



wwPDB X-ray Structure Validation Summary Report ⓘ

Oct 17, 2022 – 08:29 pm BST

PDB ID : 7NVP
Title : Trypanothione reductase from Trypanosoma brucei in complex with N-{4-methoxy-3-[(4-methoxyphenyl)sulfamoyl]phenyl}-5-nitrothiophene-2-carboxamide
Authors : Battista, T.; Fiorillo, A.; Colotti, G.; Ilari, A.
Deposited on : 2021-03-15
Resolution : 2.15 Å(reported)

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

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

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

MolProbity : 4.02b-467
Mogul : 1.8.4, CSD as541be (2020)
Xtrriage (Phenix) : 1.13
EDS : 2.31.2
buster-report : 1.1.7 (2018)
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac : 5.8.0267
CCP4 : 7.1.010 (Gargrove)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.31.2

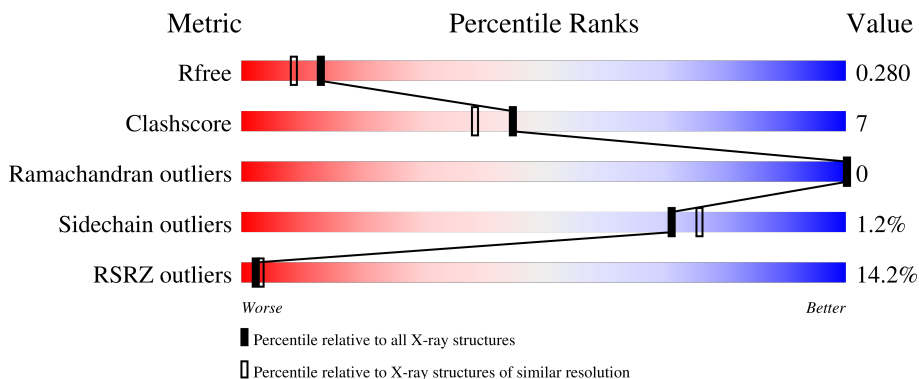
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.15 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	AAA	493	
1	BBB	493	

2 Entry composition [i](#)

There are 6 unique types of molecules in this entry. The entry contains 7868 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.

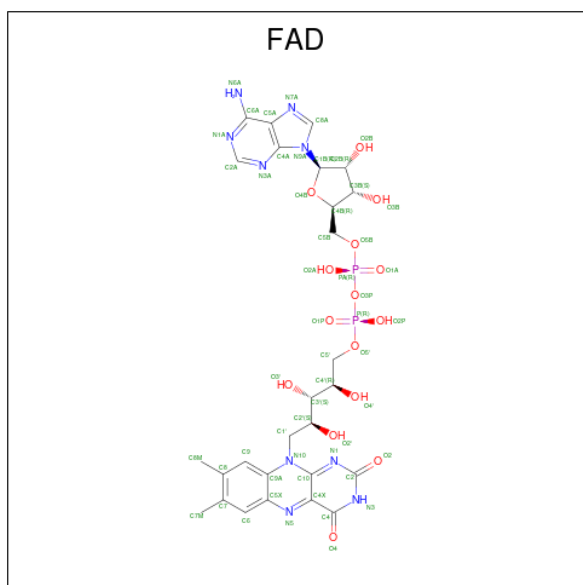
- Molecule 1 is a protein called N(1),N(8)-bis(glutathionyl)spermidine reductase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	AAA	490	Total 3753	C 2390	N 635	O 708	S 20	0	4	0
1	BBB	489	Total 3733	C 2378	N 631	O 704	S 20	0	3	0

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
AAA	0	HIS	-	expression tag	UNP Q389T8
BBB	0	HIS	-	expression tag	UNP Q389T8

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



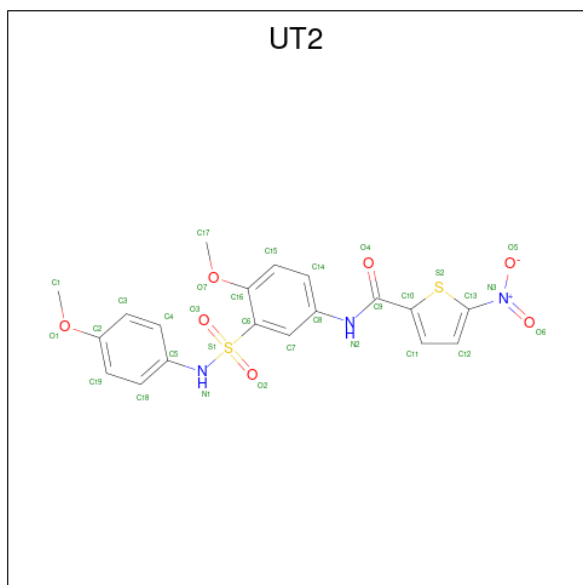
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
			Total	C	N	O	P		
2	AAA	1	Total 53	C 27	N 9	O 15	P 2	0	0

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

- Molecule 3 is N-{4-methoxy-3-[(4-methoxyphenyl)sulfamoyl]phenyl}-5-nitrothiophene-2-carboxamide (three-letter code: UT2) (formula: C₁₉H₁₇N₃O₇S₂) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
			Total	C	N	O	S		
3	AAA	1	31	19	3	7	2	0	0
3	BBB	1	31	19	3	7	2	0	0

- Molecule 4 is GLYCEROL (three-letter code: GOL) (formula: C₃H₈O₃).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	AAA	1	Total	C	O	0	0
			6	3	3		

- Molecule 5 is SULFATE ION (three-letter code: SO₄) (formula: O₄S).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	AAA	1	Total	O	S	0	0
			5	4	1		
5	AAA	1	Total	O	S	0	0
			5	4	1		
5	AAA	1	Total	O	S	0	0
			5	4	1		

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	AAA	1	Total O S 5 4 1	0	0
5	BBB	1	Total O S 5 4 1	0	0
5	BBB	1	Total O S 5 4 1	0	0
5	BBB	1	Total O S 5 4 1	0	0

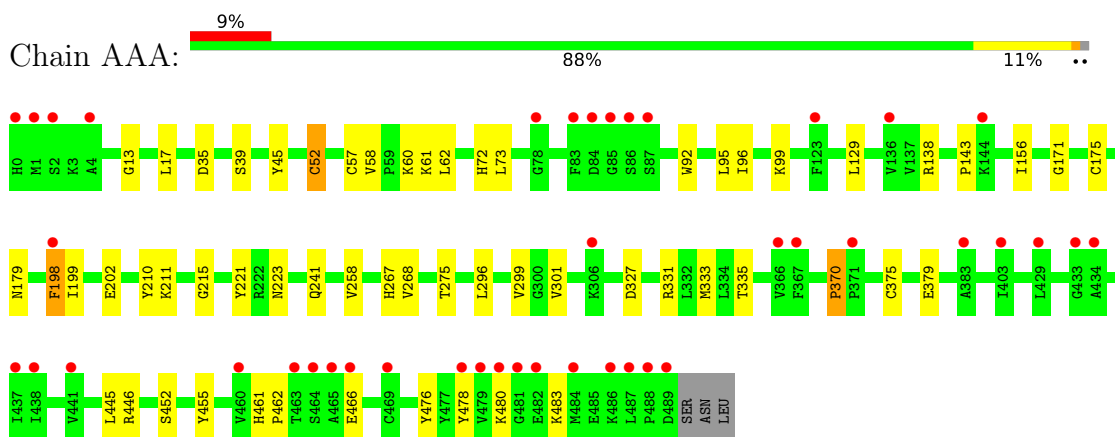
- Molecule 6 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	AAA	110	Total O 110 110	0	0
6	BBB	63	Total O 63 63	0	0

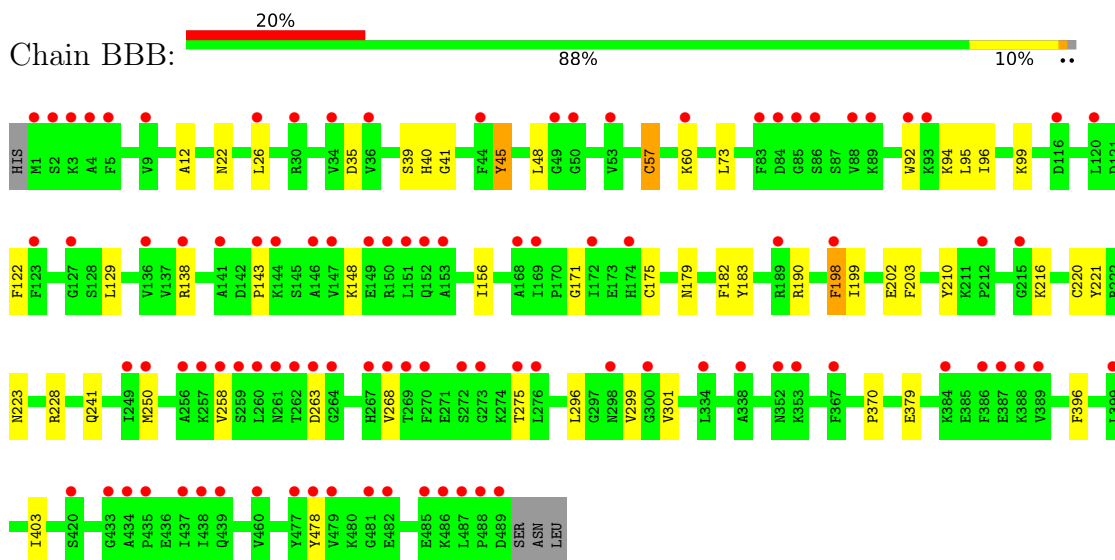
3 Residue-property plots [i](#)

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

- Molecule 1: N(1),N(8)-bis(glutathionyl)spermidine reductase



- Molecule 1: N(1),N(8)-bis(glutathionyl)spermidine reductase



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	66.10Å 133.33Å 158.91Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	102.14 – 2.15 47.48 – 2.15	Depositor EDS
% Data completeness (in resolution range)	99.7 (102.14-2.15) 99.7 (47.48-2.15)	Depositor EDS
R_{merge}	0.14	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.32 (at 2.16Å)	Xtriage
Refinement program	REFMAC 5.8.0267	Depositor
R, R_{free}	0.240 , 0.278 0.243 , 0.280	Depositor DCC
R_{free} test set	3832 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å ²)	41.4	Xtriage
Anisotropy	0.093	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	(Not available) , (Not available)	EDS
L-test for twinning ²	$\langle L \rangle = 0.43$, $\langle L^2 \rangle = 0.25$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	7868	wwPDB-VP
Average B, all atoms (Å ²)	54.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.24% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

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

5 Model quality [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: FAD, UT2, SO4, GOL

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	AAA	0.75	0/3842	0.85	0/5210
1	BBB	0.71	0/3821	0.82	0/5182
All	All	0.73	0/7663	0.84	0/10392

There are no bond length outliers.

There are no bond angle outliers.

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	AAA	3753	0	3764	48	0
1	BBB	3733	0	3750	53	0
2	AAA	53	0	31	3	0
2	BBB	53	0	31	6	0
3	AAA	31	0	0	1	0
3	BBB	31	0	0	4	0
4	AAA	6	0	8	0	0
5	AAA	20	0	0	1	0
5	BBB	15	0	0	0	0
6	AAA	110	0	0	5	1
6	BBB	63	0	0	3	1
All	All	7868	0	7584	100	1

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 7.

The worst 5 of 100 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)
2:AAA:501:FAD:H5'2	6:AAA:606:HOH:O	1.43	1.15
1:AAA:480[B]:LYS:HA	1:AAA:480[B]:LYS:CE	1.80	1.10
1:AAA:480[B]:LYS:HA	1:AAA:480[B]:LYS:HE3	1.05	1.04
1:BBB:45:TYR:CD1	1:BBB:179:ASN:HB3	1.95	1.01
1:AAA:45:TYR:CD1	1:AAA:179:ASN:HB3	2.04	0.93

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:AAA:618:HOH:O	6:BBB:647:HOH:O[3_654]	1.39	0.81

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	AAA	492/493 (100%)	462 (94%)	30 (6%)	0	100	100
1	BBB	490/493 (99%)	461 (94%)	29 (6%)	0	100	100
All	All	982/986 (100%)	923 (94%)	59 (6%)	0	100	100

There are no Ramachandran outliers to report.

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	AAA	407/406 (100%)	402 (99%)	5 (1%)	71	76
1	BBB	405/406 (100%)	400 (99%)	5 (1%)	71	76
All	All	812/812 (100%)	802 (99%)	10 (1%)	71	76

5 of 10 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	BBB	57	CYS
1	BBB	99	LYS
1	BBB	198	PHE
1	AAA	198	PHE
1	AAA	370	PRO

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

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no monosaccharides in this entry.

5.6 Ligand geometry [i](#)

12 ligands are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the

expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
3	UT2	BBB	502	-	29,33,33	1.45	2 (6%)	35,47,47	1.10	2 (5%)
5	SO4	AAA	505	-	4,4,4	0.32	0	6,6,6	0.07	0
4	GOL	AAA	503	-	5,5,5	0.10	0	5,5,5	0.32	0
5	SO4	AAA	504	-	4,4,4	0.39	0	6,6,6	0.10	0
3	UT2	AAA	502	-	29,33,33	1.33	1 (3%)	35,47,47	0.87	0
2	FAD	AAA	501	-	53,58,58	0.81	2 (3%)	68,89,89	0.93	2 (2%)
5	SO4	AAA	507	-	4,4,4	0.35	0	6,6,6	0.11	0
5	SO4	BBB	504	-	4,4,4	0.38	0	6,6,6	0.09	0
5	SO4	BBB	505	-	4,4,4	0.35	0	6,6,6	0.07	0
5	SO4	AAA	506	-	4,4,4	0.28	0	6,6,6	0.15	0
2	FAD	BBB	501	-	53,58,58	0.82	2 (3%)	68,89,89	0.82	1 (1%)
5	SO4	BBB	503	-	4,4,4	0.35	0	6,6,6	0.13	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
3	UT2	BBB	502	-	-	10/21/27/27	0/3/3/3
4	GOL	AAA	503	-	-	2/4/4/4	-
3	UT2	AAA	502	-	-	6/21/27/27	0/3/3/3
2	FAD	AAA	501	-	-	2/30/50/50	0/6/6/6
2	FAD	BBB	501	-	-	3/30/50/50	0/6/6/6

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

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	BBB	502	UT2	C13-N3	-7.30	1.32	1.45
3	AAA	502	UT2	C13-N3	-6.76	1.33	1.45
2	BBB	501	FAD	C1'-C2'	-3.25	1.48	1.52
2	AAA	501	FAD	C2-N3	-2.50	1.33	1.39
2	AAA	501	FAD	C1'-C2'	-2.49	1.49	1.52

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	BBB	502	UT2	O4-C9-C10	-4.07	112.22	121.08
2	BBB	501	FAD	O2P-P-O1P	2.56	124.89	112.24
3	BBB	502	UT2	C10-C9-N2	2.56	117.91	113.93
2	AAA	501	FAD	O5'-C5'-C4'	2.52	116.10	109.36
2	AAA	501	FAD	O2A-PA-O1A	2.41	124.15	112.24

There are no chirality outliers.

5 of 23 torsion outliers are listed below:

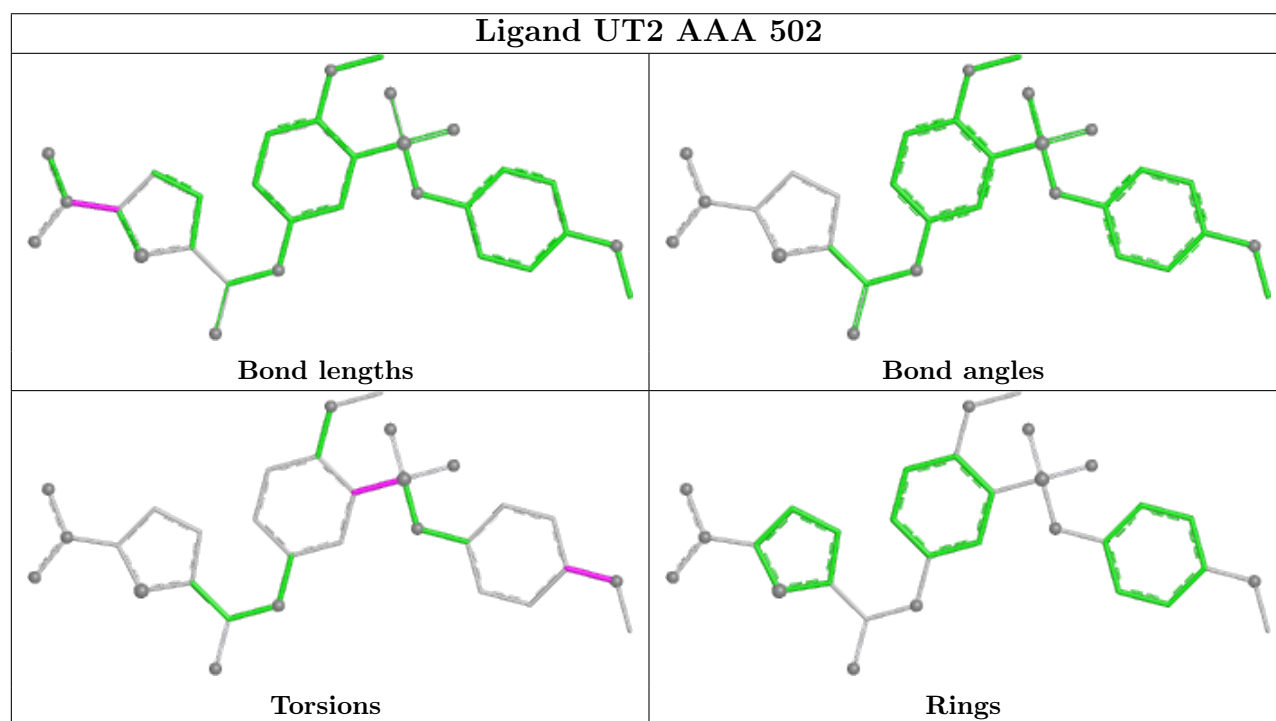
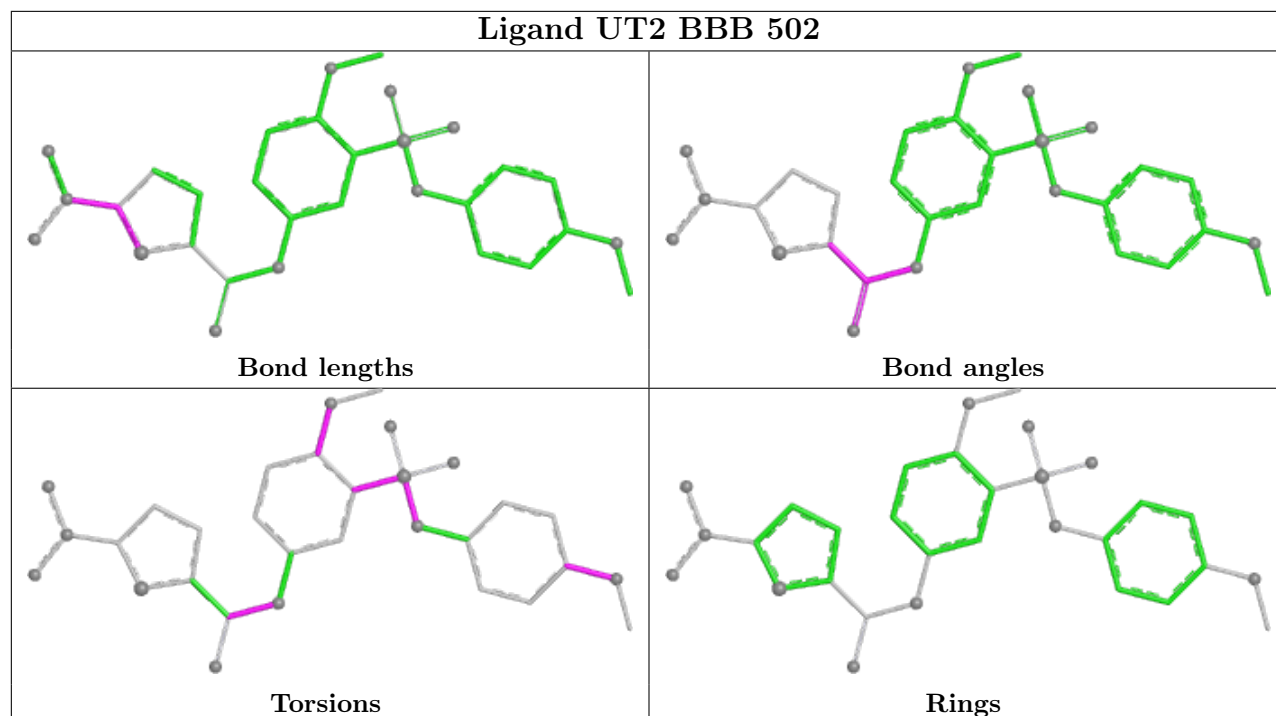
Mol	Chain	Res	Type	Atoms
2	AAA	501	FAD	PA-O3P-P-O5'
3	AAA	502	UT2	C16-C6-S1-N1
3	AAA	502	UT2	C16-C6-S1-O2
3	AAA	502	UT2	C16-C6-S1-O3
3	BBB	502	UT2	C6-C16-O7-C17

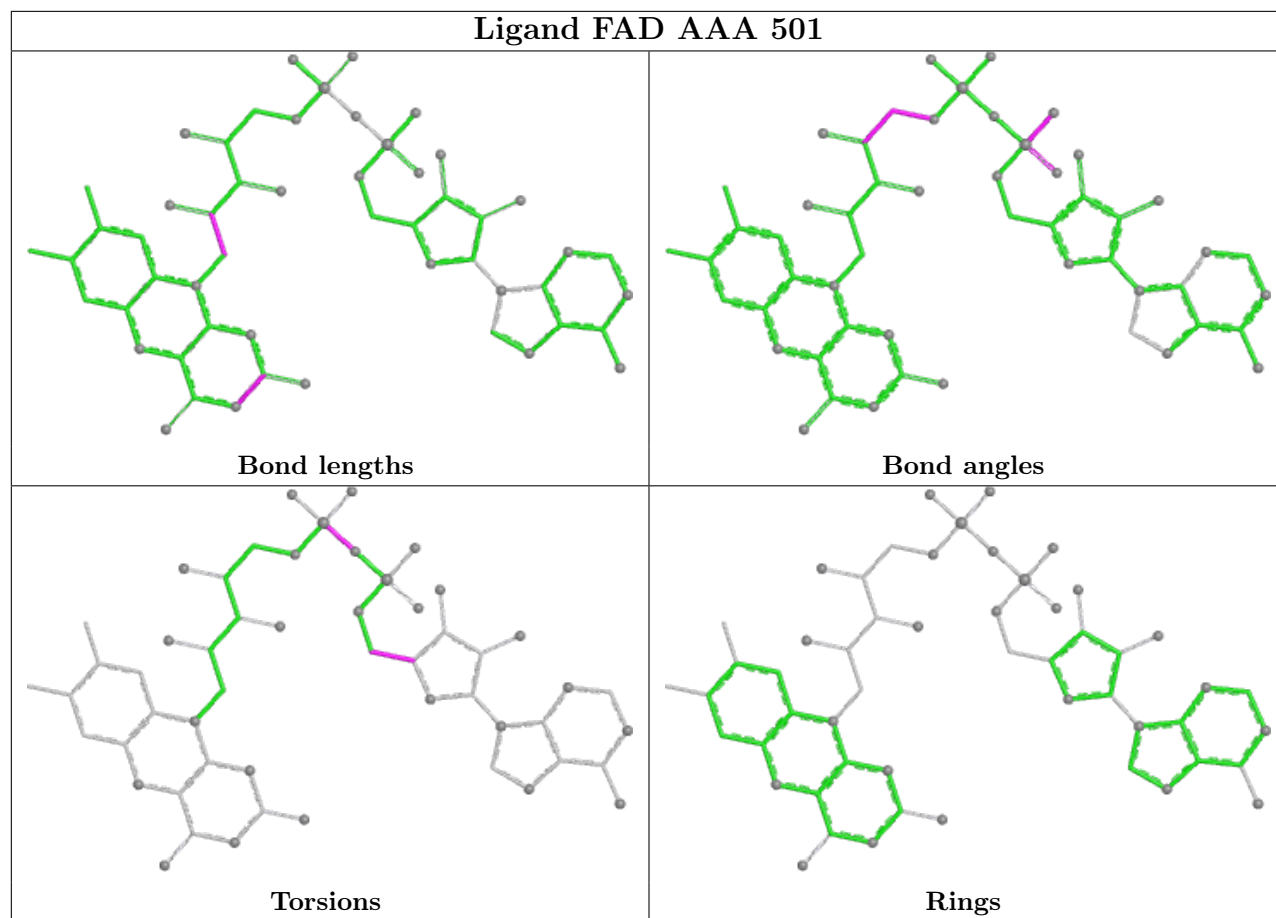
There are no ring outliers.

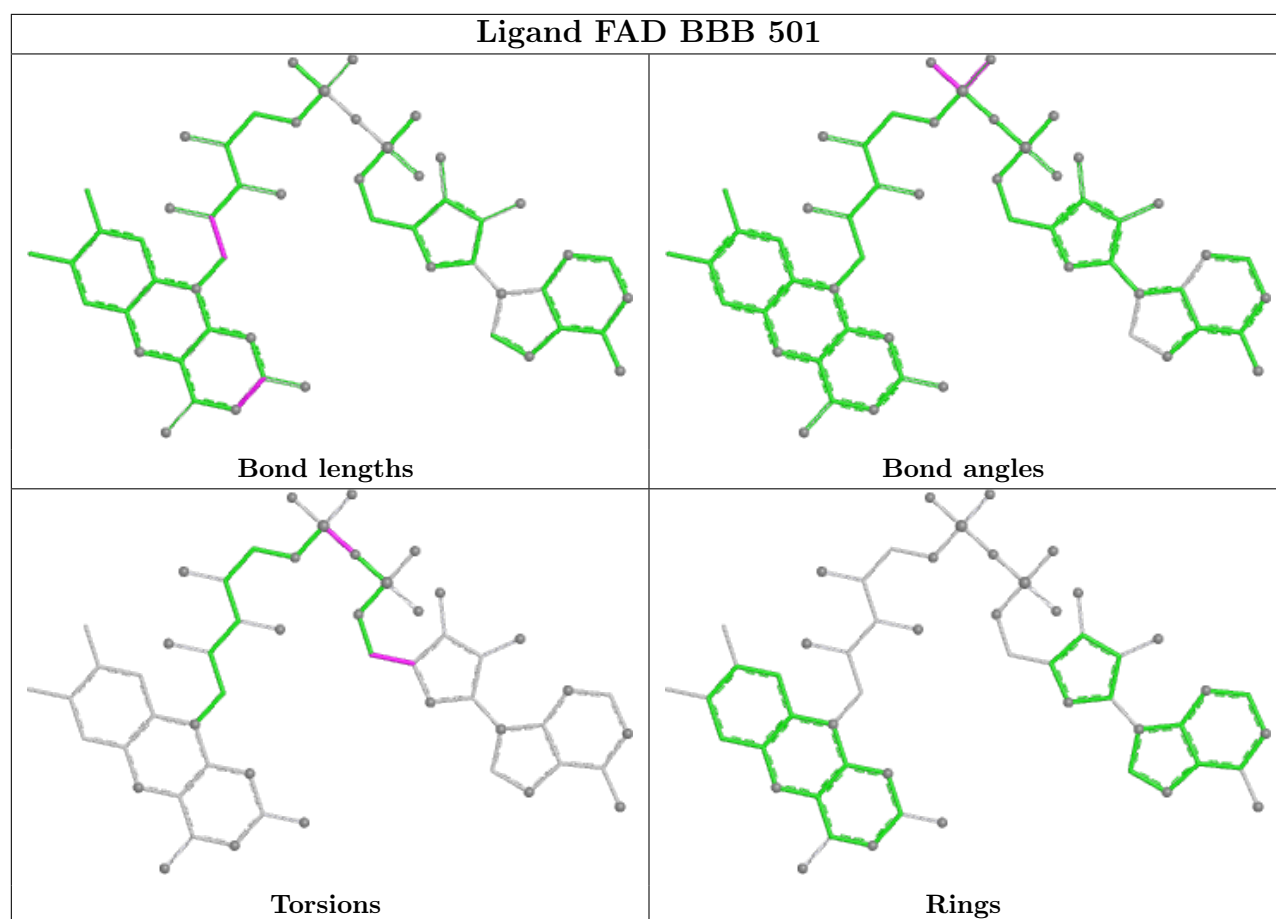
5 monomers are involved in 15 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	BBB	502	UT2	4	0
3	AAA	502	UT2	1	0
2	AAA	501	FAD	3	0
5	AAA	506	SO4	1	0
2	BBB	501	FAD	6	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	AAA	490/493 (99%)	0.56	42 (8%) 10 15	23, 44, 74, 110	0
1	BBB	489/493 (99%)	1.22	97 (19%) 1 1	28, 58, 99, 122	0
All	All	979/986 (99%)	0.89	139 (14%) 2 3	23, 50, 92, 122	0

The worst 5 of 139 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	BBB	273	GLY	8.0
1	BBB	262	THR	7.7
1	BBB	1	MET	6.9
1	AAA	0	HIS	6.8
1	BBB	489	ASP	6.1

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](#)

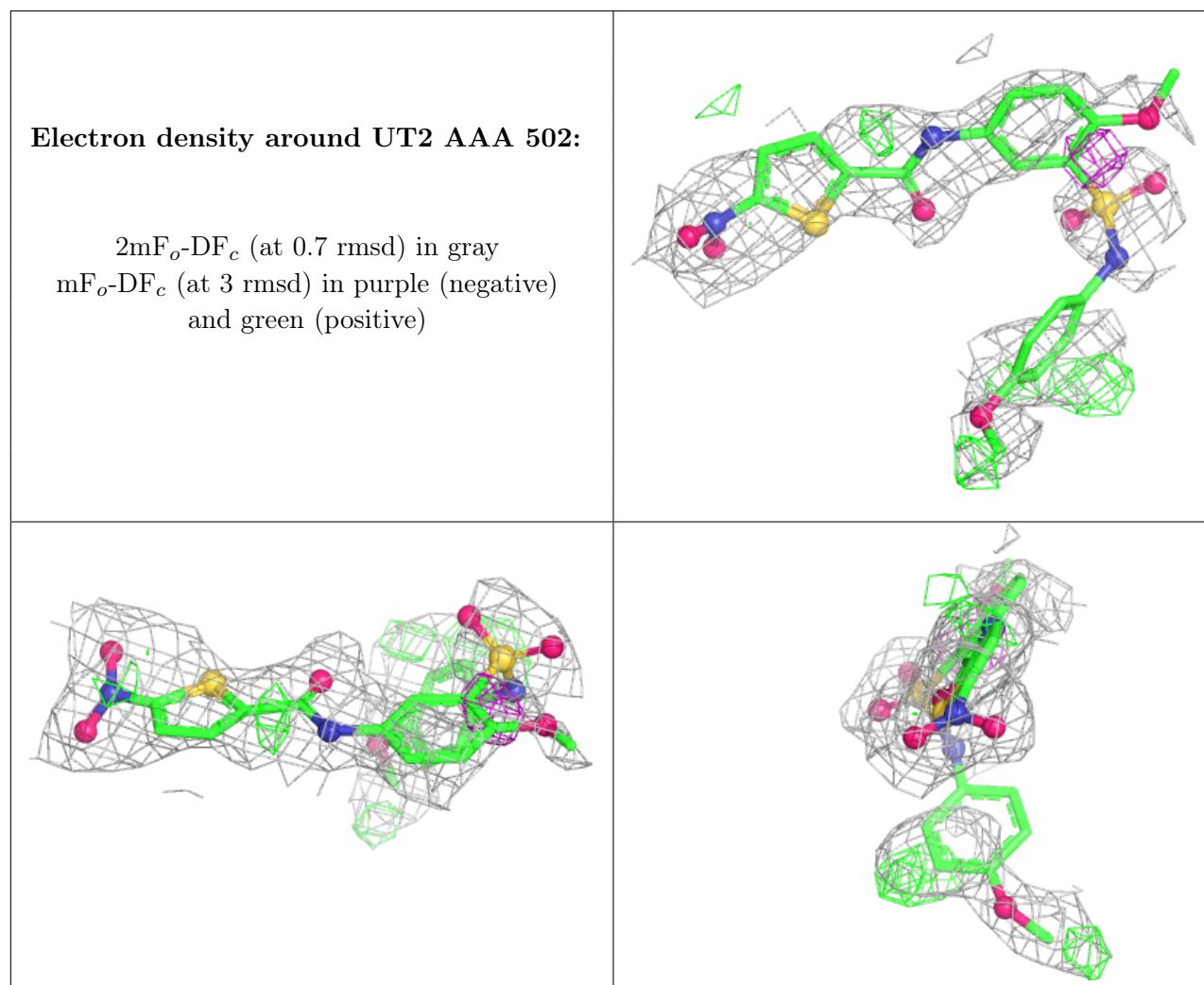
There are no monosaccharides in this entry.

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.

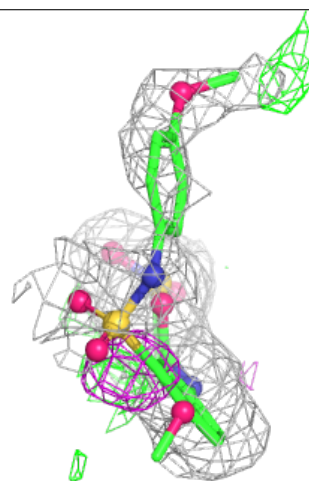
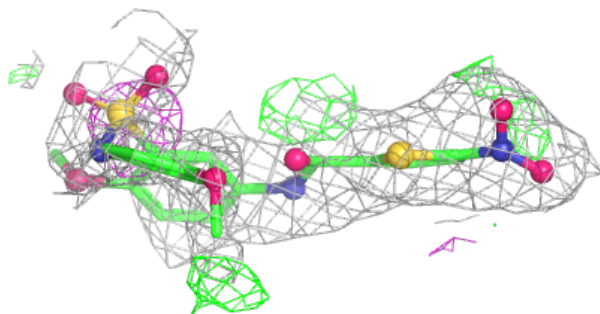
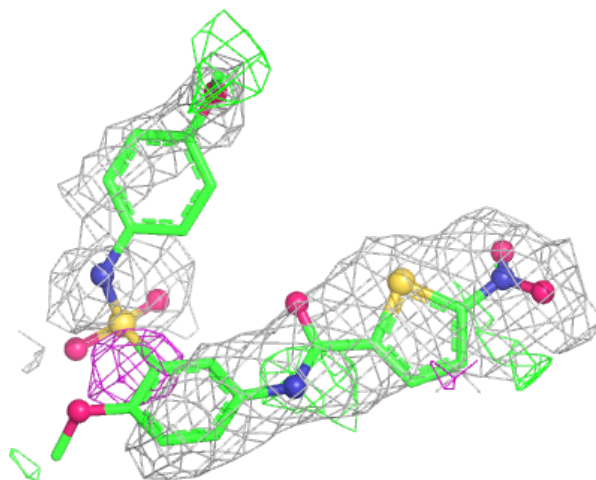
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
3	UT2	AAA	502	31/31	0.66	0.40	53,87,111,120	31
3	UT2	BBB	502	31/31	0.72	0.39	47,72,115,117	31
4	GOL	AAA	503	6/6	0.81	0.12	65,67,69,72	0
5	SO4	BBB	503	5/5	0.86	0.17	77,87,96,96	0
5	SO4	AAA	507	5/5	0.91	0.13	75,75,80,83	0
5	SO4	AAA	504	5/5	0.91	0.10	81,85,92,99	0
5	SO4	BBB	505	5/5	0.91	0.15	85,86,90,90	0
5	SO4	AAA	505	5/5	0.93	0.16	73,84,88,89	0
2	FAD	BBB	501	53/53	0.94	0.17	32,48,76,78	0
5	SO4	BBB	504	5/5	0.95	0.12	81,84,86,97	0
5	SO4	AAA	506	5/5	0.95	0.10	60,69,77,82	0
2	FAD	AAA	501	53/53	0.96	0.13	20,31,42,49	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.



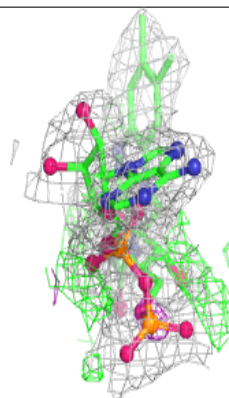
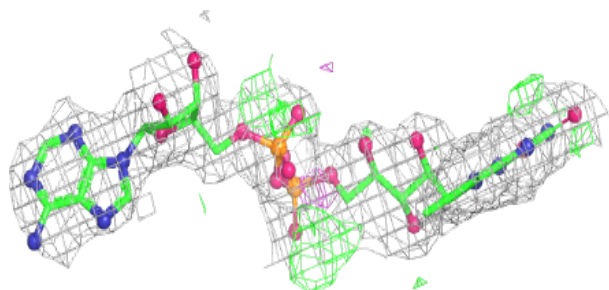
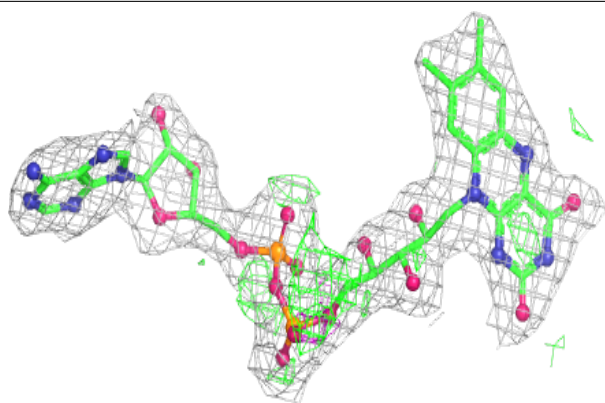
Electron density around UT2 BBB 502:

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

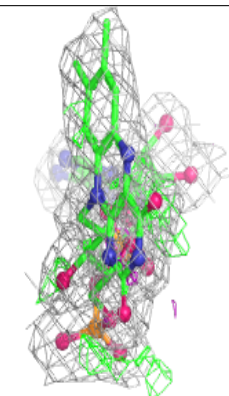
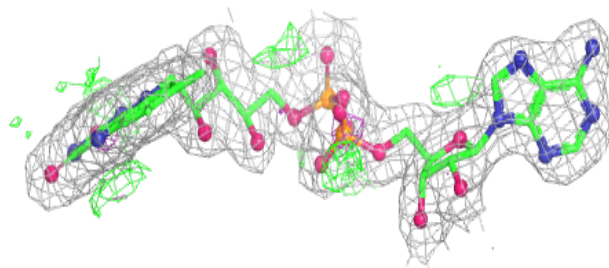
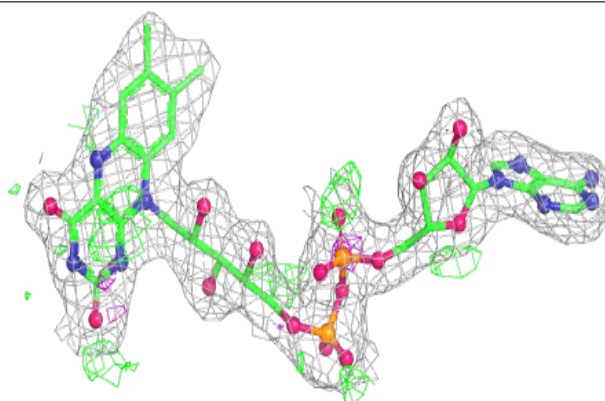


Electron density around FAD BBB 501:

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

**Electron density around FAD AAA 501:**

$2mF_o-DF_c$ (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.