



# Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 09:49 PM UTC

PDB ID : 9IFI / pdb\_00009ifi  
Title : PANDDA analysis - Crystal structure of Trypanosoma brucei trypanothione reductase in complex with Z32399802  
Authors : Exertier, C.; Antonelli, L.; Ilari, A.; Fiorillo, A.  
Deposited on : 2025-02-18  
Resolution : 1.67 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 : 4-5-2 with Phenix2.0  
Mogul : 2022.3.0, CSD as543be (2022)  
Xtriage (Phenix) : 2.0  
EDS : 3.0  
Buster-report : wwPDB partial adaption of 1.1.7 (2018)  
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)  
CCP4 : 9.0.010 (Gargrove)  
Density-Fitness : 1.0.12  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.49

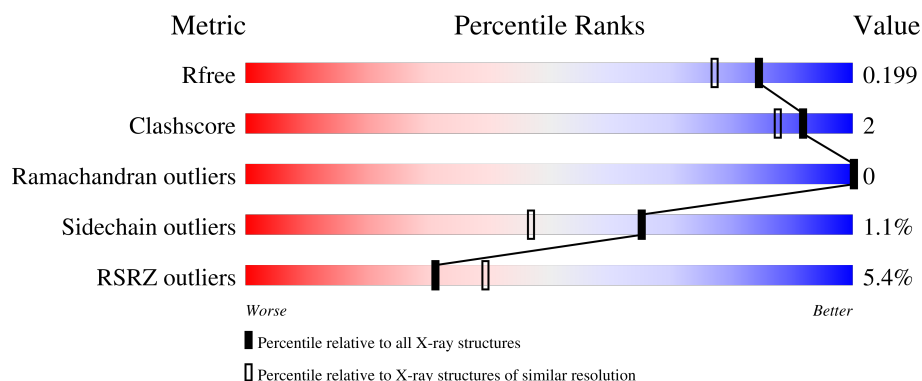
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 1.67 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
$R_{free}$	180053	1054 (1.68-1.68)
Clashscore	190562	1078 (1.68-1.68)
Ramachandran outliers	187476	1068 (1.68-1.68)
Sidechain outliers	187428	1067 (1.68-1.68)
RSRZ outliers	180081	1055 (1.68-1.68)

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	A	495	<div> <div>2%</div> <div>96%</div> <div>5%</div> <div>2%</div> </div>
1	B	495	<div> <div>6%</div> <div>93%</div> <div>5%</div> <div>6%</div> </div>
1	C	495	<div> <div>10%</div> <div>92%</div> <div>6%</div> <div>4%</div> </div>
1	D	495	<div> <div>3%</div> <div>94%</div> <div>5%</div> <div>8%</div> </div>

## 2 Entry composition

There are 7 unique types of molecules in this entry. The entry contains 16084 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 Trypanothione reductase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	489	Total	C	N	O	S	0	0	0
			3716	2364	632	700	20			
1	B	487	Total	C	N	O	S	0	0	0
			3698	2353	628	698	19			
1	C	486	Total	C	N	O	S	0	1	0
			3700	2354	629	698	19			
1	D	490	Total	C	N	O	S	0	0	0
			3719	2364	633	702	20			

There are 12 discrepancies between the modelled and reference sequences:

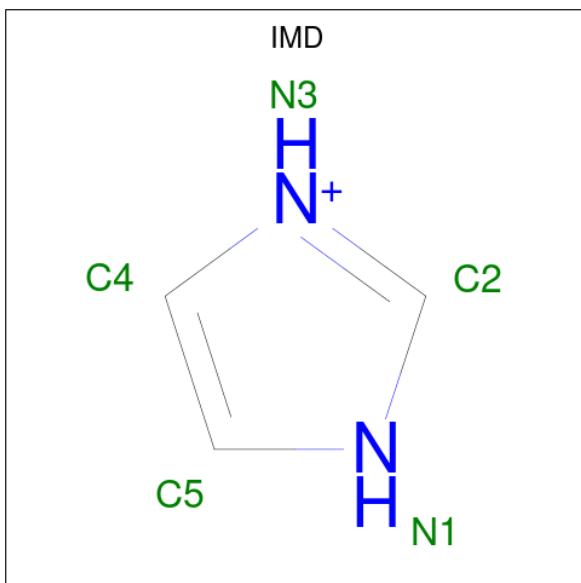
Chain	Residue	Modelled	Actual	Comment	Reference
A	-2	GLY	-	expression tag	UNP Q389T8
A	-1	SER	-	expression tag	UNP Q389T8
A	0	HIS	-	expression tag	UNP Q389T8
B	-2	GLY	-	expression tag	UNP Q389T8
B	-1	SER	-	expression tag	UNP Q389T8
B	0	HIS	-	expression tag	UNP Q389T8
C	-2	GLY	-	expression tag	UNP Q389T8
C	-1	SER	-	expression tag	UNP Q389T8
C	0	HIS	-	expression tag	UNP Q389T8
D	-2	GLY	-	expression tag	UNP Q389T8
D	-1	SER	-	expression tag	UNP Q389T8
D	0	HIS	-	expression tag	UNP Q389T8

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



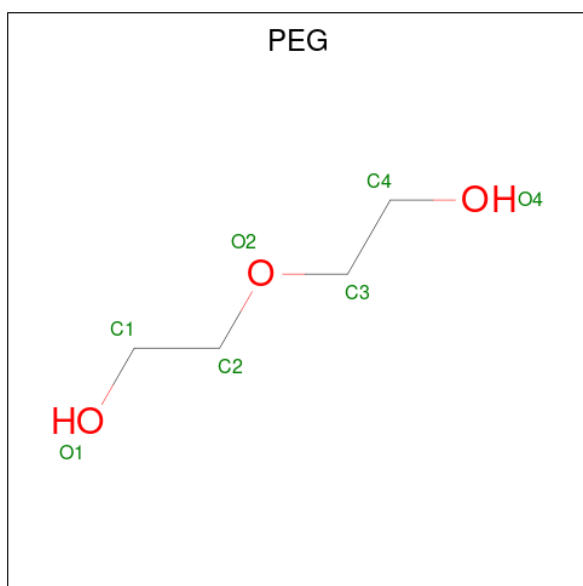
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total 53	C 27	N 9	O 15	P 2	0	0
2	B	1	Total 53	C 27	N 9	O 15	P 2	0	0
2	C	1	Total 53	C 27	N 9	O 15	P 2	0	0
2	D	1	Total 53	C 27	N 9	O 15	P 2	0	0

- Molecule 3 is IMIDAZOLE (CCD ID: IMD) (formula:  $\text{C}_3\text{H}_5\text{N}_2$ ).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	1	Total C N 5 3 2	0	0
3	B	1	Total C N 5 3 2	0	0
3	C	1	Total C N 5 3 2	0	0
3	C	1	Total C N 5 3 2	0	0
3	D	1	Total C N 5 3 2	0	0

- Molecule 4 is DI(HYDROXYETHYL)ETHER (CCD ID: PEG) (formula:  $C_4H_{10}O_3$ ).

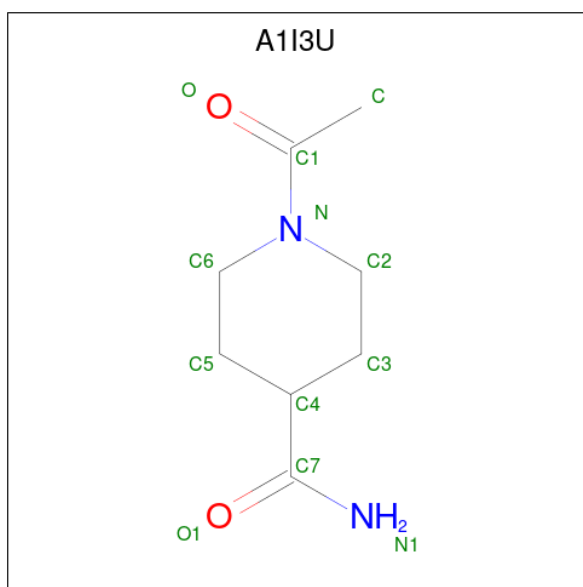


Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	1	Total C O 7 4 3	0	0
4	A	1	Total C O 7 4 3	0	0
4	C	1	Total C O 7 4 3	0	0
4	C	1	Total C O 7 4 3	0	0
4	D	1	Total C O 7 4 3	0	0

- Molecule 5 is BROMIDE ION (CCD ID: BR) (formula: Br).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	2	Total	Br	0	0
			2	2		
5	B	2	Total	Br	0	0
			2	2		
5	D	2	Total	Br	0	0
			2	2		

- Molecule 6 is 1-ethanoylpiperidine-4-carboxamide (CCD ID: A1I3U) (formula:  $C_8H_{14}N_2O_2$ ) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
6	B	1	Total	C	N	O	0	0
			12	8	2	2		
6	C	1	Total	C	N	O	0	0
			12	8	2	2		
6	D	1	Total	C	N	O	0	0
			12	8	2	2		

- Molecule 7 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	A	259	Total	O	0	0
			259	259		
7	B	191	Total	O	0	0
			191	191		
7	C	227	Total	O	0	0
			227	227		

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	D	260	Total 260	O 260	0	0

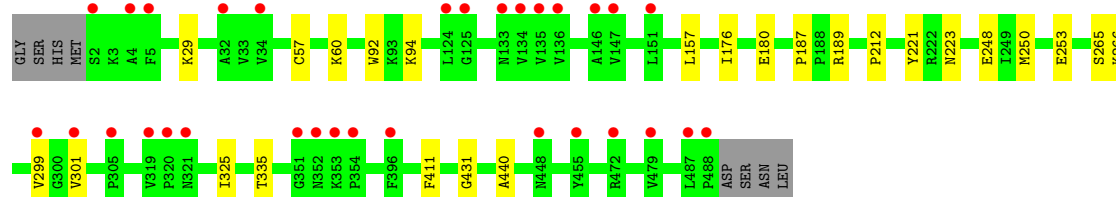
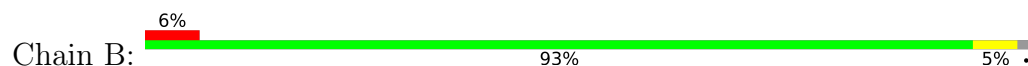
### 3 Residue-property plots [i](#)

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.

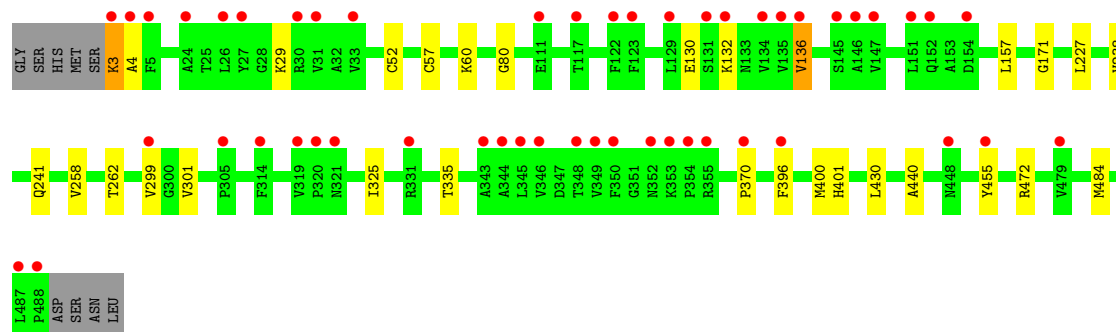
#### • Molecule 1: Trypanothione reductase



#### • Molecule 1: Trypanothione reductase



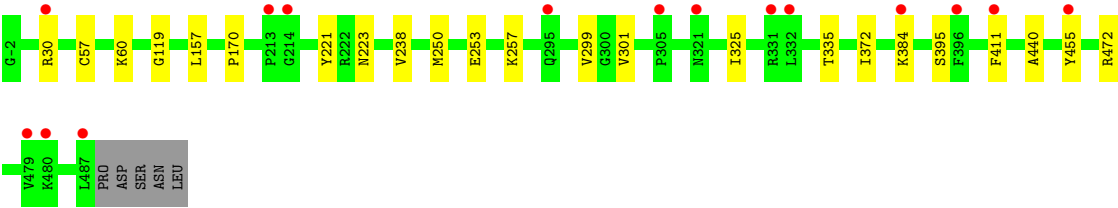
#### • Molecule 1: Trypanothione reductase



#### • Molecule 1: Trypanothione reductase







## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	102.22Å 63.98Å 171.12Å 90.00° 97.75° 90.00°	Depositor
Resolution (Å)	92.63 – 1.67 92.63 – 1.67	Depositor EDS
% Data completeness (in resolution range)	99.2 (92.63-1.67) 99.2 (92.63-1.67)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.00 (at 1.67Å)	Xtriage
Refinement program	PHENIX 1.21.2	Depositor
R, $R_{free}$	0.201 , 0.229 (Not available) , 0.199	Depositor DCC
$R_{free}$ test set	12558 reflections (4.94%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	27.9	Xtriage
Anisotropy	0.054	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.33 , 27.6	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.50$ , $\langle L^2 \rangle = 0.34$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.96	EDS
Total number of atoms	16084	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	32.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 9.15% 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 [i](#)

### 5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: A1I3U, IMD, FAD, PEG, BR

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	0.32	0/3795	0.48	0/5148
1	B	0.28	0/3776	0.47	0/5123
1	C	0.28	0/3778	0.47	0/5126
1	D	0.30	0/3797	0.48	0/5149
All	All	0.30	0/15146	0.47	0/20546

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	A	3716	0	3727	8	0
1	B	3698	0	3708	13	0
1	C	3700	0	3708	17	0
1	D	3719	0	3728	11	0
2	A	53	0	31	0	0
2	B	53	0	31	0	0
2	C	53	0	31	0	0
2	D	53	0	31	0	0
3	A	5	0	5	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	B	5	0	5	0	0
3	C	10	0	10	0	0
3	D	5	0	5	0	0
4	A	14	0	20	1	0
4	C	14	0	20	0	0
4	D	7	0	10	0	0
5	A	2	0	0	1	0
5	B	2	0	0	0	0
5	D	2	0	0	0	0
6	B	12	0	0	0	0
6	C	12	0	0	0	0
6	D	12	0	0	0	0
7	A	259	0	0	2	0
7	B	191	0	0	0	0
7	C	227	0	0	1	0
7	D	260	0	0	1	0
All	All	16084	0	15070	48	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 2.

All (48) 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:C:132:LYS:HD3	1:C:132:LYS:H	1.53	0.73
1:C:3:LYS:HG2	1:C:4:ALA:H	1.57	0.70
1:A:472:ARG:O	1:A:472:ARG:HD3	1.93	0.67
1:C:130:GLU:HB2	1:C:136:VAL:HG22	1.79	0.64
1:A:129:LEU:HD23	1:A:299:VAL:HG21	1.79	0.62
1:D:250:MET:HE2	1:D:253:GLU:HG3	1.86	0.58
1:B:299:VAL:HG23	1:B:301:VAL:HG23	1.87	0.57
1:C:370:PRO:HG2	1:C:430:LEU:HD11	1.87	0.57
1:D:455:TYR:CZ	1:D:472:ARG:HD2	2.41	0.56
1:D:221:TYR:CE2	1:D:223:ASN:HB2	2.41	0.55
1:C:130:GLU:HB2	1:C:136:VAL:CG2	2.38	0.54
1:D:384:LYS:N	1:D:384:LYS:HD3	2.23	0.54
1:B:250:MET:HE2	1:B:253:GLU:HG3	1.90	0.53
1:A:440:ALA:HB3	1:B:440:ALA:HB3	1.91	0.52
1:B:189:ARG:HA	1:B:212:PRO:HD2	1.92	0.52
1:C:80:GLY:HA2	7:D:698:HOH:O	2.10	0.51
1:C:157:LEU:HD11	1:C:325:ILE:HG12	1.92	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:238:VAL:HG21	1:D:372:ILE:HD11	1.93	0.50
1:B:157:LEU:HD11	1:B:325:ILE:HG12	1.93	0.50
1:A:400:MET:HE2	1:A:401:HIS:CE1	2.48	0.49
1:C:455:TYR:CZ	1:C:472:ARG:HD3	2.48	0.49
1:D:157:LEU:HD11	1:D:325:ILE:HG12	1.94	0.49
7:A:655:HOH:O	1:B:94:LYS:HD3	2.12	0.48
1:B:221:TYR:CE2	1:B:223:ASN:HB2	2.49	0.48
1:A:221:TYR:CE2	1:A:223:ASN:HB2	2.50	0.47
1:B:29:LYS:HA	1:B:29:LYS:HD3	1.78	0.47
1:C:241:GLN:OE1	1:C:370:PRO:HG3	2.14	0.47
1:D:395:SER:HA	1:D:411:PHE:O	2.15	0.47
1:C:396:PHE:C	1:C:396:PHE:CD1	2.94	0.46
1:C:440:ALA:HB3	1:D:440:ALA:HB3	1.97	0.46
1:C:400:MET:HE2	1:C:401:HIS:CE1	2.51	0.45
1:C:484:MET:HE2	1:C:484:MET:HB3	1.86	0.45
1:D:299:VAL:HG23	1:D:301:VAL:HG23	1.98	0.45
1:C:171:GLY:HA3	1:C:258:VAL:O	2.18	0.44
1:D:170:PRO:HG2	1:D:257:LYS:HB3	1.99	0.43
1:D:30:ARG:CZ	1:D:119:GLY:HA2	2.49	0.43
1:C:52:CYS:HB3	7:C:639:HOH:O	2.19	0.42
1:B:92:TRP:HB3	1:B:187:PRO:HD3	2.00	0.42
1:B:266:LYS:HD2	1:B:266:LYS:N	2.34	0.42
1:B:411:PHE:CD2	1:B:431:GLY:HA3	2.55	0.42
1:A:130:GLU:HB2	1:A:136:VAL:HG23	2.02	0.41
1:C:299:VAL:HG23	1:C:301:VAL:HG23	2.03	0.41
4:A:504:PEG:H22	7:A:764:HOH:O	2.20	0.41
1:B:176:ILE:HB	1:B:180:GLU:HB2	2.03	0.41
1:B:265:SER:C	1:B:266:LYS:HD2	2.45	0.40
1:A:92:TRP:N	5:A:505:BR:BR	3.08	0.40
1:A:411:PHE:CD2	1:A:431:GLY:HA3	2.57	0.40
1:C:227:LEU:HD12	1:C:238:VAL:HG11	2.03	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	487/495 (98%)	476 (98%)	11 (2%)	0	100	100
1	B	485/495 (98%)	475 (98%)	10 (2%)	0	100	100
1	C	485/495 (98%)	475 (98%)	10 (2%)	0	100	100
1	D	488/495 (99%)	477 (98%)	11 (2%)	0	100	100
All	All	1945/1980 (98%)	1903 (98%)	42 (2%)	0	100	100

There are no Ramachandran outliers to report.

### 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	402/407 (99%)	399 (99%)	3 (1%)	76	62
1	B	400/407 (98%)	396 (99%)	4 (1%)	68	52
1	C	400/407 (98%)	393 (98%)	7 (2%)	51	27
1	D	402/407 (99%)	399 (99%)	3 (1%)	76	62
All	All	1604/1628 (98%)	1587 (99%)	17 (1%)	65	47

All (17) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	57	CYS
1	A	60	LYS
1	A	335	THR
1	B	57	CYS
1	B	60	LYS
1	B	248	GLU
1	B	335	THR
1	C	3	LYS
1	C	29	LYS
1	C	57	CYS

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Mol	Chain	Res	Type
1	C	60	LYS
1	C	136	VAL
1	C	262	THR
1	C	335	THR
1	D	57	CYS
1	D	60	LYS
1	D	335	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (18) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	152	GLN
1	A	223	ASN
1	A	224	ASN
1	A	252	ASN
1	A	340	ASN
1	B	68	GLN
1	B	107	ASN
1	B	223	ASN
1	B	224	ASN
1	B	252	ASN
1	B	292	ASN
1	B	295	GLN
1	C	223	ASN
1	D	107	ASN
1	D	223	ASN
1	D	224	ASN
1	D	252	ASN
1	D	352	ASN

### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

## 5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

## 5.6 Ligand geometry [i](#)

Of 23 ligands modelled in this entry, 6 are monoatomic - leaving 17 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
2	FAD	B	501	-	58,58,58	0.89	1 (1%)	85,89,89	0.90	2 (2%)
4	PEG	C	503	-	6,6,6	0.24	0	5,5,5	0.34	0
4	PEG	A	504	-	6,6,6	0.24	0	5,5,5	0.22	0
2	FAD	C	501	-	58,58,58	0.91	2 (3%)	85,89,89	0.83	3 (3%)
3	IMD	C	505	-	5,5,5	0.30	0	5,5,5	0.95	0
3	IMD	D	502	-	5,5,5	0.33	0	5,5,5	0.77	0
3	IMD	A	502	-	5,5,5	0.29	0	5,5,5	0.85	0
6	A1I3U	C	506	-	12,12,12	0.18	0	16,16,16	0.24	0
6	A1I3U	D	504	-	12,12,12	0.18	0	16,16,16	0.21	0
6	A1I3U	B	503	-	12,12,12	0.20	0	16,16,16	0.24	0
2	FAD	A	501	-	58,58,58	0.88	2 (3%)	85,89,89	0.90	4 (4%)
3	IMD	B	502	-	5,5,5	0.32	0	5,5,5	0.82	0
4	PEG	D	503	-	6,6,6	0.24	0	5,5,5	0.33	0
2	FAD	D	501	-	58,58,58	0.93	2 (3%)	85,89,89	0.88	5 (5%)
3	IMD	C	502	-	5,5,5	0.26	0	5,5,5	0.83	0
4	PEG	A	503	-	6,6,6	0.25	0	5,5,5	0.24	0
4	PEG	C	504	-	6,6,6	0.25	0	5,5,5	0.19	0

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	FAD	B	501	-	-	4/34/50/50	0/6/6/6
4	PEG	C	503	-	-	1/4/4/4	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	PEG	A	504	-	-	3/4/4/4	-
2	FAD	C	501	-	-	4/34/50/50	0/6/6/6
3	IMD	C	505	-	-	-	0/1/1/1
3	IMD	D	502	-	-	-	0/1/1/1
6	A1I3U	C	506	-	-	2/8/18/18	0/1/1/1
6	A1I3U	D	504	-	-	2/8/18/18	0/1/1/1
3	IMD	A	502	-	-	-	0/1/1/1
6	A1I3U	B	503	-	-	1/8/18/18	0/1/1/1
2	FAD	A	501	-	-	4/34/50/50	0/6/6/6
3	IMD	B	502	-	-	-	0/1/1/1
4	PEG	D	503	-	-	3/4/4/4	-
2	FAD	D	501	-	-	5/34/50/50	0/6/6/6
3	IMD	C	502	-	-	-	0/1/1/1
4	PEG	A	503	-	-	2/4/4/4	-
4	PEG	C	504	-	-	3/4/4/4	-

All (7) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	501	FAD	P-O3P	3.82	1.63	1.59
2	A	501	FAD	P-O3P	3.50	1.63	1.59
2	C	501	FAD	P-O3P	3.37	1.63	1.59
2	B	501	FAD	P-O3P	3.30	1.63	1.59
2	D	501	FAD	PA-O3P	2.36	1.62	1.59
2	A	501	FAD	PA-O3P	2.35	1.62	1.59
2	C	501	FAD	PA-O3P	2.30	1.62	1.59

All (14) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	501	FAD	O2P-P-O1P	2.99	126.36	112.44
2	C	501	FAD	O2P-P-O1P	2.99	126.34	112.44
2	A	501	FAD	O3P-PA-O1A	-2.75	102.42	110.70
2	D	501	FAD	O2P-P-O3P	-2.56	100.34	107.27
2	D	501	FAD	O2P-P-O1P	2.51	124.14	112.44
2	D	501	FAD	O2A-PA-O1A	2.48	124.00	112.44
2	D	501	FAD	O3P-PA-O1A	-2.41	103.46	110.70
2	A	501	FAD	C2B-C1B-N9A	2.26	118.92	113.30
2	C	501	FAD	O3P-PA-O1A	-2.18	104.13	110.70
2	C	501	FAD	O2A-PA-O1A	2.18	122.59	112.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	501	FAD	O2A-PA-O1A	2.18	122.56	112.44
2	D	501	FAD	C2B-C1B-N9A	2.10	118.53	113.30
2	B	501	FAD	O2P-P-O1P	2.06	122.04	112.44
2	B	501	FAD	O3P-PA-O1A	-2.02	104.62	110.70

There are no chirality outliers.

All (34) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
6	C	506	A1I3U	C-C1-N-C2
4	A	504	PEG	O2-C3-C4-O4
6	C	506	A1I3U	O-C1-N-C2
4	C	504	PEG	O1-C1-C2-O2
4	C	504	PEG	O2-C3-C4-O4
2	C	501	FAD	O4B-C4B-C5B-O5B
2	A	501	FAD	PA-O3P-P-O5'
2	B	501	FAD	PA-O3P-P-O5'
2	C	501	FAD	PA-O3P-P-O5'
2	D	501	FAD	PA-O3P-P-O5'
4	A	503	PEG	C1-C2-O2-C3
2	C	501	FAD	C3B-C4B-C5B-O5B
4	A	504	PEG	C4-C3-O2-C2
2	A	501	FAD	P-O3P-PA-O2A
2	D	501	FAD	P-O3P-PA-O2A
4	D	503	PEG	O2-C3-C4-O4
4	D	503	PEG	C4-C3-O2-C2
2	B	501	FAD	P-O3P-PA-O2A
2	C	501	FAD	P-O3P-PA-O2A
6	D	504	A1I3U	C5-C4-C7-O1
2	D	501	FAD	O4B-C4B-C5B-O5B
6	B	503	A1I3U	O-C1-N-C6
4	C	504	PEG	C4-C3-O2-C2
6	D	504	A1I3U	C5-C4-C7-N1
2	B	501	FAD	O4B-C4B-C5B-O5B
4	A	504	PEG	C1-C2-O2-C3
2	A	501	FAD	O4B-C4B-C5B-O5B
2	A	501	FAD	P-O3P-PA-O1A
2	B	501	FAD	P-O3P-PA-O1A
2	D	501	FAD	C3B-C4B-C5B-O5B
4	A	503	PEG	O2-C3-C4-O4
4	C	503	PEG	O2-C3-C4-O4
4	D	503	PEG	C1-C2-O2-C3

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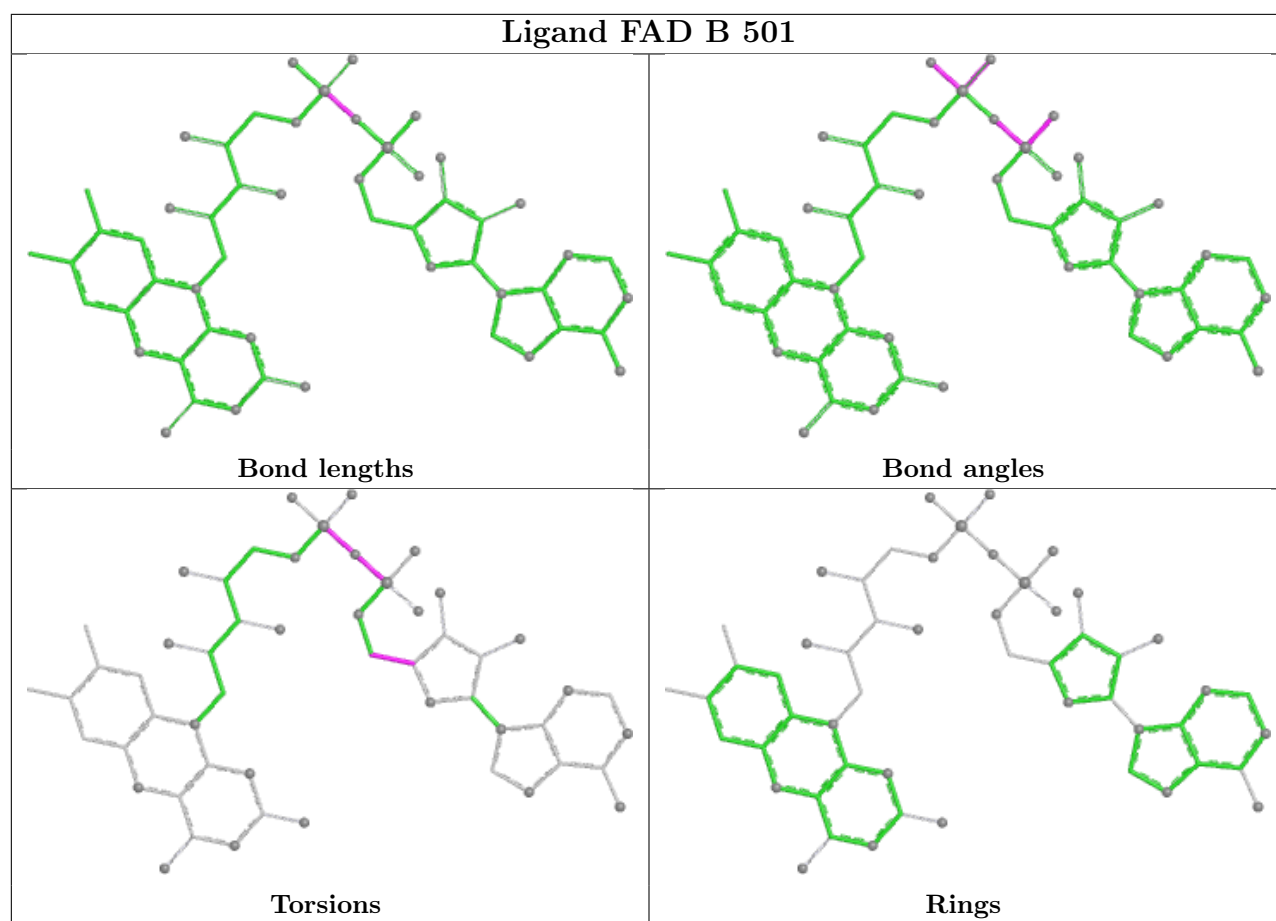
Mol	Chain	Res	Type	Atoms
2	D	501	FAD	P-O3P-PA-O1A

There are no ring outliers.

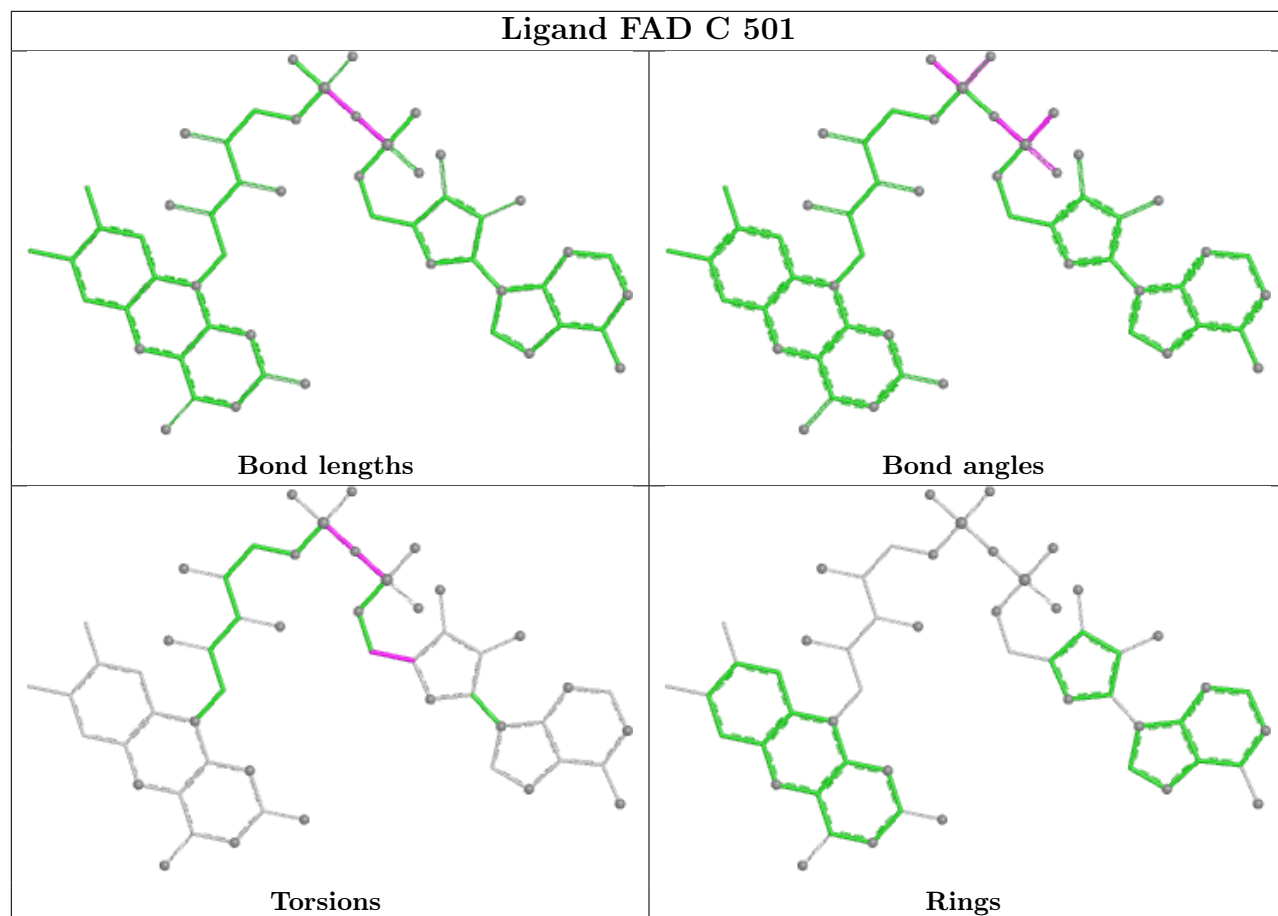
1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	504	PEG	1	0

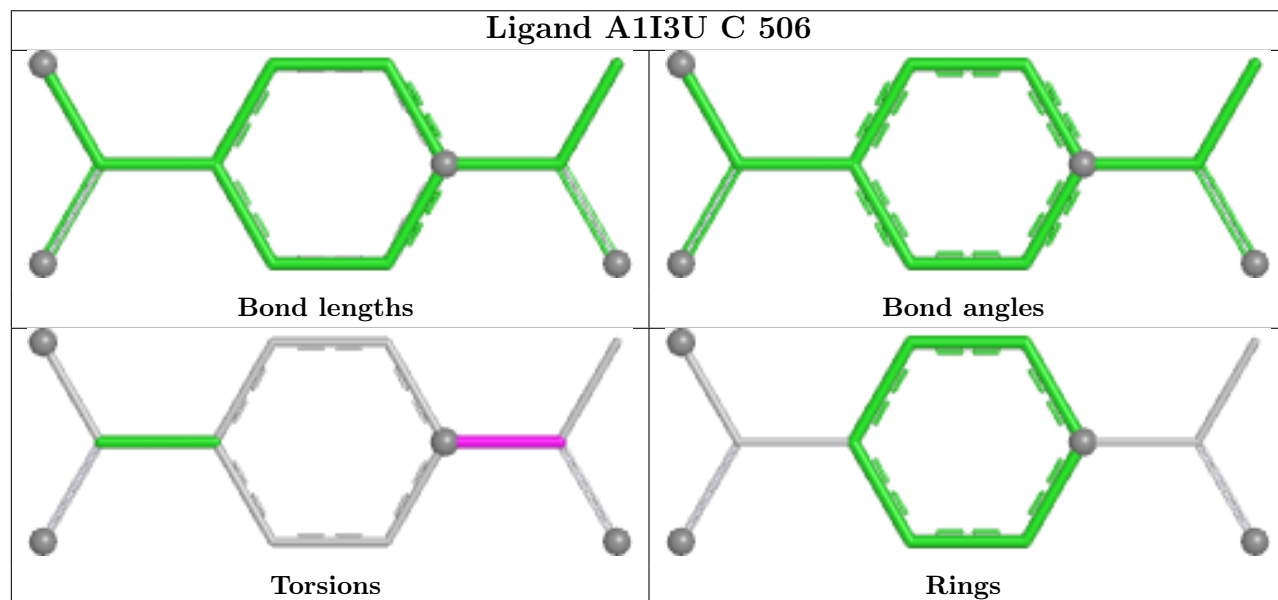
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

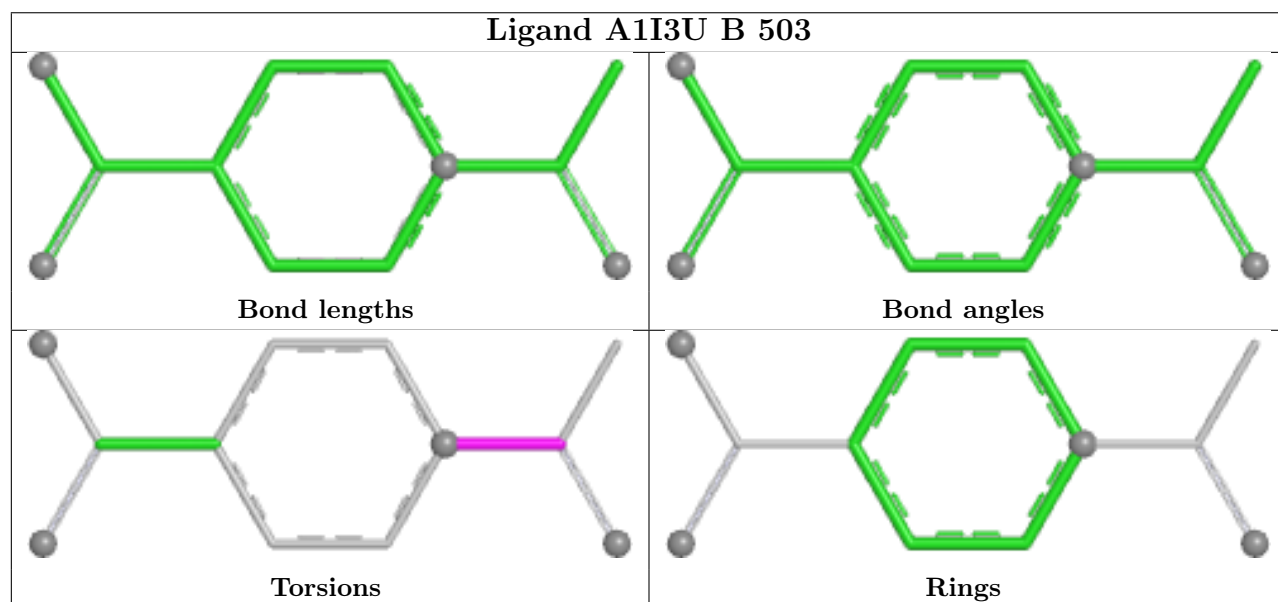
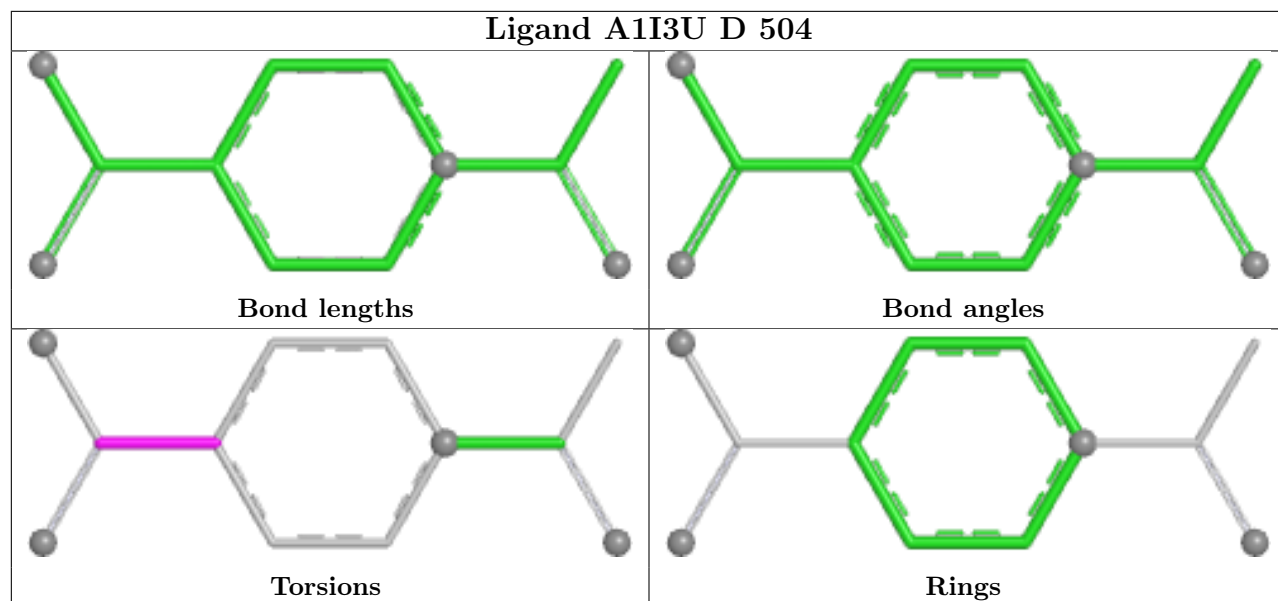


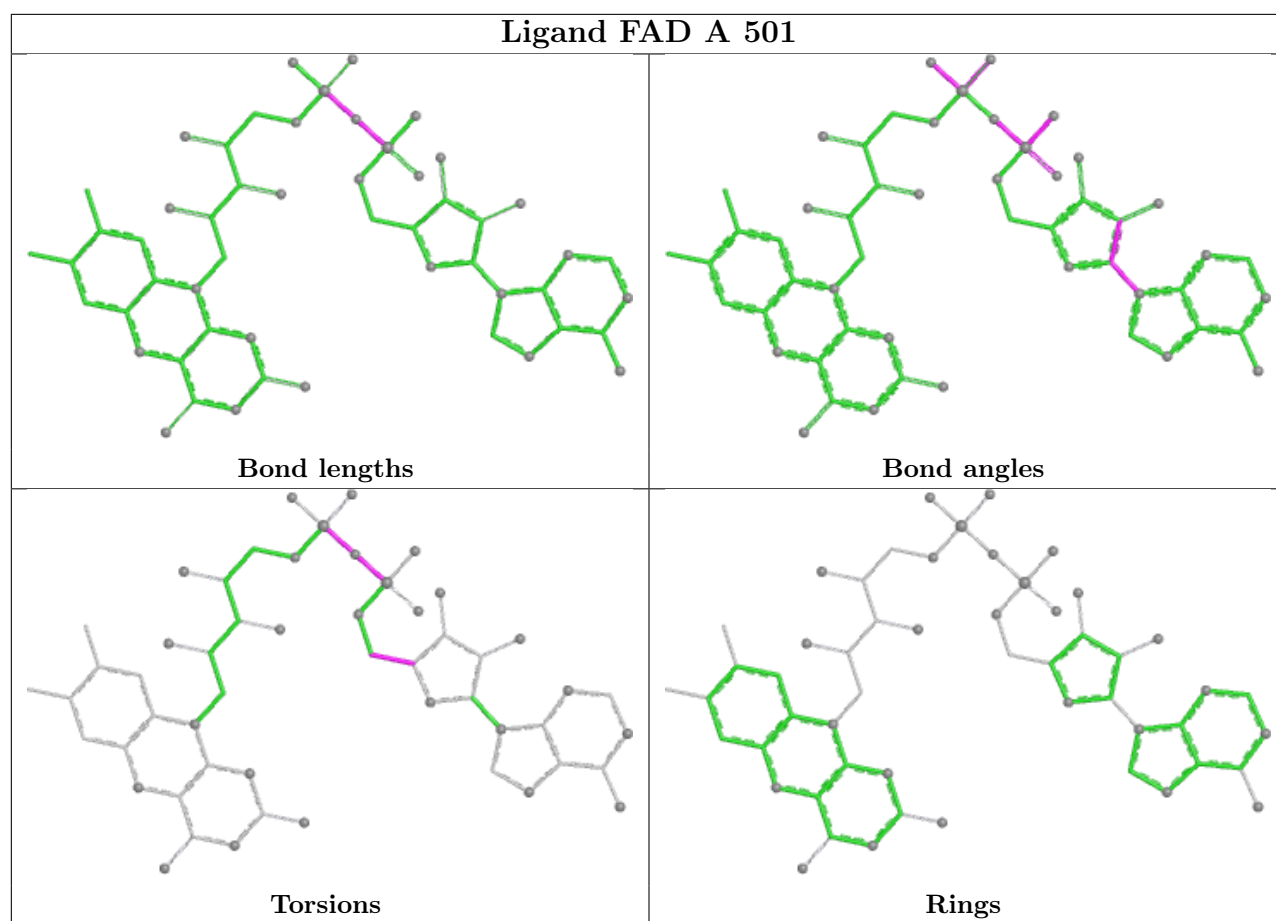
## Ligand FAD C 501

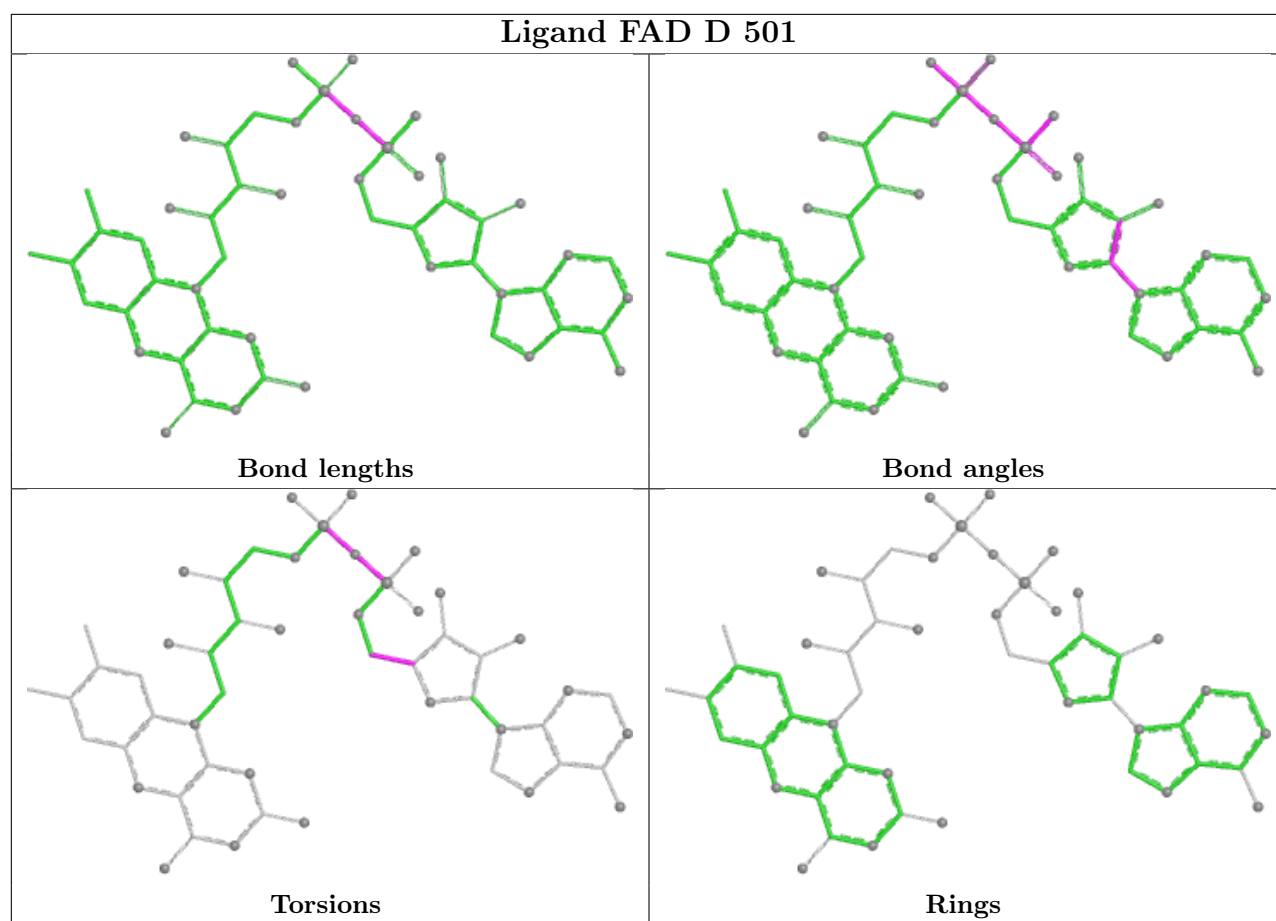


## Ligand A1I3U C 506









## 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

### 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, 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	A	489/495 (98%)	0.14	10 (2%) 65 73	20, 28, 41, 58	0
1	B	487/495 (98%)	0.46	31 (6%) 25 32	22, 31, 49, 74	0
1	C	486/495 (98%)	0.56	50 (10%) 12 15	20, 32, 54, 81	1 (0%)
1	D	490/495 (98%)	0.25	15 (3%) 51 58	21, 29, 42, 58	0
All	All	1952/1980 (98%)	0.35	106 (5%) 31 39	20, 30, 49, 81	1 (0%)

All (106) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	455	TYR	4.5
1	C	396	PHE	4.3
1	B	4	ALA	4.2
1	D	487	LEU	3.8
1	C	4	ALA	3.7
1	C	354	PRO	3.7
1	B	396	PHE	3.6
1	B	352	ASN	3.5
1	A	396	PHE	3.5
1	C	321[A]	ASN	3.4
1	C	331	ARG	3.4
1	B	353	LYS	3.4
1	B	147	VAL	3.4
1	B	146	ALA	3.3
1	A	0	HIS	3.3
1	A	488	PRO	3.2
1	C	111	GLU	3.2
1	B	488	PRO	3.1
1	C	31	VAL	3.1
1	C	134	VAL	3.0
1	A	352	ASN	3.0

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Mol	Chain	Res	Type	RSRZ
1	B	321	ASN	3.0
1	C	350	PHE	3.0
1	C	353	LYS	2.9
1	B	2	SER	2.9
1	A	306	LYS	2.9
1	C	135	VAL	2.9
1	C	488	PRO	2.9
1	C	455	TYR	2.9
1	B	124	LEU	2.9
1	C	26	LEU	2.9
1	C	147	VAL	2.8
1	B	319	VAL	2.8
1	B	354	PRO	2.8
1	C	305	PRO	2.8
1	C	5	PHE	2.8
1	C	448	ASN	2.8
1	D	455	TYR	2.7
1	D	321	ASN	2.7
1	C	299	VAL	2.7
1	C	146	ALA	2.6
1	D	332	LEU	2.5
1	D	30	ARG	2.5
1	C	319	VAL	2.5
1	C	349	VAL	2.5
1	D	213	PRO	2.5
1	D	305	PRO	2.5
1	C	154	ASP	2.5
1	C	343	ALA	2.5
1	C	355	ARG	2.5
1	C	352	ASN	2.4
1	C	314	PHE	2.4
1	D	384	LYS	2.4
1	A	116	ASP	2.4
1	B	448	ASN	2.4
1	A	262	THR	2.4
1	C	152	GLN	2.3
1	C	24	ALA	2.3
1	B	34	VAL	2.3
1	C	346	VAL	2.3
1	D	411	PHE	2.3
1	B	134	VAL	2.3
1	B	136	VAL	2.3

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Mol	Chain	Res	Type	RSRZ
1	C	348	THR	2.3
1	C	320	PRO	2.2
1	C	3	LYS	2.2
1	C	151	LEU	2.2
1	C	487	LEU	2.2
1	B	125	GLY	2.2
1	D	214	GLY	2.2
1	B	351	GLY	2.2
1	C	117	THR	2.2
1	D	479	VAL	2.1
1	A	480	LYS	2.1
1	A	305	PRO	2.1
1	B	305	PRO	2.1
1	B	32	ALA	2.1
1	B	135	VAL	2.1
1	C	136	VAL	2.1
1	C	344	ALA	2.1
1	B	133	ASN	2.1
1	C	345	LEU	2.1
1	C	370	PRO	2.1
1	D	331	ARG	2.1
1	C	123	PHE	2.1
1	D	396	PHE	2.1
1	C	27	TYR	2.1
1	B	299	VAL	2.1
1	A	115	ASN	2.1
1	B	472	ARG	2.1
1	B	487	LEU	2.1
1	B	320	PRO	2.1
1	B	5	PHE	2.1
1	B	301	VAL	2.0
1	B	151	LEU	2.0
1	C	129	LEU	2.0
1	C	132	LYS	2.0
1	D	295	GLN	2.0
1	C	30	ARG	2.0
1	C	122	PHE	2.0
1	C	131	SER	2.0
1	C	145	SER	2.0
1	B	479	VAL	2.0
1	C	33	VAL	2.0
1	C	479	VAL	2.0

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Mol	Chain	Res	Type	RSRZ
1	D	480	LYS	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 oligosaccharides 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, 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	IMD	C	505	5/5	0.62	0.20	42,43,48,52	0
3	IMD	D	502	5/5	0.65	0.25	48,52,61,66	0
6	A1I3U	C	506	12/12	0.65	0.25	37,43,49,50	12
6	A1I3U	B	503	12/12	0.66	0.19	37,47,53,56	0
4	PEG	A	503	7/7	0.69	0.20	44,52,56,58	0
3	IMD	A	502	5/5	0.76	0.18	40,46,48,51	0
4	PEG	C	504	7/7	0.76	0.16	51,53,56,58	0
4	PEG	A	504	7/7	0.77	0.17	43,45,51,54	0
4	PEG	C	503	7/7	0.78	0.17	39,48,64,71	0
4	PEG	D	503	7/7	0.78	0.20	46,53,60,61	0
3	IMD	C	502	5/5	0.80	0.15	36,40,44,46	0
6	A1I3U	D	504	12/12	0.81	0.19	34,38,41,42	12
3	IMD	B	502	5/5	0.82	0.14	38,41,47,48	0
5	BR	D	505	1/1	0.89	0.12	102,102,102,102	0
5	BR	B	504	1/1	0.89	0.16	82,82,82,82	0
5	BR	A	505	1/1	0.90	0.21	88,88,88,88	0
5	BR	A	506	1/1	0.93	0.11	90,90,90,90	0
2	FAD	C	501	53/53	0.97	0.06	23,27,34,36	0
2	FAD	D	501	53/53	0.97	0.06	19,22,25,26	0
2	FAD	B	501	53/53	0.97	0.06	21,25,34,35	0
5	BR	B	505	1/1	0.97	0.21	66,66,66,66	0
5	BR	D	506	1/1	0.98	0.17	59,59,59,59	0

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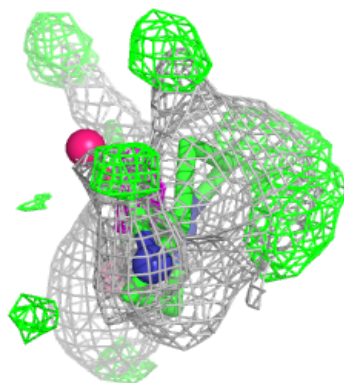
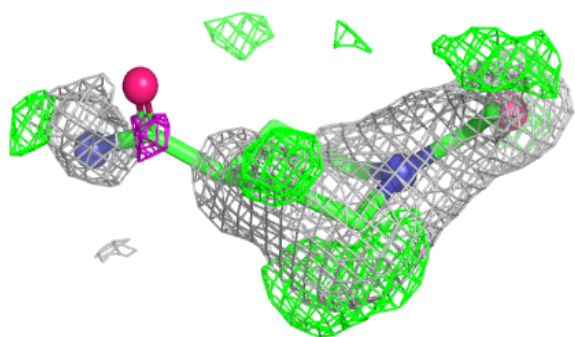
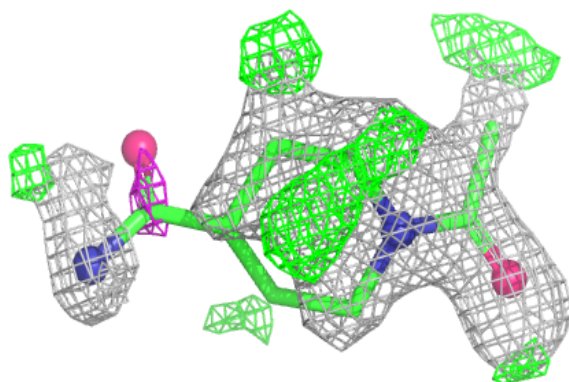
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
2	FAD	A	501	53/53	0.98	0.05	18,21,23,23	0

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.

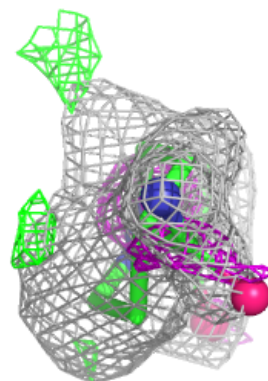
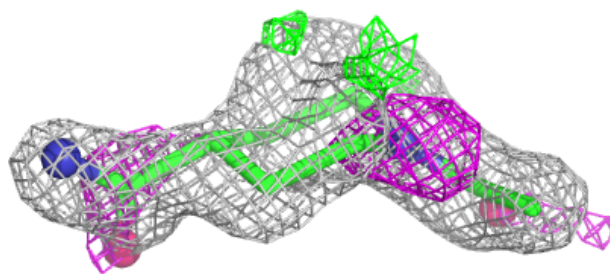
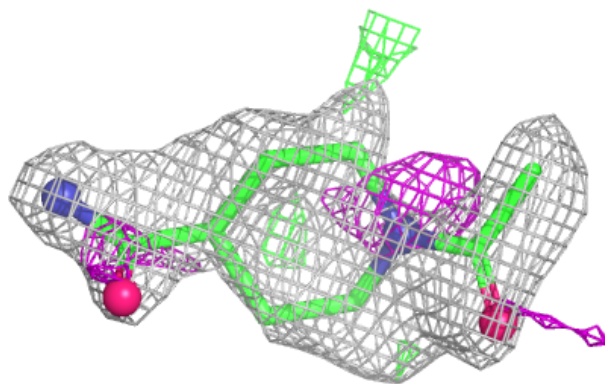
**Electron density around A1I3U C 506:**

2mF<sub>o</sub>-DF<sub>c</sub> (at 0.7 rmsd) in gray  
mF<sub>o</sub>-DF<sub>c</sub> (at 3 rmsd) in purple (negative)  
and green (positive)

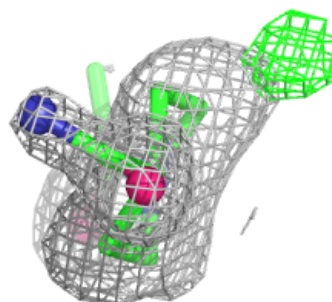
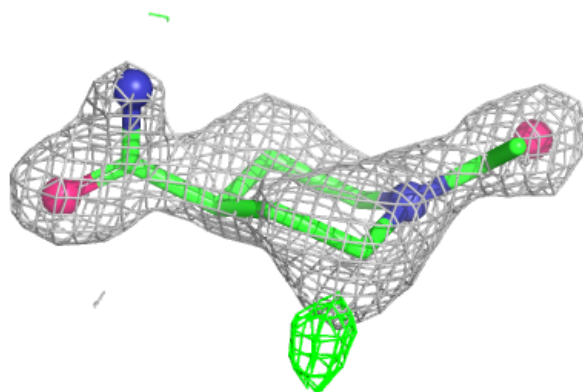
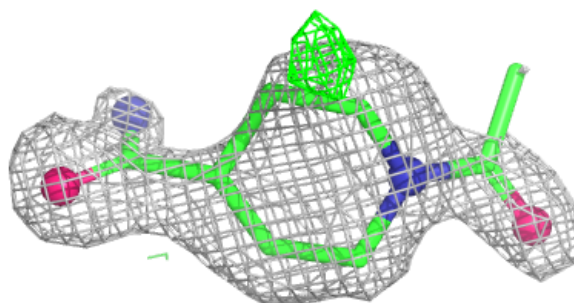


**Electron density around A1I3U B 503:**

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

**Electron density around A1I3U D 504:**

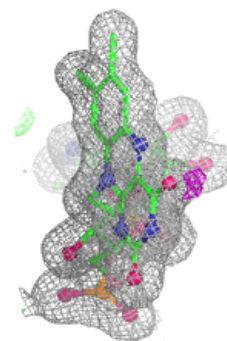
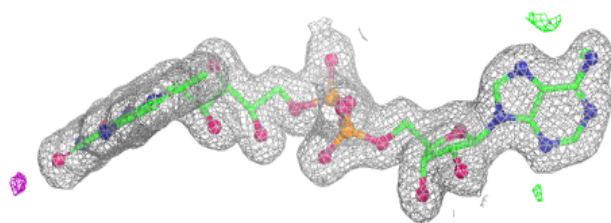
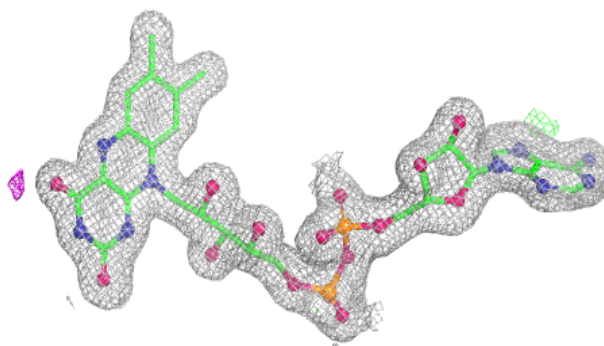
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 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



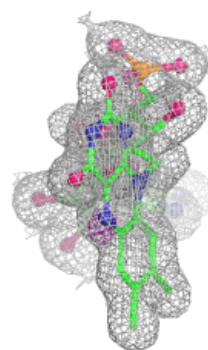
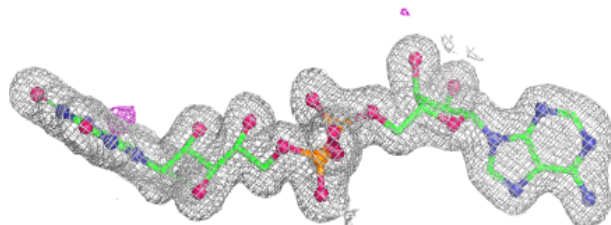
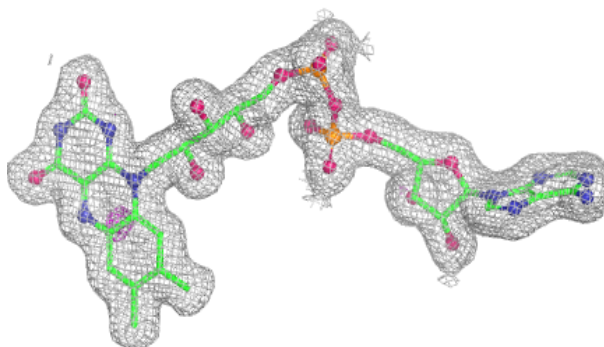


**Electron density around FAD C 501:**

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

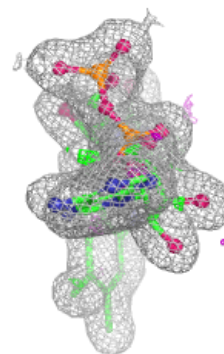
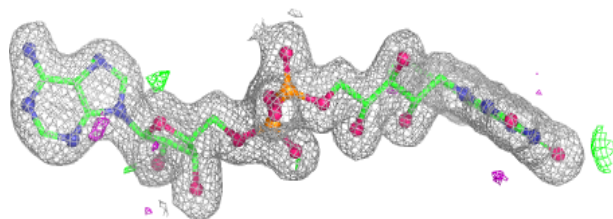
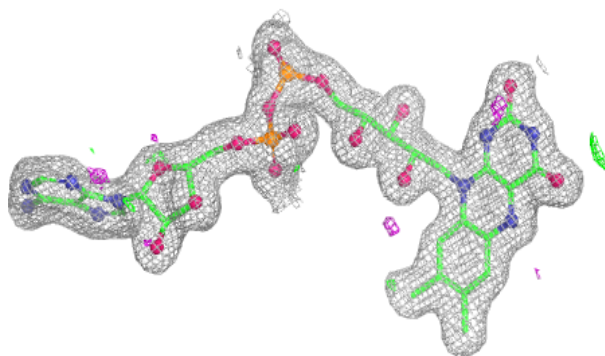
**Electron density around FAD D 501:**

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

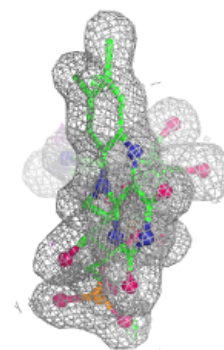
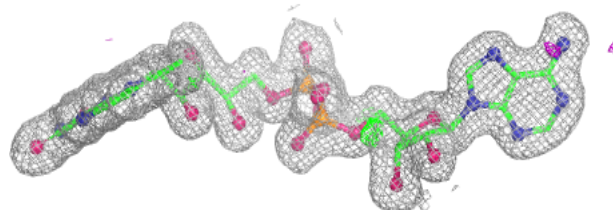
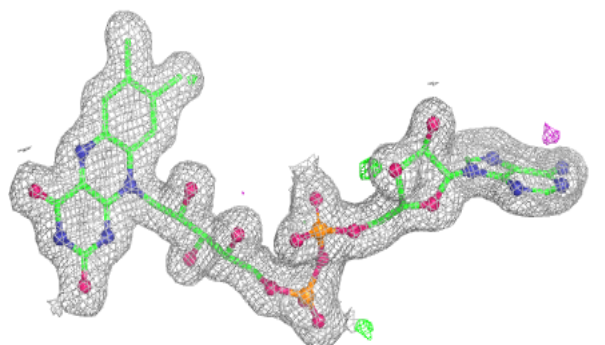


**Electron density around FAD B 501:**

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

**Electron density around FAD A 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.