



Full wwPDB X-ray Structure Validation Report ⓘ

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PDB ID : 5JWA
Title : the structure of malaria PfNDH2
Authors : Yu, Y.; Yang, Y.Q.; Li, X.L.; Yu, J.; Ge, J.P.; Li, J.; Rao, Y.; Yang, M.J.
Deposited on : 2016-05-11
Resolution : 2.16 Å(reported)

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

We welcome your comments at validation@mail.wwpdb.org

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 : 1.8.5 (274361), 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

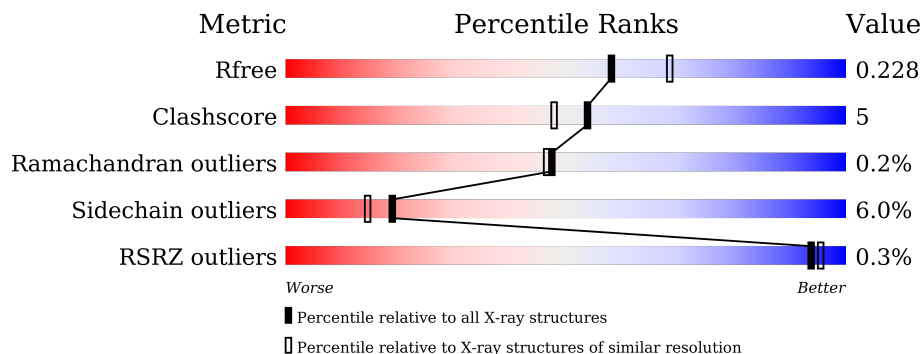
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION



The reported resolution of this entry is 2.16 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	1479 (2.16-2.16)
Clashscore	141614	1585 (2.16-2.16)
Ramachandran outliers	138981	1560 (2.16-2.16)
Sidechain outliers	138945	1559 (2.16-2.16)
RSRZ outliers	127900	1456 (2.16-2.16)

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	521	 82% 12% • 5%
1	H	521	 79% 13% • 5%

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
5	ACT	A	612	-	-	X	-
5	ACT	A	613	-	-	X	-

2 Entry composition [i](#)

There are 6 unique types of molecules in this entry. The entry contains 8671 atoms, of which 0 are hydrogens and 0 are deuteriums.

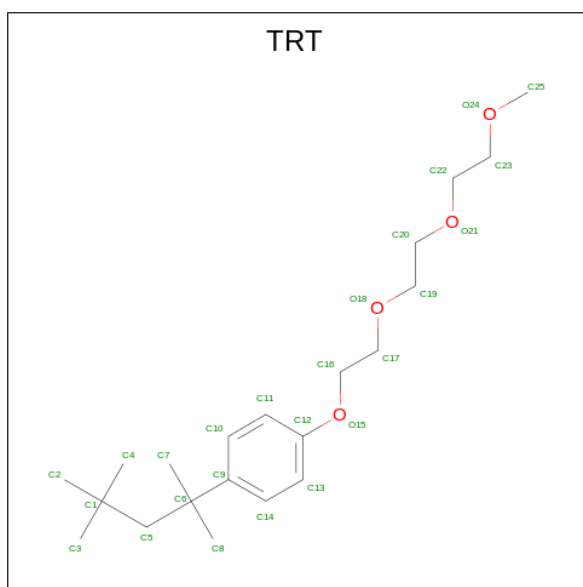
In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called NADH dehydrogenase, putative.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	495	4043	2641	662	730	10	0	0	0
1	H	495	4050	2645	664	731	10	0	0	0

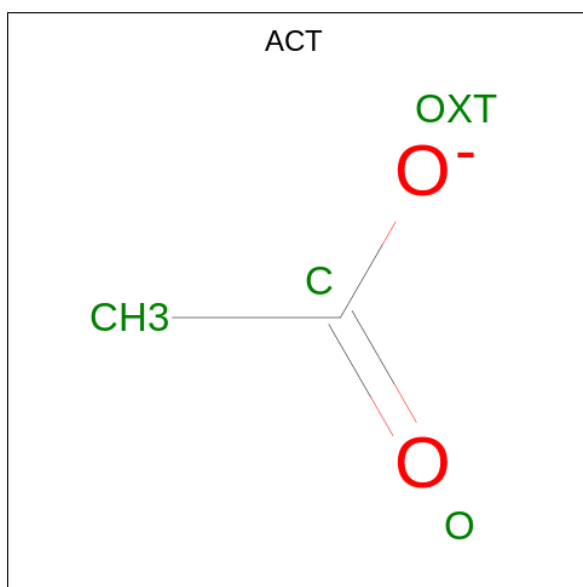
There are 24 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	13	MET	-	initiating methionine	UNP Q8I302
A	14	ARG	-	expression tag	UNP Q8I302
A	15	GLY	-	expression tag	UNP Q8I302
A	16	SER	-	expression tag	UNP Q8I302
A	17	HIS	-	expression tag	UNP Q8I302
A	18	HIS	-	expression tag	UNP Q8I302
A	19	HIS	-	expression tag	UNP Q8I302
A	20	HIS	-	expression tag	UNP Q8I302
A	21	HIS	-	expression tag	UNP Q8I302
A	22	HIS	-	expression tag	UNP Q8I302
A	23	GLY	-	expression tag	UNP Q8I302
A	24	SER	-	expression tag	UNP Q8I302
H	13	MET	-	initiating methionine	UNP Q8I302
H	14	ARG	-	expression tag	UNP Q8I302
H	15	GLY	-	expression tag	UNP Q8I302
H	16	SER	-	expression tag	UNP Q8I302
H	17	HIS	-	expression tag	UNP Q8I302
H	18	HIS	-	expression tag	UNP Q8I302
H	19	HIS	-	expression tag	UNP Q8I302
H	20	HIS	-	expression tag	UNP Q8I302
H	21	HIS	-	expression tag	UNP Q8I302
H	22	HIS	-	expression tag	UNP Q8I302
H	23	GLY	-	expression tag	UNP Q8I302
H	24	SER	-	expression tag	UNP Q8I302



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	1	Total C O 20 18 2	0	0
4	A	1	Total C O 20 18 2	0	0
4	A	1	Total C O 20 18 2	0	0
4	H	1	Total C O 20 18 2	0	0
4	H	1	Total C O 17 16 1	0	0
4	H	1	Total C O 20 18 2	0	0

- Molecule 5 is ACETATE ION (three-letter code: ACT) (formula: C₂H₃O₂).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	1	Total C O 4 2 2	0	0
5	A	1	Total C O 4 2 2	0	0
5	A	1	Total C O 4 2 2	0	0
5	A	1	Total C O 4 2 2	0	0
5	A	1	Total C O 4 2 2	0	0
5	H	1	Total C O 4 2 2	0	0
5	H	1	Total C O 4 2 2	0	0
5	H	1	Total C O 4 2 2	0	0
5	H	1	Total C O 4 2 2	0	0
5	H	1	Total C O 4 2 2	0	0
5	H	1	Total C O 4 2 2	0	0
5	H	1	Total C O 4 2 2	0	0

- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	153	Total 153	O 153	0	0
6	H	146	Total 146	O 146	0	0

4 Data and refinement statistics i

Property	Value	Source
Space group	I 41	Depositor
Cell constants a, b, c, α , β , γ	191.67Å 191.67Å 91.39Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	45.18 – 2.16 45.18 – 2.16	Depositor EDS
% Data completeness (in resolution range)	98.4 (45.18-2.16) 98.3 (45.18-2.16)	Depositor EDS
R_{merge}	0.08	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.80 (at 2.16Å)	Xtrriage
Refinement program	PHENIX phenix.refine: 1.8.4_1496	Depositor
R, R_{free}	0.188 , 0.228 0.191 , 0.228	Depositor DCC
R_{free} test set	4380 reflections (5.03%)	wwPDB-VP
Wilson B-factor (Å ²)	38.1	Xtrriage
Anisotropy	0.045	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.35 , 26.1	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.34$	Xtrriage
Estimated twinning fraction	0.488 for -k,-h,-l	Xtrriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	8671	wwPDB-VP
Average B, all atoms (Å ²)	41.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.58% 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: MG, ACT, FAD, TRT

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	0.41	0/4141	0.54	1/5598 (0.0%)
1	H	0.41	0/4148	0.55	1/5606 (0.0%)
All	All	0.41	0/8289	0.55	2/11204 (0.0%)

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	363	LEU	CA-CB-CG	6.10	129.34	115.30
1	H	363	LEU	CA-CB-CG	5.47	127.89	115.30

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	4043	0	4085	39	0
1	H	4050	0	4100	44	0
2	A	53	0	31	2	0
2	H	53	0	31	1	0
3	A	4	0	0	0	0
3	H	4	0	0	0	0
4	A	60	0	81	5	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	H	57	0	77	11	0
5	A	20	0	15	6	0
5	H	28	0	21	1	0
6	A	153	0	0	3	0
6	H	146	0	0	2	0
All	All	8671	0	8441	89	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 5.

All (89) 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:501:LYS:HB3	4:H:607:TRT:H7C3	1.47	0.97
1:H:521:PHE:HB2	4:H:607:TRT:H13	1.59	0.85
1:H:458:GLN:OE1	1:H:461:ASN:ND2	2.27	0.68
1:H:518:PHE:HD1	4:H:607:TRT:H8C2	1.64	0.63
1:A:459:LYS:NZ	6:A:703:HOH:O	2.32	0.61
1:H:336:ASP:HB3	1:H:338:LYS:H	1.66	0.60
1:A:456:THR:O	1:A:459:LYS:HG3	2.00	0.60
1:H:223:ILE:HD12	1:H:240:ILE:HD11	1.85	0.59
4:A:607:TRT:H2C2	4:A:608:TRT:H5C2	1.86	0.57
1:H:313:GLN:OE1	1:H:332:ILE:HA	2.04	0.57
1:H:377:ASN:OD1	1:H:377:ASN:N	2.24	0.57
4:H:607:TRT:H2C2	4:H:607:TRT:H8C1	1.87	0.57
1:A:264:ASN:ND2	6:A:702:HOH:O	2.28	0.55
1:H:521:PHE:CB	4:H:607:TRT:H13	2.35	0.55
1:A:223:ILE:HD12	1:A:240:ILE:HD11	1.89	0.54
1:A:518:PHE:CD2	4:H:606:TRT:H2C2	2.42	0.54
1:A:182:ASP:OD2	1:A:533:LYS:NZ	2.38	0.53
1:A:523:LYS:HG2	5:A:613:ACT:H3	1.90	0.53
1:A:523:LYS:HG2	5:A:613:ACT:CH3	2.38	0.53
1:H:122:TYR:HE2	1:H:323:THR:HG22	1.75	0.52
1:H:223:ILE:HA	1:H:227:VAL:HB	1.92	0.52
1:H:493:GLY:O	1:H:496:SER:HB2	2.09	0.52
1:H:440:LYS:HE2	1:H:444:TYR:CE2	2.46	0.51
1:H:479:HIS:CE1	5:H:610:ACT:H1	2.46	0.51
1:H:382:GLU:OE1	1:H:409:LYS:NZ	2.44	0.50
1:H:48:SER:HB2	1:H:98:ILE:HD11	1.93	0.50
1:H:388:GLN:O	1:H:392:THR:HB	2.12	0.50
1:A:313:GLN:OE1	1:A:332:ILE:HA	2.12	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:A:607:TRT:H2C3	4:A:608:TRT:H2C2	1.94	0.49
1:H:518:PHE:HD1	4:H:607:TRT:C8	2.26	0.49
1:A:223:ILE:HA	1:A:227:VAL:HB	1.95	0.49
1:A:519:ILE:HG21	1:H:519:ILE:HG21	1.94	0.48
1:H:372:LYS:O	1:H:375:THR:HG23	2.13	0.48
1:H:435:THR:HB	2:H:601:FAD:O2	2.14	0.48
1:A:363:LEU:HB2	1:A:426:ASP:OD1	2.14	0.48
1:H:392:THR:HG23	1:H:466:ILE:CD1	2.43	0.48
1:A:435:THR:HB	2:A:601:FAD:O2	2.14	0.48
1:A:138:LYS:HE2	1:A:140:PHE:CZ	2.49	0.47
1:A:498:THR:O	1:A:502:VAL:HG13	2.14	0.47
1:H:78:THR:HA	1:H:81:LEU:HD22	1.95	0.47
1:A:363:LEU:HD11	1:A:398:LEU:HD11	1.96	0.47
1:H:166:PHE:O	1:H:172:ASP:HB3	2.14	0.47
1:H:485:LEU:HD12	1:H:488:TYR:CE2	2.48	0.47
1:A:93:VAL:HG22	1:A:516:HIS:HB3	1.96	0.47
1:A:50:TRP:CD2	1:A:436:ALA:HB1	2.50	0.46
1:H:356:LYS:HG2	1:H:357:LYS:N	2.30	0.46
1:H:369:GLU:O	1:H:373:ILE:HG23	2.15	0.46
1:H:336:ASP:OD1	1:H:340:ARG:NH2	2.48	0.46
1:H:50:TRP:CD2	1:H:436:ALA:HB1	2.51	0.46
1:A:178:LYS:HD3	1:A:533:LYS:HB2	1.97	0.46
1:A:500:TRP:CE3	5:A:609:ACT:H2	2.51	0.46
1:H:388:GLN:HE21	1:H:388:GLN:HB3	1.46	0.46
1:H:518:PHE:CD1	4:H:607:TRT:H8C2	2.47	0.46
1:A:232:LYS:N	5:A:612:ACT:H2	2.30	0.45
1:H:498:THR:O	1:H:502:VAL:HG23	2.16	0.45
1:A:232:LYS:H	5:A:612:ACT:H2	1.82	0.45
1:A:458:GLN:OE1	1:A:461:ASN:ND2	2.42	0.45
1:A:501:LYS:NZ	4:A:608:TRT:H161	2.30	0.45
1:A:200:MET:O	1:A:303:GLY:HA3	2.16	0.45
1:H:326:VAL:HB	6:H:755:HOH:O	2.16	0.45
1:A:436:ALA:HB2	2:A:601:FAD:H2'	1.99	0.45
1:H:279:ILE:HD13	1:H:289:GLN:HB2	1.99	0.45
1:H:363:LEU:HD11	1:H:398:LEU:HD11	1.99	0.45
1:A:520:ASP:OD1	6:A:701:HOH:O	2.21	0.44
1:A:122:TYR:HE2	1:A:323:THR:HG22	1.83	0.44
1:A:455:HIS:HA	1:A:459:LYS:HE2	2.00	0.44
1:H:520:ASP:OD1	6:H:701:HOH:O	2.21	0.44
1:H:200:MET:O	1:H:303:GLY:HA3	2.18	0.43
1:H:363:LEU:HD13	1:H:395:PHE:CD1	2.53	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:520:ASP:OD1	5:A:613:ACT:H2	2.18	0.43
1:A:388:GLN:HE21	1:A:388:GLN:HB3	1.44	0.43
1:A:471:GLY:HA3	1:A:485:LEU:HD23	2.01	0.43
4:H:607:TRT:H2C1	4:H:608:TRT:H4C2	2.01	0.42
1:H:373:ILE:HD12	1:H:387:LYS:HG2	2.02	0.42
1:H:469:TRP:CZ2	1:H:471:GLY:HA2	2.55	0.42
1:A:465:PHE:CE2	1:A:467:GLU:HG3	2.55	0.42
4:H:607:TRT:H5C2	4:H:607:TRT:H10	1.40	0.42
1:H:501:LYS:NZ	4:H:607:TRT:H162	2.35	0.41
1:A:166:PHE:O	1:A:172:ASP:HB3	2.20	0.41
1:A:294:LYS:H	1:A:294:LYS:HG3	1.67	0.41
1:A:469:TRP:CZ2	1:A:471:GLY:HA2	2.56	0.41
1:H:50:TRP:CE2	1:H:436:ALA:HB1	2.56	0.41
1:A:50:TRP:CE2	1:A:436:ALA:HB1	2.56	0.41
1:H:232:LYS:HB2	1:H:232:LYS:HE3	1.83	0.41
1:A:369:GLU:O	1:A:373:ILE:HG13	2.20	0.41
1:H:471:GLY:HA3	1:H:485:LEU:HD23	2.02	0.40
1:A:243:ILE:N	1:A:243:ILE:HD13	2.35	0.40
4:A:608:TRT:H11	4:A:608:TRT:H162	1.79	0.40
4:A:607:TRT:H8C1	4:A:608:TRT:H3C3	2.04	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	A	493/521 (95%)	480 (97%)	12 (2%)	1 (0%)	47 46
1	H	493/521 (95%)	481 (98%)	11 (2%)	1 (0%)	47 46
All	All	986/1042 (95%)	961 (98%)	23 (2%)	2 (0%)	47 46

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	H	336	ASP
1	A	459	LYS

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	449/474 (95%)	427 (95%)	22 (5%)	25	21
1	H	451/474 (95%)	419 (93%)	32 (7%)	14	9
All	All	900/948 (95%)	846 (94%)	54 (6%)	19	14

All (54) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	57	LEU
1	A	81	LEU
1	A	137	VAL
1	A	167	VAL
1	A	174	LEU
1	A	268	LEU
1	A	292	LEU
1	A	316	LEU
1	A	321	LEU
1	A	326	VAL
1	A	363	LEU
1	A	379	LEU
1	A	387	LYS
1	A	388	GLN
1	A	394	THR
1	A	422	LEU
1	A	467	GLU
1	A	470	LYS
1	A	472	SER
1	A	488	TYR
1	A	490	LEU
1	A	507	LEU

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Mol	Chain	Res	Type
1	H	57	LEU
1	H	81	LEU
1	H	137	VAL
1	H	160	VAL
1	H	161	ASP
1	H	167	VAL
1	H	168	LYS
1	H	174	LEU
1	H	195	GLU
1	H	268	LEU
1	H	273	LEU
1	H	292	LEU
1	H	316	LEU
1	H	321	LEU
1	H	326	VAL
1	H	356	LYS
1	H	363	LEU
1	H	372	LYS
1	H	373	ILE
1	H	374	LEU
1	H	377	ASN
1	H	379	LEU
1	H	388	GLN
1	H	391	LEU
1	H	392	THR
1	H	394	THR
1	H	422	LEU
1	H	472	SER
1	H	490	LEU
1	H	496	SER
1	H	507	LEU
1	H	523	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (2) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	388	GLN
1	H	479	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](#)

Of 28 ligands modelled in this entry, 8 are monoatomic - leaving 20 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
5	ACT	A	613	-	3,3,3	0.69	0	3,3,3	1.11	0
5	ACT	A	611	-	3,3,3	0.77	0	3,3,3	1.26	0
5	ACT	H	609	-	3,3,3	0.74	0	3,3,3	1.21	0
5	ACT	A	612	-	3,3,3	0.77	0	3,3,3	1.27	0
4	TRT	A	606	-	20,20,25	1.17	2 (10%)	28,28,33	0.80	0
4	TRT	A	608	-	20,20,25	1.12	1 (5%)	28,28,33	0.93	1 (3%)
2	FAD	A	601	3	53,58,58	1.05	4 (7%)	68,89,89	1.34	9 (13%)
4	TRT	H	607	-	17,17,25	1.23	1 (5%)	25,25,33	1.27	4 (16%)
5	ACT	H	614	-	3,3,3	0.79	0	3,3,3	1.14	0
5	ACT	H	613	-	3,3,3	0.77	0	3,3,3	1.32	0
5	ACT	A	610	-	3,3,3	0.79	0	3,3,3	1.49	0
4	TRT	H	606	-	20,20,25	1.27	2 (10%)	28,28,33	0.76	0
4	TRT	H	608	-	20,20,25	1.24	2 (10%)	28,28,33	0.79	0
5	ACT	H	610	-	3,3,3	0.72	0	3,3,3	1.31	0
5	ACT	H	615	-	3,3,3	0.76	0	3,3,3	1.43	0
5	ACT	H	611	-	3,3,3	0.76	0	3,3,3	1.28	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
5	ACT	A	609	-	3,3,3	0.77	0	3,3,3	1.22	0
4	TRT	A	607	-	20,20,25	1.19	1 (5%)	28,28,33	0.69	0
2	FAD	H	601	3	53,58,58	1.10	4 (7%)	68,89,89	1.28	6 (8%)
5	ACT	H	612	-	3,3,3	0.76	0	3,3,3	1.17	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
4	TRT	A	608	-	-	12/18/18/23	0/1/1/1
2	FAD	A	601	3	-	1/30/50/50	0/6/6/6
4	TRT	H	607	-	-	8/15/15/23	0/1/1/1
4	TRT	H	606	-	-	3/18/18/23	0/1/1/1
4	TRT	H	608	-	-	7/18/18/23	0/1/1/1
4	TRT	A	607	-	-	2/18/18/23	0/1/1/1
2	FAD	H	601	3	-	1/30/50/50	0/6/6/6
4	TRT	A	606	-	-	3/18/18/23	0/1/1/1

All (17) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	H	601	FAD	C4X-N5	3.81	1.38	1.30
2	H	601	FAD	C2A-N3A	3.77	1.38	1.32
2	A	601	FAD	C4X-N5	3.64	1.37	1.30
2	A	601	FAD	C2A-N3A	3.59	1.37	1.32
4	H	607	TRT	O15-C12	3.54	1.45	1.37
4	H	608	TRT	O15-C12	3.48	1.45	1.37
4	H	606	TRT	O15-C12	3.30	1.45	1.37
4	A	607	TRT	O15-C12	3.22	1.45	1.37
4	A	606	TRT	O15-C12	3.12	1.44	1.37
2	H	601	FAD	C2A-N1A	2.51	1.38	1.33
4	A	608	TRT	O15-C12	2.48	1.43	1.37
4	H	606	TRT	C13-C12	2.29	1.43	1.38
2	A	601	FAD	C2A-N1A	2.18	1.38	1.33
2	A	601	FAD	C10-N1	2.15	1.37	1.33
2	H	601	FAD	C10-N1	2.13	1.37	1.33
4	A	606	TRT	C13-C12	2.12	1.42	1.38
4	H	608	TRT	C13-C12	2.00	1.42	1.38

All (20) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	601	FAD	N3A-C2A-N1A	-5.58	119.95	128.68
2	H	601	FAD	N3A-C2A-N1A	-5.47	120.13	128.68
2	H	601	FAD	C4'-C3'-C2'	-3.38	106.32	113.36
2	A	601	FAD	C4'-C3'-C2'	-3.36	106.37	113.36
4	H	607	TRT	C5-C6-C9	-2.87	105.59	111.93
2	H	601	FAD	C4X-C10-N10	2.72	120.45	116.48
4	H	607	TRT	C13-C14-C9	-2.60	117.74	121.22
2	A	601	FAD	C9A-C5X-N5	-2.59	119.61	122.43
2	A	601	FAD	C4X-C10-N10	2.56	120.22	116.48
4	H	607	TRT	C8-C6-C9	-2.54	103.84	110.20
4	A	608	TRT	C16-O15-C12	-2.54	111.30	117.93
4	H	607	TRT	C14-C13-C12	2.35	122.60	119.73
2	A	601	FAD	C4-N3-C2	-2.26	121.46	125.64
2	A	601	FAD	C4X-C4-N3	2.20	118.77	113.19
2	H	601	FAD	C4-N3-C2	-2.19	121.59	125.64
2	A	601	FAD	C10-C4X-N5	-2.19	120.21	124.86
2	H	601	FAD	C4X-C4-N3	2.15	118.66	113.19
2	H	601	FAD	C10-C4X-N5	-2.12	120.37	124.86
2	A	601	FAD	C4A-C5A-N7A	-2.02	107.30	109.40
2	A	601	FAD	C1B-N9A-C4A	-2.01	123.11	126.64

There are no chirality outliers.

All (37) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	H	607	TRT	C1-C5-C6-C9
4	A	606	TRT	C13-C12-O15-C16
4	A	606	TRT	C11-C12-O15-C16
4	A	608	TRT	O15-C16-C17-O18
4	H	607	TRT	C13-C12-O15-C16
4	H	607	TRT	C11-C12-O15-C16
4	H	606	TRT	C11-C12-O15-C16
4	H	607	TRT	C1-C5-C6-C8
4	H	607	TRT	C17-C16-O15-C12
4	H	606	TRT	C13-C12-O15-C16
4	H	607	TRT	C5-C6-C9-C14
4	H	607	TRT	C5-C6-C9-C10
4	A	607	TRT	C11-C12-O15-C16
4	A	608	TRT	C13-C12-O15-C16
4	A	607	TRT	C13-C12-O15-C16
4	H	608	TRT	C13-C12-O15-C16

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Mol	Chain	Res	Type	Atoms
4	H	608	TRT	C11-C12-O15-C16
4	A	608	TRT	C11-C12-O15-C16
4	A	608	TRT	C17-C16-O15-C12
4	H	607	TRT	C1-C5-C6-C7
4	H	606	TRT	O15-C16-C17-O18
4	A	608	TRT	C1-C5-C6-C7
4	H	608	TRT	C16-C17-O18-C19
4	A	608	TRT	C1-C5-C6-C9
4	A	608	TRT	C16-C17-O18-C19
2	H	601	FAD	O4B-C4B-C5B-O5B
2	A	601	FAD	O4B-C4B-C5B-O5B
4	A	606	TRT	C20-C19-O18-C17
4	A	608	TRT	C20-C19-O18-C17
4	A	608	TRT	C1-C5-C6-C8
4	H	608	TRT	C8-C6-C9-C10
4	A	608	TRT	C7-C6-C9-C10
4	H	608	TRT	C7-C6-C9-C14
4	H	608	TRT	C8-C6-C9-C14
4	A	608	TRT	C7-C6-C9-C14
4	A	608	TRT	C8-C6-C9-C10
4	H	608	TRT	C7-C6-C9-C10

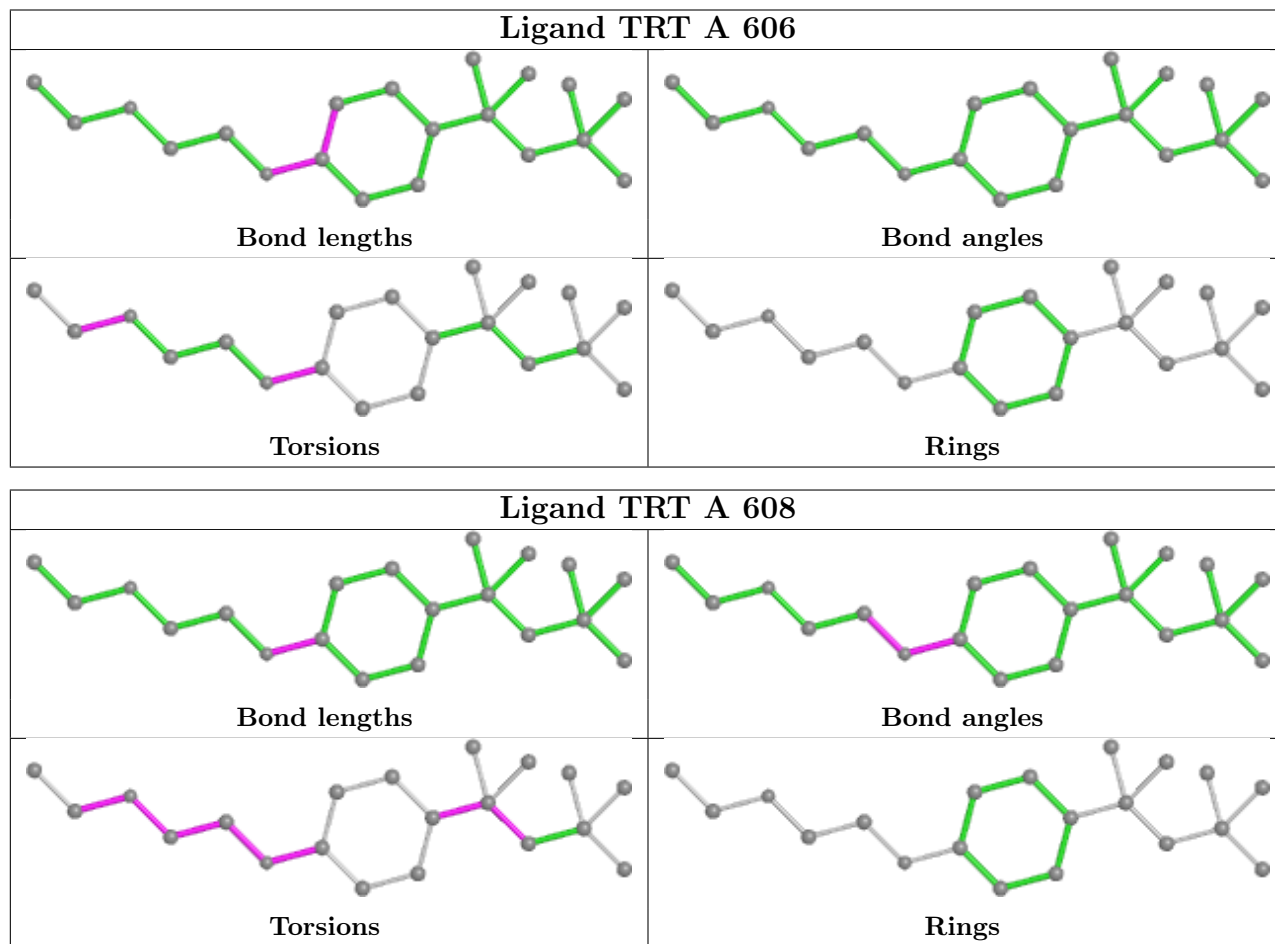
There are no ring outliers.

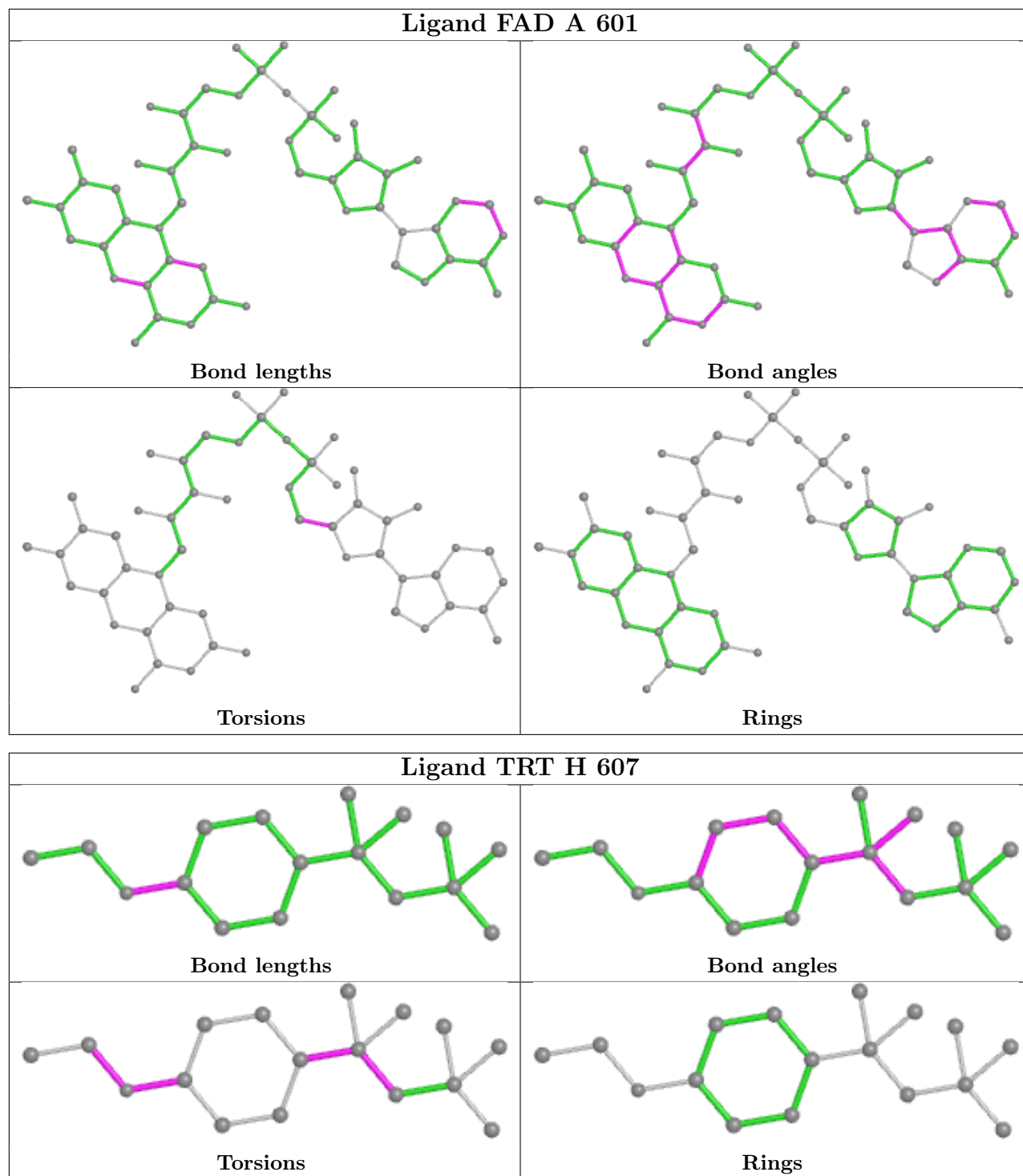
11 monomers are involved in 26 short contacts:

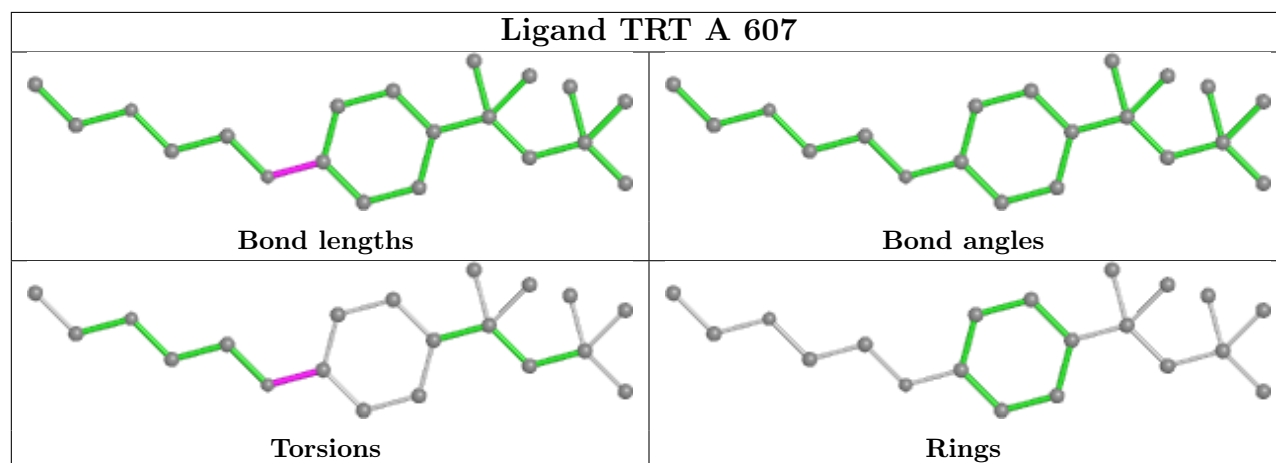
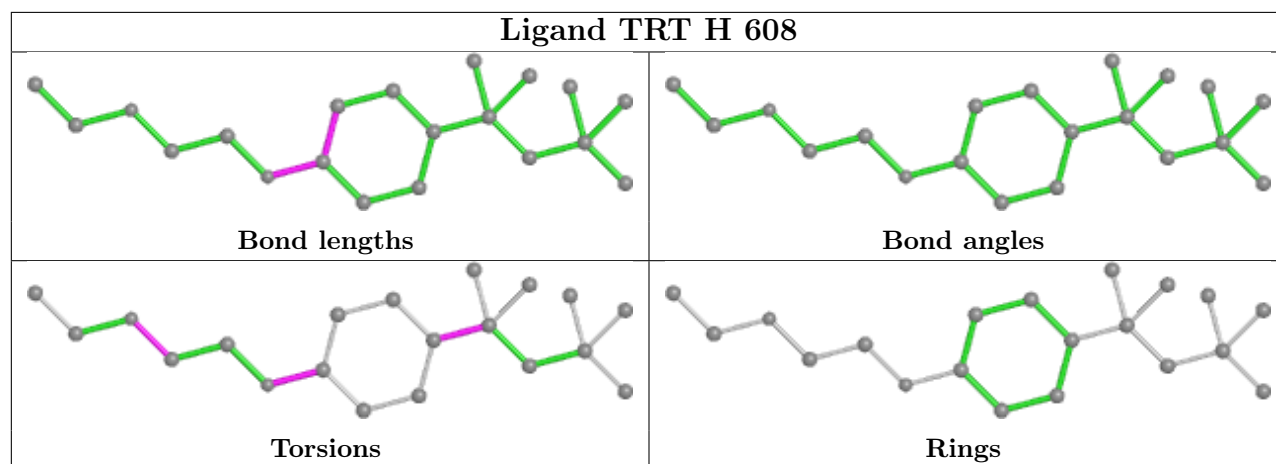
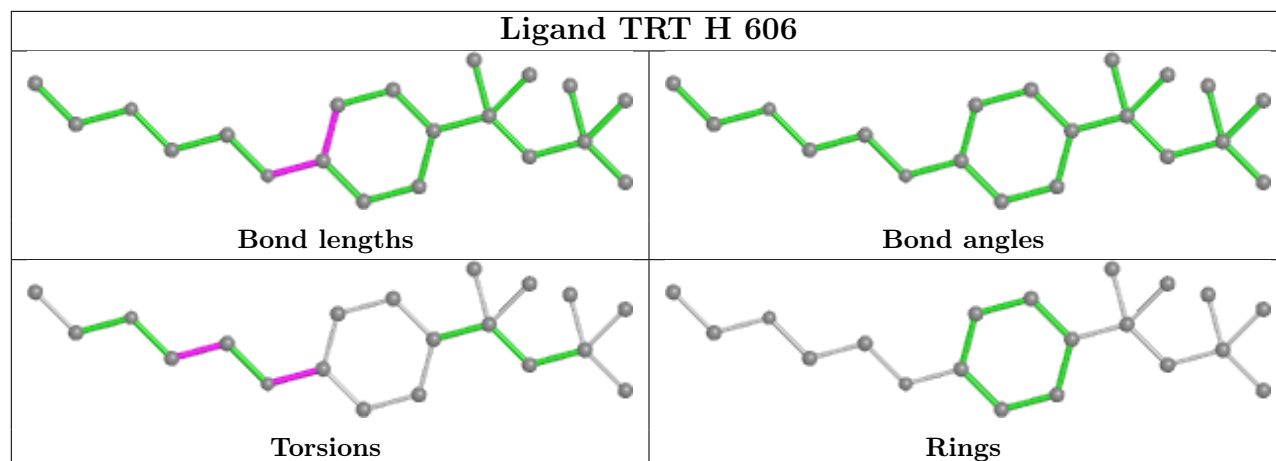
Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	A	613	ACT	3	0
5	A	612	ACT	2	0
4	A	608	TRT	5	0
2	A	601	FAD	2	0
4	H	607	TRT	10	0
4	H	606	TRT	1	0
4	H	608	TRT	1	0
5	H	610	ACT	1	0
5	A	609	ACT	1	0
4	A	607	TRT	3	0
2	H	601	FAD	1	0

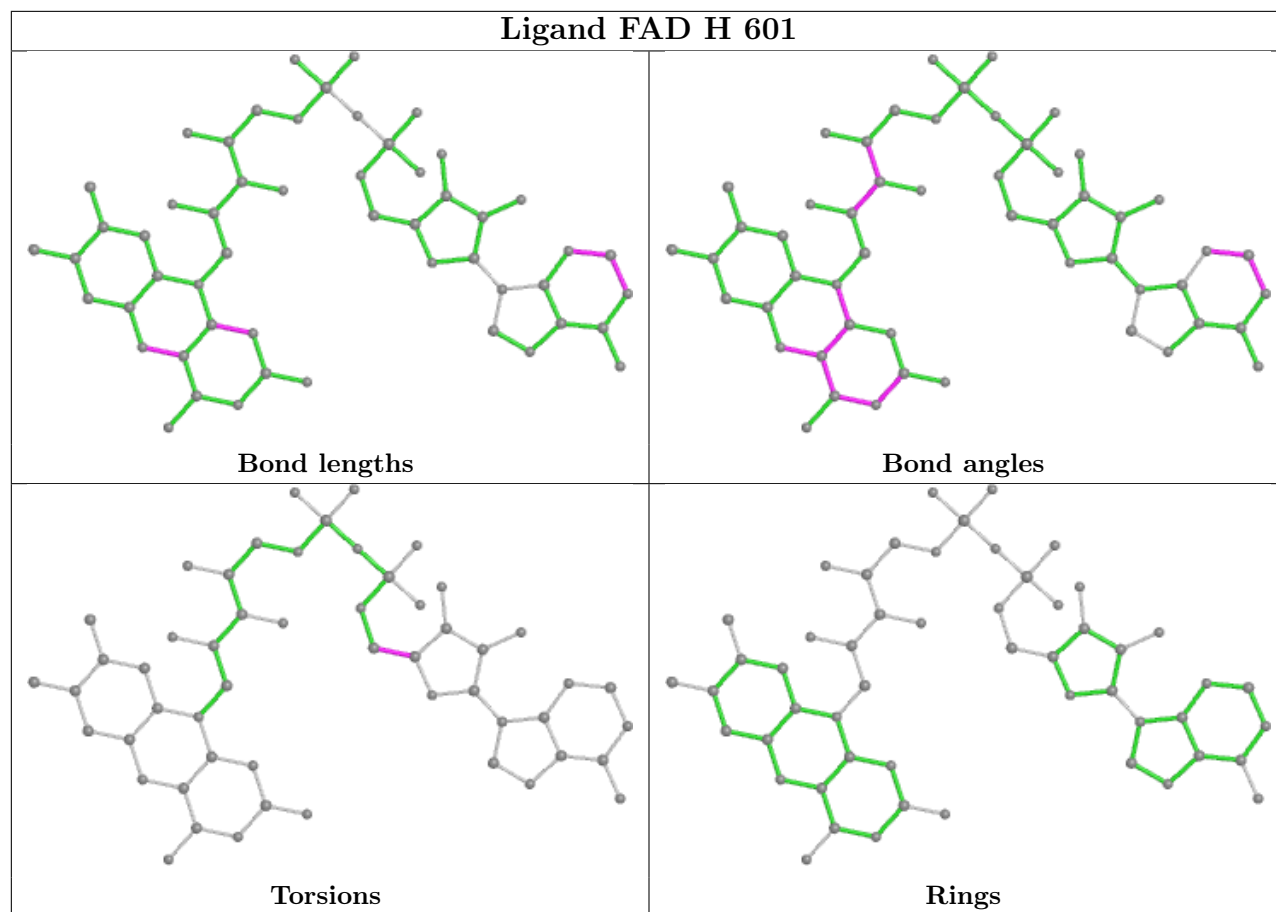
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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









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	495/521 (95%)	0.11	2 (0%) 92 94	25, 38, 57, 84	0
1	H	495/521 (95%)	0.10	1 (0%) 95 96	26, 39, 57, 86	0
All	All	990/1042 (95%)	0.10	3 (0%) 94 95	25, 39, 57, 86	0

All (3) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	39	ARG	3.6
1	A	457	ASN	2.3
1	H	105	LYS	2.3

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 [i](#)

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	TRT	H	606	20/25	0.80	0.24	43,52,57,58	0
5	ACT	A	611	4/4	0.83	0.15	47,50,55,58	0

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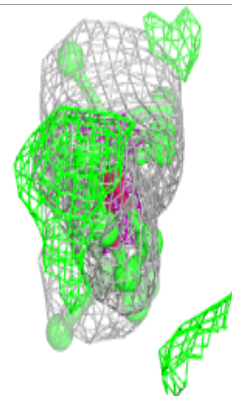
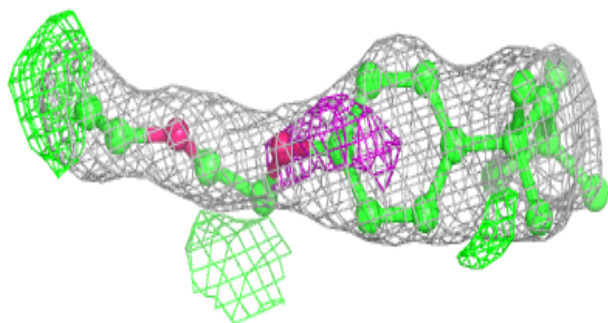
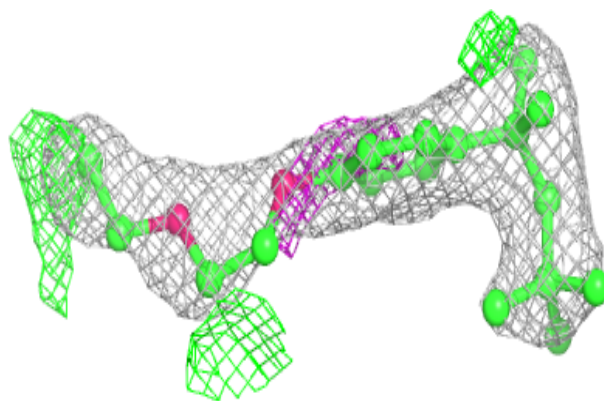
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
4	TRT	H	608	20/25	0.86	0.21	46,55,60,60	0
4	TRT	A	608	20/25	0.88	0.23	47,60,67,70	0
4	TRT	A	607	20/25	0.88	0.21	44,55,62,63	0
4	TRT	H	607	17/25	0.89	0.22	47,57,62,63	0
5	ACT	H	609	4/4	0.89	0.14	37,54,57,59	0
4	TRT	A	606	20/25	0.92	0.23	46,53,57,57	0
5	ACT	A	609	4/4	0.93	0.06	45,54,54,55	0
5	ACT	A	610	4/4	0.93	0.15	49,52,53,55	0
5	ACT	H	612	4/4	0.93	0.19	51,57,58,61	0
3	MG	H	605	1/1	0.94	0.14	43,43,43,43	0
5	ACT	A	613	4/4	0.94	0.10	50,50,50,51	0
5	ACT	H	611	4/4	0.95	0.07	48,52,53,55	0
5	ACT	H	615	4/4	0.95	0.09	55,58,60,60	0
5	ACT	H	613	4/4	0.96	0.18	53,54,54,55	0
3	MG	A	605	1/1	0.96	0.08	44,44,44,44	0
3	MG	A	603	1/1	0.97	0.09	33,33,33,33	0
5	ACT	H	614	4/4	0.97	0.20	35,38,39,52	0
5	ACT	H	610	4/4	0.97	0.12	48,50,50,59	0
3	MG	H	604	1/1	0.98	0.13	36,36,36,36	0
2	FAD	A	601	53/53	0.98	0.12	25,29,34,35	0
3	MG	A	604	1/1	0.98	0.11	38,38,38,38	0
2	FAD	H	601	53/53	0.98	0.13	24,29,34,36	0
3	MG	H	602	1/1	0.98	0.12	37,37,37,37	0
5	ACT	A	612	4/4	0.98	0.20	47,49,52,53	0
3	MG	H	603	1/1	0.98	0.08	34,34,34,34	0
3	MG	A	602	1/1	0.99	0.18	39,39,39,39	0

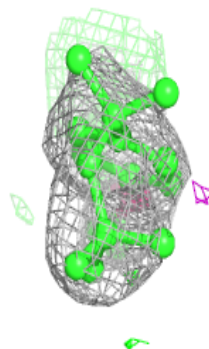
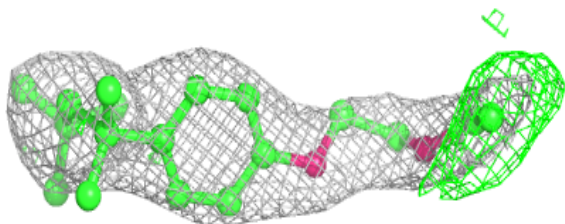
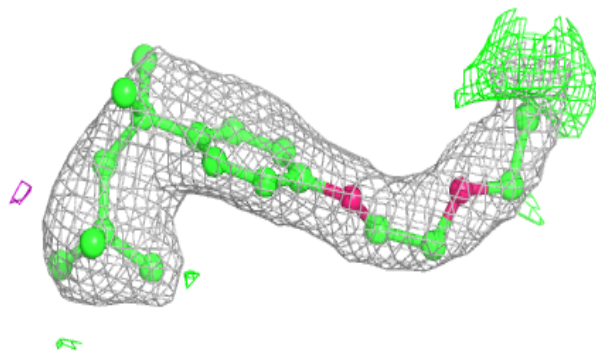
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around TRT H 606:

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

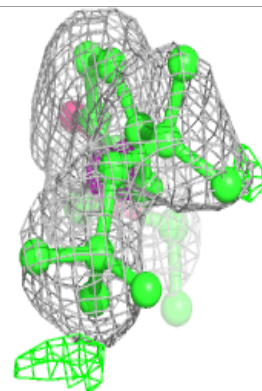
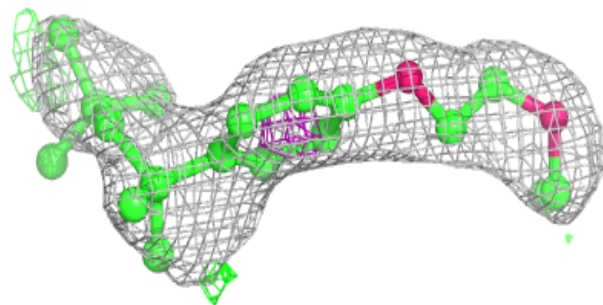
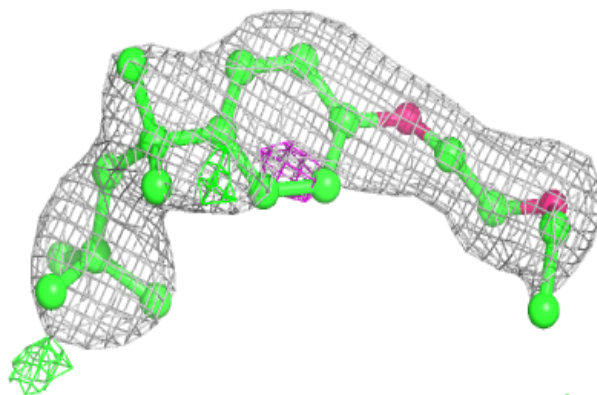
**Electron density around TRT H 608:**

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

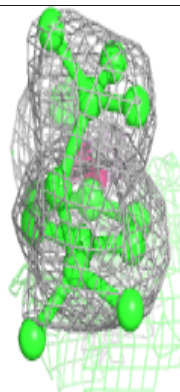
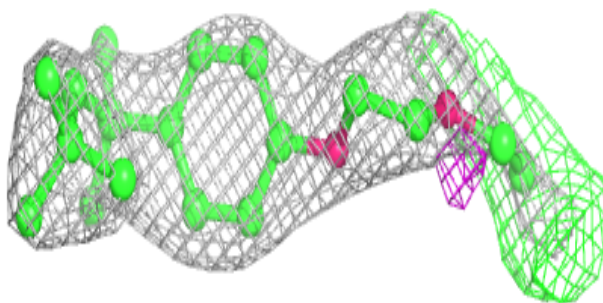
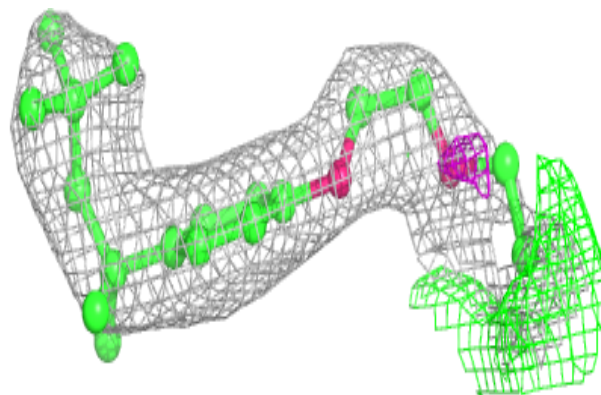


Electron density around TRT A 608:

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

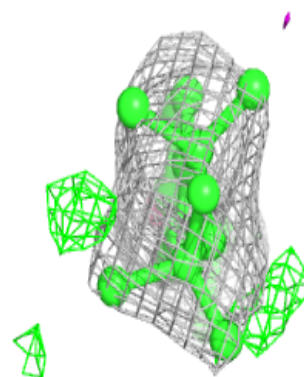
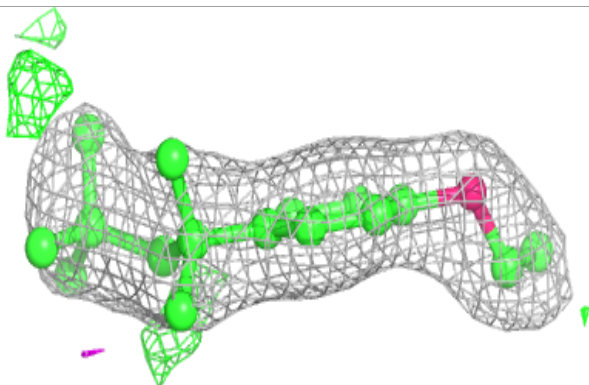
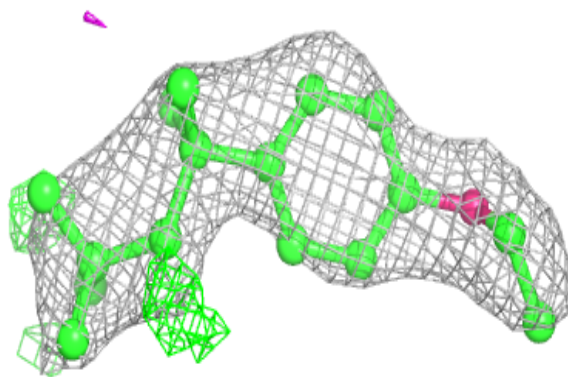
**Electron density around TRT A 607:**

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

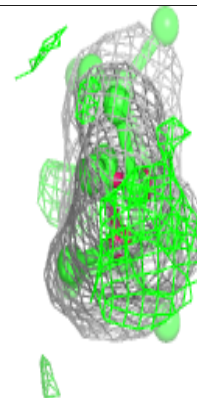
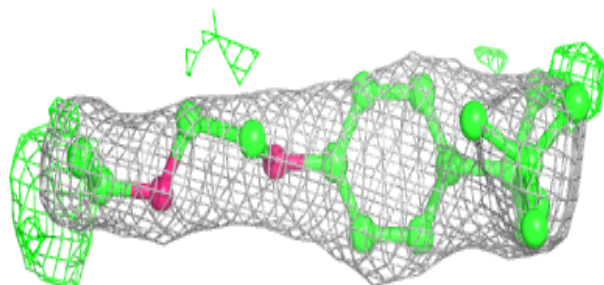
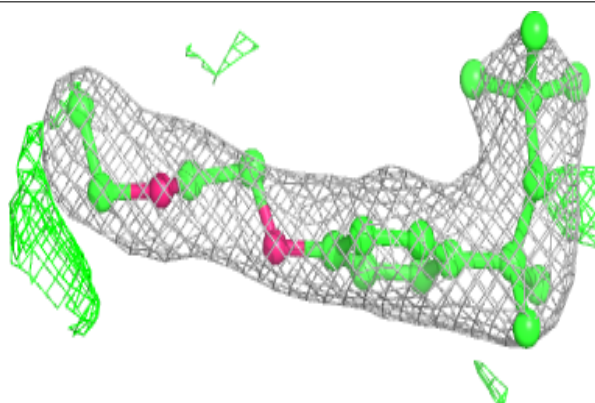


Electron density around TRT H 607:

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

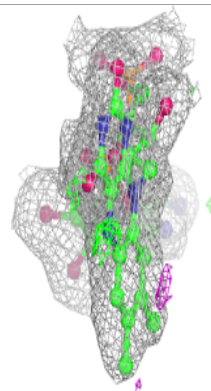
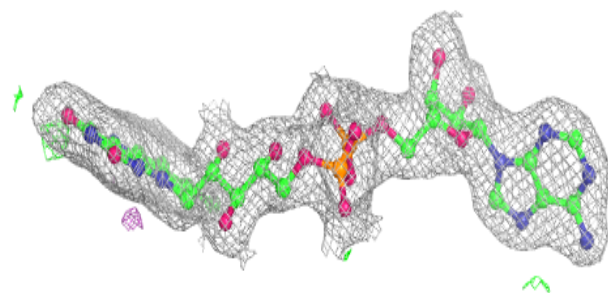
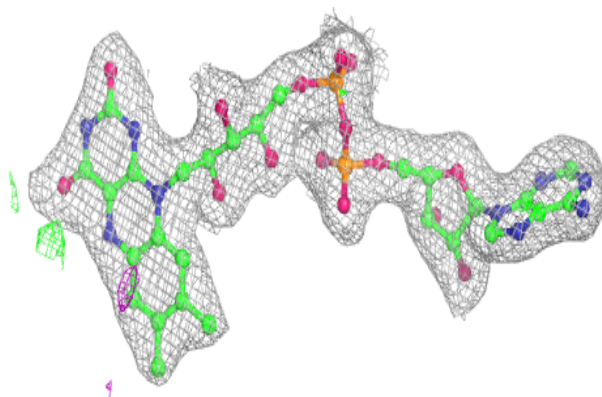
**Electron density around TRT A 606:**

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and green (positive)

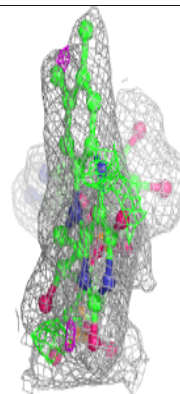
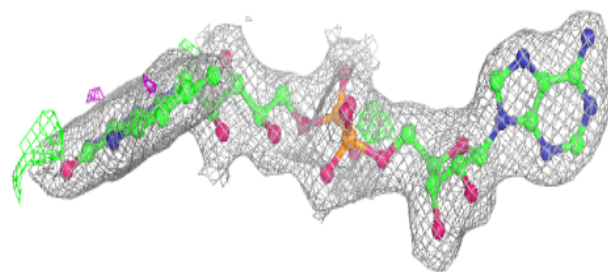
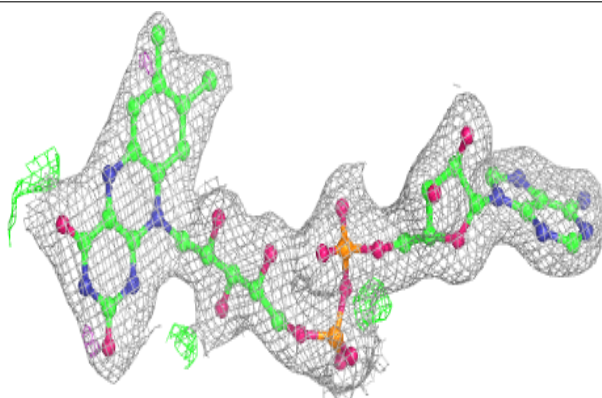


Electron density around FAD A 601:

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

**Electron density around FAD H 601:**

$2mF_o-DF_c$ (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.