



wwPDB X-ray Structure Validation Summary Report ⓘ

May 21, 2020 – 09:05 am BST

PDB ID : 3UKH
Title : Crystal structure of udp-galactopyranose mutase from *Aspergillus fumigatus* in complex with UDPGALP (non-reduced)
Authors : Van Straaten, K.E.; Sanders, D.A.R.
Deposited on : 2011-11-09
Resolution : 2.30 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 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

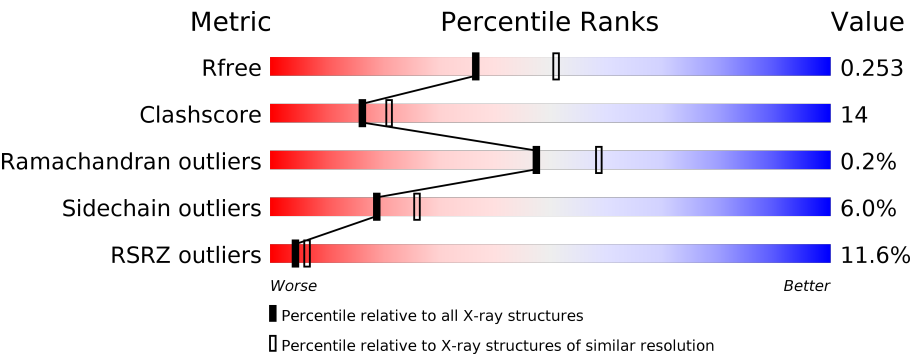
1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.30 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	5042 (2.30-2.30)
Clashscore	141614	5643 (2.30-2.30)
Ramachandran outliers	138981	5575 (2.30-2.30)
Sidechain outliers	138945	5575 (2.30-2.30)
RSRZ outliers	127900	4938 (2.30-2.30)

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 ≥ 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	<div><div>8%</div><div><div></div><div>73%</div><div>21%</div><div></div></div><div></div></div>
1	B	519	<div><div>12%</div><div><div></div><div>75%</div><div>20%</div><div></div></div><div></div></div>
1	C	519	<div><div>12%</div><div><div></div><div>70%</div><div>26%</div><div></div></div><div></div></div>
1	D	519	<div><div>10%</div><div><div></div><div>78%</div><div>17%</div><div></div></div><div></div></div>
1	E	519	<div><div>18%</div><div><div></div><div>71%</div><div>23%</div><div></div></div><div></div></div>
1	F	519	<div><div>6%</div><div><div></div><div>77%</div><div>17%</div><div></div></div><div></div></div>

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Mol	Chain	Length	Quality of chain
1	G	519	
1	H	519	

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	GDU	A	521	-	-	-	X
3	GDU	B	521	-	-	-	X
3	GDU	D	521	-	-	-	X
3	GDU	E	521	-	-	-	X
3	GDU	F	521	-	-	-	X
3	GDU	G	521	-	-	-	X

2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 34881 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 UDP-galactopyranose mutase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	504	Total	C	N	O	S	0	15	0
			4080	2590	699	768	23			
1	B	510	Total	C	N	O	S	0	15	0
			4126	2619	711	774	22			
1	C	511	Total	C	N	O	S	0	42	0
			4270	2713	734	801	22			
1	D	510	Total	C	N	O	S	0	3	0
			4035	2560	694	759	22			
1	E	510	Total	C	N	O	S	0	9	0
			4074	2586	700	767	21			
1	F	504	Total	C	N	O	S	0	8	0
			4026	2554	689	761	22			
1	G	504	Total	C	N	O	S	0	1	0
			3977	2525	680	751	21			
1	H	511	Total	C	N	O	S	0	42	0
			4301	2733	740	807	21			

There are 80 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	511	LEU	-	EXPRESSION TAG	UNP Q4W1X2
A	512	GLU	-	EXPRESSION TAG	UNP Q4W1X2
A	513	LEU	-	EXPRESSION TAG	UNP Q4W1X2
A	514	GLU	-	EXPRESSION TAG	UNP Q4W1X2
A	515	HIS	-	EXPRESSION TAG	UNP Q4W1X2
A	516	HIS	-	EXPRESSION TAG	UNP Q4W1X2
A	517	HIS	-	EXPRESSION TAG	UNP Q4W1X2
A	518	HIS	-	EXPRESSION TAG	UNP Q4W1X2
A	519	HIS	-	EXPRESSION TAG	UNP Q4W1X2
A	520	HIS	-	EXPRESSION TAG	UNP Q4W1X2
B	511	LEU	-	EXPRESSION TAG	UNP Q4W1X2
B	512	GLU	-	EXPRESSION TAG	UNP Q4W1X2
B	513	LEU	-	EXPRESSION TAG	UNP Q4W1X2

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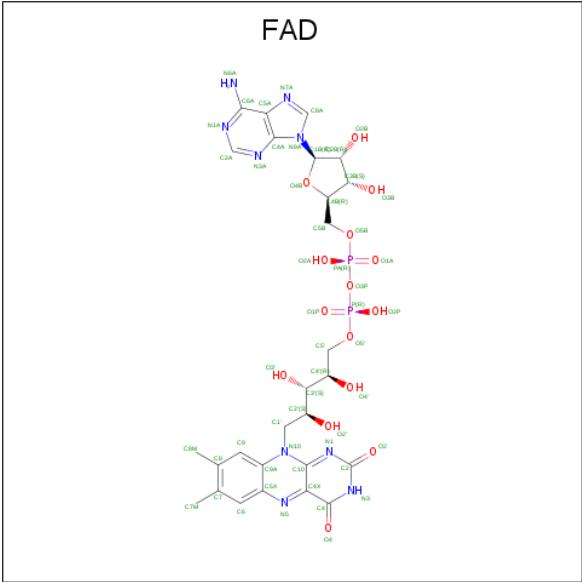
Chain	Residue	Modelled	Actual	Comment	Reference
B	514	GLU	-	EXPRESSION TAG	UNP Q4W1X2
B	515	HIS	-	EXPRESSION TAG	UNP Q4W1X2
B	516	HIS	-	EXPRESSION TAG	UNP Q4W1X2
B	517	HIS	-	EXPRESSION TAG	UNP Q4W1X2
B	518	HIS	-	EXPRESSION TAG	UNP Q4W1X2
B	519	HIS	-	EXPRESSION TAG	UNP Q4W1X2
B	520	HIS	-	EXPRESSION TAG	UNP Q4W1X2
C	511	LEU	-	EXPRESSION TAG	UNP Q4W1X2
C	512	GLU	-	EXPRESSION TAG	UNP Q4W1X2
C	513	LEU	-	EXPRESSION TAG	UNP Q4W1X2
C	514	GLU	-	EXPRESSION TAG	UNP Q4W1X2
C	515	HIS	-	EXPRESSION TAG	UNP Q4W1X2
C	516	HIS	-	EXPRESSION TAG	UNP Q4W1X2
C	517	HIS	-	EXPRESSION TAG	UNP Q4W1X2
C	518	HIS	-	EXPRESSION TAG	UNP Q4W1X2
C	519	HIS	-	EXPRESSION TAG	UNP Q4W1X2
C	520	HIS	-	EXPRESSION TAG	UNP Q4W1X2
D	511	LEU	-	EXPRESSION TAG	UNP Q4W1X2
D	512	GLU	-	EXPRESSION TAG	UNP Q4W1X2
D	513	LEU	-	EXPRESSION TAG	UNP Q4W1X2
D	514	GLU	-	EXPRESSION TAG	UNP Q4W1X2
D	515	HIS	-	EXPRESSION TAG	UNP Q4W1X2
D	516	HIS	-	EXPRESSION TAG	UNP Q4W1X2
D	517	HIS	-	EXPRESSION TAG	UNP Q4W1X2
D	518	HIS	-	EXPRESSION TAG	UNP Q4W1X2
D	519	HIS	-	EXPRESSION TAG	UNP Q4W1X2
D	520	HIS	-	EXPRESSION TAG	UNP Q4W1X2
E	511	LEU	-	EXPRESSION TAG	UNP Q4W1X2
E	512	GLU	-	EXPRESSION TAG	UNP Q4W1X2
E	513	LEU	-	EXPRESSION TAG	UNP Q4W1X2
E	514	GLU	-	EXPRESSION TAG	UNP Q4W1X2
E	515	HIS	-	EXPRESSION TAG	UNP Q4W1X2
E	516	HIS	-	EXPRESSION TAG	UNP Q4W1X2
E	517	HIS	-	EXPRESSION TAG	UNP Q4W1X2
E	518	HIS	-	EXPRESSION TAG	UNP Q4W1X2
E	519	HIS	-	EXPRESSION TAG	UNP Q4W1X2
E	520	HIS	-	EXPRESSION TAG	UNP Q4W1X2
F	511	LEU	-	EXPRESSION TAG	UNP Q4W1X2
F	512	GLU	-	EXPRESSION TAG	UNP Q4W1X2
F	513	LEU	-	EXPRESSION TAG	UNP Q4W1X2
F	514	GLU	-	EXPRESSION TAG	UNP Q4W1X2
F	515	HIS	-	EXPRESSION TAG	UNP Q4W1X2

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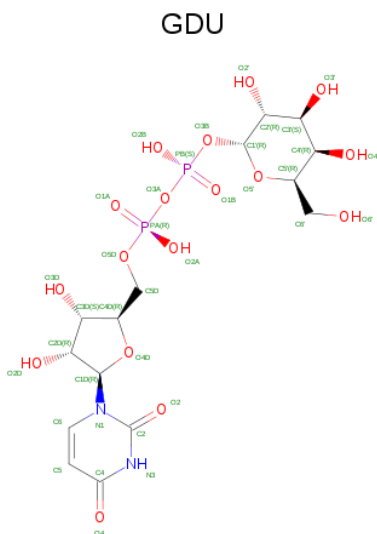
Chain	Residue	Modelled	Actual	Comment	Reference
F	516	HIS	-	EXPRESSION TAG	UNP Q4W1X2
F	517	HIS	-	EXPRESSION TAG	UNP Q4W1X2
F	518	HIS	-	EXPRESSION TAG	UNP Q4W1X2
F	519	HIS	-	EXPRESSION TAG	UNP Q4W1X2
F	520	HIS	-	EXPRESSION TAG	UNP Q4W1X2
G	511	LEU	-	EXPRESSION TAG	UNP Q4W1X2
G	512	GLU	-	EXPRESSION TAG	UNP Q4W1X2
G	513	LEU	-	EXPRESSION TAG	UNP Q4W1X2
G	514	GLU	-	EXPRESSION TAG	UNP Q4W1X2
G	515	HIS	-	EXPRESSION TAG	UNP Q4W1X2
G	516	HIS	-	EXPRESSION TAG	UNP Q4W1X2
G	517	HIS	-	EXPRESSION TAG	UNP Q4W1X2
G	518	HIS	-	EXPRESSION TAG	UNP Q4W1X2
G	519	HIS	-	EXPRESSION TAG	UNP Q4W1X2
G	520	HIS	-	EXPRESSION TAG	UNP Q4W1X2
H	511	LEU	-	EXPRESSION TAG	UNP Q4W1X2
H	512	GLU	-	EXPRESSION TAG	UNP Q4W1X2
H	513	LEU	-	EXPRESSION TAG	UNP Q4W1X2
H	514	GLU	-	EXPRESSION TAG	UNP Q4W1X2
H	515	HIS	-	EXPRESSION TAG	UNP Q4W1X2
H	516	HIS	-	EXPRESSION TAG	UNP Q4W1X2
H	517	HIS	-	EXPRESSION TAG	UNP Q4W1X2
H	518	HIS	-	EXPRESSION TAG	UNP Q4W1X2
H	519	HIS	-	EXPRESSION TAG	UNP Q4W1X2
H	520	HIS	-	EXPRESSION TAG	UNP Q4W1X2

- 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	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		
2	G	1	Total	C	N	O	P	0	0
			53	27	9	15	2		

- Molecule 3 is GALACTOSE-URIDINE-5'-DIPHOSPHATE (three-letter code: GDU) (formula: C₁₅H₂₄N₂O₁₇P₂).

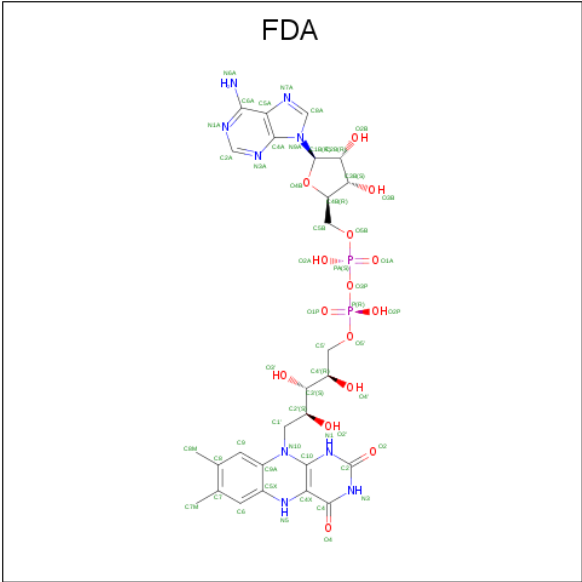


Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	A	1	Total 36	C 15	N 2	O 17	P 2	0	0
3	B	1	Total 36	C 15	N 2	O 17	P 2	0	0
3	C	1	Total 36	C 15	N 2	O 17	P 2	0	0
3	D	1	Total 36	C 15	N 2	O 17	P 2	0	0
3	E	1	Total 36	C 15	N 2	O 17	P 2	0	0
3	F	1	Total 36	C 15	N 2	O 17	P 2	0	0
3	G	1	Total 36	C 15	N 2	O 17	P 2	0	0
3	H	1	Total 36	C 15	N 2	O 17	P 2	0	0

- Molecule 4 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	B	1	Total Cl 1 1	0	0
4	A	1	Total Cl 1 1	0	0

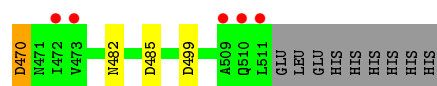
- Molecule 5 is DIHYDROFLAVINE-ADENINE DINUCLEOTIDE (three-letter code: FDA) (formula: $C_{27}H_{35}N_9O_{15}P_2$).



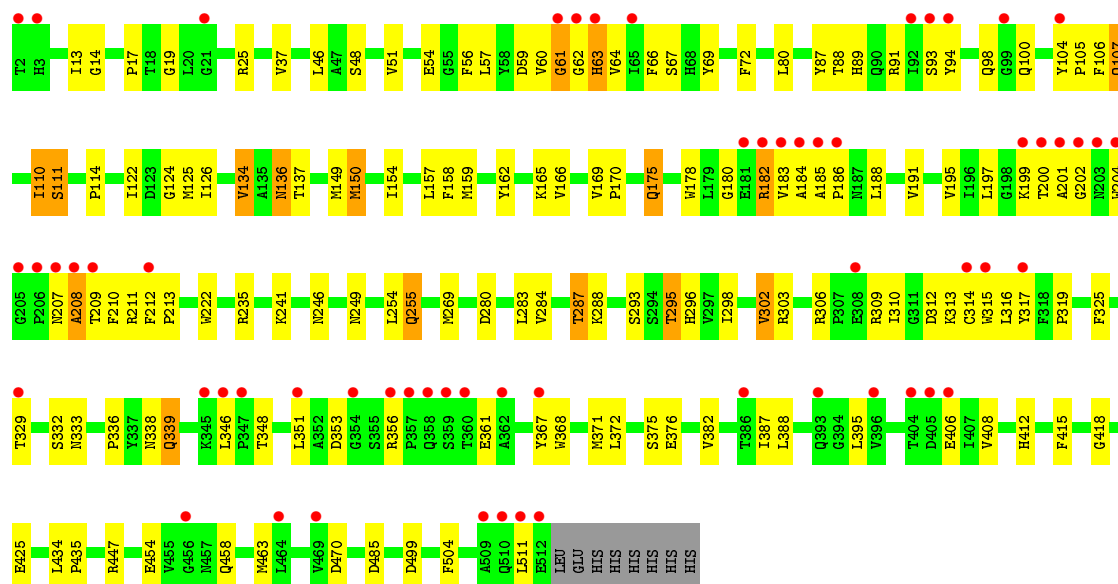
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
5	C	1	Total	C	N	O	P	0	0
			53	27	9	15	2		
5	H	1	Total	C	N	O	P	0	0
			53	27	9	15	2		

- Molecule 6 is water.

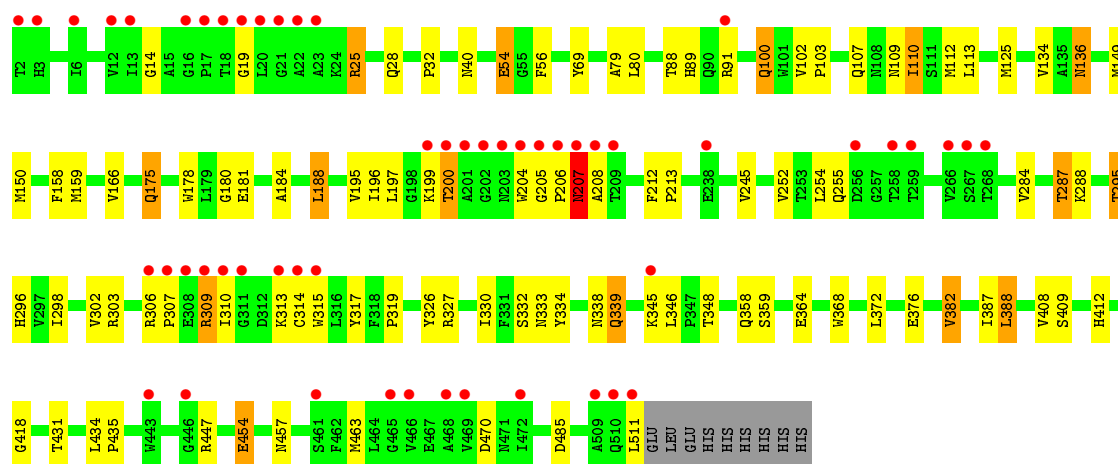
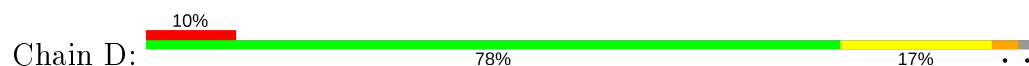
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	207	Total	O	0	0
			207	207		
6	B	180	Total	O	0	0
			180	180		
6	C	150	Total	O	0	0
			150	150		
6	D	172	Total	O	0	0
			172	172		
6	E	137	Total	O	0	0
			137	137		
6	F	126	Total	O	0	0
			126	126		
6	G	156	Total	O	0	0
			156	156		
6	H	150	Total	O	0	0
			150	150		



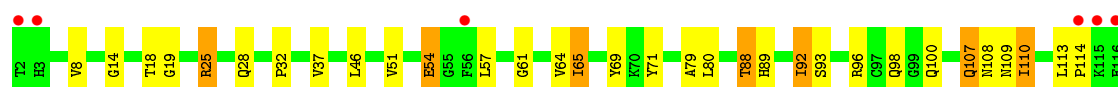
• Molecule 1: UDP-galactopyranose mutase

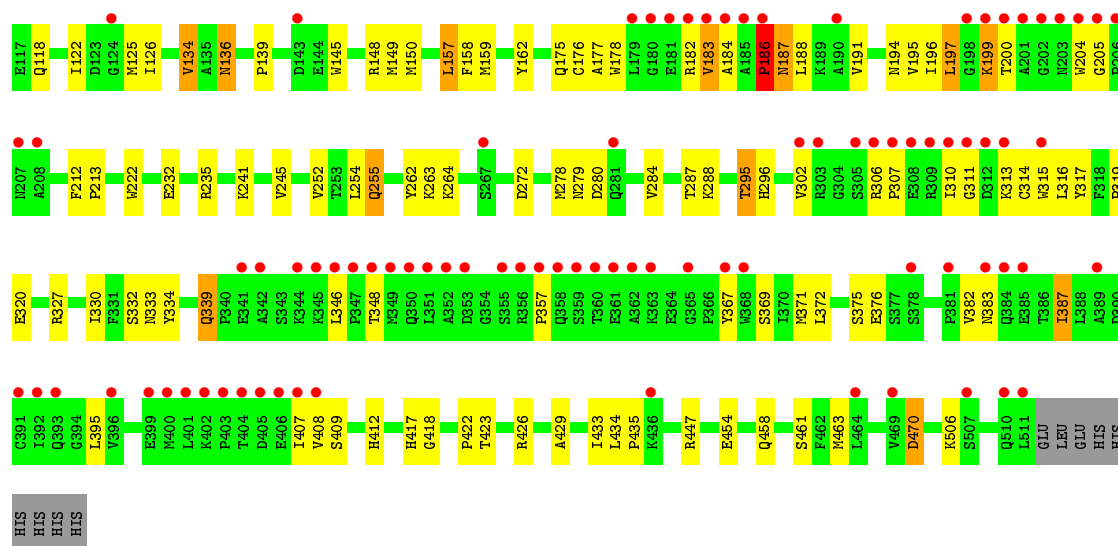


• Molecule 1: UDP-galactopyranose mutase

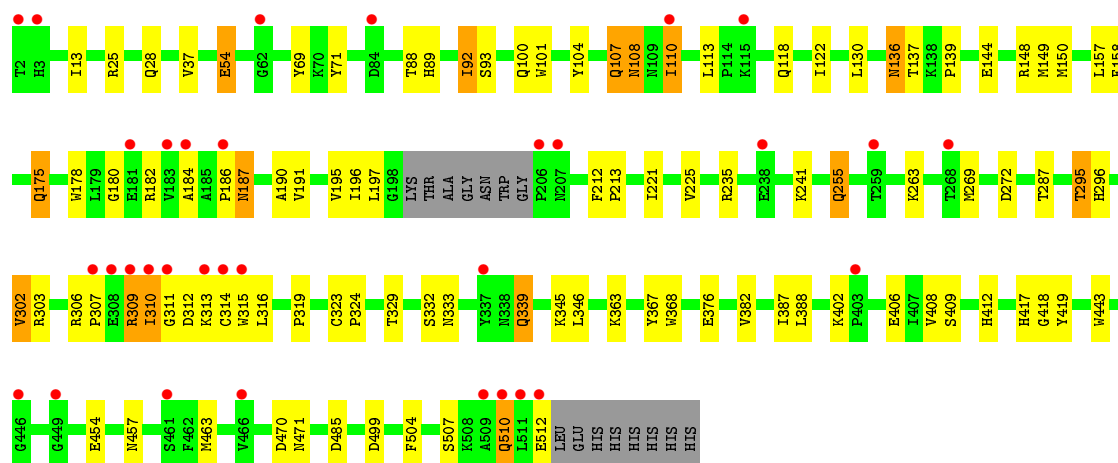
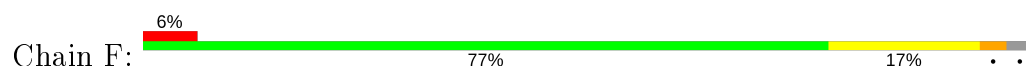


• Molecule 1: UDP-galactopyranose mutase

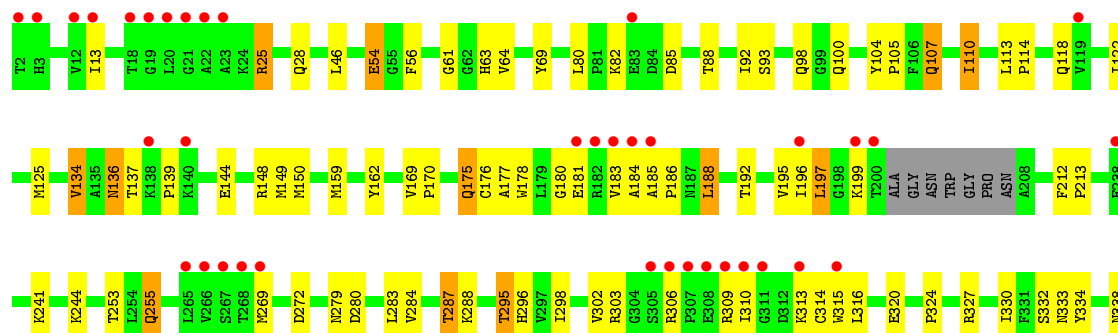
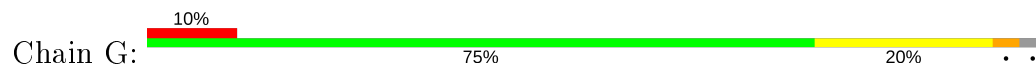


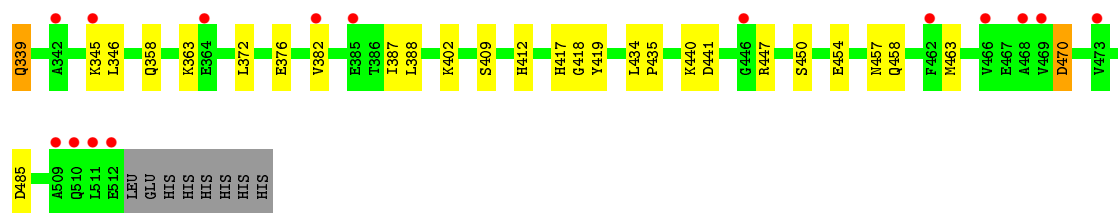


• Molecule 1: UDP-galactopyranose mutase

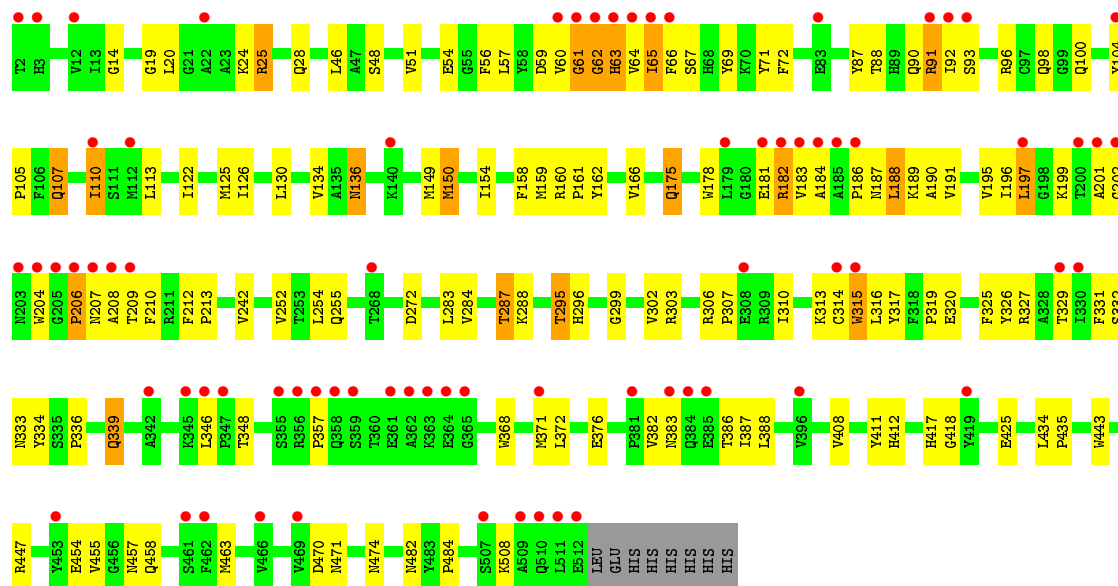


• Molecule 1: UDP-galactopyranose mutase





● Molecule 1: UDP-galactopyranose mutase



4 Data and refinement statistics

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α , β , γ	71.97Å 129.26Å 173.88Å 89.87° 84.64° 81.21°	Depositor
Resolution (Å)	35.55 – 2.30 35.55 – 2.30	Depositor EDS
% Data completeness (in resolution range)	97.3 (35.55-2.30) 97.3 (35.55-2.30)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	0.07	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.57 (at 2.29Å)	Xtriage
Refinement program	PHENIX 1.7.1 _743	Depositor
R, R_{free}	0.222 , 0.264 0.210 , 0.253	Depositor DCC
R_{free} test set	13334 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å ²)	50.3	Xtriage
Anisotropy	0.324	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 48.5	EDS
L-test for twinning ²	$\langle L \rangle = 0.51$, $\langle L^2 \rangle = 0.35$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	34881	wwPDB-VP
Average B, all atoms (Å ²)	55.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.09% 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

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: FDA, GDU, FAD, CL

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	0.25	0/4180	0.43	0/5680
1	B	0.25	0/4230	0.43	0/5751
1	C	0.25	0/4378	0.43	0/5951
1	D	0.25	0/4136	0.43	0/5621
1	E	0.25	0/4176	0.43	0/5677
1	F	0.24	0/4125	0.42	0/5603
1	G	0.25	0/4074	0.43	0/5534
1	H	0.26	0/4413	0.44	0/6000
All	All	0.25	0/33712	0.43	0/45817

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	E	0	1
1	H	0	1
All	All	0	2

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	E	186[B]	PRO	Peptide
1	H	206[A]	PRO	Peptide

5.2 Too-close contacts ⓘ

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	4080	0	3999	120	0
1	B	4126	0	4041	123	0
1	C	4270	0	4171	135	0
1	D	4035	0	3951	91	0
1	E	4074	0	3992	130	0
1	F	4026	0	3941	88	0
1	G	3977	0	3899	88	0
1	H	4301	0	4193	154	0
2	A	53	0	30	6	0
2	B	53	0	30	4	0
2	D	53	0	30	2	0
2	E	53	0	30	2	0
2	F	53	0	30	6	0
2	G	53	0	30	4	0
3	A	36	0	22	10	0
3	B	36	0	22	10	0
3	C	36	0	22	7	0
3	D	36	0	22	4	0
3	E	36	0	22	12	0
3	F	36	0	22	3	0
3	G	36	0	22	8	0
3	H	36	0	22	11	0
4	A	1	0	0	1	0
4	B	1	0	0	0	0
5	C	53	0	32	6	0
5	H	53	0	32	6	0
6	A	207	0	0	4	0
6	B	180	0	0	13	0
6	C	150	0	0	12	0
6	D	172	0	0	8	0
6	E	137	0	0	7	0
6	F	126	0	0	5	0
6	G	156	0	0	4	0
6	H	150	0	0	4	0
All	All	34881	0	32607	949	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 14.

The worst 5 of 949 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:H:104[A]:TYR:O	1:H:202[A]:GLY:HA2	1.68	0.92
1:E:175:GLN:HG2	6:E:820:HOH:O	1.67	0.92
3:B:521:GDU:O1A	6:B:1234:HOH:O	1.88	0.89
1:B:109:ASN:OD1	1:B:200:THR:HG21	1.74	0.88
1:F:296:HIS:HD2	1:F:412:HIS:HE1	1.22	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	515/519 (99%)	501 (97%)	14 (3%)	0	100	100
1	B	523/519 (101%)	501 (96%)	22 (4%)	0	100	100
1	C	541/519 (104%)	509 (94%)	28 (5%)	4 (1%)	22	26
1	D	511/519 (98%)	494 (97%)	16 (3%)	1 (0%)	47	58
1	E	517/519 (100%)	487 (94%)	27 (5%)	3 (1%)	25	31
1	F	508/519 (98%)	490 (96%)	15 (3%)	3 (1%)	25	31
1	G	501/519 (96%)	481 (96%)	20 (4%)	0	100	100
1	H	545/519 (105%)	515 (94%)	26 (5%)	4 (1%)	22	26
All	All	4161/4152 (100%)	3978 (96%)	168 (4%)	15 (0%)	47	42

5 of 15 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	E	186[A]	PRO
1	E	186[B]	PRO

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Mol	Chain	Res	Type
1	E	187	ASN
1	C	208[B]	ALA
1	H	61[A]	GLY

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	440/441 (100%)	415 (94%)	25 (6%)	20	28
1	B	443/441 (100%)	413 (93%)	30 (7%)	16	21
1	C	459/441 (104%)	428 (93%)	31 (7%)	16	21
1	D	435/441 (99%)	406 (93%)	29 (7%)	16	21
1	E	438/441 (99%)	412 (94%)	26 (6%)	19	27
1	F	436/441 (99%)	413 (95%)	23 (5%)	22	31
1	G	430/441 (98%)	406 (94%)	24 (6%)	21	29
1	H	461/441 (104%)	427 (93%)	34 (7%)	13	17
All	All	3542/3528 (100%)	3320 (94%)	222 (6%)	19	24

5 of 222 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	D	207	ASN
1	E	136	ASN
1	H	182[A]	ARG
1	D	287	THR
1	D	454	GLU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 163 such sidechains are listed below:

Mol	Chain	Res	Type
1	D	339	GLN
1	E	333	ASN

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Mol	Chain	Res	Type
1	H	175	GLN
1	D	393	GLN
1	E	98	GLN

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](#)

Of 18 ligands modelled in this entry, 2 are monoatomic - leaving 16 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	$\# Z > 2$
3	GDU	C	521	-	31,38,38	1.86	9 (29%)	41,58,58	1.35	5 (12%)
3	GDU	D	521	-	31,38,38	1.82	9 (29%)	41,58,58	1.55	6 (14%)
3	GDU	E	521	-	31,38,38	1.78	8 (25%)	41,58,58	1.67	8 (19%)
5	FDA	H	600	-	51,58,58	2.48	16 (31%)	60,89,89	1.91	16 (26%)
2	FAD	D	600	-	51,58,58	2.52	15 (29%)	60,89,89	1.85	16 (26%)
2	FAD	B	600	-	51,58,58	2.51	16 (31%)	60,89,89	1.86	17 (28%)
3	GDU	A	521	-	31,38,38	1.83	8 (25%)	41,58,58	1.48	5 (12%)
5	FDA	C	600	-	51,58,58	2.42	14 (27%)	60,89,89	1.85	13 (21%)
3	GDU	G	521	-	31,38,38	1.83	9 (29%)	41,58,58	1.51	5 (12%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	FAD	G	600	-	51,58,58	2.58	15 (29%)	60,89,89	2.04	20 (33%)
2	FAD	E	600	-	51,58,58	2.51	14 (27%)	60,89,89	1.87	16 (26%)
2	FAD	F	600	-	51,58,58	2.52	15 (29%)	60,89,89	1.95	14 (23%)
3	GDU	F	521	-	31,38,38	1.81	9 (29%)	41,58,58	1.42	5 (12%)
3	GDU	H	521	-	31,38,38	1.86	8 (25%)	41,58,58	1.45	5 (12%)
2	FAD	A	600	-	51,58,58	2.44	15 (29%)	60,89,89	1.87	17 (28%)
3	GDU	B	521	-	31,38,38	1.84	9 (29%)	41,58,58	1.47	5 (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	GDU	C	521	-	-	12/21/59/59	0/3/3/3
3	GDU	D	521	-	-	9/21/59/59	0/3/3/3
3	GDU	E	521	-	-	11/21/59/59	0/3/3/3
5	FDA	H	600	-	-	9/30/50/50	0/6/6/6
2	FAD	D	600	-	-	13/30/50/50	0/6/6/6
2	FAD	B	600	-	-	11/30/50/50	0/6/6/6
3	GDU	A	521	-	-	8/21/59/59	0/3/3/3
5	FDA	C	600	-	-	9/30/50/50	0/6/6/6
3	GDU	G	521	-	-	11/21/59/59	0/3/3/3
2	FAD	G	600	-	-	12/30/50/50	0/6/6/6
2	FAD	E	600	-	-	13/30/50/50	0/6/6/6
2	FAD	F	600	-	-	15/30/50/50	0/6/6/6
3	GDU	F	521	-	-	10/21/59/59	0/3/3/3
3	GDU	H	521	-	-	10/21/59/59	0/3/3/3
2	FAD	A	600	-	-	13/30/50/50	0/6/6/6
3	GDU	B	521	-	-	10/21/59/59	0/3/3/3

The worst 5 of 189 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	G	600	FAD	C10-N1	8.64	1.44	1.33
2	F	600	FAD	C10-N1	8.63	1.44	1.33
2	G	600	FAD	C1'-N10	-8.41	1.39	1.48

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	H	600	FDA	C1'-N10	-8.32	1.39	1.48
2	B	600	FAD	C10-N1	8.29	1.43	1.33

The worst 5 of 173 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	C	600	FDA	C4-N3-C2	6.36	120.51	115.14
2	A	600	FAD	C4-N3-C2	6.22	120.40	115.14
2	F	600	FAD	C4-N3-C2	6.07	120.27	115.14
2	D	600	FAD	C4-N3-C2	5.94	120.16	115.14
2	B	600	FAD	C4-N3-C2	5.93	120.14	115.14

There are no chirality outliers.

5 of 176 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	H	600	FDA	C2'-C1'-N10-C9A
5	H	600	FDA	C1'-C2'-C3'-O3'
5	H	600	FDA	C1'-C2'-C3'-C4'
5	H	600	FDA	O2'-C2'-C3'-O3'
5	H	600	FDA	O2'-C2'-C3'-C4'

There are no ring outliers.

16 monomers are involved in 90 short contacts:

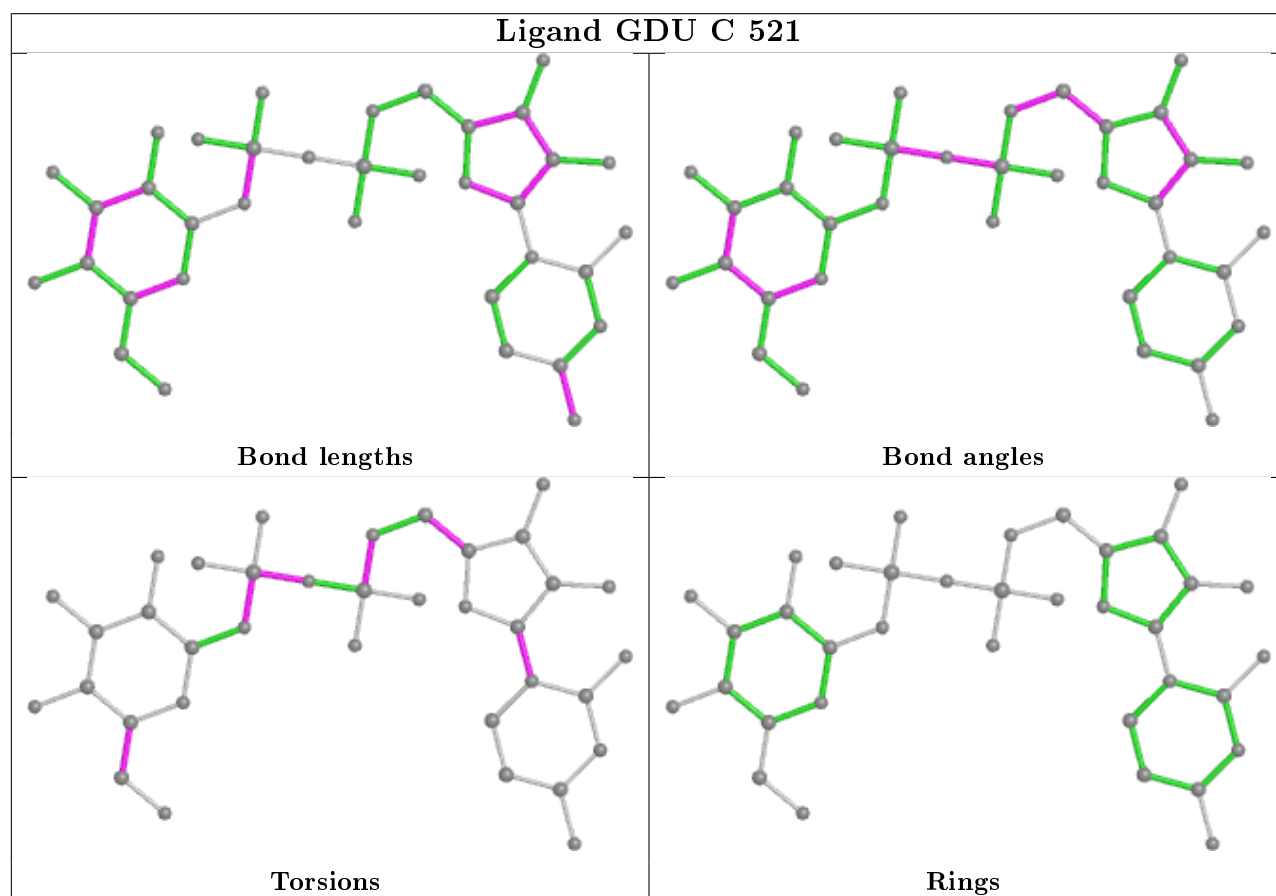
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	C	521	GDU	7	0
3	D	521	GDU	4	0
3	E	521	GDU	12	0
5	H	600	FDA	6	0
2	D	600	FAD	2	0
2	B	600	FAD	4	0
3	A	521	GDU	10	0
5	C	600	FDA	6	0
3	G	521	GDU	8	0
2	G	600	FAD	4	0
2	E	600	FAD	2	0
2	F	600	FAD	6	0
3	F	521	GDU	3	0
3	H	521	GDU	11	0
2	A	600	FAD	6	0

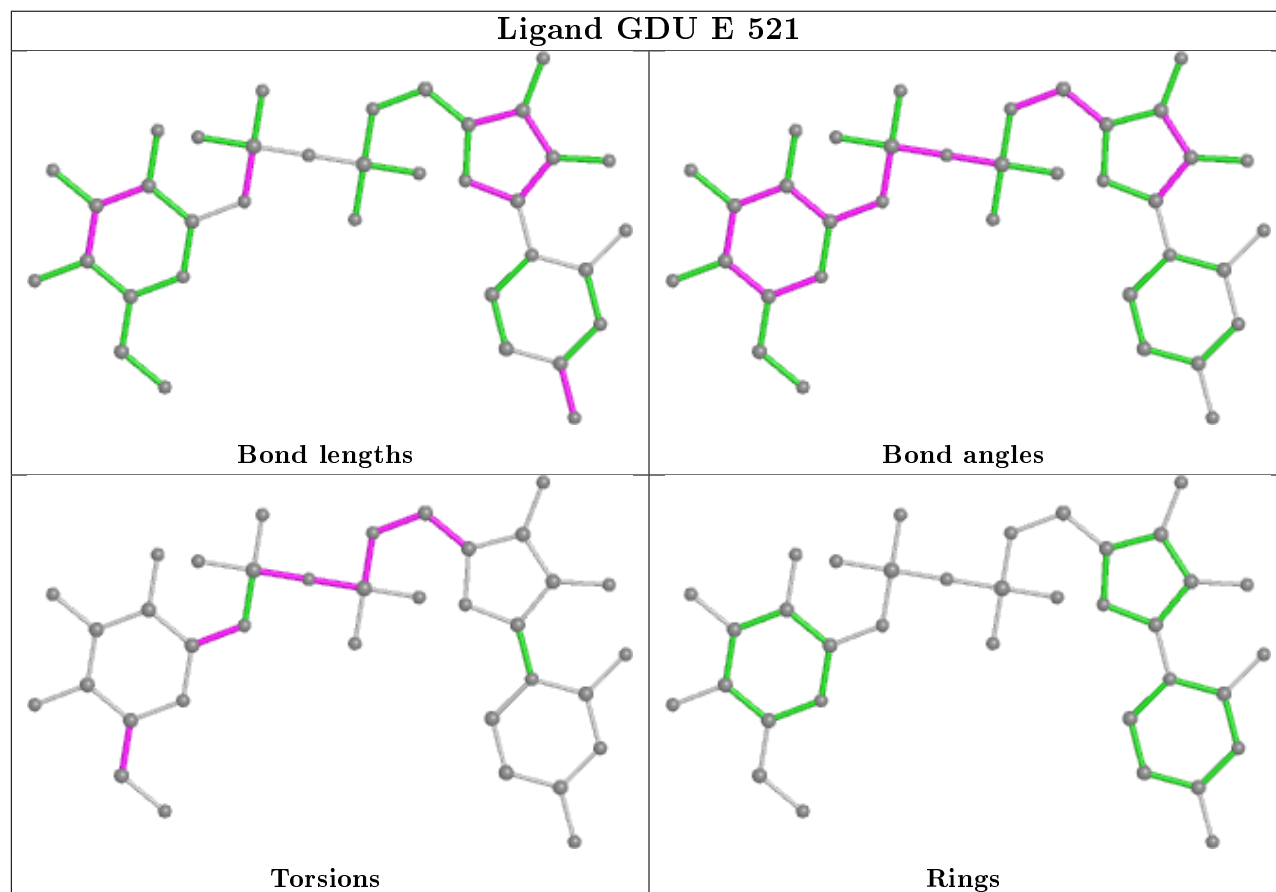
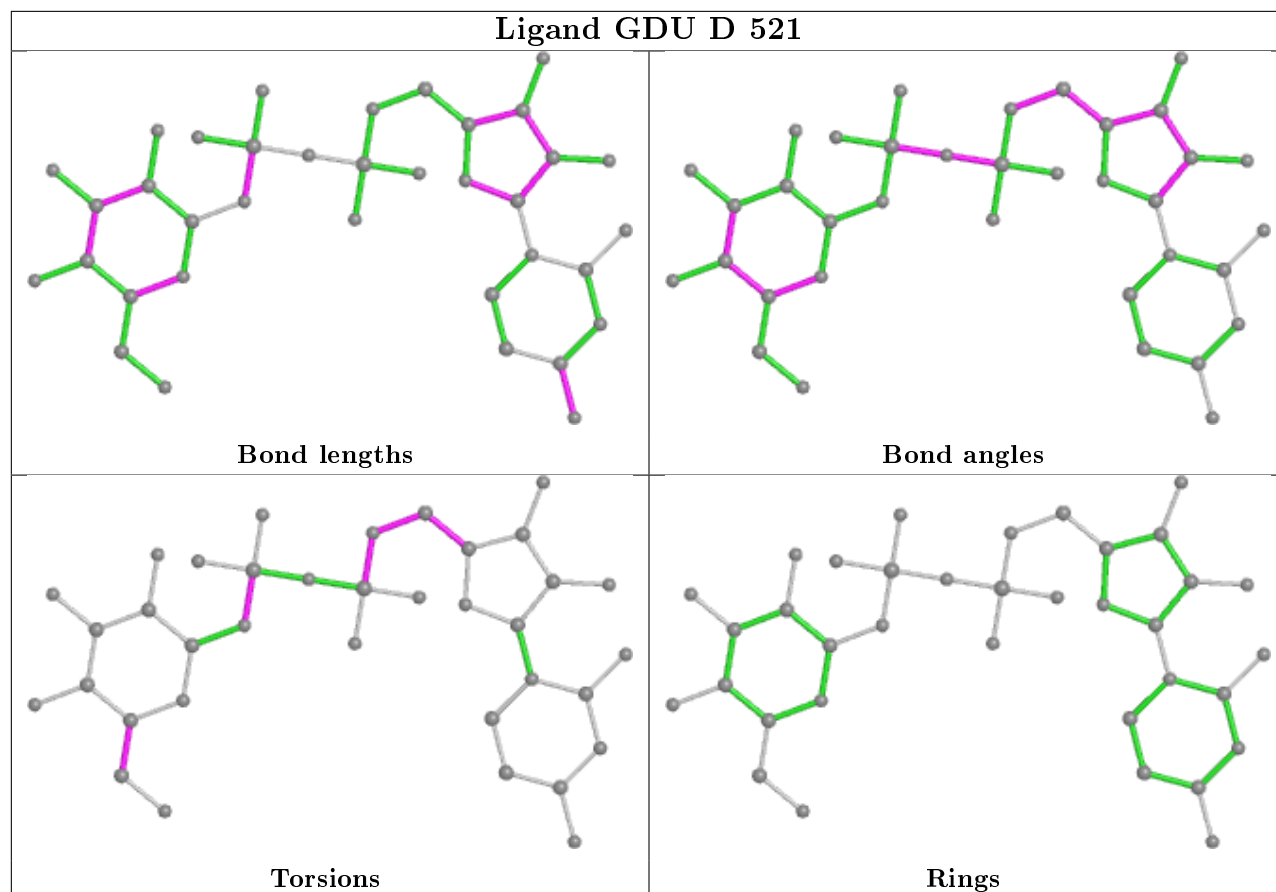
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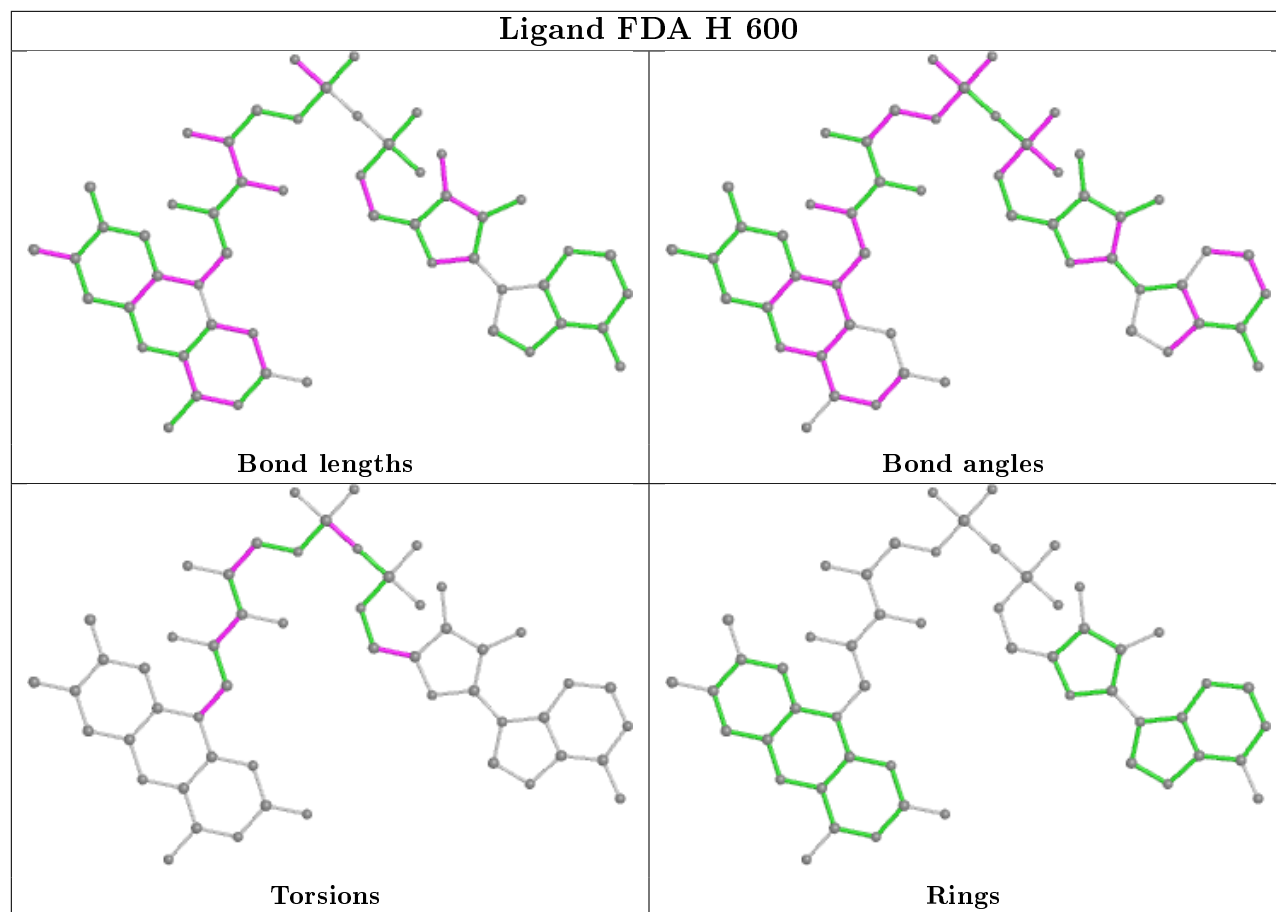
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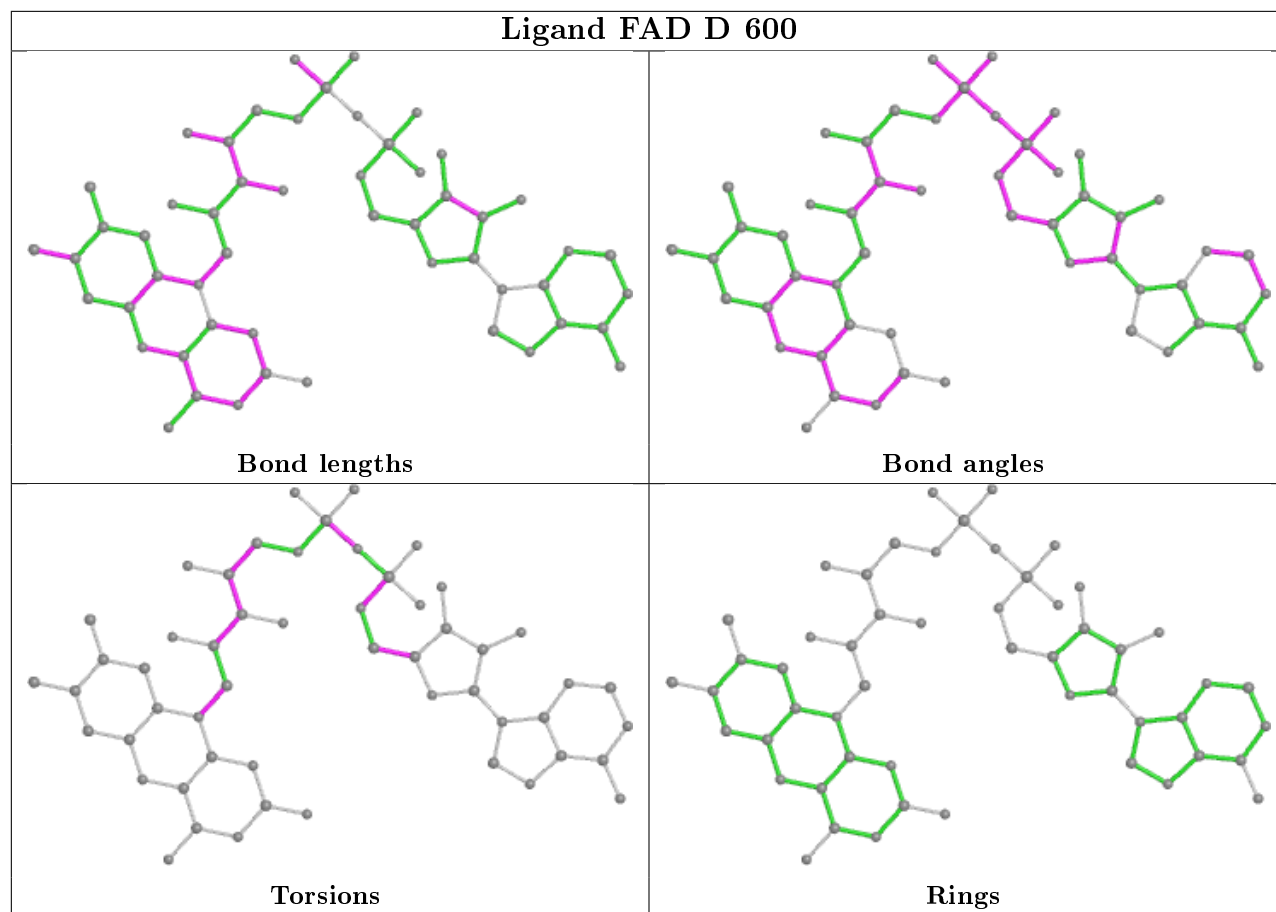
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	B	521	GDU	10	0

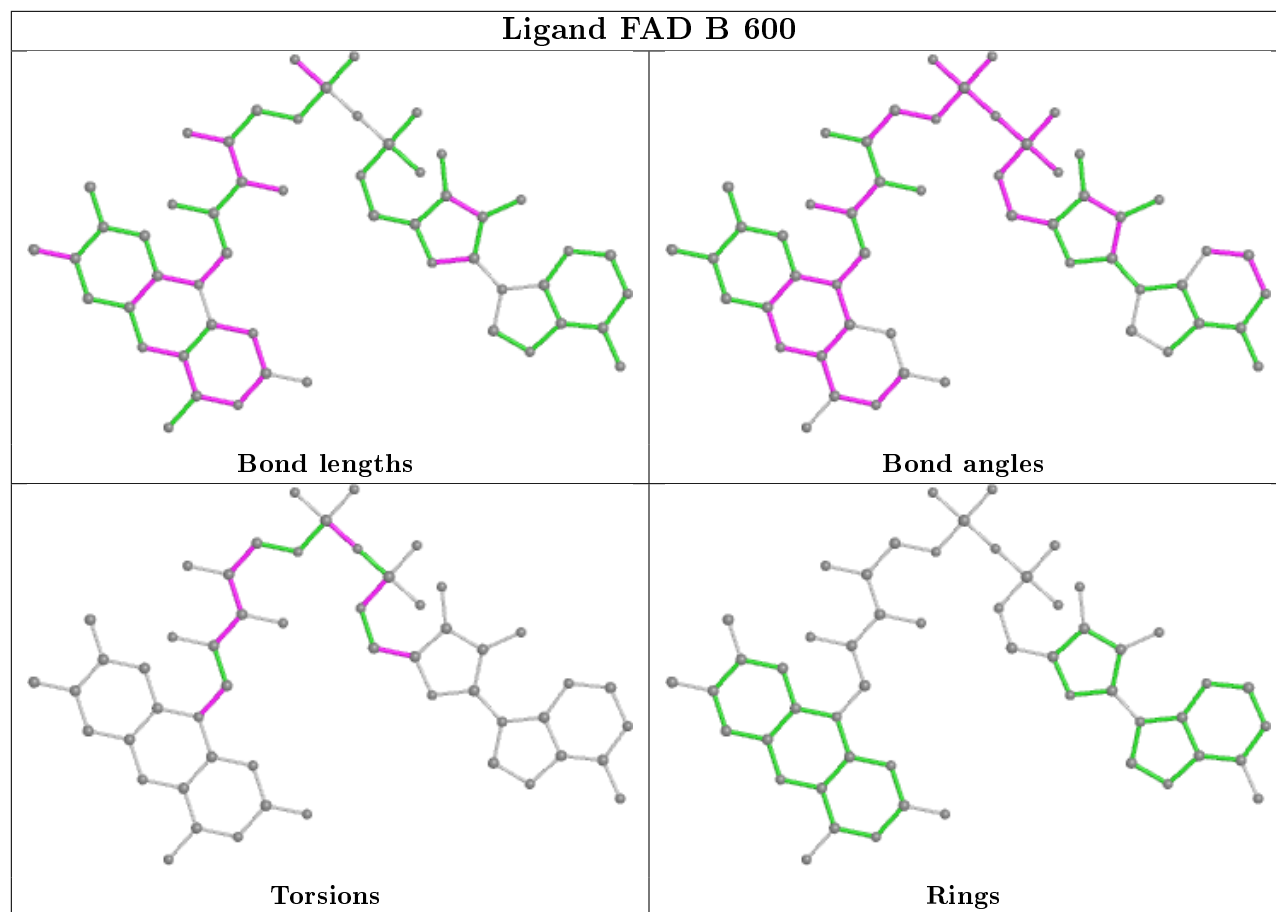
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

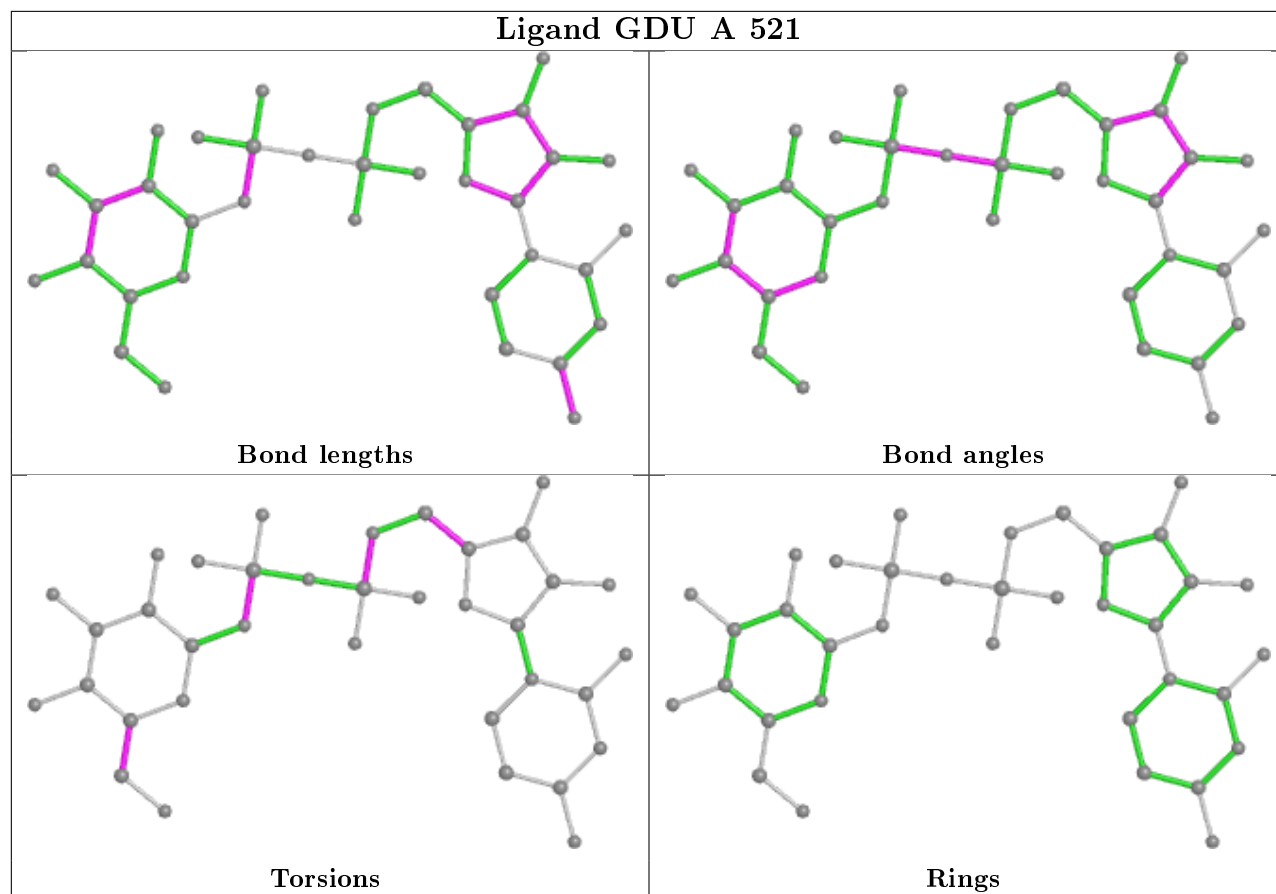


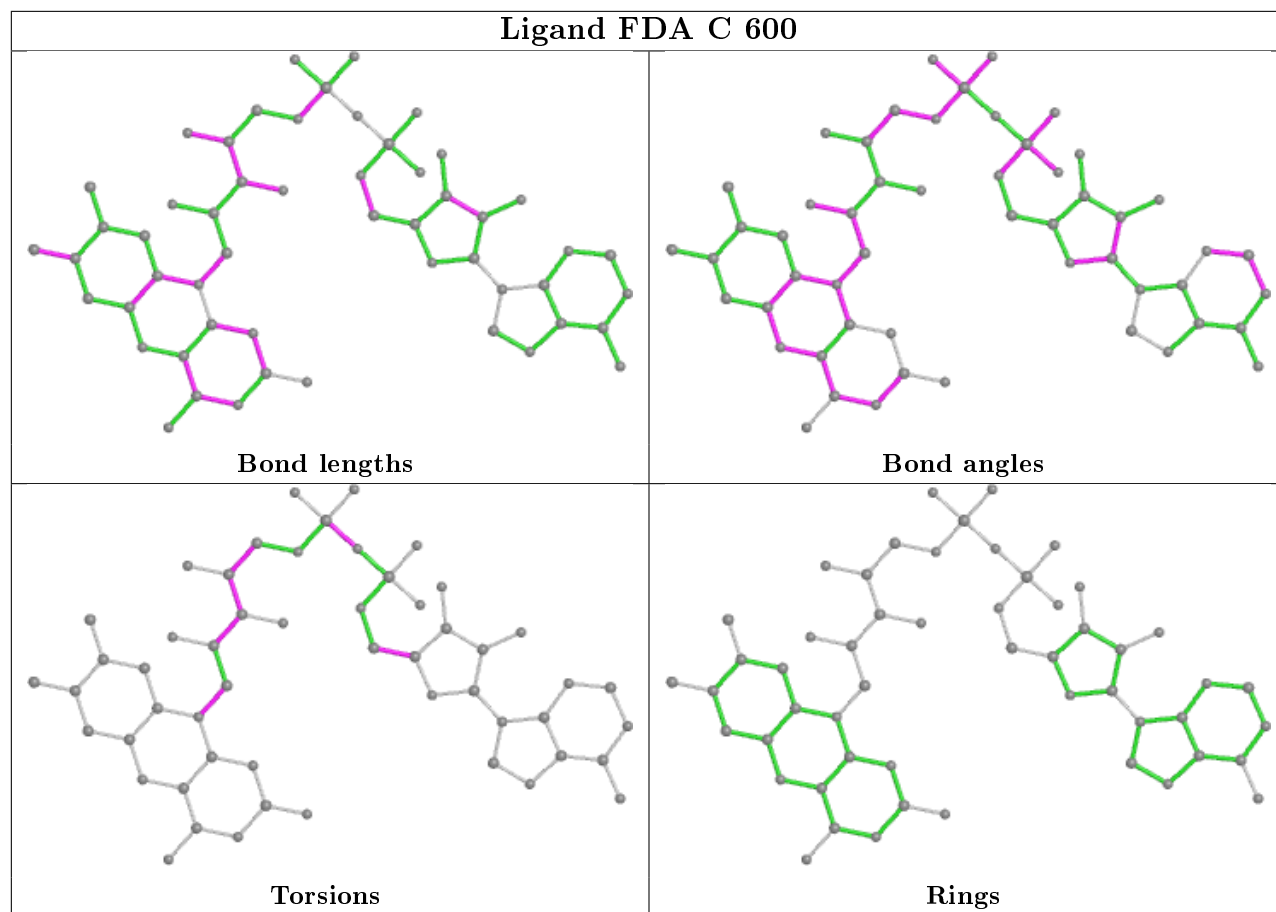


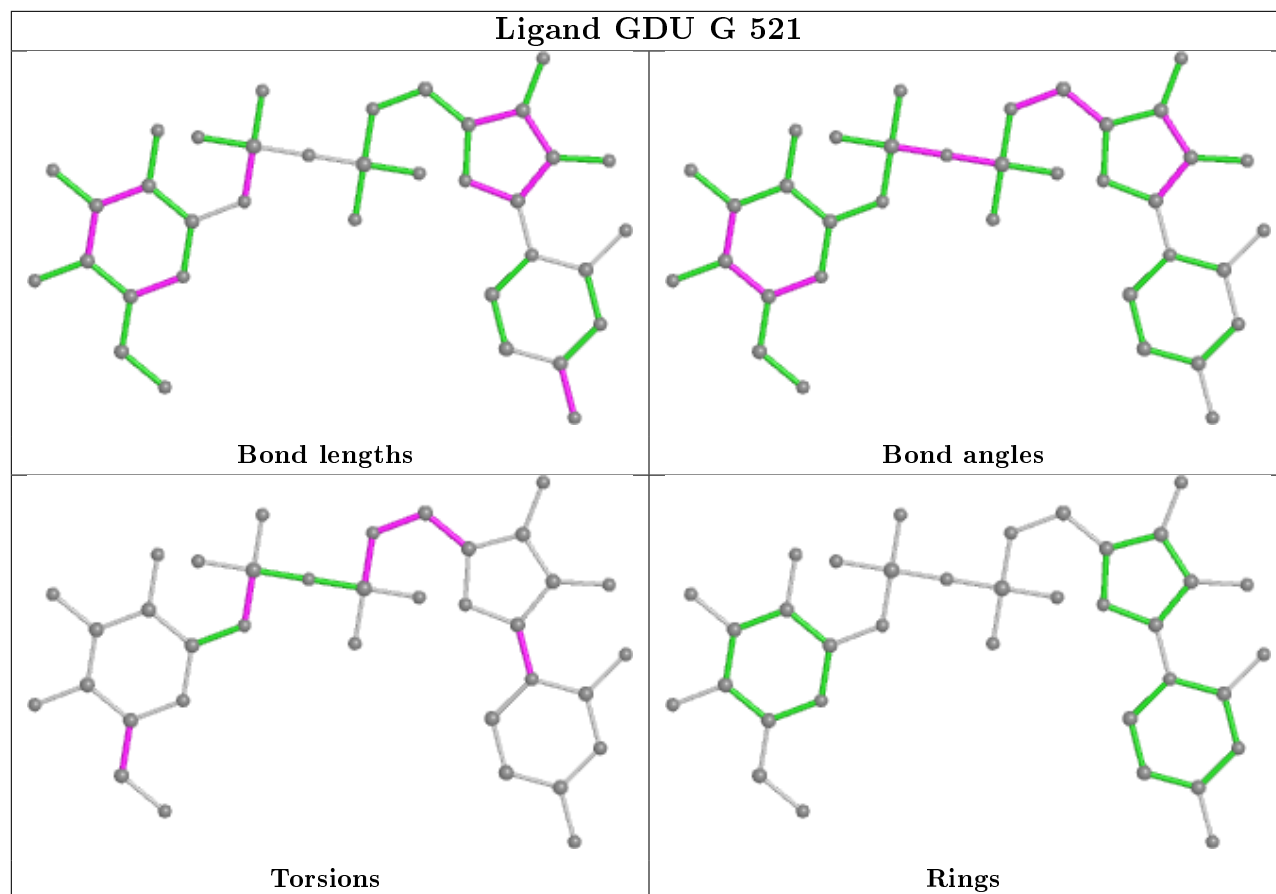


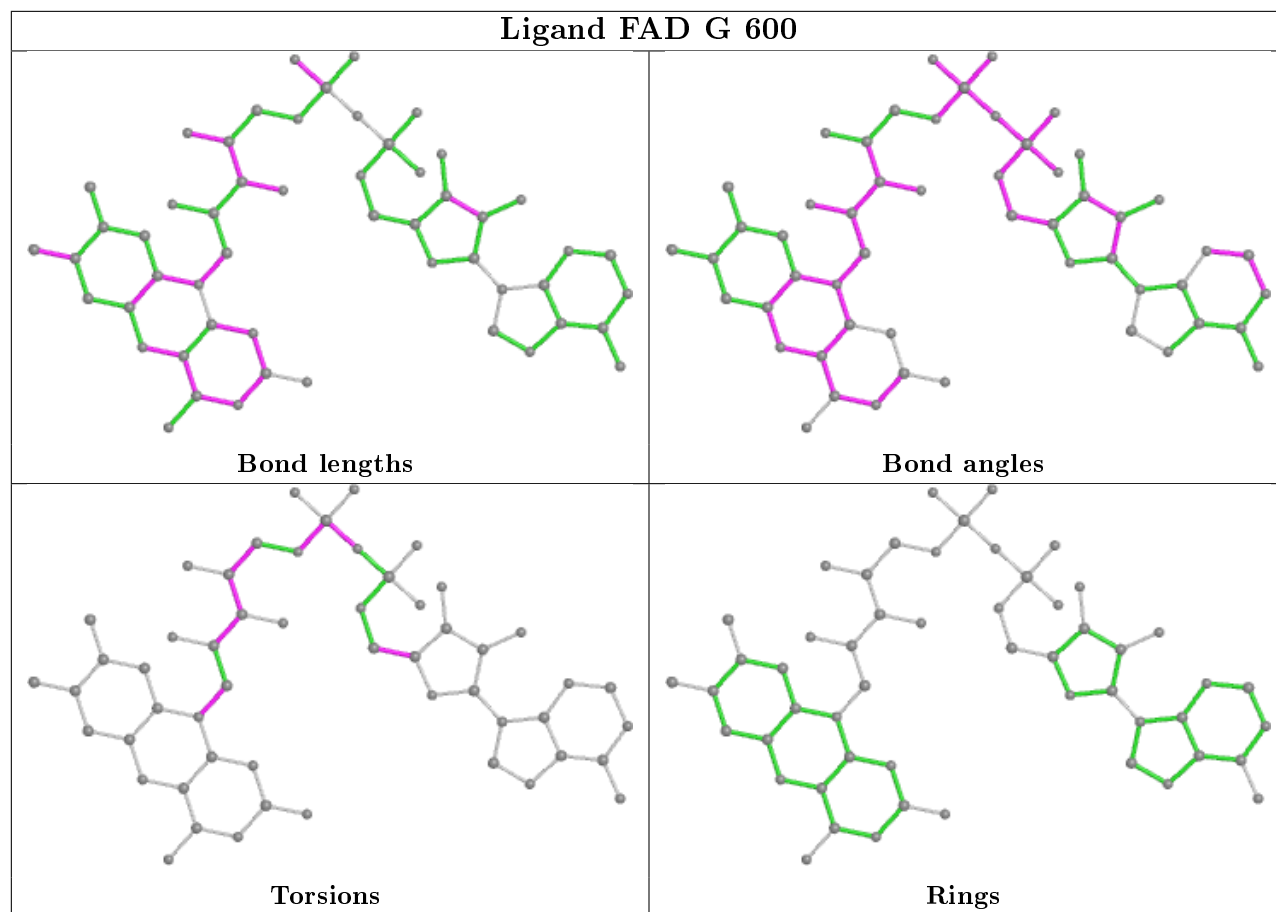


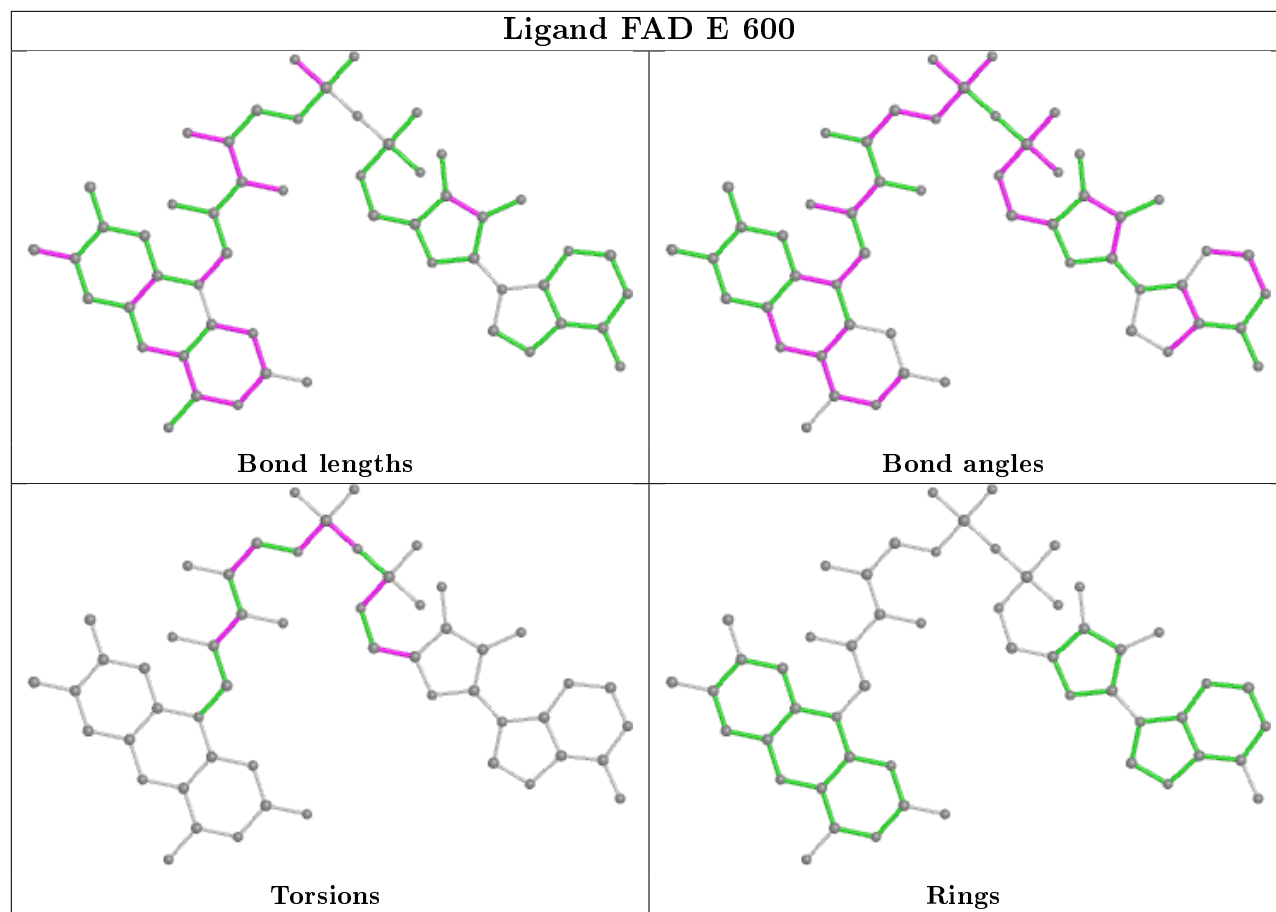


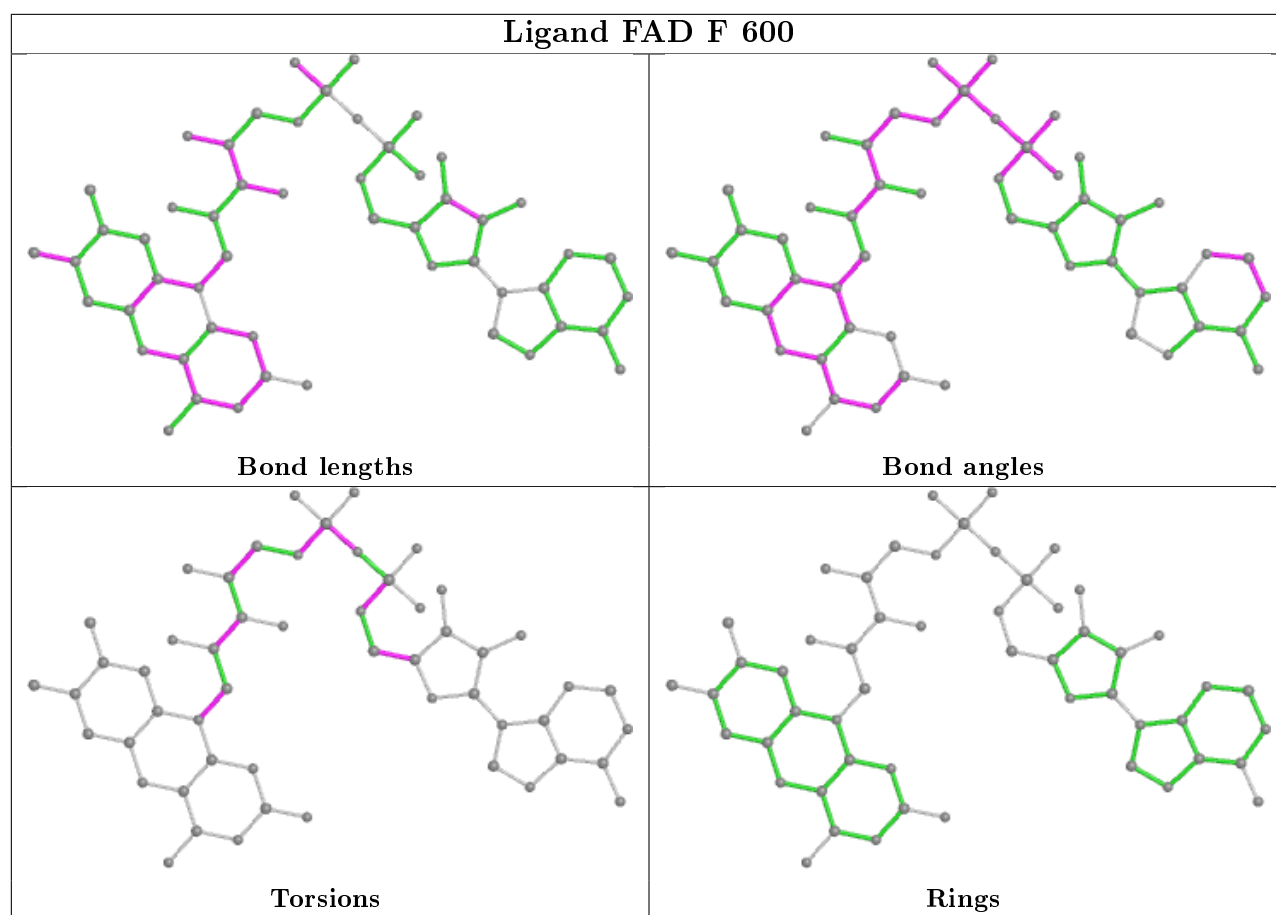


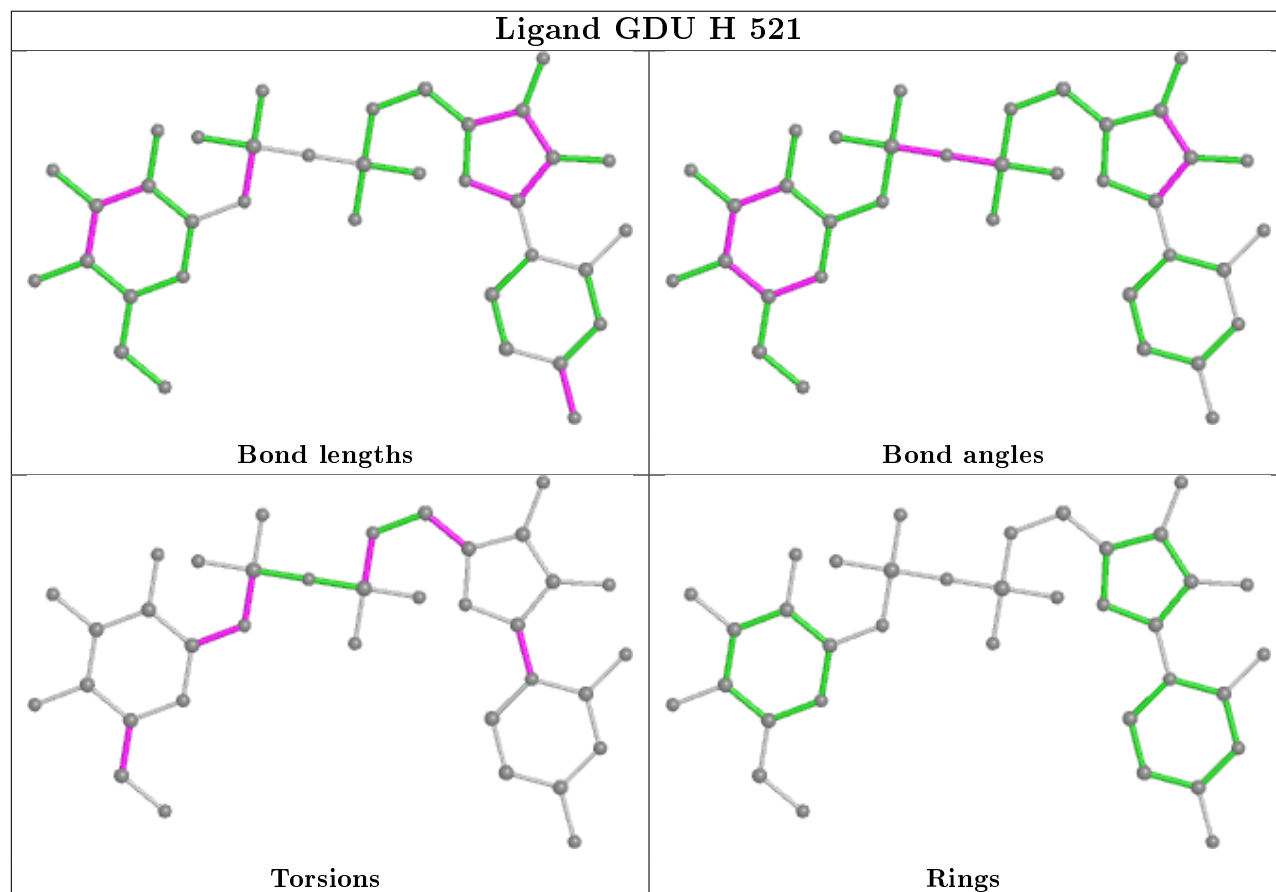
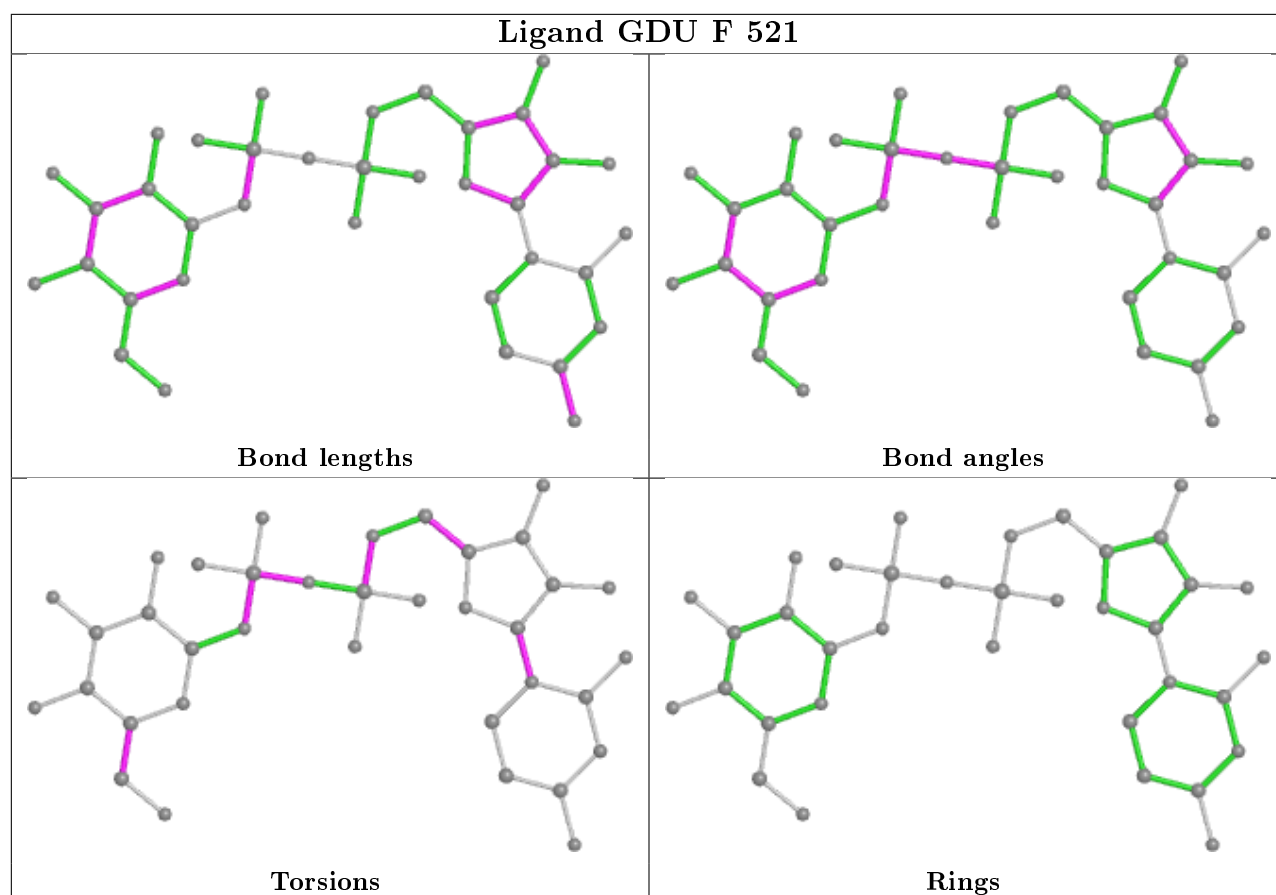


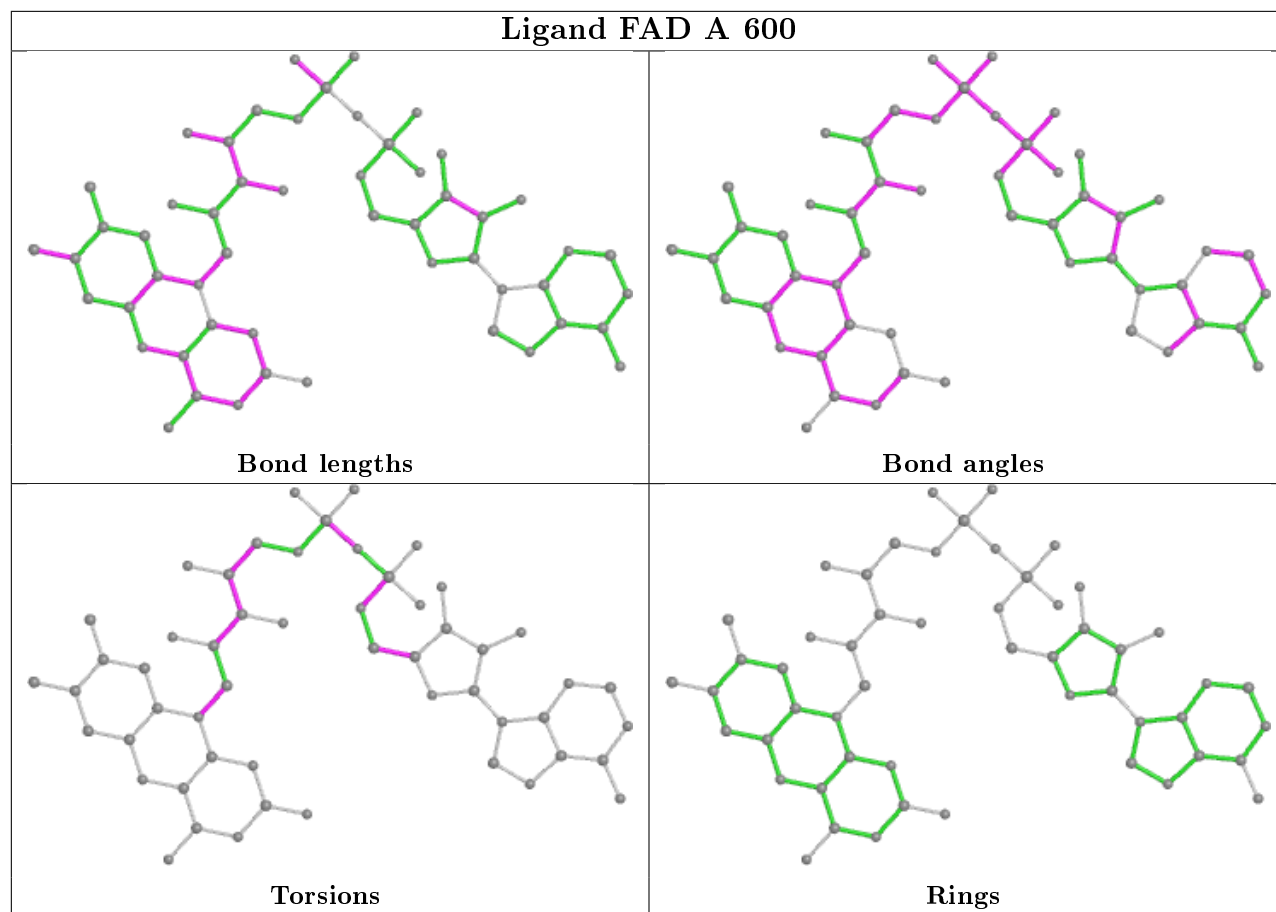


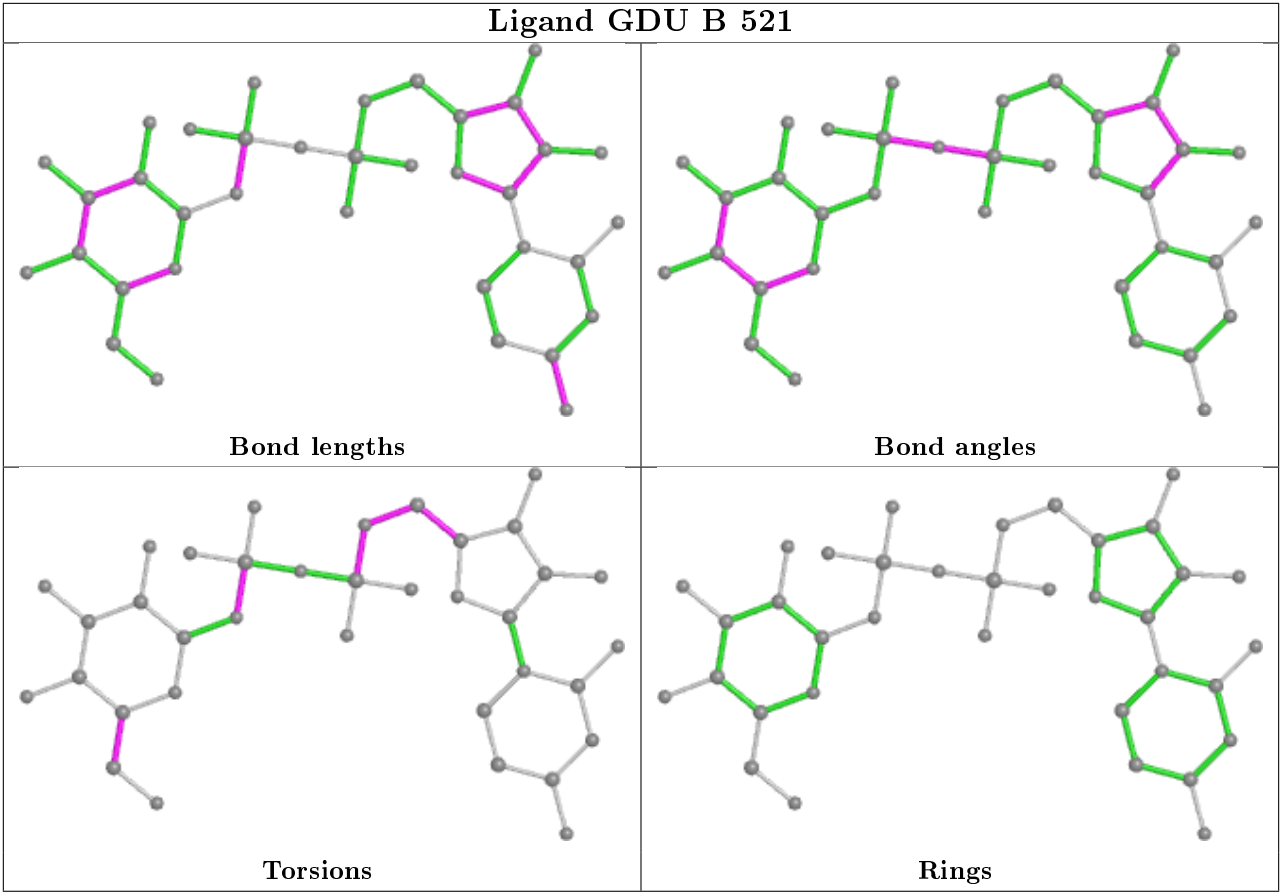












5.7 Other polymers ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

The following chains have linkage breaks:

Mol	Chain	Number of breaks
1	F	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	F	185:ALA	C	186[B]:PRO	N	4.49

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 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	504/519 (97%)	0.51	42 (8%) 11 15	27, 50, 80, 137	0
1	B	510/519 (98%)	0.77	64 (12%) 3 5	28, 53, 88, 163	0
1	C	511/519 (98%)	0.81	60 (11%) 4 6	28, 54, 84, 138	10 (1%)
1	D	510/519 (98%)	0.56	53 (10%) 6 9	30, 52, 87, 150	0
1	E	510/519 (98%)	0.97	92 (18%) 1 1	30, 56, 89, 147	2 (0%)
1	F	504/519 (97%)	0.44	33 (6%) 18 24	31, 53, 85, 137	0
1	G	504/519 (97%)	0.59	52 (10%) 6 9	28, 53, 85, 140	0
1	H	511/519 (98%)	0.85	74 (14%) 2 3	27, 54, 82, 137	6 (1%)
All	All	4064/4152 (97%)	0.69	470 (11%) 4 6	27, 53, 85, 163	18 (0%)

The worst 5 of 470 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	202	GLY	16.2
1	C	204[B]	TRP	14.8
1	E	202	GLY	13.1
1	H	204[A]	TRP	12.5
1	E	201	ALA	12.2

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

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

6.3 Carbohydrates ⓘ

There are no carbohydrates in this entry.

6.4 Ligands

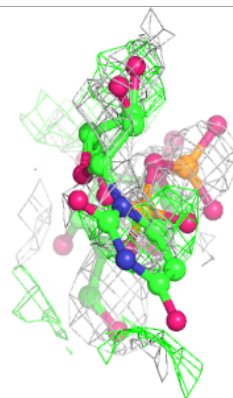
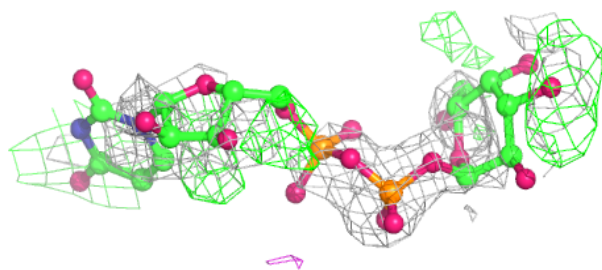
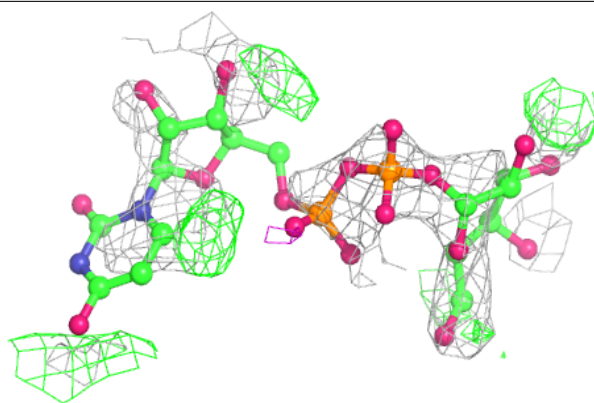
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
4	CL	A	522	1/1	0.52	0.19	103,103,103,103	0
3	GDU	F	521	36/36	0.55	0.71	41,69,87,93	36
4	CL	B	1	1/1	0.60	0.15	99,99,99,99	0
3	GDU	E	521	36/36	0.62	0.58	48,69,78,84	36
3	GDU	B	521	36/36	0.64	0.58	43,62,81,86	36
3	GDU	D	521	36/36	0.67	0.53	49,70,84,88	36
3	GDU	A	521	36/36	0.67	0.67	48,67,79,83	36
3	GDU	G	521	36/36	0.73	0.41	56,75,90,90	36
3	GDU	H	521	36/36	0.82	0.57	45,67,85,85	36
3	GDU	C	521	36/36	0.85	0.47	31,57,76,85	36
2	FAD	F	600	53/53	0.93	0.19	34,50,63,69	0
5	FDA	C	600	53/53	0.93	0.17	33,51,64,82	0
2	FAD	B	600	53/53	0.94	0.17	36,48,62,70	0
5	FDA	H	600	53/53	0.94	0.19	28,53,65,76	0
2	FAD	D	600	53/53	0.94	0.19	30,47,56,60	0
2	FAD	A	600	53/53	0.95	0.19	30,42,57,66	0
2	FAD	G	600	53/53	0.95	0.17	34,48,60,63	0
2	FAD	E	600	53/53	0.95	0.16	36,55,64,69	0

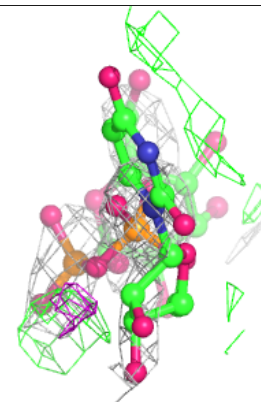
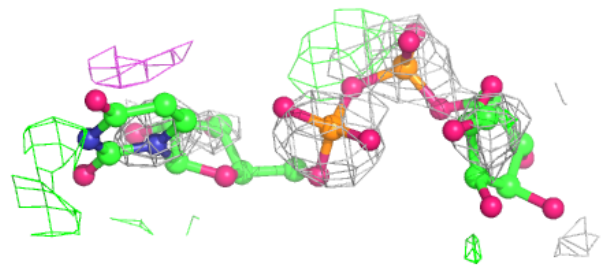
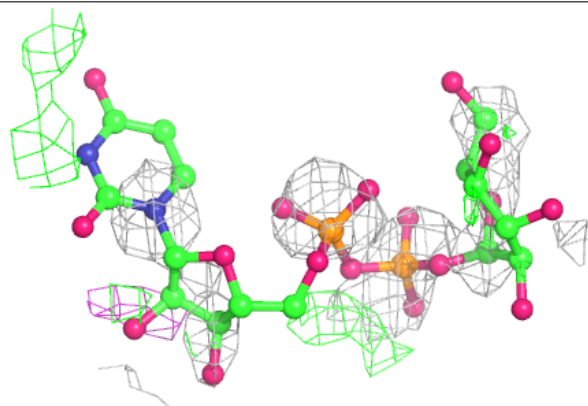
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around GDU F 521:

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

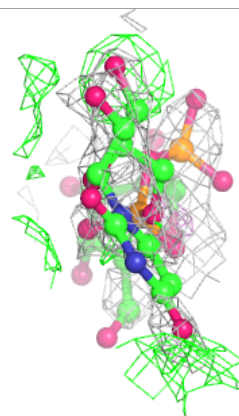
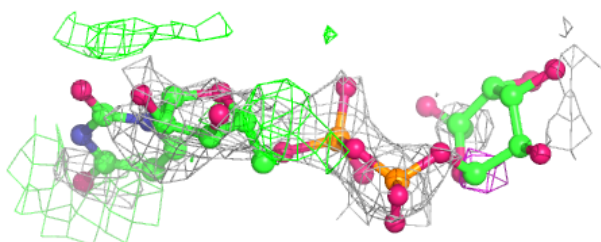
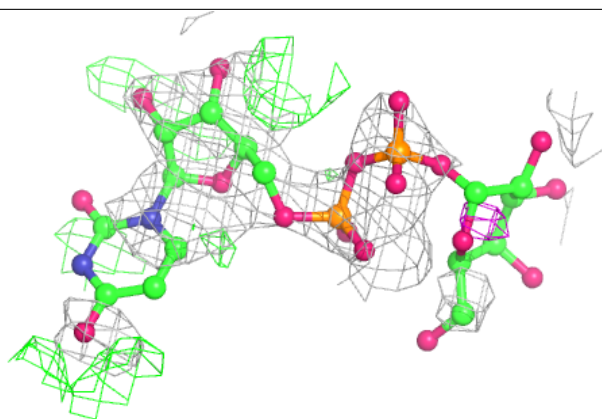
**Electron density around GDU E 521:**

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

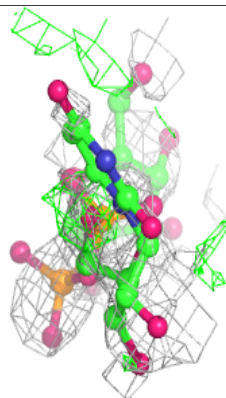
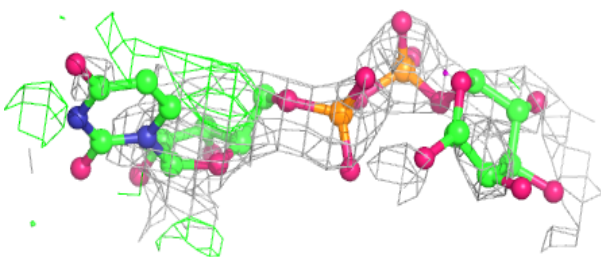
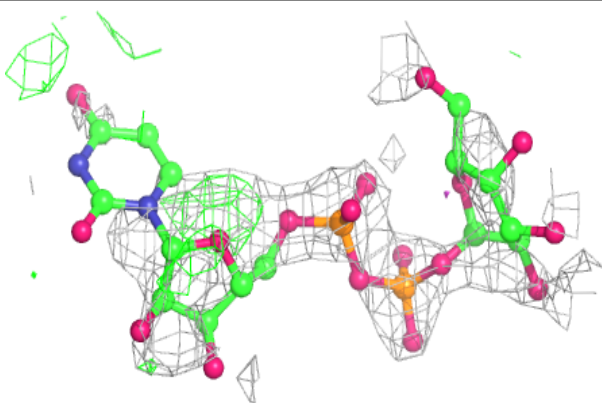


Electron density around GDU B 521:

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

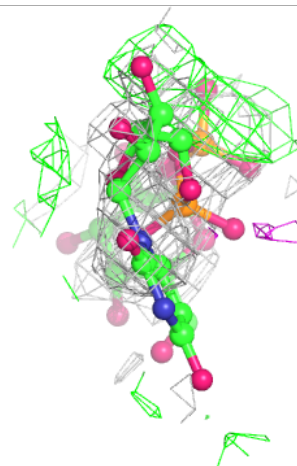
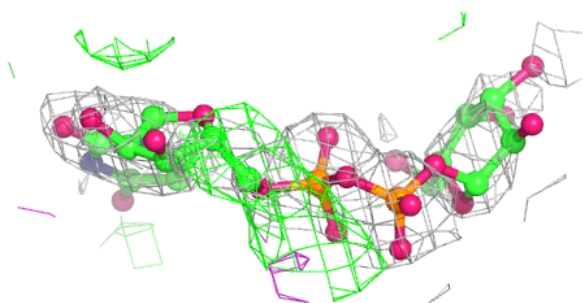
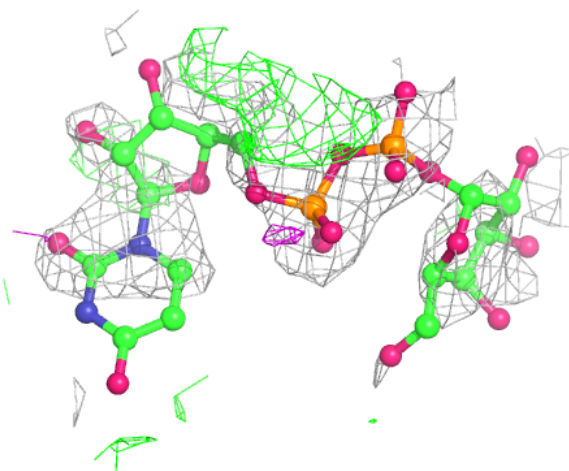
**Electron density around GDU D 521:**

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



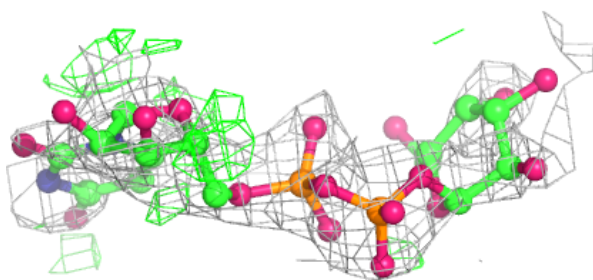
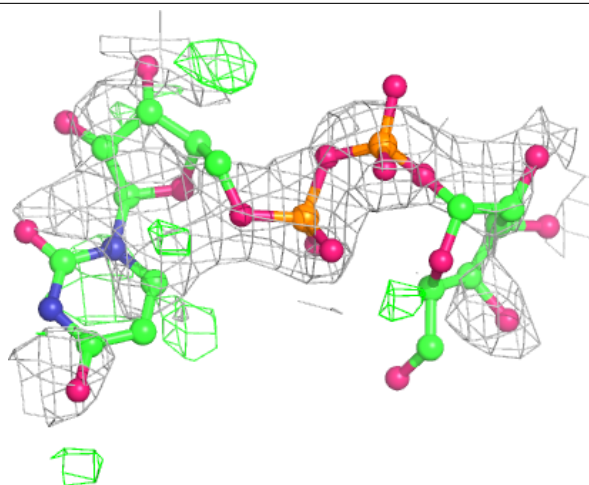
Electron density around GDU A 521:

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



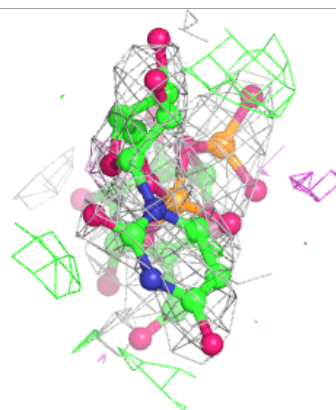
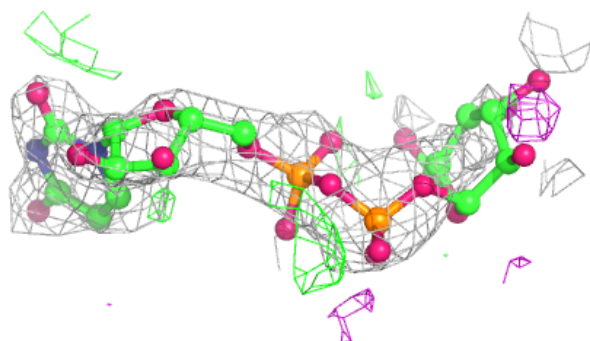
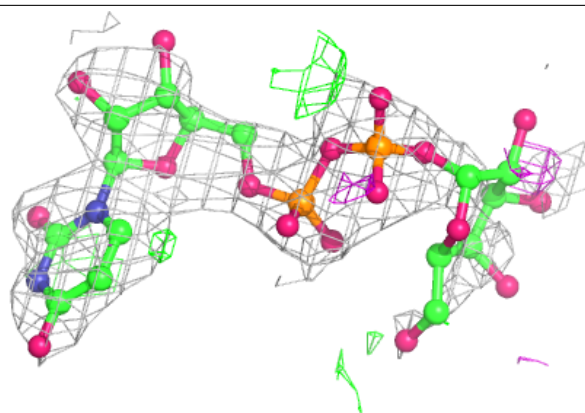
Electron density around GDU G 521:

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

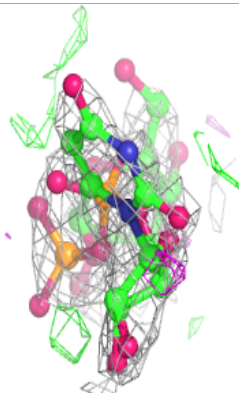
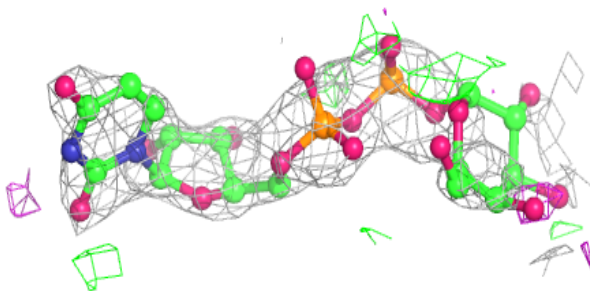
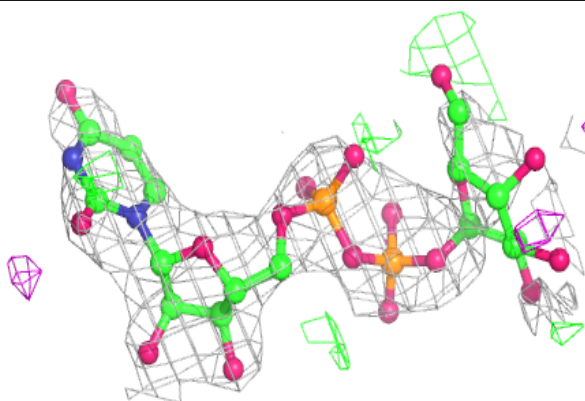


Electron density around GDU H 521:

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

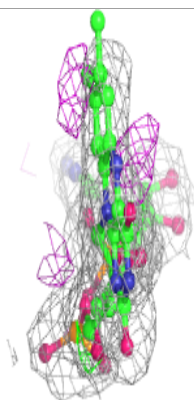
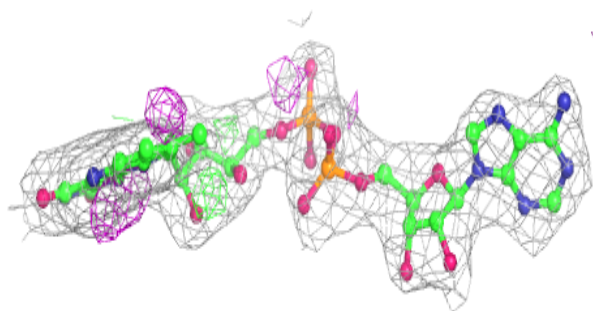
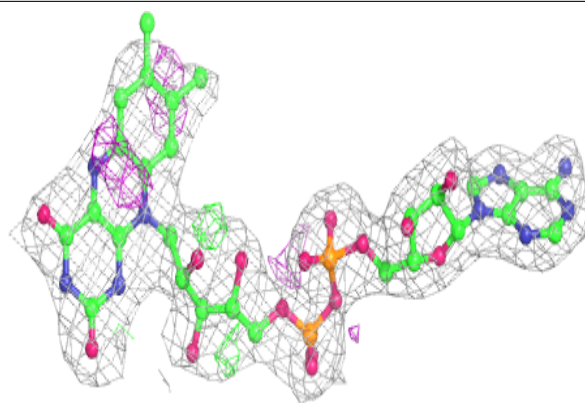
**Electron density around GDU C 521:**

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

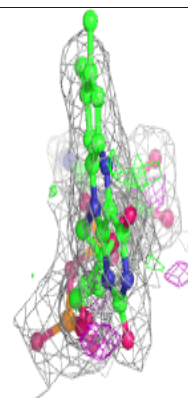
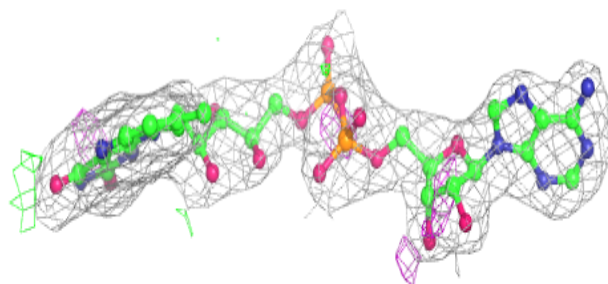
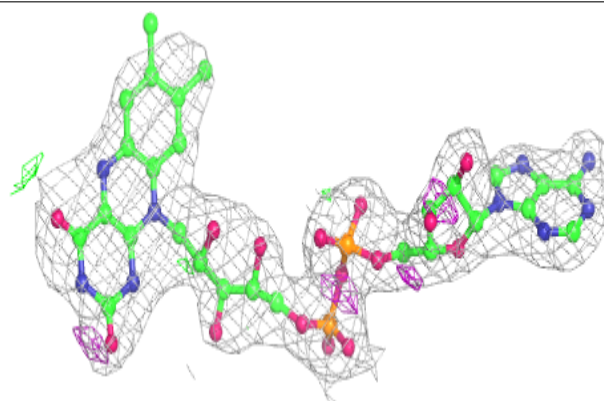


Electron density around FAD F 600:

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

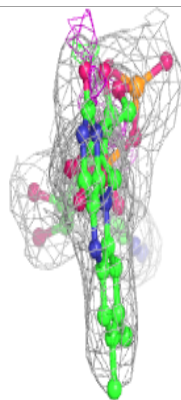
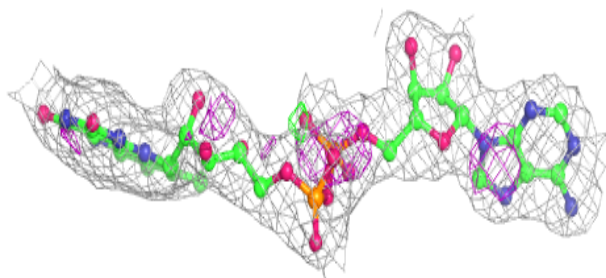
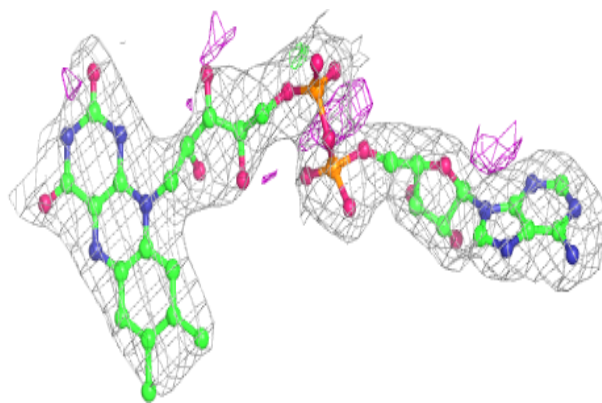
**Electron density around FDA C 600:**

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

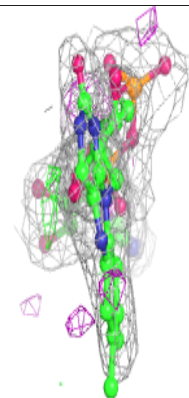
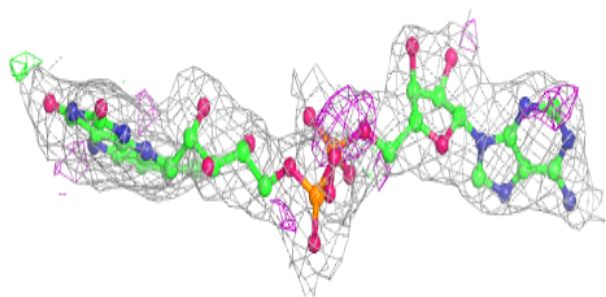
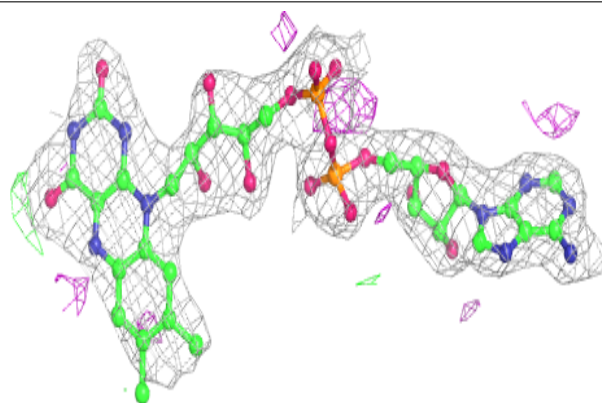


Electron density around FAD B 600:

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

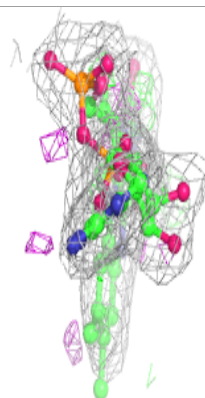
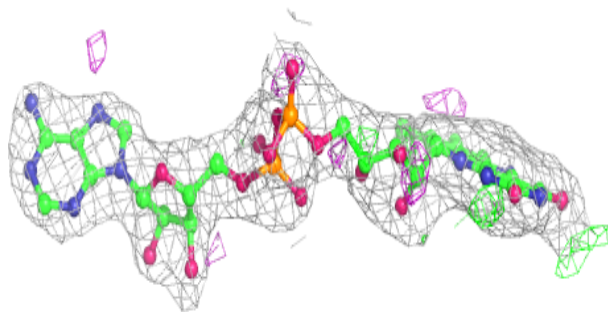
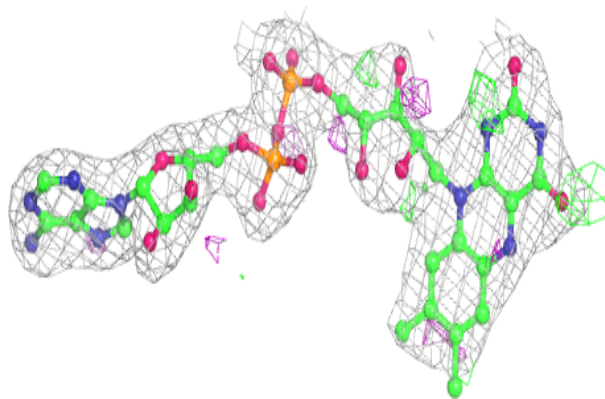
**Electron density around FDA H 600:**

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

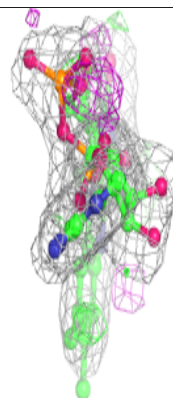
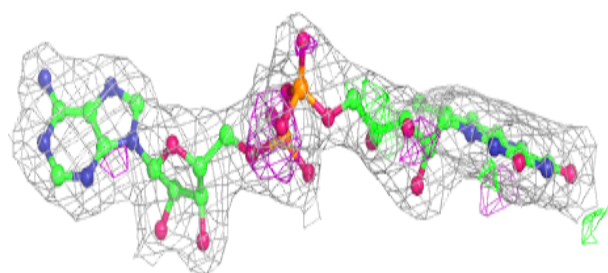
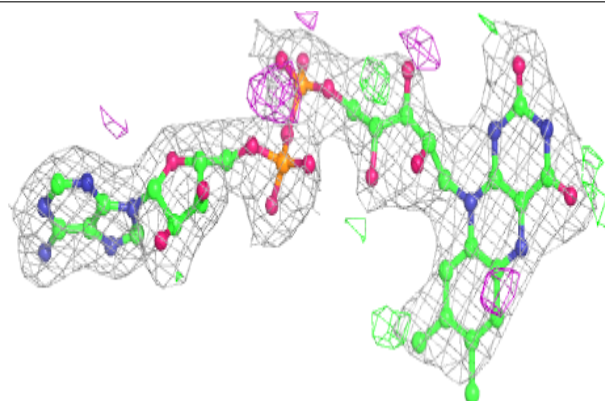


Electron density around FAD D 600:

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

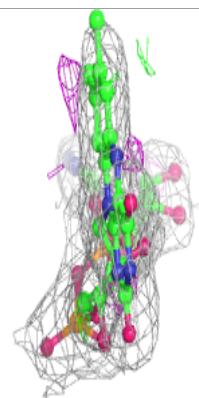
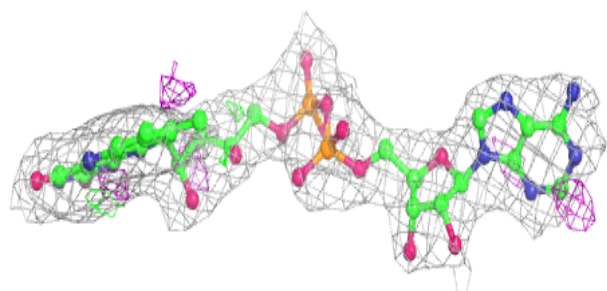
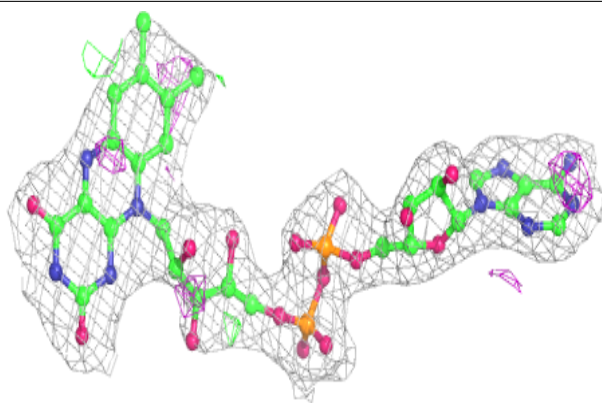
**Electron density around FAD A 600:**

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

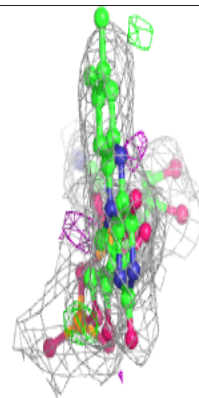
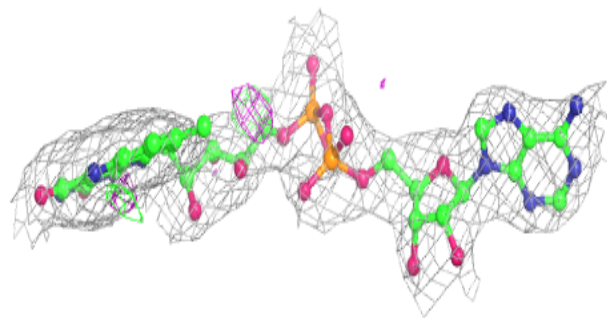
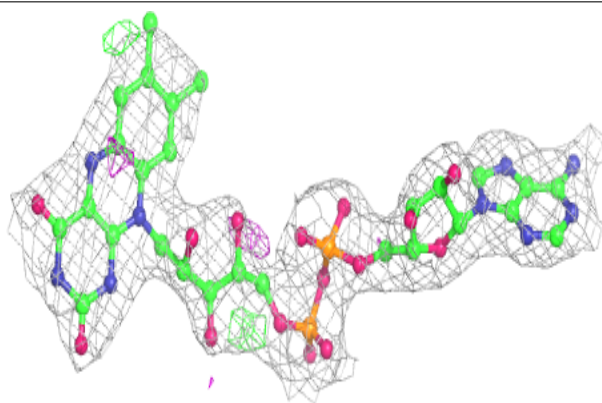


Electron density around FAD G 600:

$2mF_o-DF_c$ (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)



6.5 Other polymers [i](#)

There are no such residues in this entry.