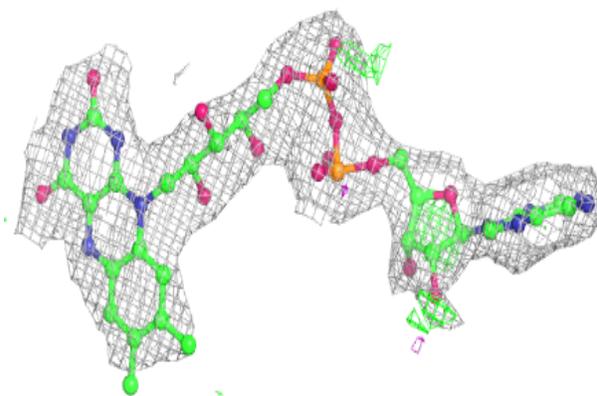


Electron density around FAD F 600:

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

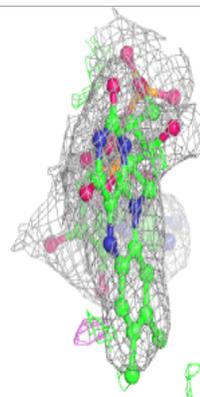
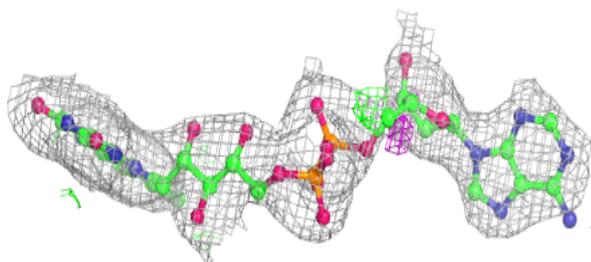
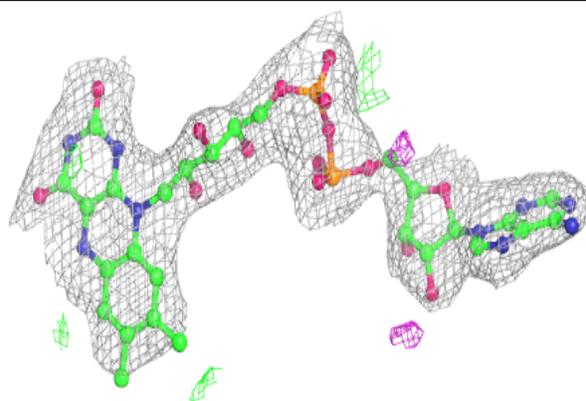
**Electron density around FAD B 600:**

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

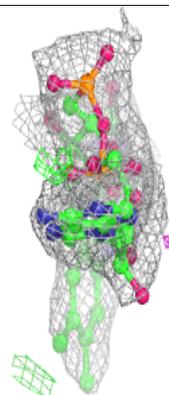
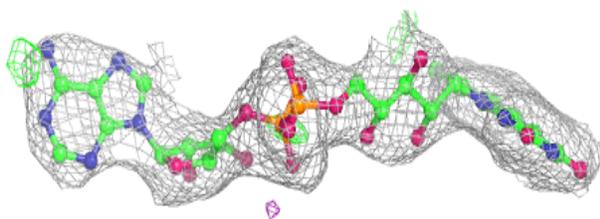
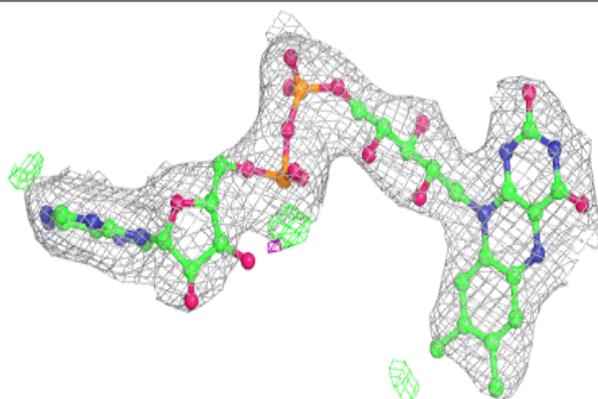


Electron density around FAD A 600:

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

**Electron density around FAD C 600:**

$2mF_o-DF_c$ (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.