



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

We welcome your comments at [validation@mail.wwpdb.org](mailto: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>.

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

MolProbity : 4.02b-467  
Mogul : 1.8.4, CSD as541be (2020)  
Xtriage (Phenix) : 1.13  
EDS : 2.31.2  
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

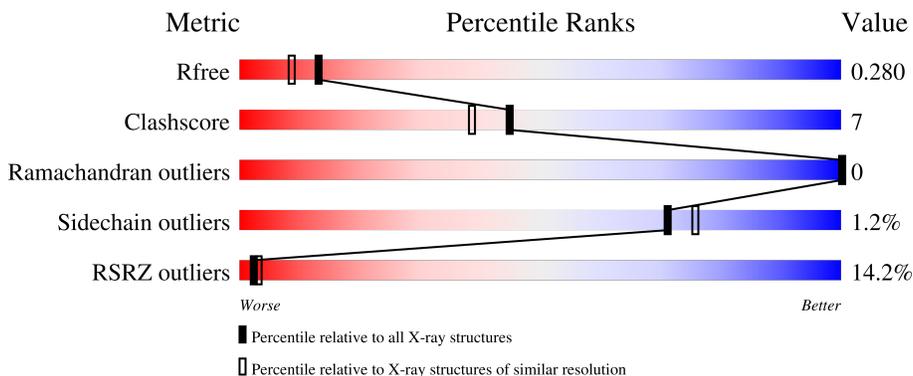
# 1 Overall quality at a glance

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  $\geq 3$ , 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.

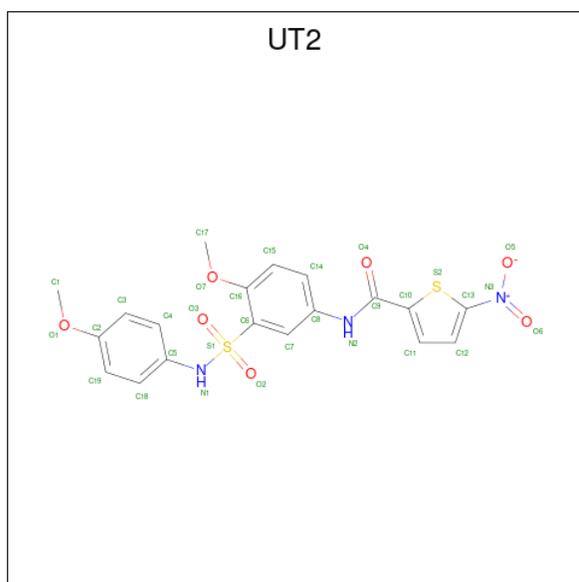
Mol	Chain	Length	Quality of chain
1	AAA	493	
1	BBB	493	



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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: C<sub>19</sub>H<sub>17</sub>N<sub>3</sub>O<sub>7</sub>S<sub>2</sub>) (labeled as "Ligand of Interest" by depositor).



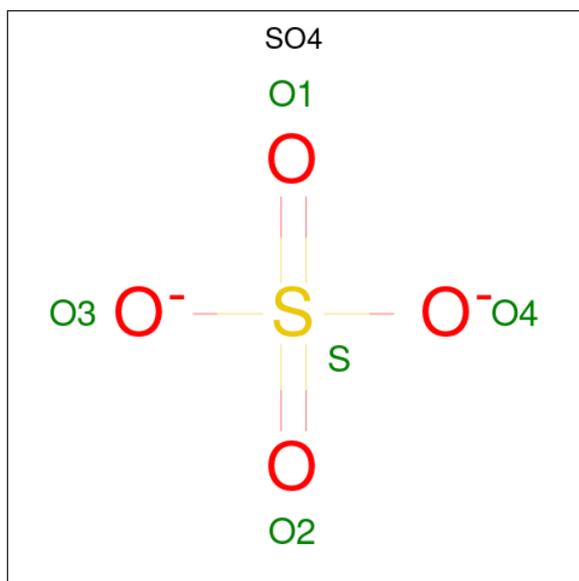
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
			Total	C	N	O	S		
3	AAA	1	31	19	3	7	2	0	0
3	BBB	1	31	19	3	7	2	0	0

- Molecule 4 is GLYCEROL (three-letter code: GOL) (formula: C<sub>3</sub>H<sub>8</sub>O<sub>3</sub>).



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: O<sub>4</sub>S).



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	0	0
			5	4	1		
5	BBB	1	Total	O	S	0	0
			5	4	1		
5	BBB	1	Total	O	S	0	0
			5	4	1		
5	BBB	1	Total	O	S	0	0
			5	4	1		

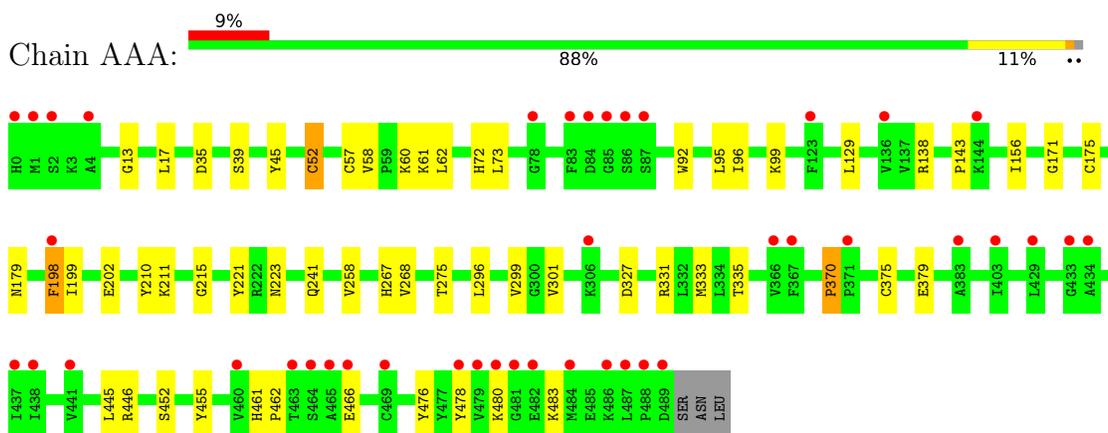
- Molecule 6 is water.

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

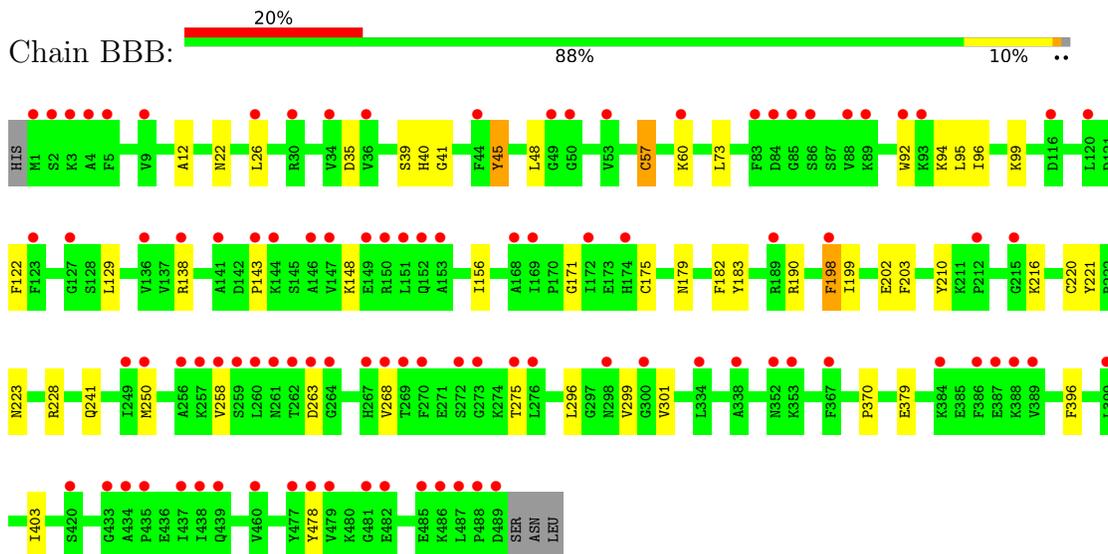
### 3 Residue-property plots [i](#)

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, $\alpha$ , $\beta$ , $\gamma$	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
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	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 <sup>2</sup> )	41.4	Xtriage
Anisotropy	0.093	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	(Not available) , (Not available)	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.43$ , $\langle L^2 \rangle = 0.25$	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 <sup>2</sup> )	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.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical 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: 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

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.

All (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
1:BBB:60[A]:LYS:HD2	1:BBB:202:GLU:OE1	1.74	0.87
1:AAA:480[B]:LYS:HE3	1:AAA:480[B]:LYS:CA	2.00	0.83
1:AAA:198:PHE:CE1	1:AAA:199:ILE:HG13	2.17	0.79
1:BBB:198:PHE:CE1	1:BBB:199:ILE:HG13	2.20	0.77
1:AAA:480[B]:LYS:CE	1:AAA:480[B]:LYS:CA	2.63	0.72
1:AAA:461:HIS:HA	1:AAA:466[A]:GLU:OE2	1.91	0.70
1:BBB:138:ARG:NE	1:BBB:143:PRO:O	2.19	0.69
1:BBB:35[B]:ASP:OD1	1:BBB:122:PHE:CZ	2.47	0.68
1:BBB:396[A]:PHE:CE2	3:BBB:502:UT2:C11	2.77	0.67
1:BBB:12:ALA:HB3	1:BBB:35[B]:ASP:OD2	1.99	0.62
1:AAA:129:LEU:HD13	1:AAA:299:VAL:HG21	1.82	0.62
1:AAA:198:PHE:CD1	1:AAA:199:ILE:HG13	2.35	0.62
1:AAA:138:ARG:NE	1:AAA:143:PRO:O	2.28	0.61
1:BBB:198:PHE:CD1	1:BBB:199:ILE:HG13	2.36	0.61
1:AAA:72:HIS:HD2	6:AAA:620:HOH:O	1.85	0.60
3:AAA:502:UT2:C14	6:AAA:661:HOH:O	2.50	0.60
1:BBB:129:LEU:HD13	1:BBB:299:VAL:HG21	1.85	0.59
1:BBB:175:CYS:SG	1:BBB:258:VAL:HG21	2.43	0.59
1:BBB:129:LEU:HD12	1:BBB:296:LEU:HD23	1.87	0.57
1:AAA:129:LEU:HD12	1:AAA:296:LEU:HD23	1.86	0.56
1:AAA:221:TYR:CE2	1:AAA:223:ASN:HB2	2.41	0.56
1:BBB:35[B]:ASP:OD1	1:BBB:122:PHE:CE1	2.60	0.55
1:BBB:35[B]:ASP:OD1	1:BBB:122:PHE:HZ	1.87	0.55
1:BBB:60[B]:LYS:NZ	1:BBB:199:ILE:HA	2.22	0.54
1:BBB:228:ARG:NH2	6:BBB:606:HOH:O	2.38	0.54
1:BBB:263:ASP:O	6:BBB:602:HOH:O	2.19	0.53
1:AAA:241:GLN:OE1	1:AAA:370:PRO:HG3	2.08	0.53
1:AAA:92:TRP:CZ2	1:AAA:96:ILE:HD11	2.44	0.52
1:BBB:92:TRP:CZ2	1:BBB:96:ILE:HD11	2.45	0.52
1:BBB:57:CYS:HB3	2:BBB:501:FAD:C4	2.40	0.52
1:AAA:62:LEU:HD22	1:BBB:403:ILE:CD1	2.40	0.50
1:BBB:35[A]:ASP:CG	2:BBB:501:FAD:H1B	2.32	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:BBB:95:LEU:HD22	1:BBB:210:TYR:CZ	2.47	0.50
1:AAA:299:VAL:HG23	1:AAA:301:VAL:HG23	1.92	0.50
1:BBB:171:GLY:HA3	1:BBB:258:VAL:O	2.11	0.50
1:AAA:60:LYS:HG3	1:AAA:61:LYS:N	2.24	0.50
1:BBB:241:GLN:OE1	1:BBB:370:PRO:HG3	2.11	0.50
1:BBB:35[A]:ASP:OD1	2:BBB:501:FAD:H1B	2.12	0.50
1:AAA:446:ARG:NH1	6:AAA:601:HOH:O	2.26	0.50
1:BBB:45:TYR:HD1	1:BBB:179:ASN:HB3	1.66	0.49
1:BBB:60[A]:LYS:CD	1:BBB:202:GLU:OE1	2.54	0.49
1:BBB:299:VAL:HG23	1:BBB:301:VAL:HG23	1.94	0.49
1:BBB:379:GLU:HB2	1:BBB:478:TYR:HE2	1.77	0.49
1:AAA:52:CYS:SG	1:AAA:335:THR:OG1	2.58	0.49
1:BBB:22:ASN:O	1:BBB:26:LEU:HB3	2.13	0.48
1:BBB:220:CYS:HA	1:BBB:250:MET:O	2.13	0.48
1:AAA:95:LEU:HD22	1:AAA:210:TYR:CZ	2.48	0.48
1:BBB:60[B]:LYS:HG3	1:BBB:182:PHE:CZ	2.49	0.48
1:BBB:148:LYS:NZ	6:BBB:608:HOH:O	2.45	0.48
1:BBB:221:TYR:CE2	1:BBB:223:ASN:HB2	2.49	0.47
1:AAA:327:ASP:OD1	1:AAA:333:MET:HA	2.14	0.47
1:AAA:73:LEU:CD2	1:BBB:73:LEU:CD2	2.93	0.47
1:AAA:175:CYS:SG	1:AAA:258:VAL:HG21	2.55	0.47
1:AAA:331:ARG:NH2	5:AAA:506:SO4:O4	2.42	0.47
1:AAA:129:LEU:HD21	1:AAA:156:ILE:HG21	1.97	0.46
1:BBB:60[B]:LYS:HD2	2:BBB:501:FAD:C7M	2.45	0.46
1:BBB:60[B]:LYS:HD2	2:BBB:501:FAD:HM72	1.96	0.46
1:AAA:13:GLY:O	1:AAA:17:LEU:HD12	2.16	0.46
1:AAA:211:LYS:HD2	1:AAA:215:GLY:C	2.36	0.46
1:AAA:57:CYS:HB3	2:AAA:501:FAD:C4	2.45	0.46
1:AAA:221:TYR:CZ	1:AAA:223:ASN:HB2	2.51	0.46
1:BBB:268:VAL:O	1:BBB:275:THR:HA	2.16	0.45
1:AAA:171:GLY:HA3	1:AAA:258:VAL:O	2.16	0.45
1:AAA:375:CYS:SG	1:AAA:445:LEU:HD22	2.57	0.44
2:BBB:501:FAD:H9	2:BBB:501:FAD:H1'1	1.78	0.44
1:BBB:396[A]:PHE:HE2	3:BBB:502:UT2:C11	2.31	0.44
1:AAA:379:GLU:HB2	1:AAA:478:TYR:HE2	1.82	0.44
1:BBB:35[B]:ASP:OD2	1:BBB:48:LEU:HA	2.18	0.44
1:BBB:94:LYS:HA	1:BBB:94:LYS:HD2	1.73	0.44
1:BBB:129:LEU:HD21	1:BBB:156:ILE:HG21	1.99	0.44
1:AAA:476:TYR:CD1	1:AAA:483:LYS:HE3	2.53	0.43
1:BBB:60[B]:LYS:HG3	1:BBB:182:PHE:HZ	1.81	0.43
1:AAA:198:PHE:CD1	1:AAA:199:ILE:N	2.86	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:BBB:41:GLY:HA2	1:BBB:183:TYR:CZ	2.54	0.43
1:AAA:45:TYR:CD2	1:AAA:45:TYR:N	2.87	0.43
1:AAA:268:VAL:O	1:AAA:275:THR:HA	2.19	0.43
1:BBB:45:TYR:CE1	1:BBB:179:ASN:HB3	2.47	0.43
1:AAA:73:LEU:CD2	1:BBB:73:LEU:HD23	2.49	0.43
1:AAA:60:LYS:CG	1:AAA:61:LYS:N	2.81	0.42
1:BBB:60[B]:LYS:HZ1	1:BBB:199:ILE:HA	1.84	0.42
1:AAA:461:HIS:HA	1:AAA:462:PRO:HA	1.76	0.42
1:AAA:452:SER:HA	1:AAA:455:TYR:CZ	2.55	0.42
1:AAA:198:PHE:CE1	1:AAA:199:ILE:CG1	2.97	0.42
1:BBB:396[A]:PHE:HE2	3:BBB:502:UT2:C12	2.33	0.42
1:AAA:35:ASP:HA	2:AAA:501:FAD:N3A	2.35	0.42
1:BBB:57:CYS:HA	1:BBB:60[A]:LYS:HE3	2.02	0.42
1:BBB:60[B]:LYS:HE3	1:BBB:203:PHE:CE2	2.55	0.41
1:AAA:60:LYS:CD	1:AAA:202:GLU:OE1	2.68	0.41
1:AAA:57:CYS:SG	1:AAA:58:VAL:N	2.94	0.41
1:BBB:190:ARG:HA	1:BBB:216:LYS:O	2.21	0.41
1:BBB:40:HIS:ND1	1:BBB:183:TYR:OH	2.35	0.41
3:BBB:502:UT2:O4	3:BBB:502:UT2:C7	2.67	0.41
1:AAA:73:LEU:HD23	1:BBB:73:LEU:CD2	2.51	0.41
1:AAA:267:HIS:CE1	6:AAA:667:HOH:O	2.74	0.40
1:AAA:73:LEU:HD23	1:BBB:73:LEU:HD23	2.03	0.40

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

All (10) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	AAA	39	SER
1	AAA	52	CYS
1	AAA	99	LYS
1	AAA	198	PHE
1	AAA	370	PRO
1	BBB	39	SER
1	BBB	45	TYR
1	BBB	57	CYS
1	BBB	99	LYS
1	BBB	198	PHE

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	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
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

All (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
2	BBB	501	FAD	C2-N3	-2.23	1.33	1.39
3	BBB	502	UT2	C13-S2	-2.18	1.70	1.74

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.

All (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
3	BBB	502	UT2	C3-C2-O1-C1
3	BBB	502	UT2	C19-C2-O1-C1
3	AAA	502	UT2	C3-C2-O1-C1
3	AAA	502	UT2	C19-C2-O1-C1
2	BBB	501	FAD	O4B-C4B-C5B-O5B
2	BBB	501	FAD	C3B-C4B-C5B-O5B
3	BBB	502	UT2	O4-C9-N2-C8

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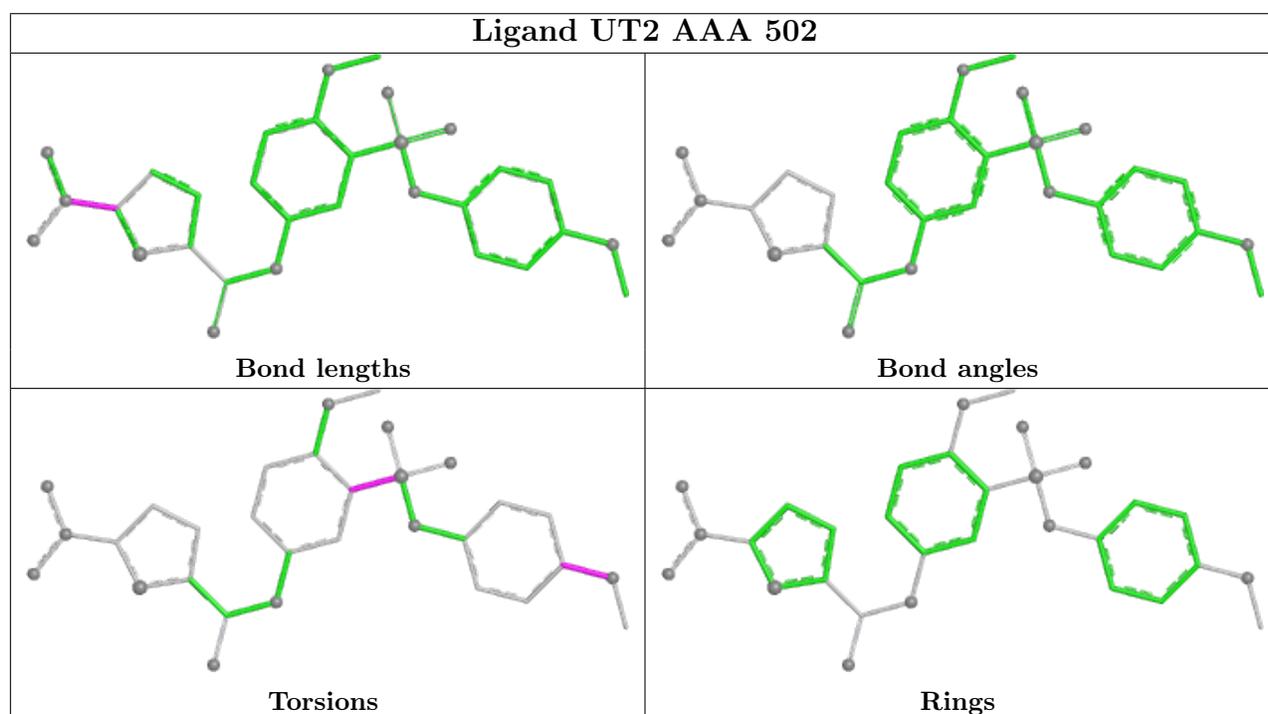
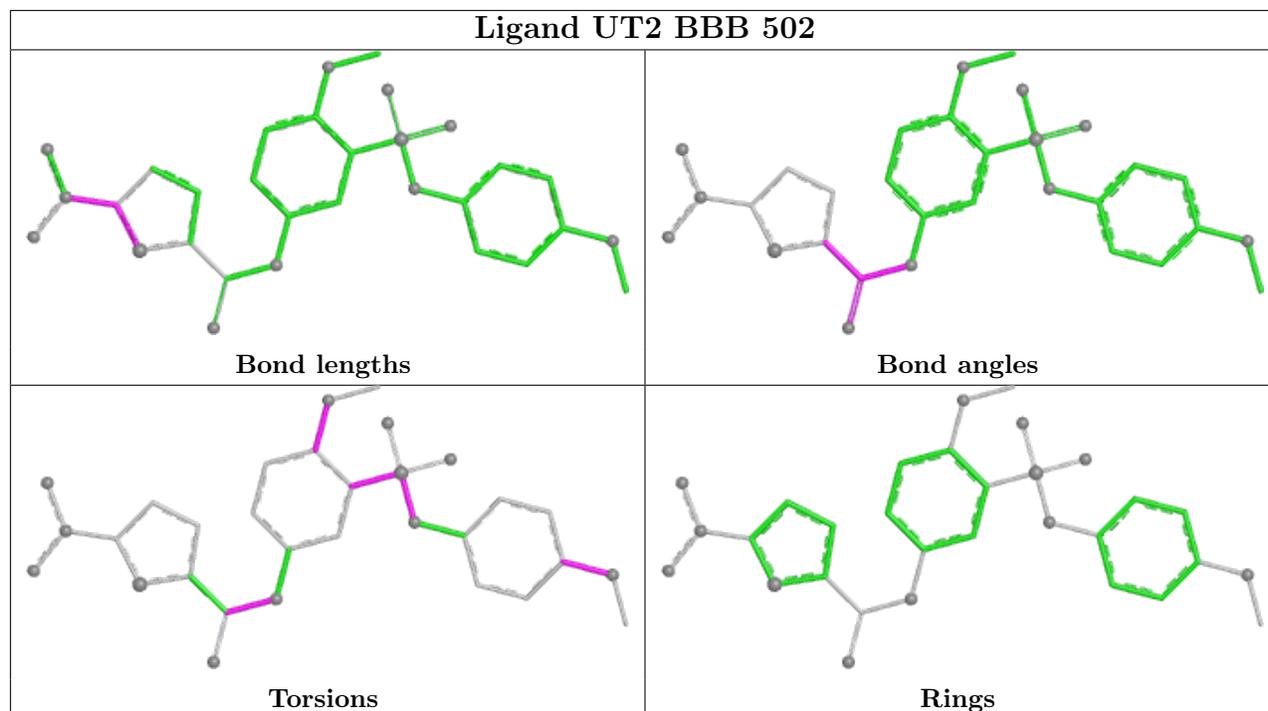
Mol	Chain	Res	Type	Atoms
3	BBB	502	UT2	C15-C16-O7-C17
4	AAA	503	GOL	C1-C2-C3-O3
3	BBB	502	UT2	C16-C6-S1-O3
3	BBB	502	UT2	C5-N1-S1-O3
3	BBB	502	UT2	C5-N1-S1-O2
2	BBB	501	FAD	PA-O3P-P-O5'
3	BBB	502	UT2	C16-C6-S1-N1
2	AAA	501	FAD	O4B-C4B-C5B-O5B
3	BBB	502	UT2	C5-N1-S1-C6
4	AAA	503	GOL	O2-C2-C3-O3
3	AAA	502	UT2	C7-C6-S1-O3

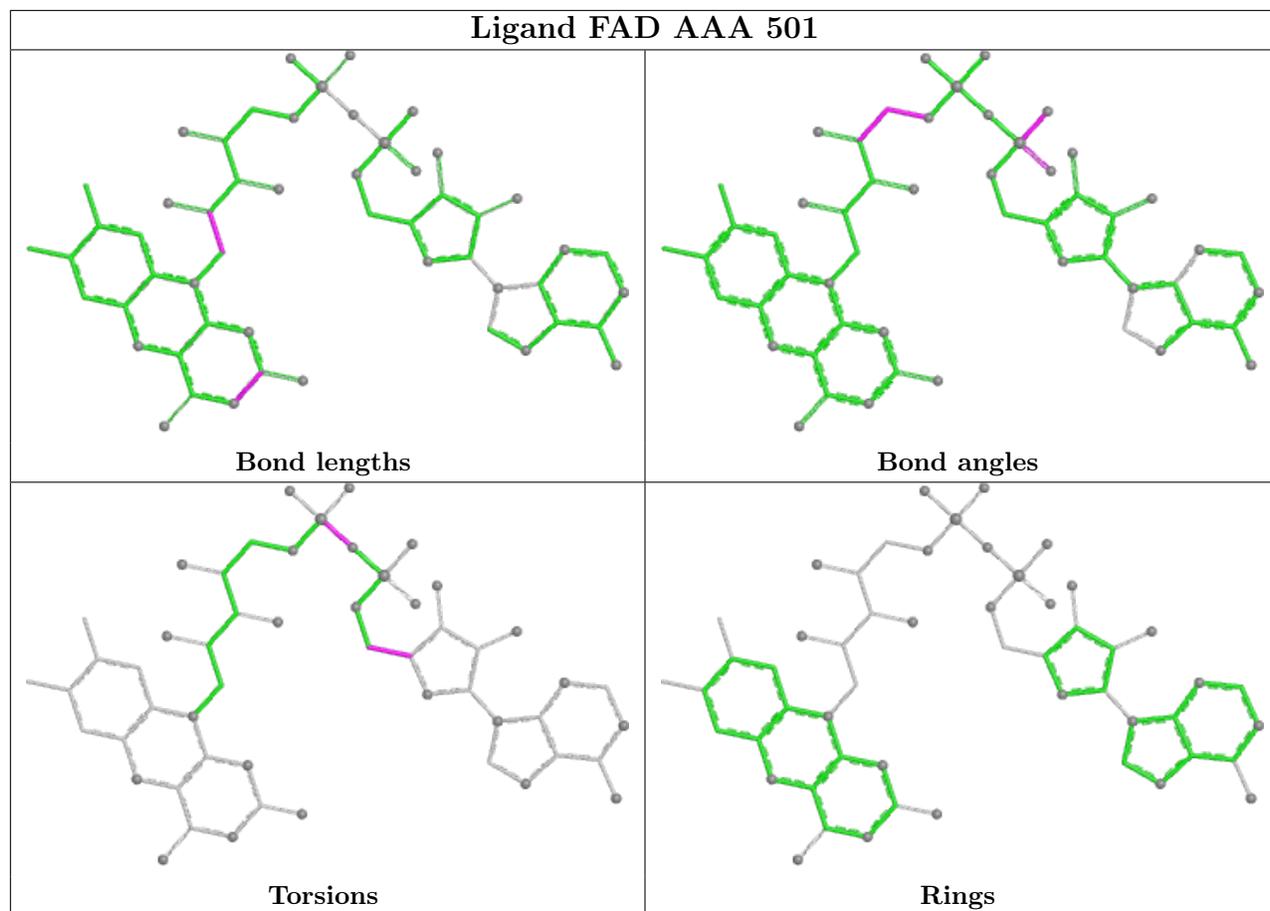
There are no ring outliers.

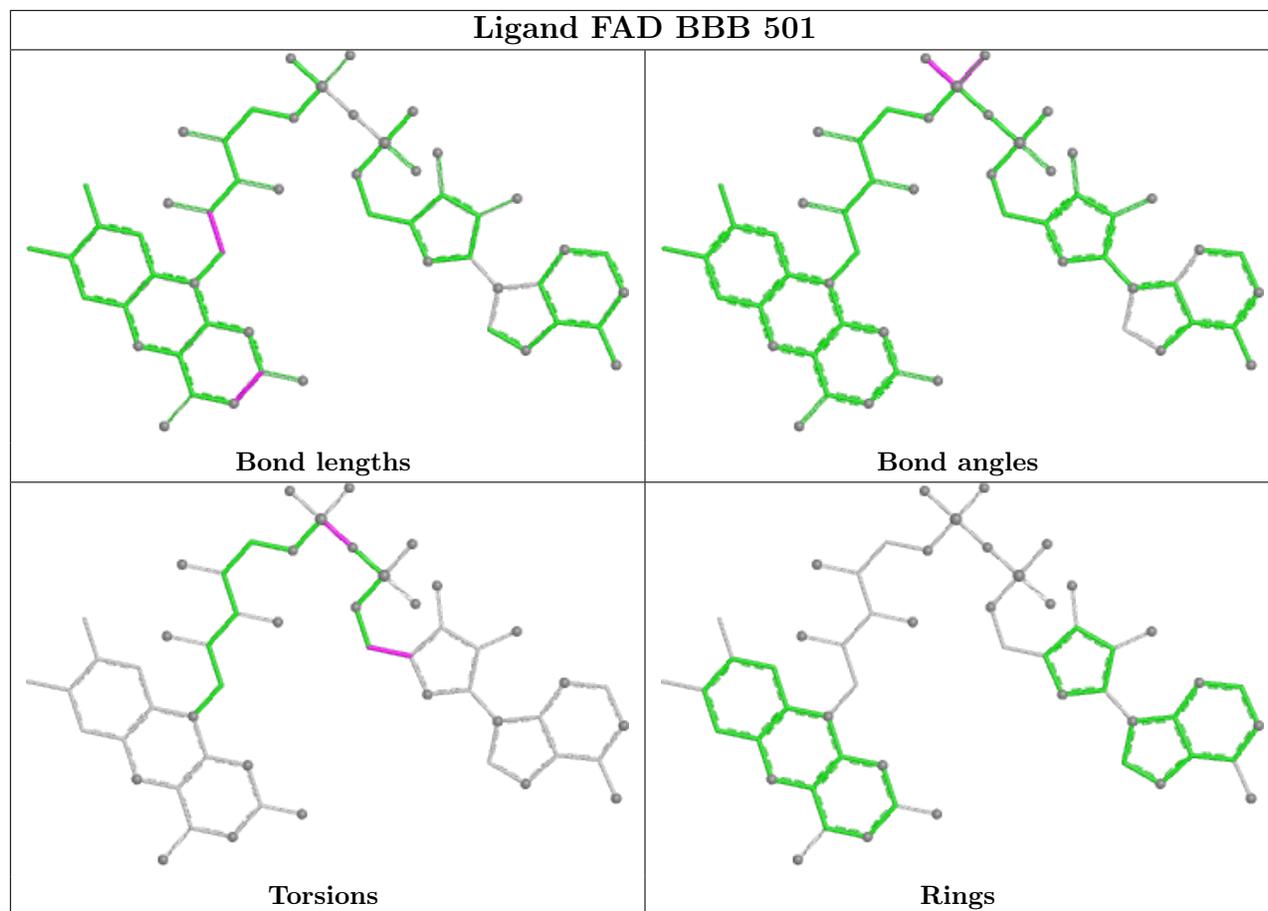
5 monomers are involved in 15 short contacts:

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, 95<sup>th</sup> 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 <sup>2</sup> )	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

All (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
1	BBB	2	SER	6.1
1	AAA	489	ASP	5.9
1	BBB	256	ALA	5.8
1	BBB	264	GLY	5.6
1	AAA	488	PRO	5.1
1	BBB	144	LYS	5.1
1	AAA	487	LEU	5.0
1	AAA	144	LYS	4.8
1	BBB	85	GLY	4.7
1	BBB	168	ALA	4.7
1	BBB	260	LEU	4.7
1	BBB	153	ALA	4.6
1	BBB	174	HIS	4.6
1	BBB	258	VAL	4.6
1	AAA	480[A]	LYS	4.3
1	BBB	138	ARG	4.2
1	BBB	151	LEU	4.1
1	BBB	5	PHE	4.1
1	BBB	89	LYS	4.1

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>	<b>RSRZ</b>
1	BBB	123	PHE	4.1
1	BBB	276	LEU	4.0
1	BBB	352	ASN	4.0
1	AAA	478	TYR	4.0
1	AAA	434	ALA	4.0
1	AAA	1	MET	4.0
1	BBB	146	ALA	3.9
1	AAA	460	VAL	3.8
1	BBB	270	PHE	3.8
1	BBB	34	VAL	3.8
1	BBB	26	LEU	3.7
1	BBB	147	VAL	3.7
1	BBB	268	VAL	3.7
1	BBB	172	ILE	3.7
1	BBB	261	ASN	3.7
1	AAA	429	LEU	3.7
1	AAA	486	LYS	3.7
1	BBB	88	VAL	3.7
1	BBB	150	ARG	3.6
1	BBB	434	ALA	3.6
1	AAA	84	ASP	3.5
1	AAA	437	ILE	3.5
1	AAA	481	GLY	3.4
1	BBB	479	VAL	3.4
1	BBB	4	ALA	3.4
1	BBB	386	PHE	3.4
1	BBB	212	PRO	3.4
1	BBB	389	VAL	3.4
1	AAA	463	THR	3.3
1	BBB	488	PRO	3.3
1	BBB	249	ILE	3.3
1	BBB	257	LYS	3.3
1	BBB	478	TYR	3.3
1	BBB	86	SER	3.2
1	BBB	141	ALA	3.2
1	BBB	269	THR	3.2
1	AAA	469	CYS	3.1
1	BBB	437	ILE	3.1
1	BBB	136	VAL	3.0
1	BBB	384	LYS	2.9
1	AAA	465	ALA	2.9
1	BBB	267	HIS	2.8

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>	<b>RSRZ</b>
1	AAA	433	GLY	2.8
1	BBB	60[A]	LYS	2.8
1	BBB	272	SER	2.8
1	AAA	86	SER	2.8
1	BBB	120	LEU	2.8
1	BBB	486	LYS	2.7
1	BBB	298	ASN	2.7
1	AAA	371	PRO	2.7
1	BBB	189	ARG	2.7
1	BBB	50	GLY	2.7
1	BBB	438	ILE	2.7
1	BBB	300	GLY	2.7
1	BBB	460	VAL	2.6
1	BBB	127	GLY	2.6
1	AAA	383	ALA	2.6
1	BBB	152	GLN	2.6
1	BBB	93	LYS	2.6
1	AAA	198	PHE	2.6
1	BBB	116	ASP	2.6
1	BBB	387	GLU	2.6
1	BBB	433	GLY	2.5
1	BBB	275	THR	2.5
1	AAA	482	GLU	2.5
1	AAA	83	PHE	2.5
1	BBB	83	PHE	2.5
1	AAA	466[A]	GLU	2.4
1	BBB	388	LYS	2.4
1	BBB	198	PHE	2.4
1	BBB	487	LEU	2.4
1	BBB	169	ILE	2.4
1	BBB	482	GLU	2.4
1	AAA	85	GLY	2.4
1	BBB	215	GLY	2.4
1	BBB	9	VAL	2.4
1	BBB	53	VAL	2.4
1	BBB	3	LYS	2.3
1	BBB	30	ARG	2.3
1	BBB	485	GLU	2.3
1	BBB	420	SER	2.3
1	AAA	367	PHE	2.3
1	BBB	92	TRP	2.3
1	BBB	367	PHE	2.3

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Mol	Chain	Res	Type	RSRZ
1	BBB	84	ASP	2.3
1	AAA	87	SER	2.2
1	AAA	464	SER	2.2
1	AAA	403	ILE	2.2
1	BBB	477	TYR	2.2
1	AAA	438	ILE	2.2
1	BBB	250	MET	2.2
1	AAA	2	SER	2.2
1	AAA	306	LYS	2.2
1	AAA	123	PHE	2.1
1	AAA	479	VAL	2.1
1	BBB	259	SER	2.1
1	BBB	334	LEU	2.1
1	AAA	441	VAL	2.1
1	BBB	44	PHE	2.1
1	BBB	143	PRO	2.1
1	AAA	366	VAL	2.1
1	BBB	338	ALA	2.1
1	BBB	149	GLU	2.1
1	BBB	481	GLY	2.1
1	BBB	399	LEU	2.1
1	BBB	263	ASP	2.1
1	AAA	4	ALA	2.0
1	AAA	136	VAL	2.0
1	BBB	439	GLN	2.0
1	BBB	353	LYS	2.0
1	AAA	484	MET	2.0
1	BBB	435	PRO	2.0
1	BBB	36	VAL	2.0
1	AAA	78	GLY	2.0
1	BBB	49	GLY	2.0

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

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

## 6.3 Carbohydrates [i](#)

There are no monosaccharides in this entry.

## 6.4 Ligands

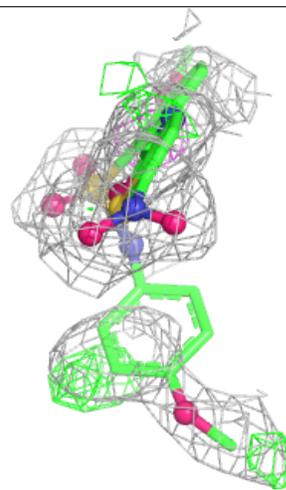
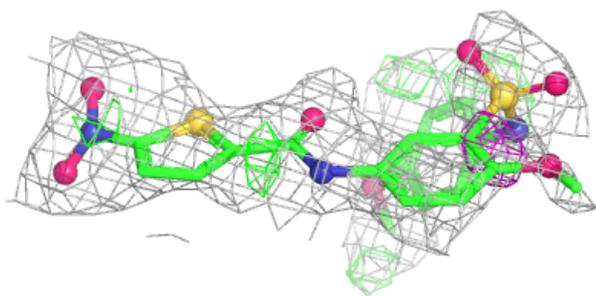
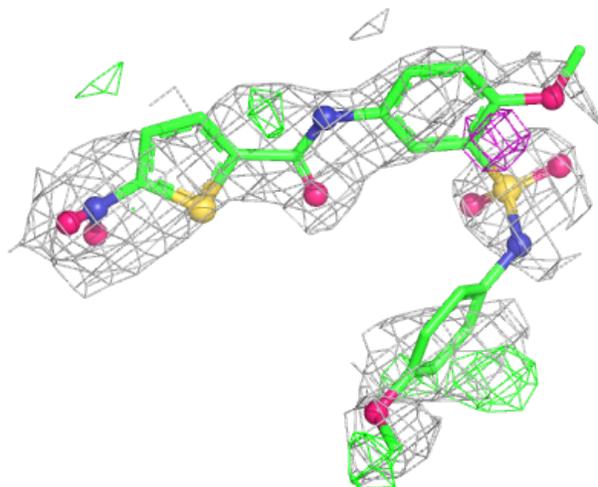
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled 'Q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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å <sup>2</sup> )	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.

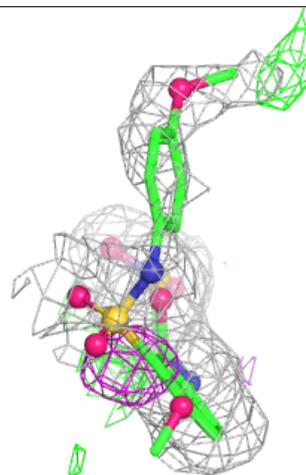
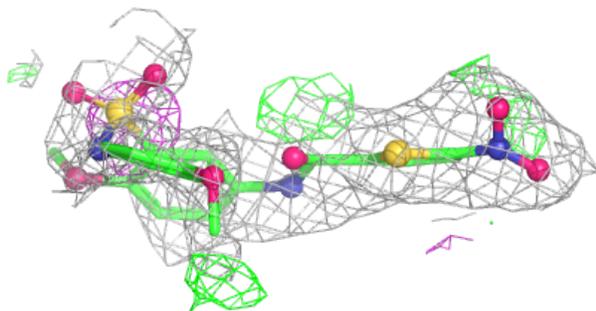
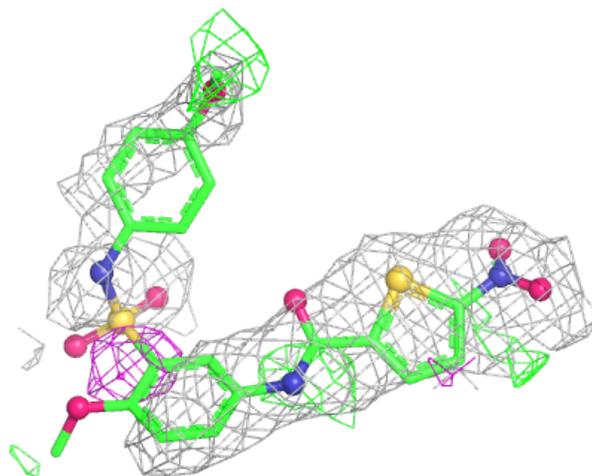
**Electron density around UT2 AAA 502:**

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



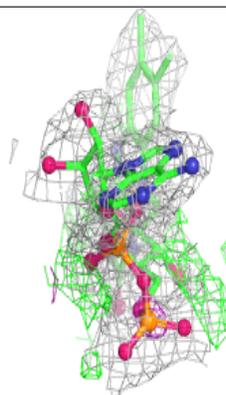
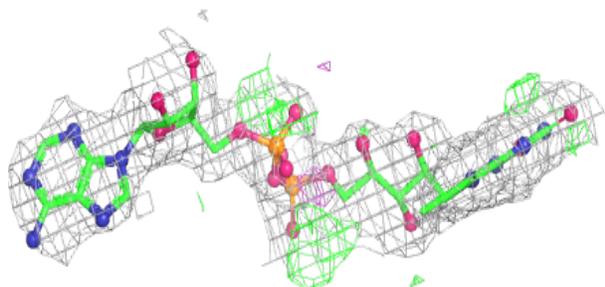
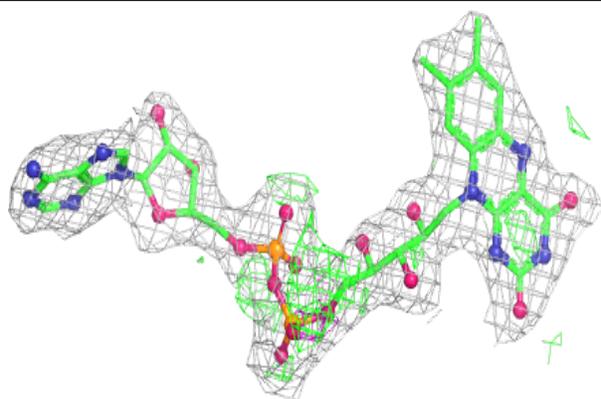
**Electron density around UT2 BBB 502:**

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

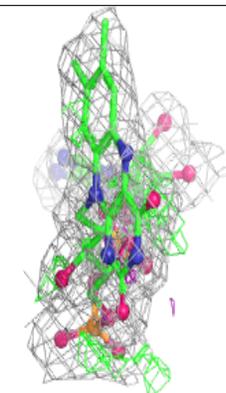
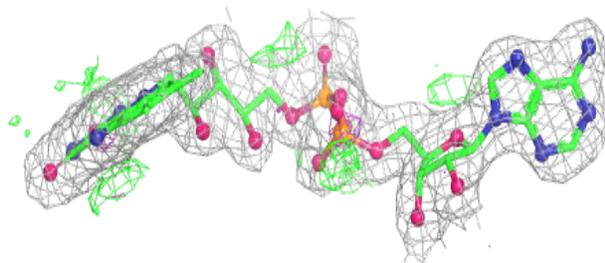
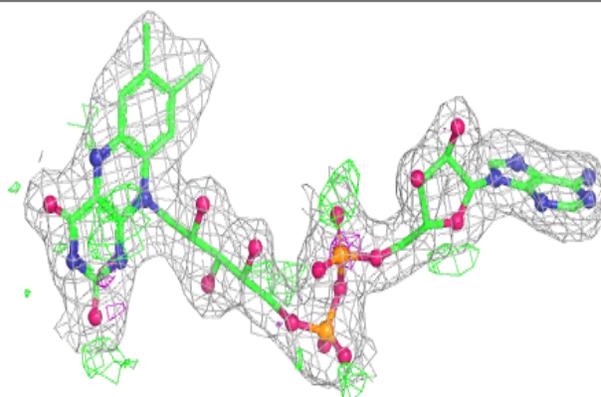


**Electron density around FAD BBB 501:**

$2mF_o-DF_c$  (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.