



wwPDB X-ray Structure Validation Summary Report ⓘ

Mar 12, 2026 – 02:59 AM UTC

PDB ID : 8RPH / pdb_00008rph
Title : JanthE from Janthinobacterium sp. HH01,ketobutyryl-ThDP
Authors : Lanza, L.; Leogrande, C.; Rabe von Pappenheim, F.; Tittmann, K.; Mueller, M.
Deposited on : 2024-01-16
Resolution : 2.96 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 : 4-5-2 with Phenix2.0
Mogul : 2022.3.0, CSD as543be (2022)
Xtriage (Phenix) : 2.0
EDS : 3.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4 : 9.0.010 (Gargrove)
Density-Fitness : 1.0.12
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

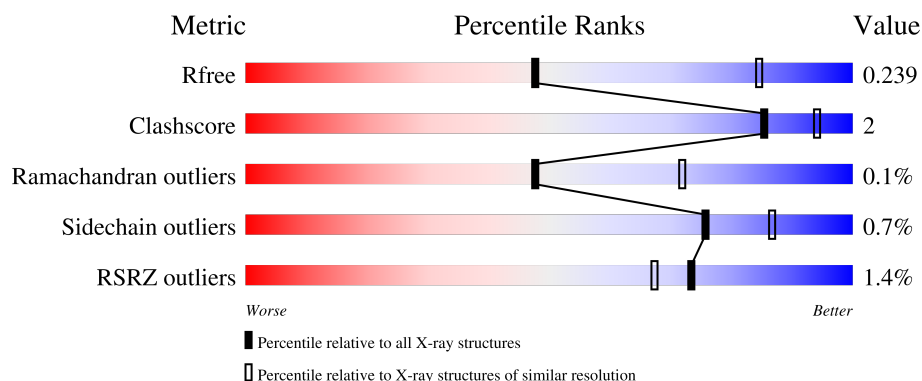
1 Overall quality at a glance ⓘ

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.96 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}	180053	1130 (2.98-2.94)
Clashscore	190562	1157 (2.98-2.94)
Ramachandran outliers	187476	1101 (2.98-2.94)
Sidechain outliers	187428	1101 (2.98-2.94)
RSRZ outliers	180081	1130 (2.98-2.94)

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	619	% 94% 5% 5%
1	B	619	% 93% 5% 5%
1	C	619	94% 5% 5%
1	D	619	% 93% 5% 5%
1	E	619	92% 5% 5%

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Mol	Chain	Length	Quality of chain
1	F	619	5% 76% 7% 16%

2 Entry composition [i](#)

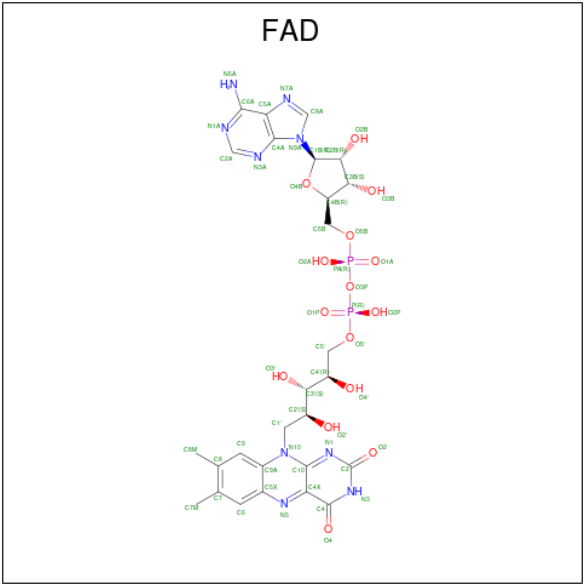
There are 6 unique types of molecules in this entry. The entry contains 55155 atoms, of which 27279 are hydrogens and 0 are deuteriums.

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 Thiamine pyrophosphate-binding protein.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	605	Total	C	H	N	O	S	0	4	0
			9296	2959	4629	814	862	32			
1	B	599	Total	C	H	N	O	S	0	5	0
			9198	2930	4576	806	855	31			
1	C	605	Total	C	H	N	O	S	0	4	0
			9296	2959	4629	814	862	32			
1	D	608	Total	C	H	N	O	S	0	6	0
			9351	2974	4655	822	869	31			
1	E	605	Total	C	H	N	O	S	0	4	0
			9296	2959	4629	814	862	32			
1	F	520	Total	C	H	N	O	S	0	6	0
			7984	2542	3961	703	748	30			

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

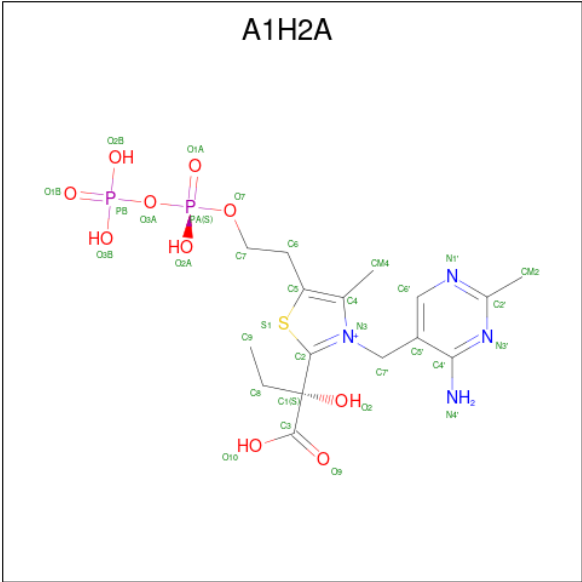


Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
2	A	1	Total	C	H	N	O	P	0	0
			84	27	31	9	15	2		
2	B	1	Total	C	H	N	O	P	0	0
			84	27	31	9	15	2		
2	C	1	Total	C	H	N	O	P	0	0
			84	27	31	9	15	2		
2	D	1	Total	C	H	N	O	P	0	0
			84	27	31	9	15	2		
2	E	1	Total	C	H	N	O	P	0	0
			84	27	31	9	15	2		
2	F	1	Total	C	H	N	O	P	0	0
			84	27	31	9	15	2		

- Molecule 3 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	1	Total	Mg	0	0
			1	1		
3	B	1	Total	Mg	0	0
			1	1		
3	C	1	Total	Mg	0	0
			1	1		
3	D	1	Total	Mg	0	0
			1	1		
3	E	1	Total	Mg	0	0
			1	1		
3	F	1	Total	Mg	0	0
			1	1		

- Molecule 4 is (2 {S})-2-[3-[(4-azanyl-2-methyl-pyrimidin-5-yl)methyl]-4-methyl-5-[2-[oxidanyl(phosphonooxy)phosphoryl]oxyethyl]-1,3-thiazol-2-yl]-2-oxidanyl-butanoic acid (CCD ID: A1H2A) (formula: C₁₆H₂₅N₄O₁₀P₂S) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
4	A	1	Total	C	N	O	P	S	0	0
			33	16	4	10	2	1		
4	B	1	Total	C	N	O	P	S	0	0
			33	16	4	10	2	1		
4	C	1	Total	C	N	O	P	S	0	0
			33	16	4	10	2	1		
4	D	1	Total	C	N	O	P	S	0	0
			33	16	4	10	2	1		
4	E	1	Total	C	N	O	P	S	0	0
			33	16	4	10	2	1		
4	F	1	Total	C	N	O	P	S	0	0
			33	16	4	10	2	1		

- Molecule 5 is TRIETHYLENE GLYCOL (CCD ID: PGE) (formula: C₆H₁₄O₄).

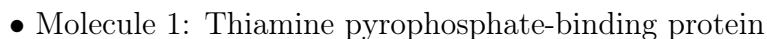


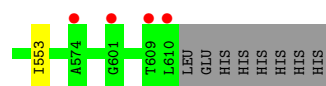
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
5	D	1	Total	C	H	O	0	0
			24	6	14	4		

- Molecule 6 is water.

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

- Molecule 1: Thiamine pyrophosphate-binding protein





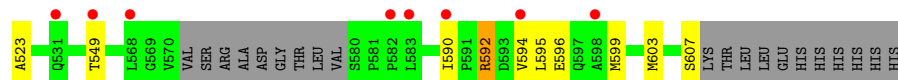
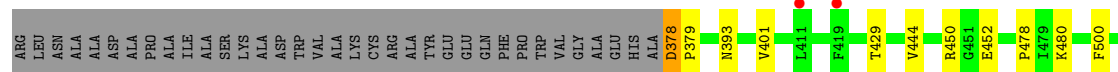
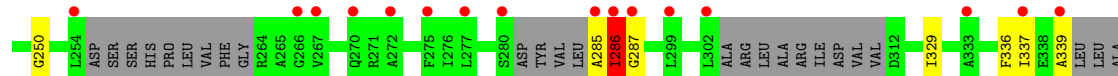
- Molecule 1: Thiamine pyrophosphate-binding protein

Chain E: 92% 5%



- Molecule 1: Thiamine pyrophosphate-binding protein

Chain F: 5% 76% 7% 16%



4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	173.33Å 118.19Å 201.17Å 90.00° 97.06° 90.00°	Depositor
Resolution (Å)	99.82 – 2.96 99.82 – 2.96	Depositor EDS
% Data completeness (in resolution range)	94.5 (99.82-2.96) 94.5 (99.82-2.96)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.42 (at 2.96Å)	Xtriage
Refinement program	PHENIX 1.20.1_4487	Depositor
R, R_{free}	0.206 , 0.240 0.207 , 0.239	Depositor DCC
R_{free} test set	3860 reflections (4.60%)	wwPDB-VP
Wilson B-factor (Å ²)	66.7	Xtriage
Anisotropy	0.235	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.40 , 39.0	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	55155	wwPDB-VP
Average B, all atoms (Å ²)	78.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.86% 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: PGE, A1H2A, MG, FAD

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	0.10	0/4779	0.25	0/6483
1	B	0.18	1/4739 (0.0%)	0.28	0/6428
1	C	0.10	0/4779	0.25	0/6483
1	D	0.10	0/4814	0.26	0/6531
1	E	0.17	0/4779	0.26	0/6483
1	F	0.23	0/4118	0.42	4/5569 (0.1%)
All	All	0.15	1/28008 (0.0%)	0.29	4/37977 (0.0%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	581	PRO	C-O	-5.32	1.18	1.24

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	F	286	ILE	N-CA-C	10.58	124.27	111.05
1	F	203	VAL	CB-CA-C	-6.64	103.47	111.97
1	F	592	ARG	N-CA-C	5.25	118.78	112.38
1	F	203	VAL	N-CA-C	-5.19	105.44	110.42

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	4667	4629	4629	15	0
1	B	4622	4576	4569	11	0
1	C	4667	4629	4629	12	0
1	D	4696	4655	4649	18	0
1	E	4667	4629	4629	20	0
1	F	4023	3961	3953	41	0
2	A	53	31	31	0	0
2	B	53	31	31	1	0
2	C	53	31	31	0	0
2	D	53	31	31	0	0
2	E	53	31	31	0	0
2	F	53	31	31	1	0
3	A	1	0	0	0	0
3	B	1	0	0	0	0
3	C	1	0	0	0	0
3	D	1	0	0	0	0
3	E	1	0	0	0	0
3	F	1	0	0	0	0
4	A	33	0	0	3	0
4	B	33	0	0	1	0
4	C	33	0	0	2	0
4	D	33	0	0	3	0
4	E	33	0	0	4	0
4	F	33	0	0	1	0
5	D	10	14	14	2	0
6	B	1	0	0	0	0
6	C	1	0	0	1	0
All	All	27876	27279	27258	122	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 2.

The worst 5 of 122 close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:239:LYS:HE2	1:E:345:ASN:OD1	1.60	0.99
1:F:595:LEU:CD2	1:F:607:SER:HB3	1.98	0.94
1:F:595:LEU:HD23	1:F:607:SER:HB3	1.52	0.90
4:E:703:A1H2A:O2	4:E:703:A1H2A:N4'	2.06	0.88
4:B:703:A1H2A:N4'	4:B:703:A1H2A:O2	2.07	0.87

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	605/619 (98%)	590 (98%)	15 (2%)	0	100	100
1	B	600/619 (97%)	583 (97%)	17 (3%)	0	100	100
1	C	605/619 (98%)	588 (97%)	17 (3%)	0	100	100
1	D	612/619 (99%)	590 (96%)	22 (4%)	0	100	100
1	E	605/619 (98%)	587 (97%)	17 (3%)	1 (0%)	43	66
1	F	510/619 (82%)	487 (96%)	22 (4%)	1 (0%)	43	66
All	All	3537/3714 (95%)	3425 (97%)	110 (3%)	2 (0%)	48	72

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	E	405	ASP
1	F	379	PRO

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	492/500 (98%)	491 (100%)	1 (0%)	87	94
1	B	486/500 (97%)	483 (99%)	3 (1%)	78	89
1	C	492/500 (98%)	491 (100%)	1 (0%)	87	94

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	D	494/500 (99%)	493 (100%)	1 (0%)	87	94
1	E	492/500 (98%)	490 (100%)	2 (0%)	84	92
1	F	425/500 (85%)	412 (97%)	13 (3%)	35	59
All	All	2881/3000 (96%)	2860 (99%)	21 (1%)	76	87

5 of 21 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	F	245	LEU
1	F	378	ASP
1	F	590	ILE
1	F	393	ASN
1	F	337	ILE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 18 such sidechains are listed below:

Mol	Chain	Res	Type
1	E	222	ASN
1	F	561	GLN
1	F	384	ASN
1	C	561	GLN
1	E	61	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry

Of 19 ligands modelled in this entry, 6 are monoatomic - leaving 13 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	FAD	D	701	-	58,58,58	0.33	0	85,89,89	0.33	0
4	A1H2A	A	703	3	29,34,34	0.78	0	34,52,52	0.95	1 (2%)
4	A1H2A	F	703	3	29,34,34	0.77	0	34,52,52	1.10	2 (5%)
4	A1H2A	B	703	3	29,34,34	1.20	3 (10%)	34,52,52	1.10	1 (2%)
2	FAD	A	701	-	58,58,58	0.30	0	85,89,89	0.33	0
5	PGE	D	703	-	9,9,9	0.11	0	8,8,8	0.22	0
2	FAD	E	701	-	58,58,58	0.33	0	85,89,89	0.31	0
4	A1H2A	D	704	3	29,34,34	0.80	0	34,52,52	0.96	1 (2%)
2	FAD	C	701	-	58,58,58	0.29	0	85,89,89	0.31	0
2	FAD	B	701	-	58,58,58	0.33	0	85,89,89	0.32	0
4	A1H2A	E	703	3	29,34,34	0.81	0	34,52,52	0.97	1 (2%)
4	A1H2A	C	703	3	29,34,34	0.81	0	34,52,52	1.04	1 (2%)
2	FAD	F	701	-	58,58,58	0.33	0	85,89,89	0.32	0

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	D	701	-	-	11/34/50/50	0/6/6/6
4	A1H2A	A	703	3	-	6/29/32/32	0/2/2/2
4	A1H2A	F	703	3	-	10/29/32/32	0/2/2/2
4	A1H2A	B	703	3	-	12/29/32/32	0/2/2/2
2	FAD	A	701	-	-	8/34/50/50	0/6/6/6
5	PGE	D	703	-	-	0/7/7/7	-
2	FAD	E	701	-	-	9/34/50/50	0/6/6/6
4	A1H2A	D	704	3	-	11/29/32/32	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	FAD	C	701	-	-	9/34/50/50	0/6/6/6
2	FAD	B	701	-	-	11/34/50/50	0/6/6/6
4	A1H2A	E	703	3	-	11/29/32/32	0/2/2/2
4	A1H2A	C	703	3	-	9/29/32/32	0/2/2/2
2	FAD	F	701	-	-	10/34/50/50	0/6/6/6

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	B	703	A1H2A	C5-S1	-3.10	1.67	1.74
4	B	703	A1H2A	C2'-N3'	-2.06	1.30	1.34
4	B	703	A1H2A	PB-O3B	-2.00	1.47	1.54

The worst 5 of 7 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	F	703	A1H2A	S1-C2-N3	-4.36	107.96	112.24
4	C	703	A1H2A	S1-C2-N3	-4.21	108.11	112.24
4	B	703	A1H2A	S1-C2-N3	-3.97	108.35	112.24
4	A	703	A1H2A	S1-C2-N3	-3.93	108.39	112.24
4	E	703	A1H2A	S1-C2-N3	-3.93	108.39	112.24

There are no chirality outliers.

5 of 117 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	701	FAD	C5B-O5B-PA-O1A
2	A	701	FAD	C5B-O5B-PA-O2A
2	A	701	FAD	C5B-O5B-PA-O3P
2	B	701	FAD	C5B-O5B-PA-O1A
2	B	701	FAD	C5B-O5B-PA-O2A

There are no ring outliers.

9 monomers are involved in 18 short contacts:

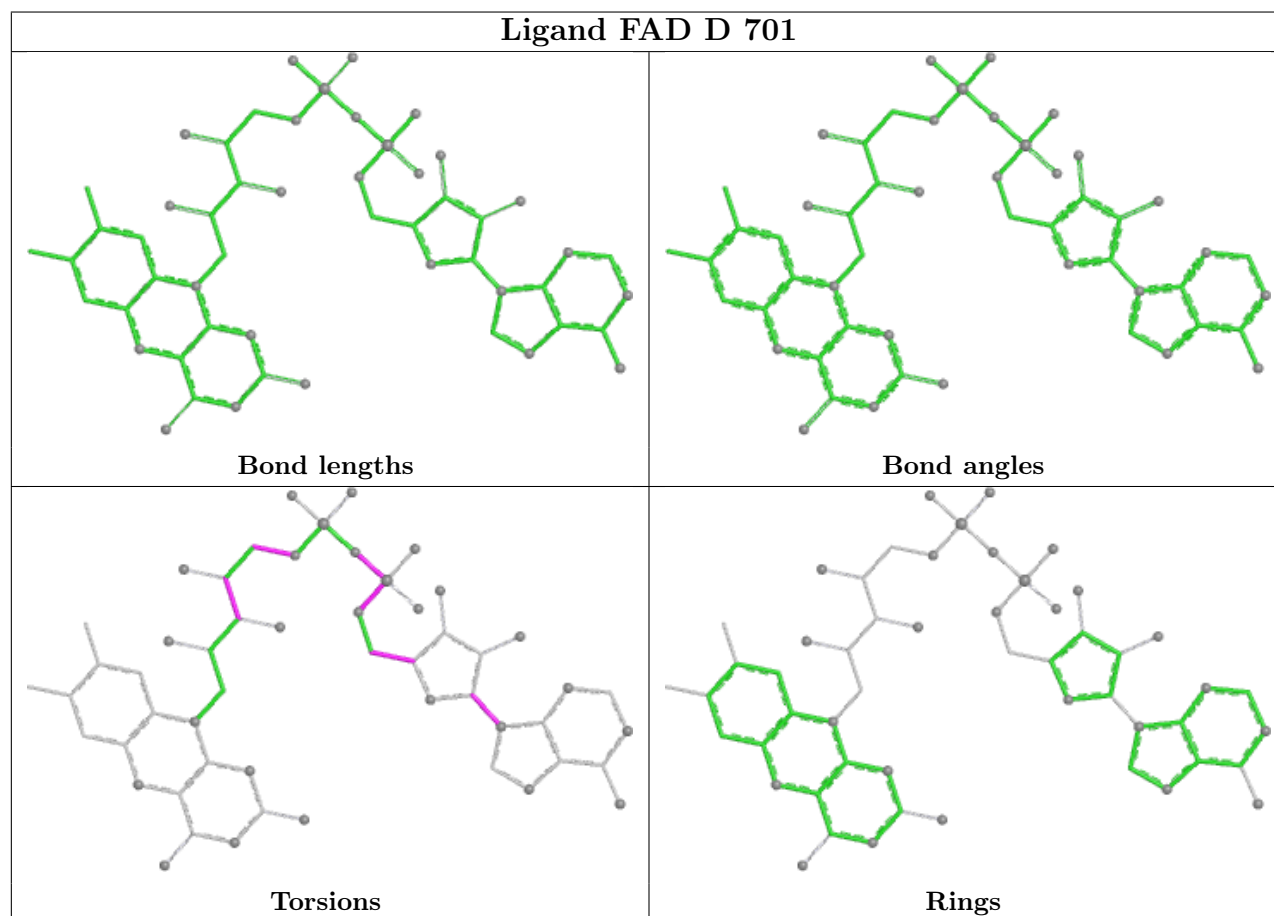
Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	703	A1H2A	3	0
4	F	703	A1H2A	1	0
4	B	703	A1H2A	1	0
5	D	703	PGE	2	0

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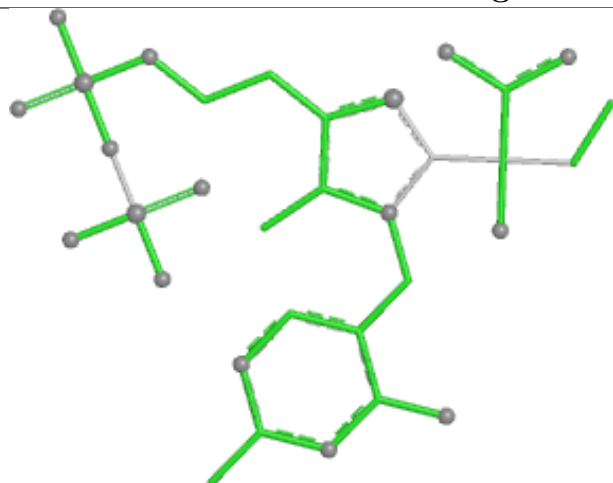
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Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	D	704	A1H2A	3	0
2	B	701	FAD	1	0
4	E	703	A1H2A	4	0
4	C	703	A1H2A	2	0
2	F	701	FAD	1	0

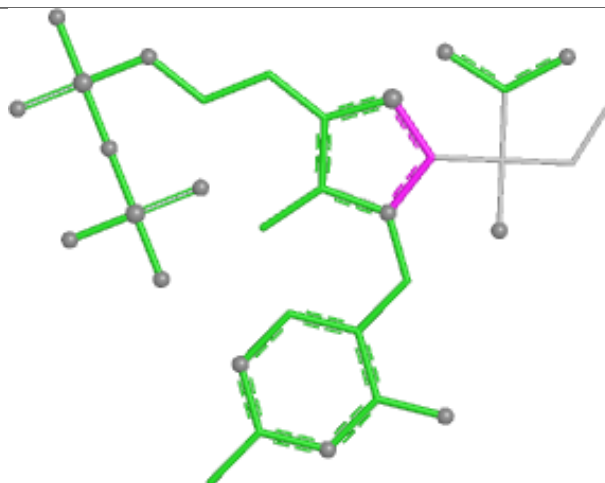
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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



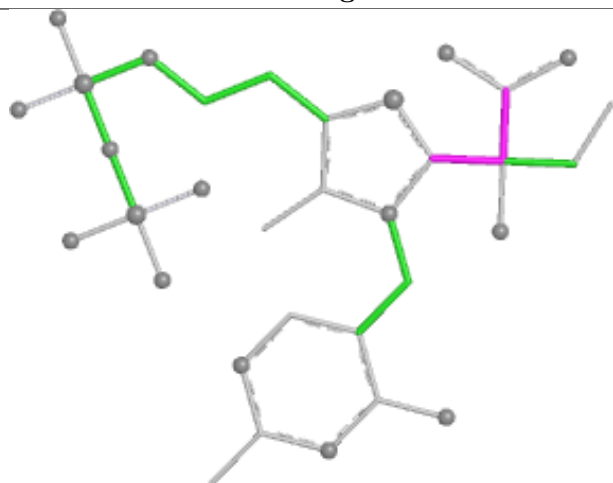
Ligand A1H2A A 703



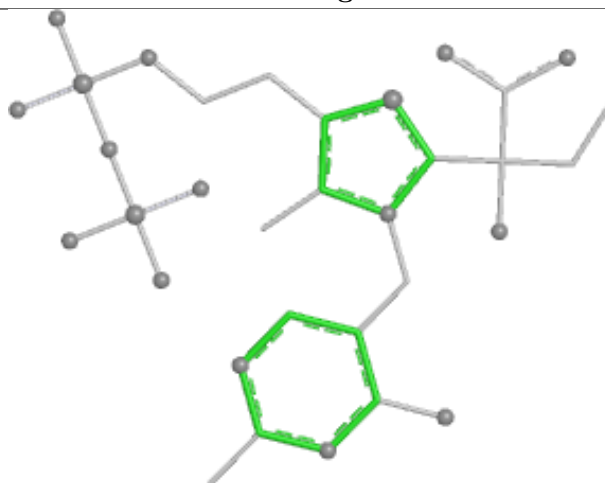
Bond lengths



Bond angles

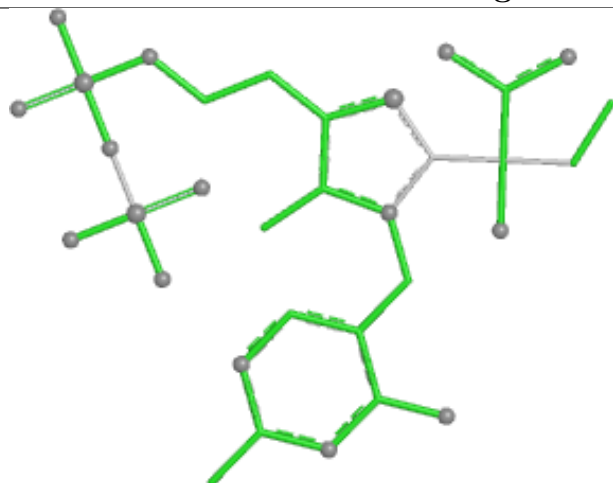


Torsions

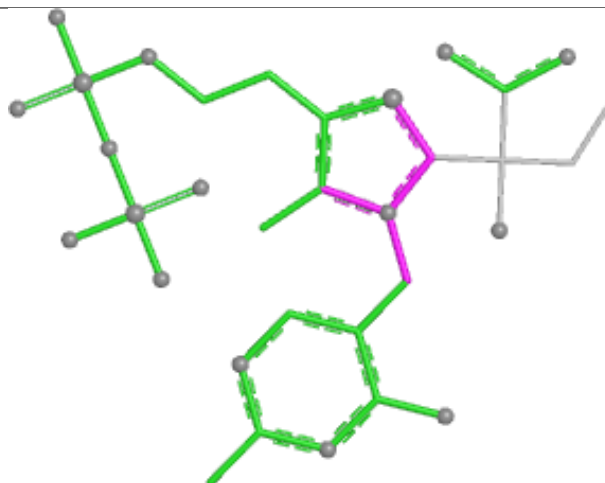


Rings

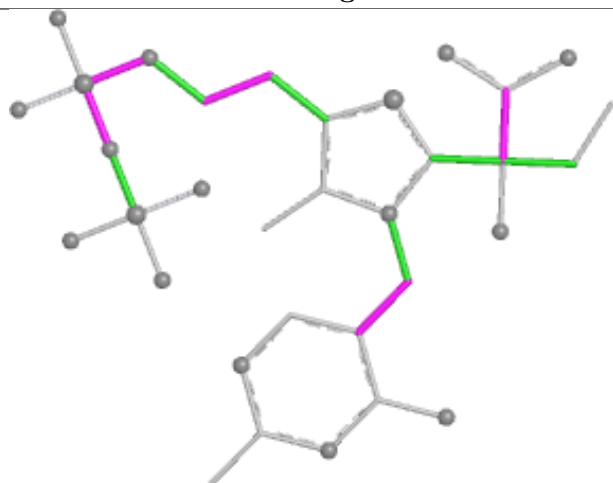
Ligand A1H2A F 703



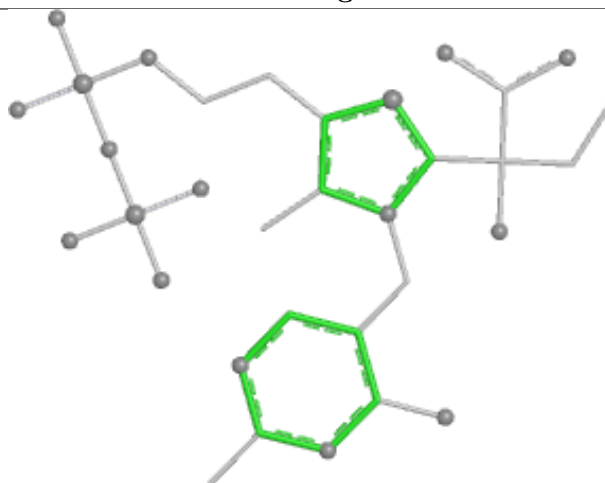
Bond lengths



Bond angles

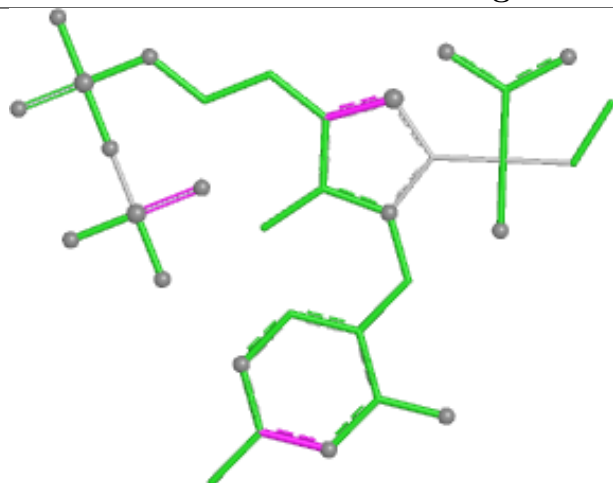


Torsions

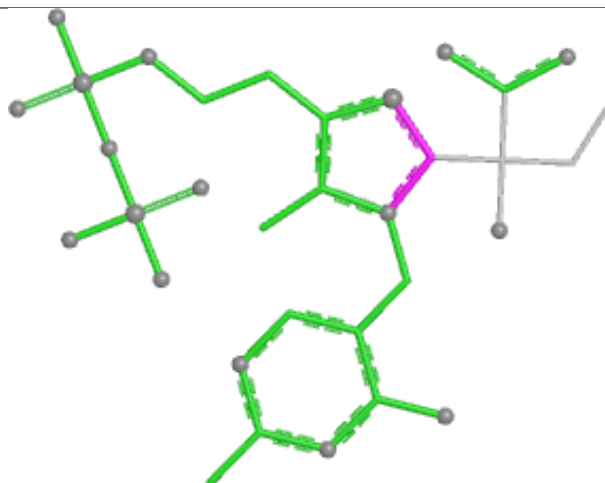


Rings

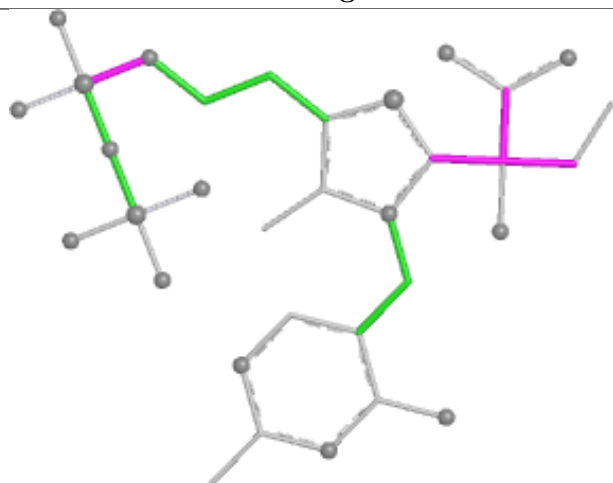
Ligand A1H2A B 703



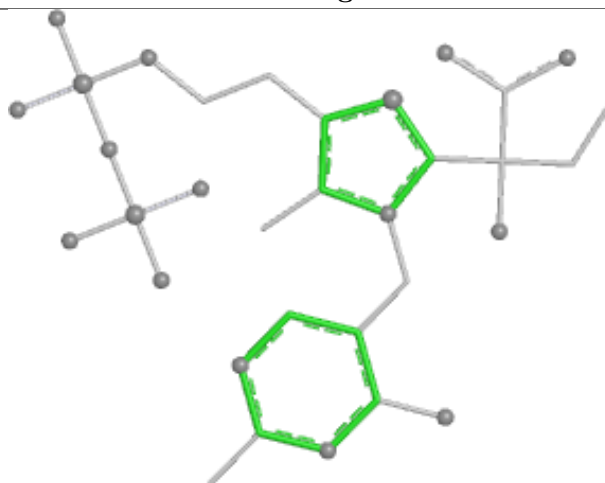
Bond lengths



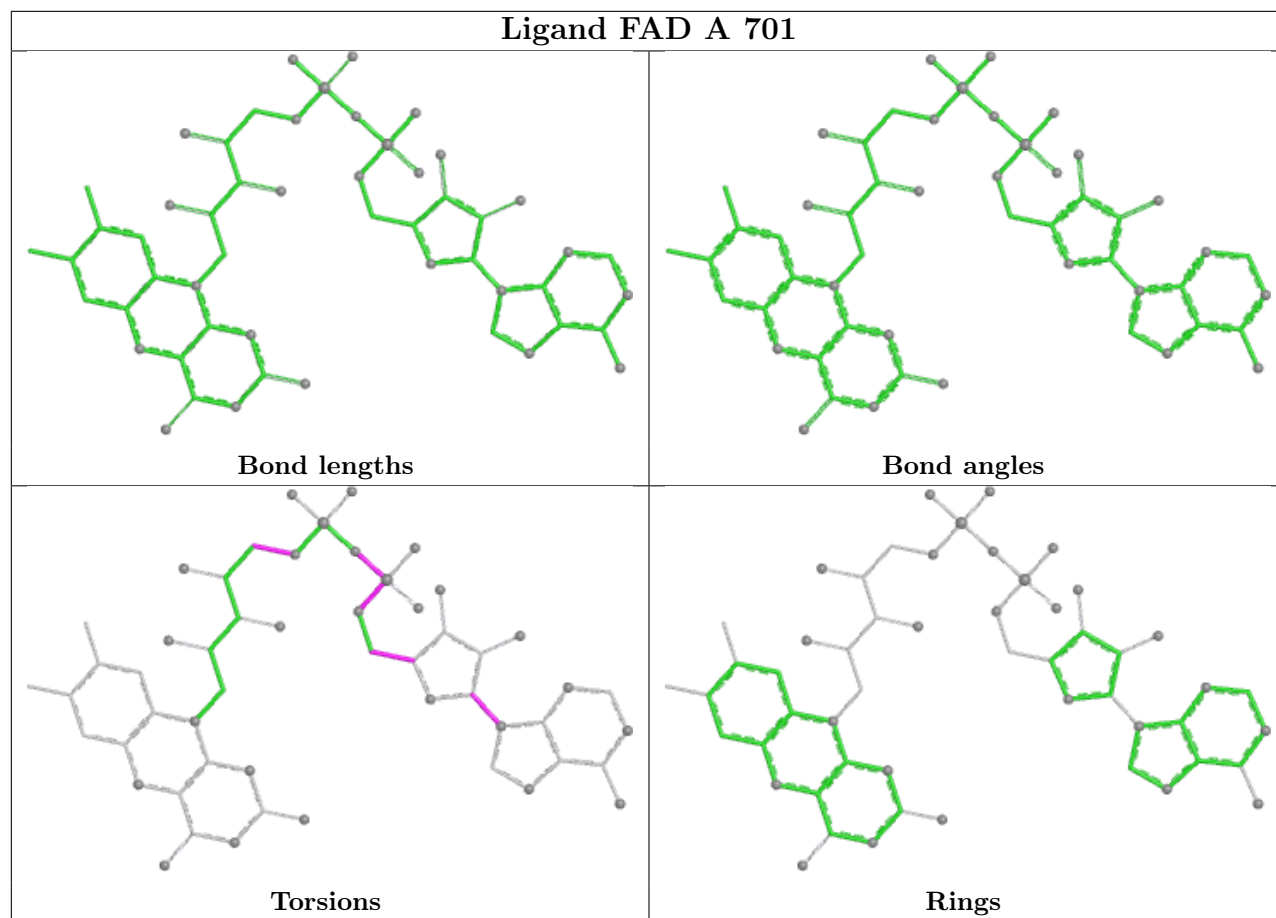
Bond angles

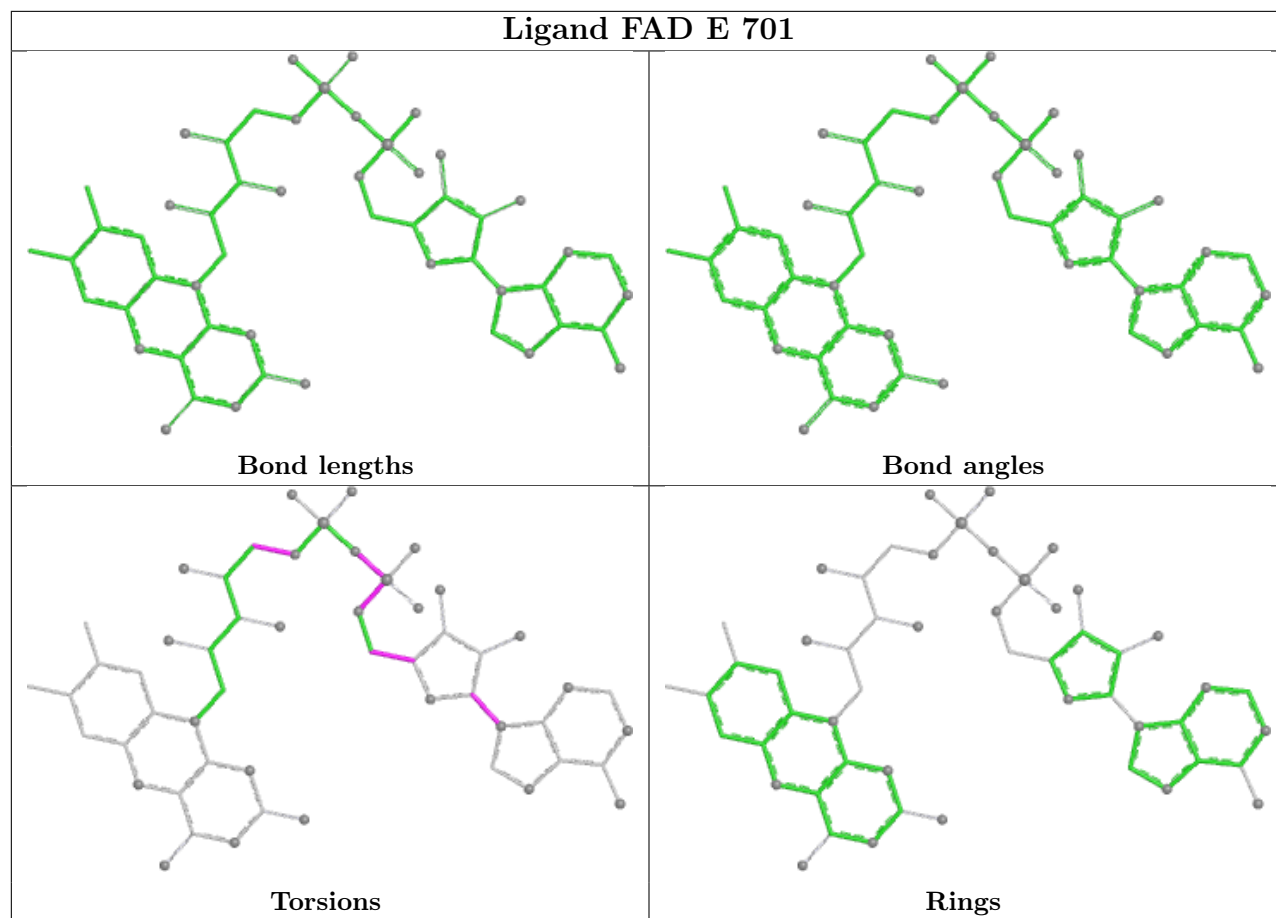


Torsions

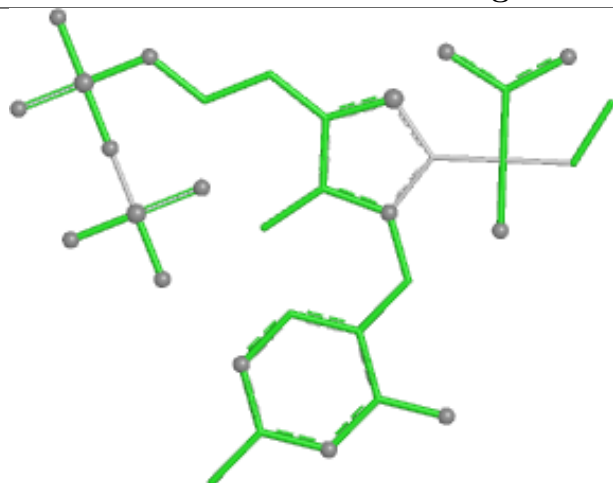


Rings

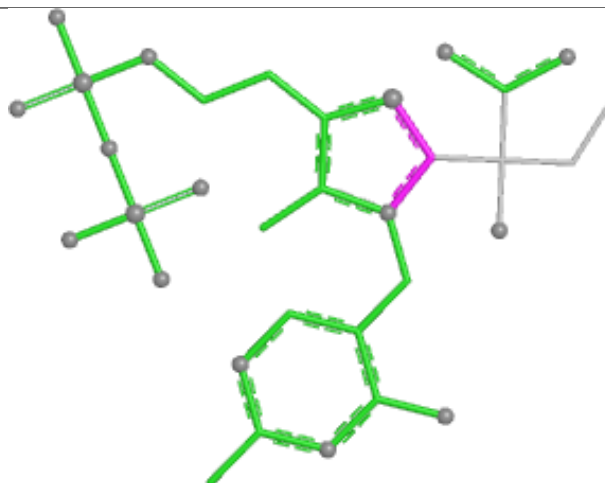




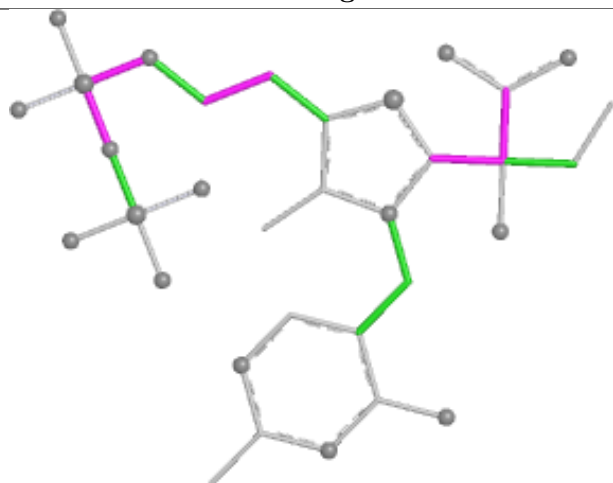
Ligand A1H2A D 704



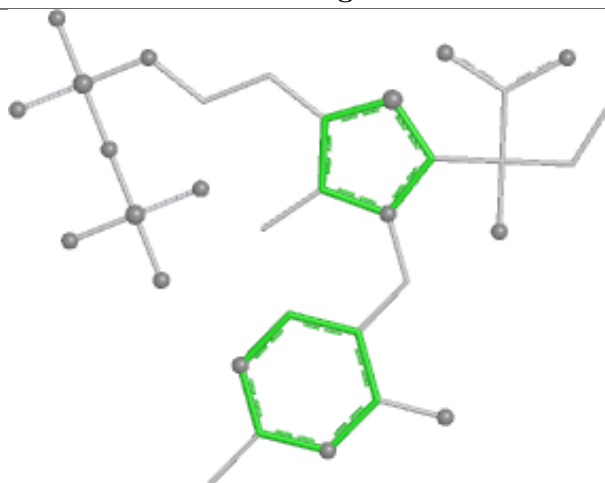
Bond lengths



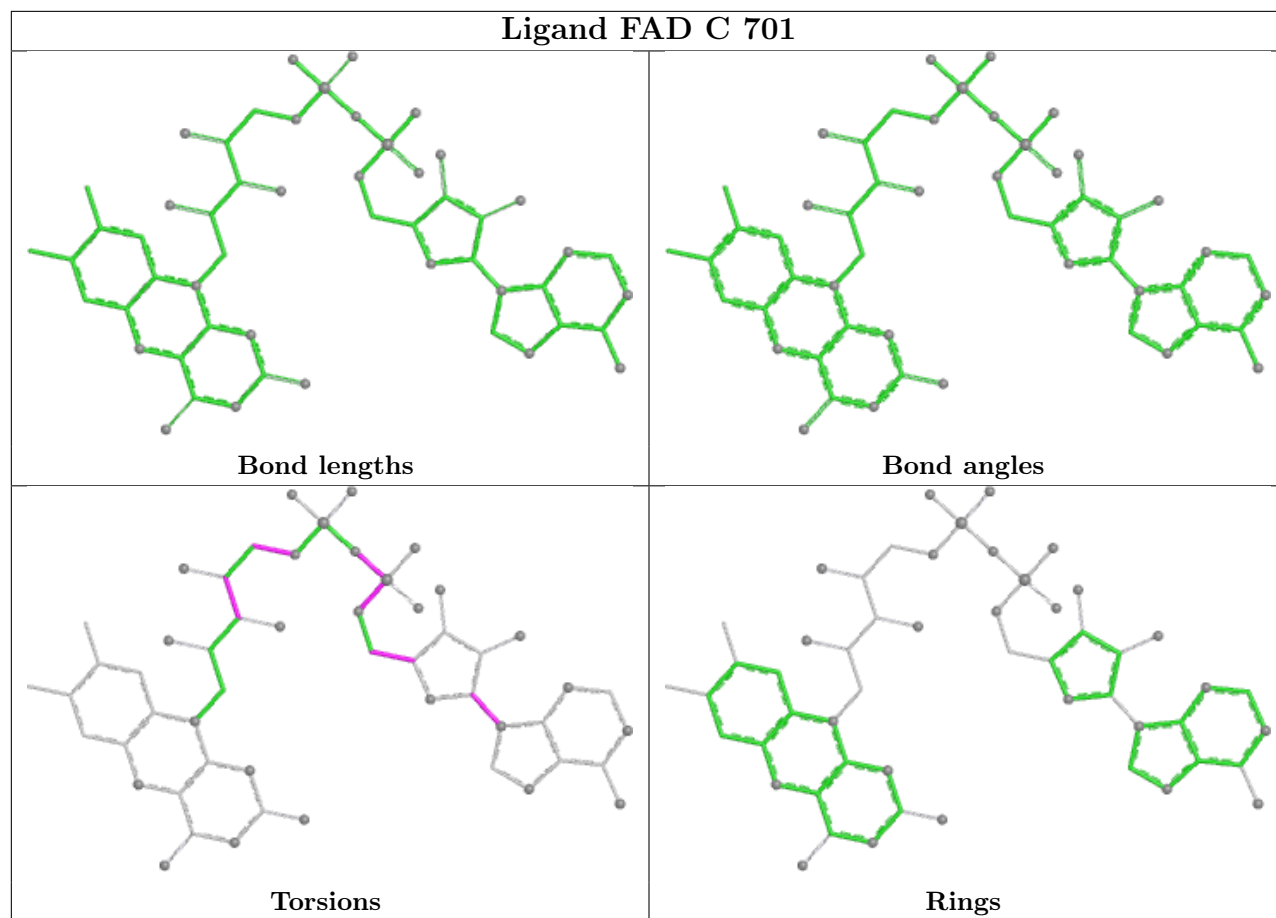
Bond angles

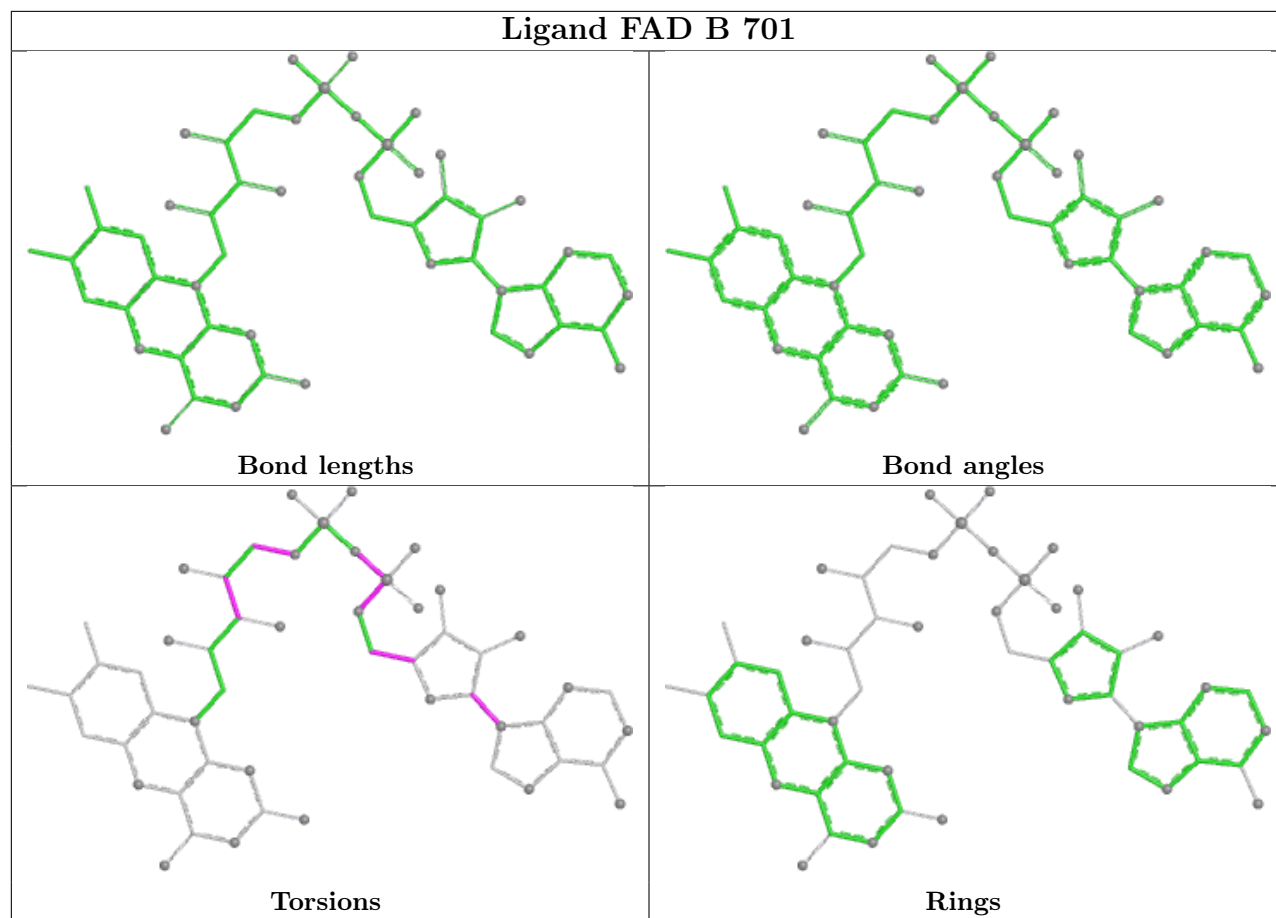


Torsions

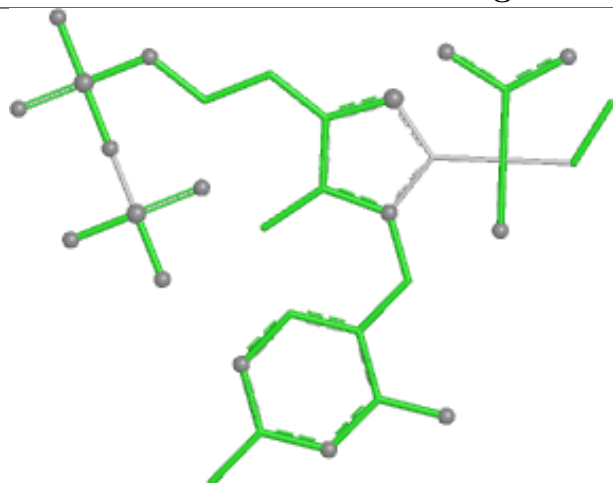


Rings

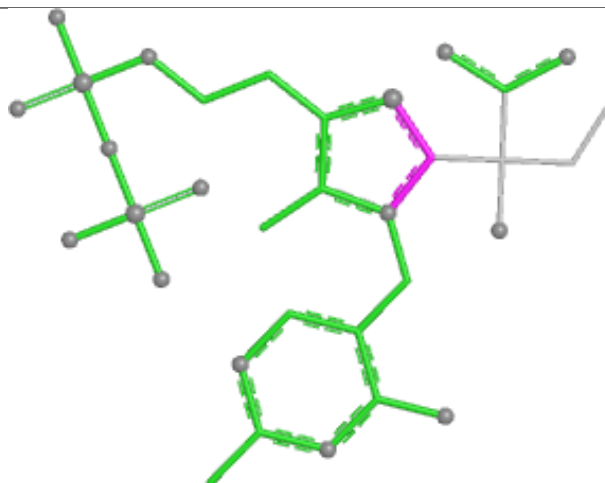




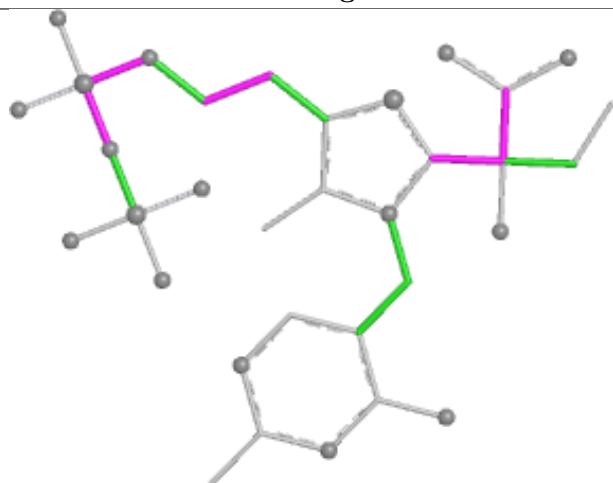
Ligand A1H2A E 703



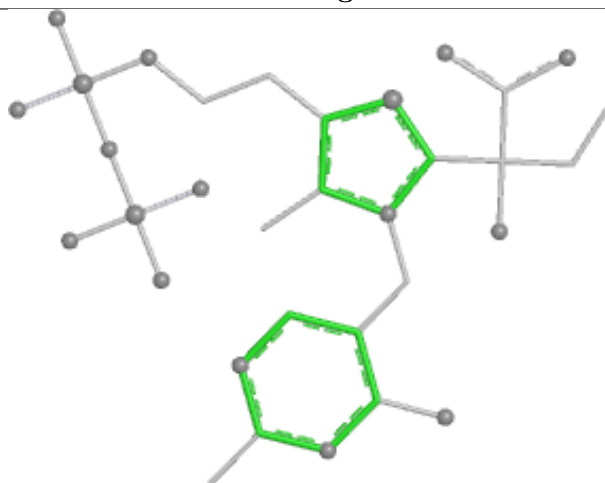
Bond lengths



Bond angles

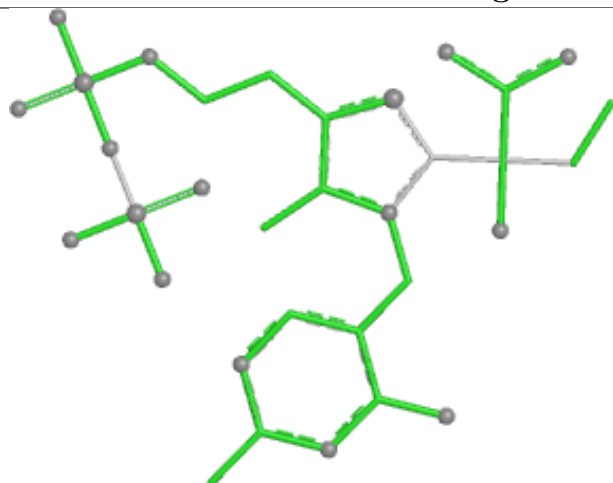


Torsions

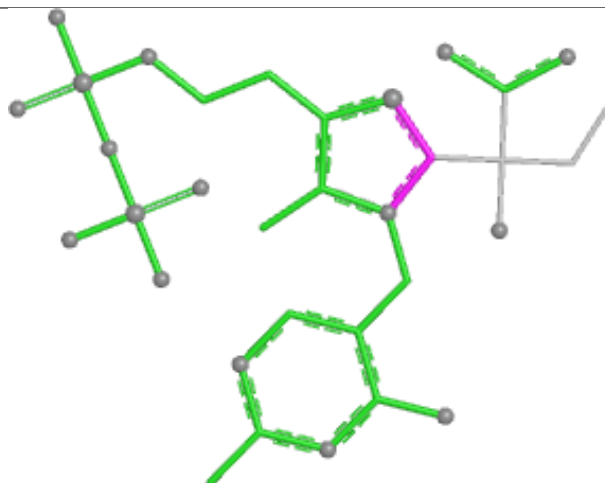


Rings

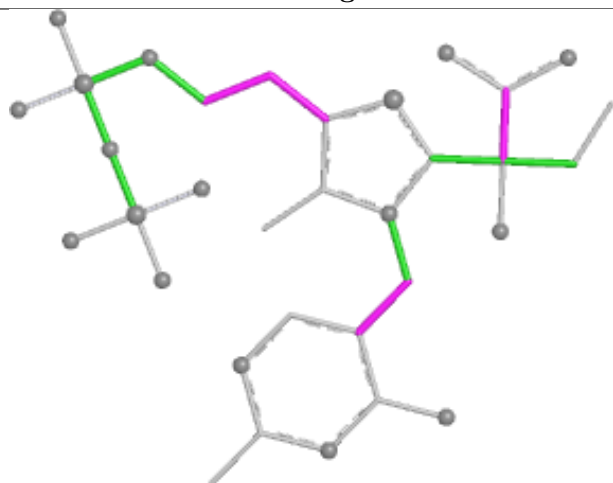
Ligand A1H2A C 703



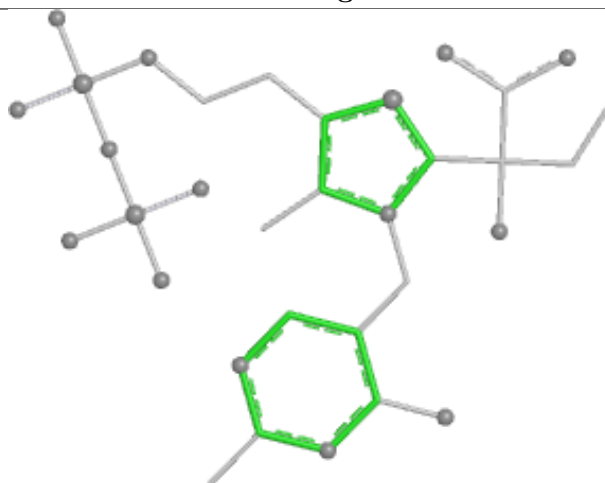
Bond lengths



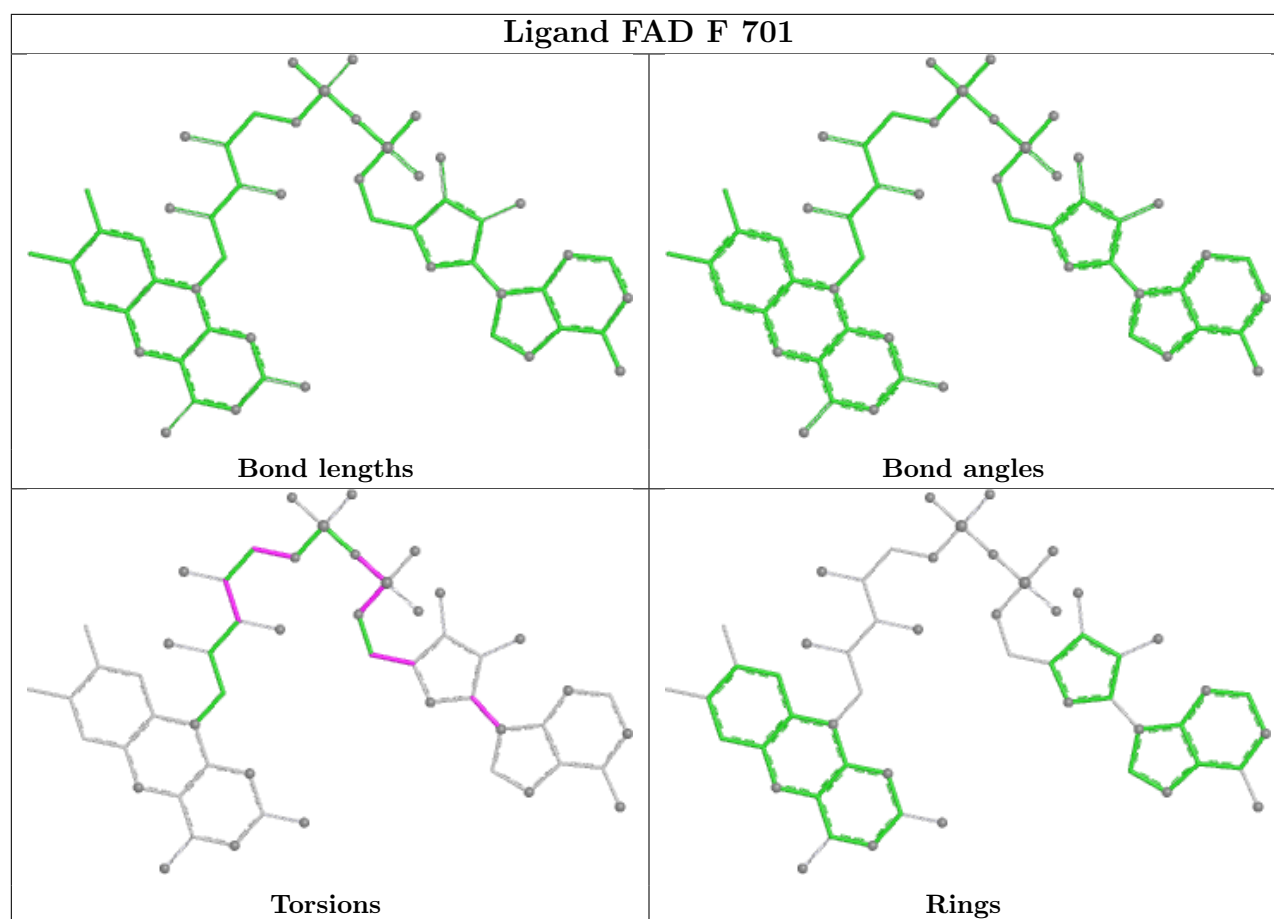
Bond angles



Torsions



Rings



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	605/619 (97%)	-0.21	5 (0%) 82 78	35, 73, 106, 136	2 (0%)
1	B	599/619 (96%)	-0.14	5 (0%) 82 78	37, 74, 100, 158	2 (0%)
1	C	605/619 (97%)	-0.17	2 (0%) 90 88	40, 73, 100, 144	2 (0%)
1	D	608/619 (98%)	-0.18	5 (0%) 82 78	36, 72, 100, 155	3 (0%)
1	E	605/619 (97%)	-0.12	3 (0%) 87 83	34, 74, 104, 165	2 (0%)
1	F	520/619 (84%)	0.39	29 (5%) 30 25	38, 91, 131, 159	3 (0%)
All	All	3542/3714 (95%)	-0.08	49 (1%) 73 67	34, 74, 112, 165	14 (0%)

The worst 5 of 49 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	570	VAL	4.3
1	F	339	ALA	4.3
1	F	210	LEU	4.0
1	F	280	SER	3.7
1	E	610	LEU	3.6

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 oligosaccharides in this entry.

6.4 Ligands

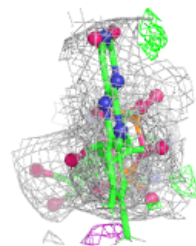
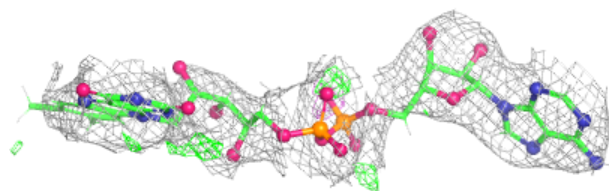
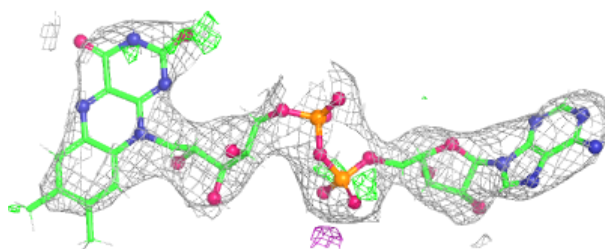
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
5	PGE	D	703	10/10	0.78	0.14	78,94,97,100	0
3	MG	F	702	1/1	0.84	0.12	85,85,85,85	0
3	MG	D	702	1/1	0.86	0.17	68,68,68,68	0
2	FAD	F	701	53/53	0.92	0.11	80,94,111,115	0
4	A1H2A	C	703	33/33	0.94	0.10	60,64,69,70	0
4	A1H2A	F	703	33/33	0.94	0.10	68,77,83,86	0
3	MG	E	702	1/1	0.94	0.15	75,75,75,75	0
4	A1H2A	A	703	33/33	0.95	0.09	61,66,68,69	0
4	A1H2A	B	703	33/33	0.95	0.09	61,65,67,68	0
2	FAD	C	701	53/53	0.95	0.07	55,61,73,76	0
4	A1H2A	E	703	33/33	0.95	0.10	62,65,69,71	0
2	FAD	B	701	53/53	0.95	0.08	57,60,72,76	0
3	MG	A	702	1/1	0.95	0.10	71,71,71,71	0
4	A1H2A	D	704	33/33	0.96	0.09	59,61,66,67	0
2	FAD	E	701	53/53	0.96	0.07	55,58,71,73	0
2	FAD	A	701	53/53	0.96	0.07	54,57,69,71	0
2	FAD	D	701	53/53	0.96	0.08	56,60,71,73	0
3	MG	B	702	1/1	0.97	0.07	67,67,67,67	0
3	MG	C	702	1/1	0.97	0.05	60,60,60,60	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.

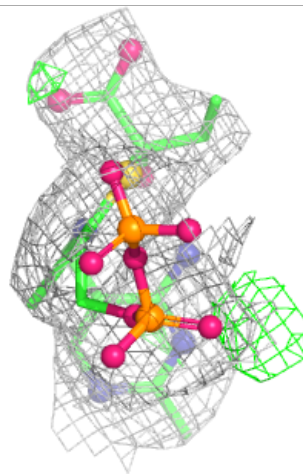
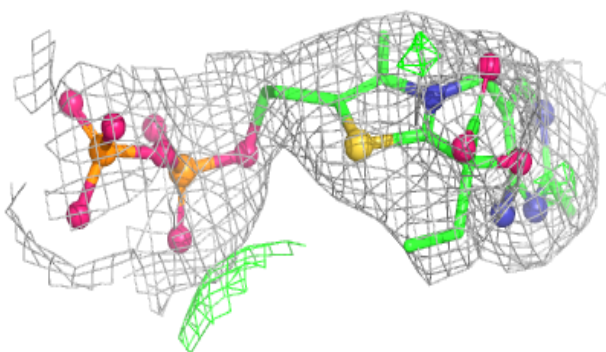
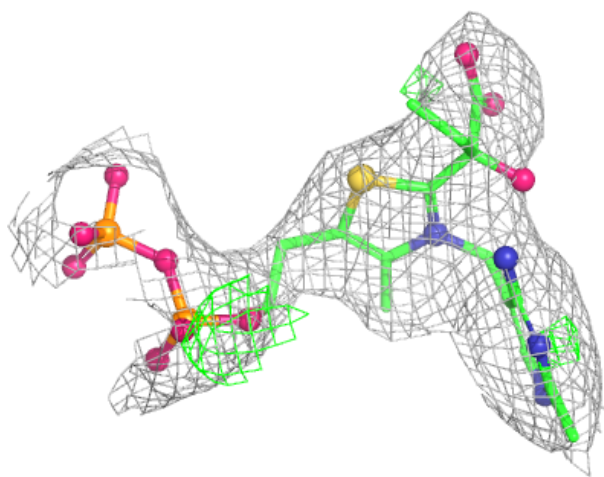
Electron density around FAD F 701:

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



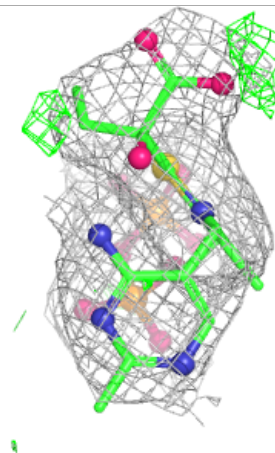
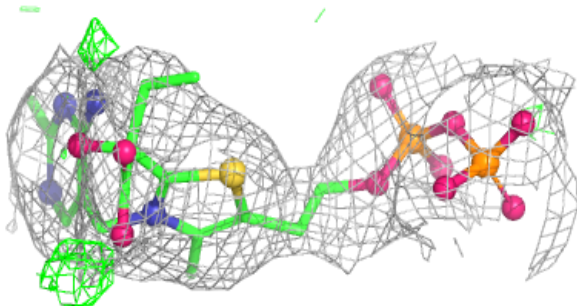
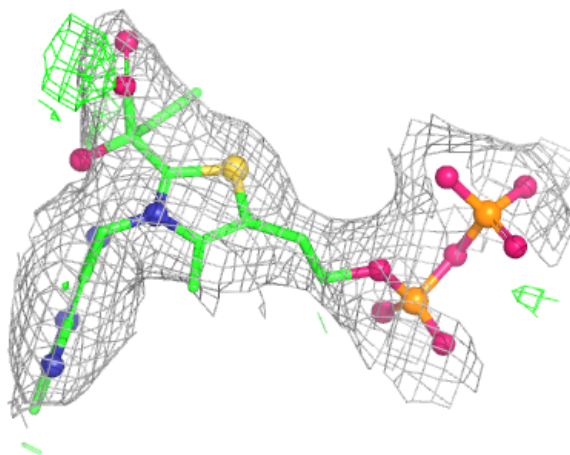
Electron density around A1H2A C 703:

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



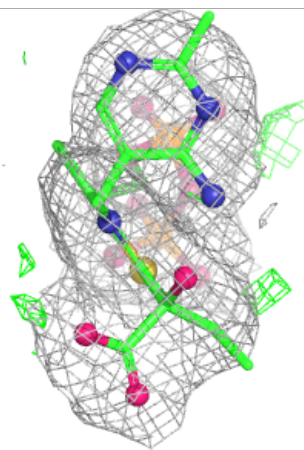
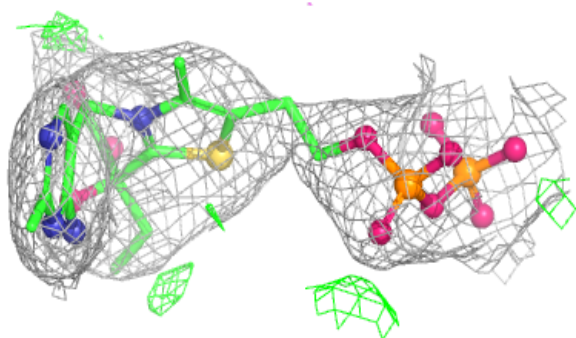
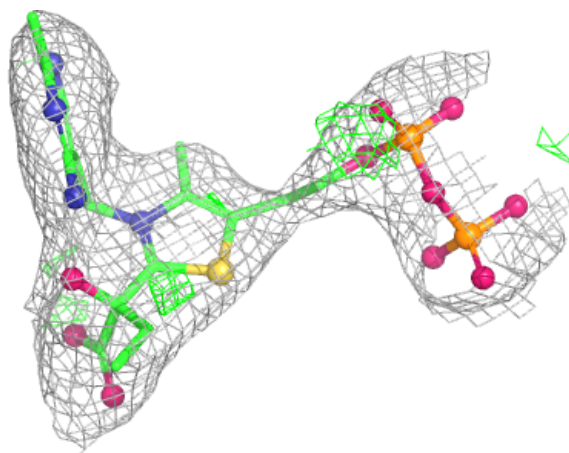
Electron density around A1H2A F 703:

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



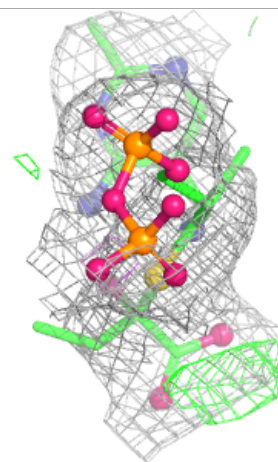
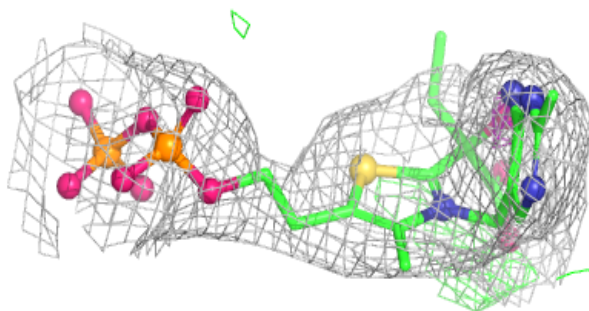
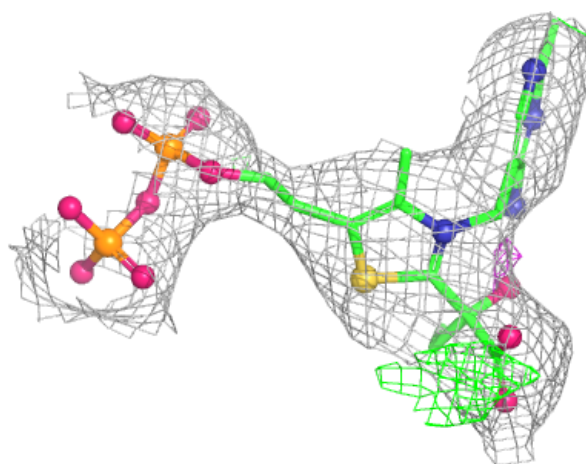
Electron density around A1H2A A 703:

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



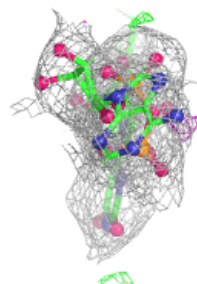
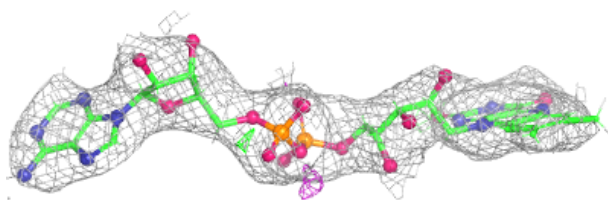
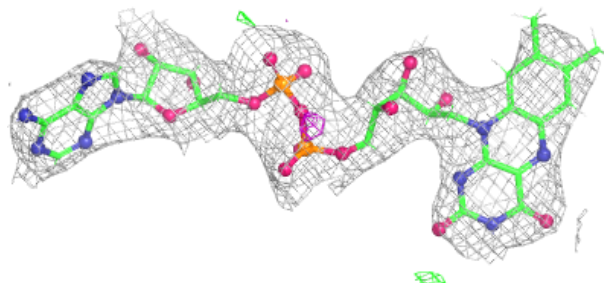
Electron density around A1H2A B 703:

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and green (positive)



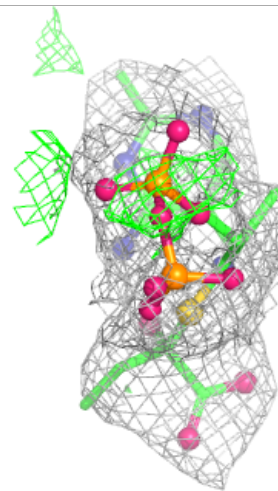
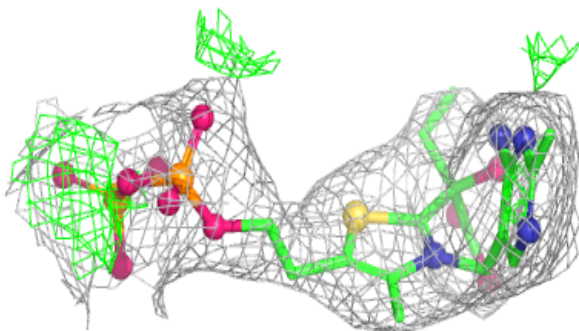
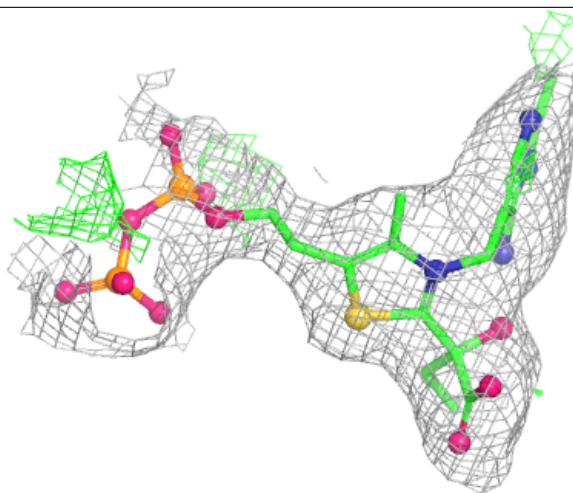
Electron density around FAD C 701:

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



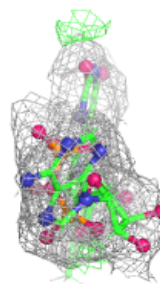
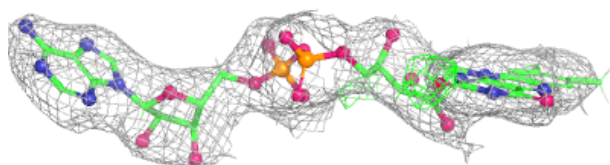
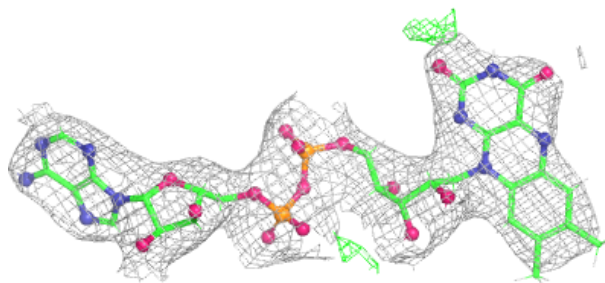
Electron density around A1H2A E 703:

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

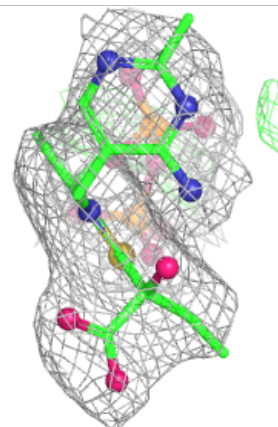
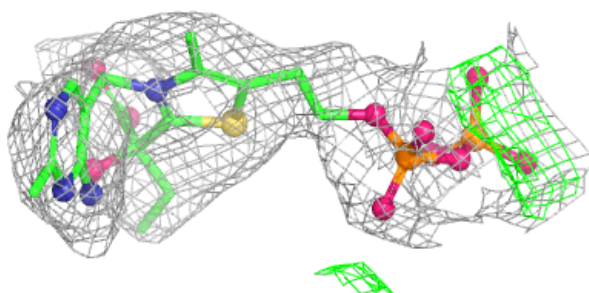
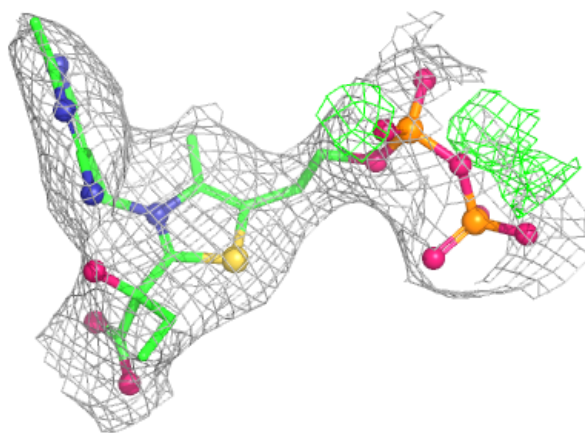


Electron density around FAD B 701:

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and green (positive)

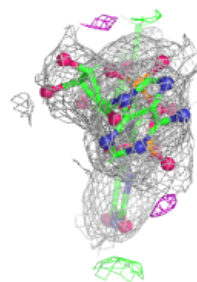
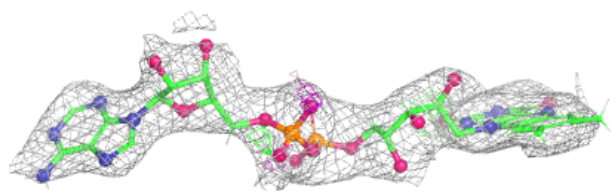
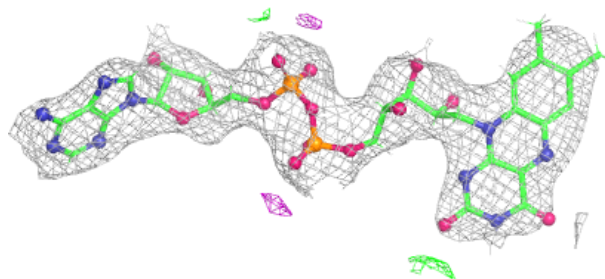
**Electron density around A1H2A D 704:**

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

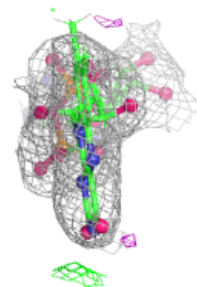
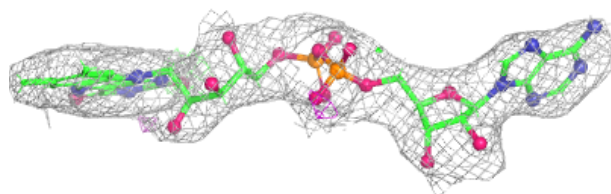
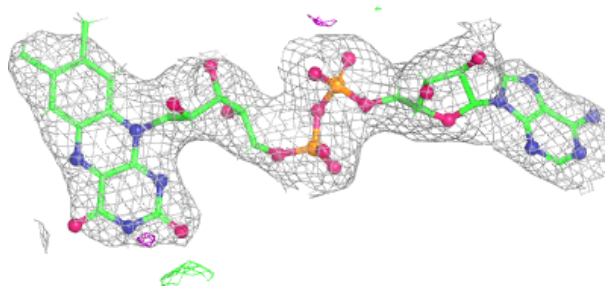


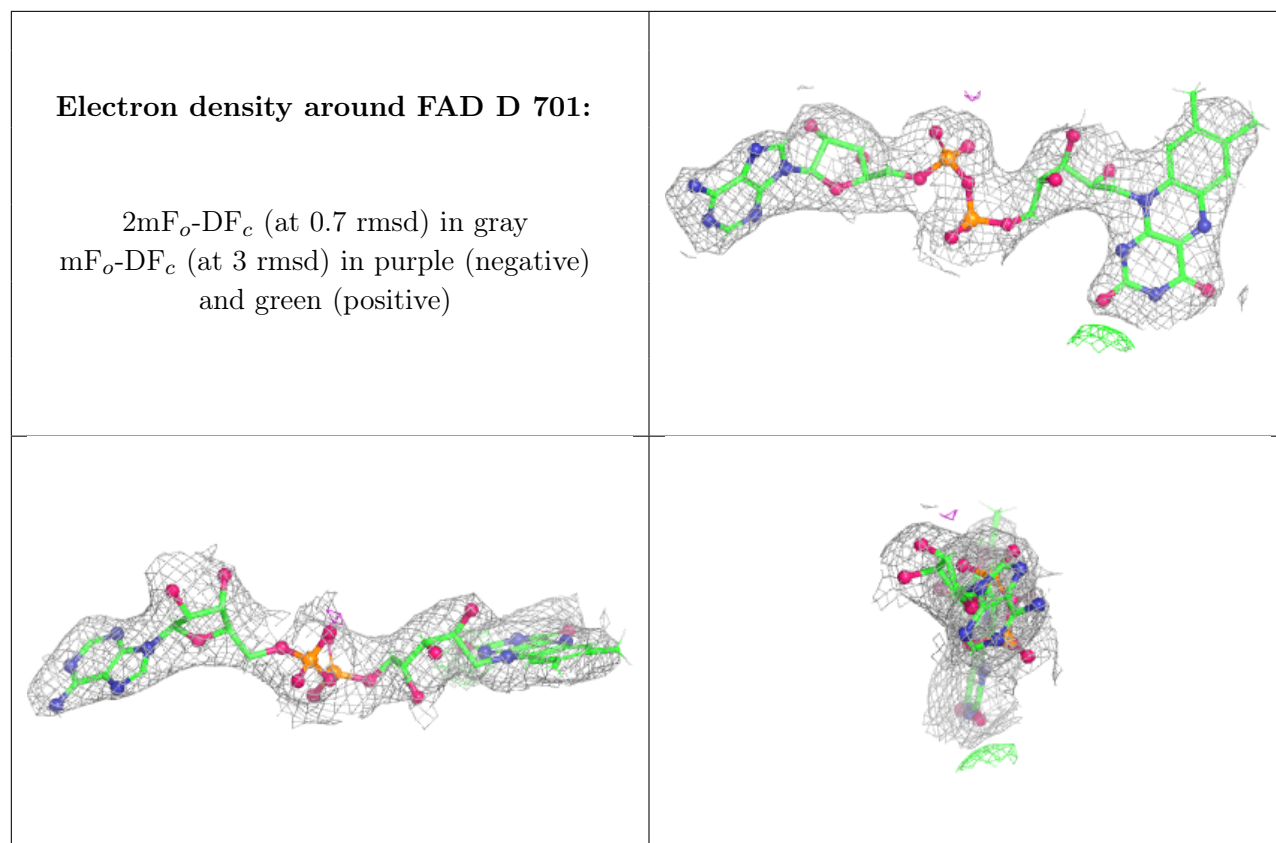
Electron density around FAD E 701:

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

**Electron density around FAD A 701:**

$2mF_o-DF_c$ (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.