



# Full wwPDB X-ray Structure Validation Report ⓘ

Mar 8, 2026 – 02:27 PM UTC

PDB ID : 9IFJ / pdb\_00009ifj  
Title : PANDDA analysis - Crystal structure of Trypanosoma brucei trypanothione reductase in complex with Z2017861827  
Authors : Exertier, C.; Fiorillo, A.; Ilari, A.; Antonelli, L.  
Deposited on : 2025-02-18  
Resolution : 1.62 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

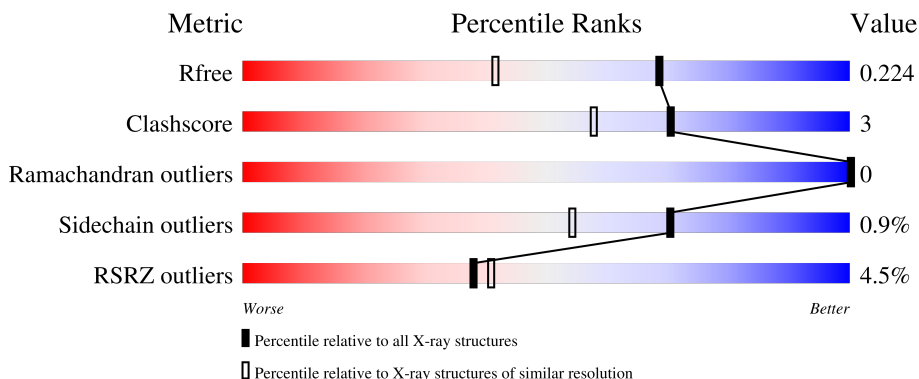
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 1.62 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	6728 (1.64-1.60)
Clashscore	190562	7023 (1.64-1.60)
Ramachandran outliers	187476	6898 (1.64-1.60)
Sidechain outliers	187428	6896 (1.64-1.60)
RSRZ outliers	180081	6727 (1.64-1.60)

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>93%</div> <div>6%</div> </div>
1	B	495	<div> <div>5%</div> <div>91%</div> <div>7%</div> </div>
1	C	495	<div> <div>9%</div> <div>87%</div> <div>11%</div> </div>
1	D	495	<div> <div>2%</div> <div>91%</div> <div>8%</div> </div>

## 2 Entry composition

There are 7 unique types of molecules in this entry. The entry contains 16082 atoms, of which 15 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	1	0
			3727	2370	636	701	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
			3716	2362	633	702	19			
1	D	489	Total	C	N	O	S	0	1	0
			3722	2364	636	702	20			

There are 12 discrepancies between the modelled and reference sequences:

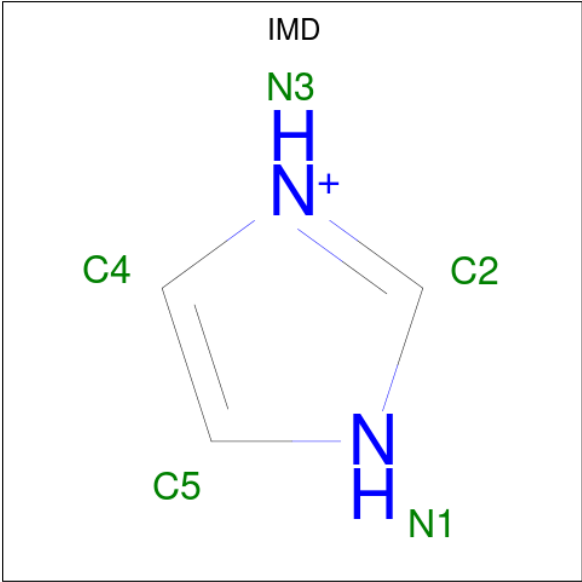
Chain	Residue	Modelled	Actual	Comment	Reference
A	-2	GLY	-	expression tag	UNP Q389T8
A	-1	SER	-	expression tag	UNP Q389T8
A	0	HIS	-	expression tag	UNP Q389T8
B	-2	GLY	-	expression tag	UNP Q389T8
B	-1	SER	-	expression tag	UNP Q389T8
B	0	HIS	-	expression tag	UNP Q389T8
C	-2	GLY	-	expression tag	UNP Q389T8
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:  $C_{27}H_{33}N_9O_{15}P_2$ ).



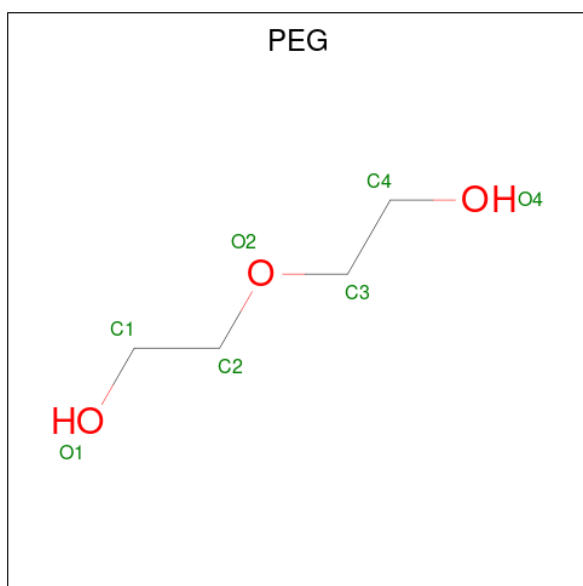
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	N	O	P	0	0
			53	27	9	15	2		
2	B	1	Total	C	N	O	P	0	0
			53	27	9	15	2		
2	C	1	Total	C	N	O	P	0	0
			53	27	9	15	2		
2	D	1	Total	C	N	O	P	0	0
			53	27	9	15	2		

- Molecule 3 is IMIDAZOLE (CCD ID: IMD) (formula: C<sub>3</sub>H<sub>5</sub>N<sub>2</sub>).



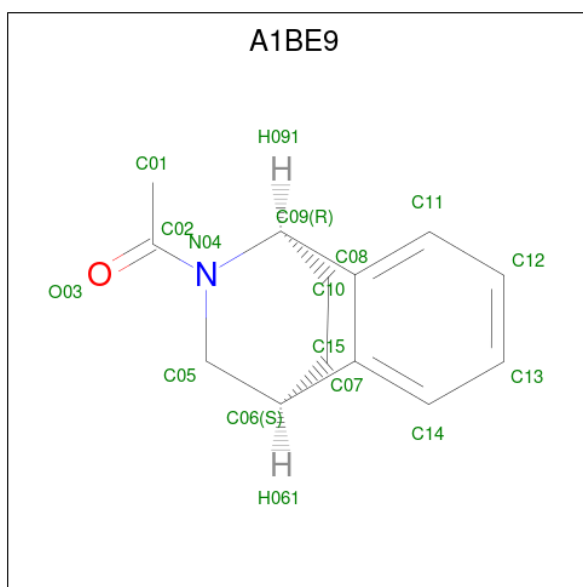
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	C	N	0	0
			5	3	2		
3	B	1	Total	C	N	0	0
			5	3	2		
3	C	1	Total	C	N	0	0
			5	3	2		
3	C	1	Total	C	N	0	0
			5	3	2		
3	D	1	Total	C	N	0	0
			5	3	2		

- 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	0	0
			7	4	3		
4	C	1	Total	C	O	0	0
			7	4	3		
4	C	1	Total	C	O	0	0
			7	4	3		
4	D	1	Total	C	O	0	0
			7	4	3		

- Molecule 5 is 1-[(1S,4S)-1,2,3,4-tetrahydro-1,4-(epiminomethano)naphthalen-10-yl]ethan-1-one (CCD ID: A1BE9) (formula:  $C_{13}H_{15}NO$ ) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
5	A	1	Total	C	H	N	O	0	0
			30	13	15	1	1		

- Molecule 6 is BROMIDE ION (CCD ID: BR) (formula: Br).

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

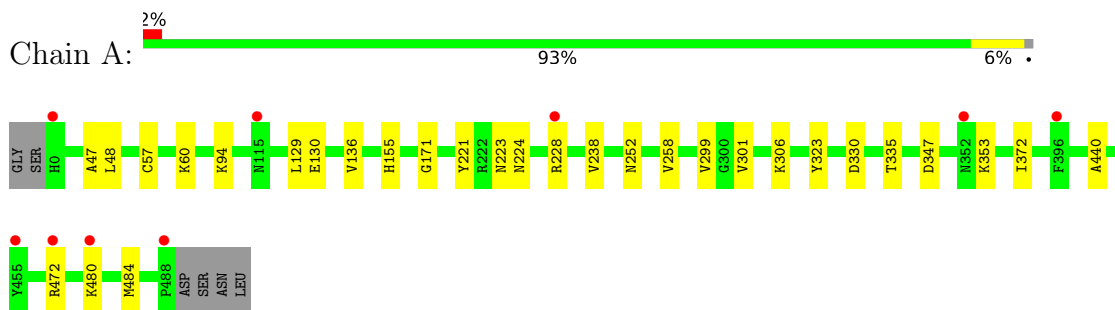
- Molecule 7 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	A	266	Total	O	0	0
			266	266		
7	B	176	Total	O	0	0
			176	176		
7	C	220	Total	O	0	0
			220	220		
7	D	256	Total	O	0	0
			256	256		

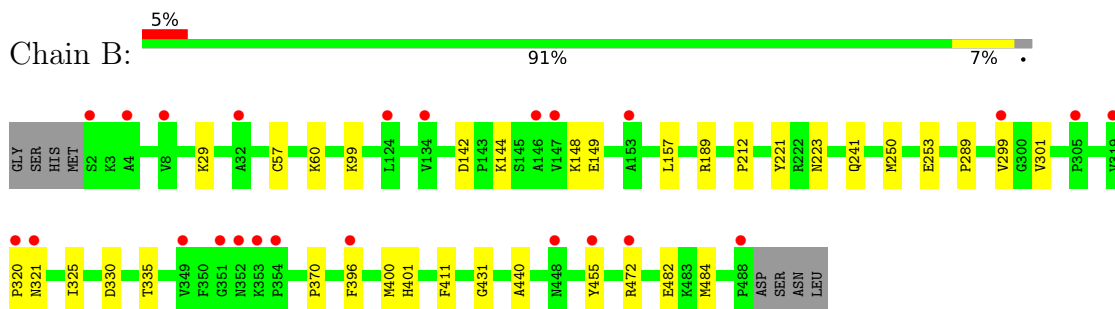
### 3 Residue-property plots [i](#)

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.

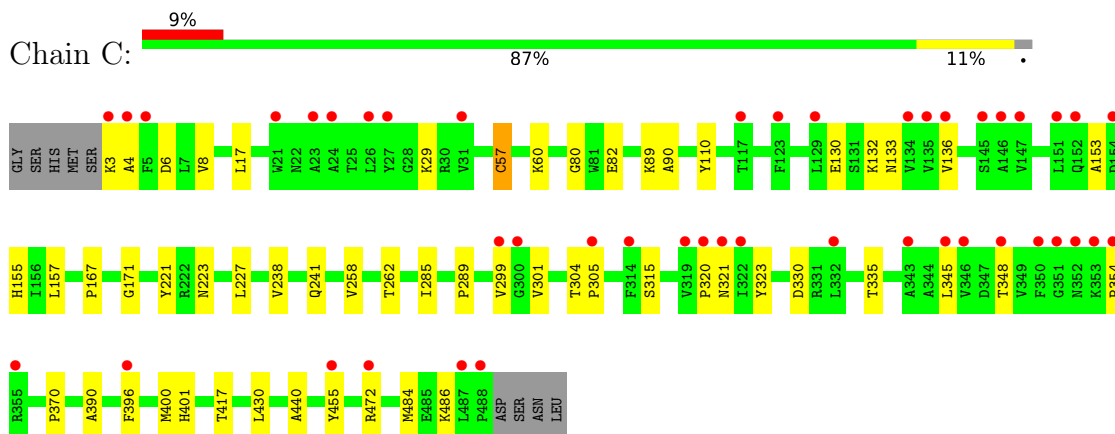
- Molecule 1: Trypanothione reductase



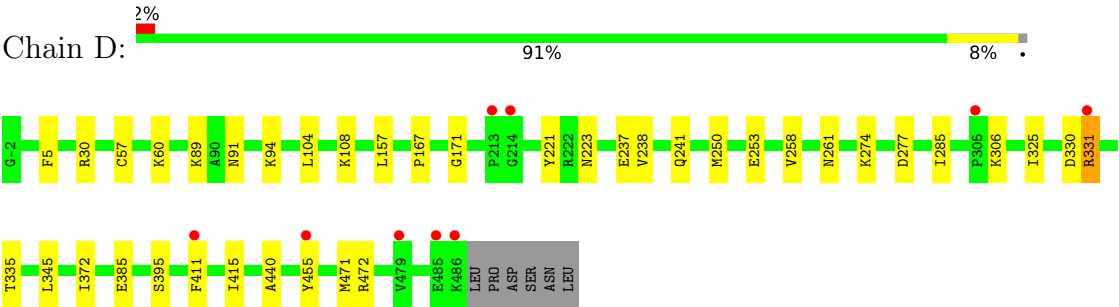
- Molecule 1: Trypanothione reductase



- 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, $\alpha$ , $\beta$ , $\gamma$	102.23Å 63.91Å 170.53Å 90.00° 97.67° 90.00°	Depositor
Resolution (Å)	84.50 – 1.62 84.50 – 1.62	Depositor EDS
% Data completeness (in resolution range)	99.4 (84.50-1.62) 99.6 (84.50-1.62)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.03 (at 1.62Å)	Xtriage
Refinement program	PHENIX 1.21.2	Depositor
R, $R_{free}$	0.197 , 0.224 0.197 , 0.224	Depositor DCC
$R_{free}$ test set	13748 reflections (4.94%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	27.1	Xtriage
Anisotropy	0.086	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.33 , 28.2	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.50$ , $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.96	EDS
Total number of atoms	16082	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 8.87% 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: FAD, A1BE9, BR, PEG, IMD

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	0.35	0/3806	0.50	0/5162
1	B	0.30	0/3776	0.48	0/5123
1	C	0.29	0/3794	0.46	0/5148
1	D	0.31	0/3800	0.48	0/5152
All	All	0.31	0/15176	0.48	0/20585

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	3727	0	3739	16	0
1	B	3698	0	3708	22	0
1	C	3716	0	3720	42	0
1	D	3722	0	3729	27	0
2	A	53	0	31	1	0
2	B	53	0	31	0	0
2	C	53	0	31	1	0
2	D	53	0	31	1	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	2	0
3	D	5	0	5	0	0
4	A	7	0	10	0	0
4	C	14	0	20	0	0
4	D	7	0	10	0	0
5	A	15	15	0	0	0
6	A	2	0	0	0	0
6	B	2	0	0	0	0
6	D	2	0	0	0	0
7	A	266	0	0	1	0
7	B	176	0	0	0	0
7	C	220	0	0	5	0
7	D	256	0	0	1	0
All	All	16067	15	15085	104	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 3.

All (104) 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)
7:C:653:HOH:O	1:D:91:ASN:HB3	1.57	1.05
1:C:130:GLU:HB2	1:C:136:VAL:CG2	2.07	0.83
1:C:3:LYS:HG3	1:C:4:ALA:H	1.46	0.80
1:A:224:ASN:HD22	1:A:252:ASN:HD21	1.29	0.80
7:C:653:HOH:O	1:D:94:LYS:HB2	1.83	0.78
1:C:80:GLY:HA2	7:C:653:HOH:O	1.89	0.72
1:C:130:GLU:HB2	1:C:136:VAL:HG23	1.73	0.70
1:A:94:LYS:HD3	7:A:764:HOH:O	1.91	0.69
1:C:82:GLU:OE1	1:D:89:LYS:HE3	1.91	0.69
1:A:129:LEU:HD23	1:A:299:VAL:HG21	1.73	0.69
1:C:370:PRO:HG2	1:C:430:LEU:HD11	1.80	0.64
1:B:299:VAL:HG23	1:B:301:VAL:HG23	1.81	0.61
1:C:484:MET:HG3	1:C:486:LYS:O	2.02	0.59
1:C:80:GLY:CA	7:C:653:HOH:O	2.50	0.58
1:C:455:TYR:HB3	3:C:505:IMD:H5	1.84	0.58
1:D:221:TYR:CE2	1:D:223:ASN:HB2	2.39	0.57
1:C:289:PRO:HG3	1:C:330:ASP:HB2	1.89	0.55
1:A:472:ARG:O	1:A:472:ARG:HD3	2.07	0.54
1:C:455:TYR:CZ	1:C:472:ARG:HD2	2.42	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:455:TYR:CB	3:C:505:IMD:H5	2.38	0.54
1:B:250:MET:HE2	1:B:253:GLU:HG3	1.90	0.53
1:C:82:GLU:CD	1:D:89:LYS:HE3	2.33	0.53
1:B:221:TYR:CE2	1:B:223:ASN:HB2	2.44	0.53
1:C:304:THR:HB	1:C:305:PRO:HD2	1.90	0.52
1:D:455:TYR:CE2	1:D:472:ARG:HB3	2.45	0.52
1:C:241:GLN:OE1	1:C:370:PRO:HG3	2.09	0.52
1:D:237:GLU:HG3	1:D:241:GLN:NE2	2.25	0.52
1:A:221:TYR:CE2	1:A:223:ASN:HB2	2.45	0.51
1:D:274:LYS:HE2	7:D:817:HOH:O	2.09	0.51
1:D:157:LEU:HD13	1:D:345:LEU:CD2	2.40	0.51
1:A:440:ALA:HB3	1:B:440:ALA:HB3	1.92	0.51
1:B:289:PRO:HG3	1:B:330:ASP:HB2	1.91	0.51
1:B:189:ARG:HA	1:B:212:PRO:HD2	1.93	0.50
1:D:306:LYS:HE2	1:D:330:ASP:OD2	2.11	0.50
1:D:415:ILE:HD12	1:D:471:MET:HE3	1.93	0.50
1:C:132:LYS:CE	1:C:133:ASN:HD21	2.25	0.49
1:D:237:GLU:HG3	1:D:241:GLN:HE21	1.77	0.49
1:D:250:MET:HE2	1:D:253:GLU:HG3	1.95	0.49
1:D:238:VAL:HG21	1:D:372:ILE:HD11	1.94	0.49
1:C:155:HIS:HB3	1:C:323:TYR:HE1	1.77	0.48
1:C:171:GLY:HA3	1:C:258:VAL:O	2.13	0.48
1:C:400:MET:HE2	1:C:401:HIS:CE1	2.48	0.48
1:C:396:PHE:C	1:C:396:PHE:CD1	2.92	0.48
1:D:167:PRO:HD3	1:D:285:ILE:CD1	2.44	0.48
1:B:455:TYR:CZ	1:B:472:ARG:CD	2.96	0.48
1:A:130:GLU:HB2	1:A:136:VAL:HG23	1.95	0.48
1:B:455:TYR:CD1	1:B:472:ARG:HG2	2.49	0.47
1:D:104:LEU:HG	1:D:108:LYS:HE3	1.96	0.47
1:C:320:PRO:O	1:C:321:ASN:OD1	2.31	0.47
1:C:82:GLU:OE1	1:D:89:LYS:CE	2.61	0.47
1:C:440:ALA:HB3	1:D:440:ALA:HB3	1.96	0.47
1:A:480:LYS:HA	1:A:480:LYS:HD2	1.65	0.47
1:D:395:SER:HA	1:D:411:PHE:O	2.15	0.46
1:C:299:VAL:HG23	1:C:301:VAL:HG23	1.97	0.46
1:B:142:ASP:CG	1:B:144:LYS:HG2	2.40	0.46
1:B:400:MET:HE2	1:B:401:HIS:CE1	2.51	0.46
1:B:157:LEU:HD11	1:B:325:ILE:HG12	1.97	0.46
1:C:3:LYS:HG3	1:C:4:ALA:N	2.24	0.45
1:A:347:ASP:HB3	1:A:353:LYS:HG3	1.97	0.45
1:B:299:VAL:CG2	1:B:301:VAL:HG23	2.45	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:221:TYR:CE2	1:C:223:ASN:HB2	2.52	0.45
1:C:132:LYS:NZ	1:C:133:ASN:HD21	2.13	0.45
1:D:306:LYS:HE2	1:D:330:ASP:CG	2.42	0.45
1:D:157:LEU:HD11	1:D:325:ILE:HG12	1.98	0.44
1:C:57:CYS:HB3	2:C:501:FAD:C4	2.47	0.44
1:C:400:MET:HE2	1:C:401:HIS:ND1	2.32	0.44
1:B:29:LYS:HA	1:B:29:LYS:HD3	1.78	0.44
1:B:396:PHE:C	1:B:396:PHE:CD1	2.95	0.44
7:C:653:HOH:O	1:D:94:LYS:CE	2.66	0.44
1:A:484:MET:HE2	1:A:484:MET:HB3	1.92	0.43
1:C:348:THR:HG23	1:C:354:PRO:HB3	2.00	0.43
1:C:89:LYS:HG3	1:C:90:ALA:N	2.31	0.43
1:B:142:ASP:OD1	1:B:144:LYS:HG2	2.19	0.43
1:C:167:PRO:HD3	1:C:285:ILE:CD1	2.49	0.43
1:C:400:MET:HE2	1:C:401:HIS:CG	2.53	0.43
1:C:455:TYR:OH	1:C:472:ARG:HD2	2.18	0.43
1:B:455:TYR:CE1	1:B:472:ARG:HG2	2.54	0.43
1:C:6:ASP:CG	1:C:29:LYS:HE2	2.45	0.42
1:C:17:LEU:HD13	1:C:110:TYR:CE1	2.55	0.42
1:D:171:GLY:HA3	1:D:258:VAL:O	2.20	0.42
1:B:148:LYS:C	1:B:149:GLU:HG2	2.44	0.42
1:C:8:VAL:CG2	1:C:153:ALA:HB2	2.49	0.42
1:D:385:GLU:O	1:D:385:GLU:HG2	2.18	0.42
1:B:241:GLN:OE1	1:B:370:PRO:HG2	2.19	0.42
1:C:315:SER:O	1:C:323:TYR:HB3	2.20	0.42
1:D:5:PHE:CD1	1:D:30:ARG:HG3	2.56	0.41
1:C:157:LEU:HD13	1:C:345:LEU:CD2	2.51	0.41
1:C:227:LEU:HD12	1:C:238:VAL:HG11	2.03	0.41
1:D:261:ASN:ND2	1:D:277:ASP:OD2	2.52	0.41
2:A:501:FAD:HM73	2:A:501:FAD:HM81	1.91	0.41
1:B:482:GLU:CG	1:B:484:MET:HE3	2.51	0.41
1:A:238:VAL:HG21	1:A:372:ILE:HD11	2.03	0.41
1:B:320:PRO:O	1:B:321:ASN:HB2	2.21	0.41
1:B:411:PHE:CD2	1:B:431:GLY:HA3	2.56	0.41
1:A:299:VAL:HG23	1:A:301:VAL:HG23	2.03	0.40
2:D:501:FAD:H9	2:D:501:FAD:H1'1	1.93	0.40
1:A:47:ALA:O	1:A:48:LEU:C	2.65	0.40
1:A:155:HIS:HB3	1:A:323:TYR:HE2	1.87	0.40
1:B:99:LYS:C	1:B:99:LYS:HD2	2.46	0.40
1:C:400:MET:CE	1:C:401:HIS:CE1	3.04	0.40
1:C:390:ALA:HB3	1:C:417:THR:OG1	2.21	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:171:GLY:HA3	1:A:258:VAL:O	2.21	0.40
1:A:306:LYS:HE2	1:A:330:ASP:OD2	2.22	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	488/495 (99%)	475 (97%)	13 (3%)	0	100	100
1	B	485/495 (98%)	471 (97%)	14 (3%)	0	100	100
1	C	487/495 (98%)	473 (97%)	14 (3%)	0	100	100
1	D	488/495 (99%)	475 (97%)	13 (3%)	0	100	100
All	All	1948/1980 (98%)	1894 (97%)	54 (3%)	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	A	403/407 (99%)	398 (99%)	5 (1%)	63	43
1	B	400/407 (98%)	397 (99%)	3 (1%)	73	59
1	C	402/407 (99%)	398 (99%)	4 (1%)	68	50

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	D	402/407 (99%)	397 (99%)	5 (1%)	63 43
All	All	1607/1628 (99%)	1590 (99%)	17 (1%)	70 46

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	228[A]	ARG
1	A	228[B]	ARG
1	A	335	THR
1	B	57	CYS
1	B	60	LYS
1	B	335	THR
1	C	57	CYS
1	C	60	LYS
1	C	262	THR
1	C	335	THR
1	D	57	CYS
1	D	60	LYS
1	D	331[C]	ARG
1	D	331[D]	ARG
1	D	335	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (25) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	223	ASN
1	A	252	ASN
1	A	295	GLN
1	A	340	ASN
1	B	68	GLN
1	B	107	ASN
1	B	174	HIS
1	B	223	ASN
1	B	224	ASN
1	B	252	ASN
1	B	292	ASN
1	B	321	ASN
1	B	419	HIS
1	C	133	ASN

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

### 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 oligosaccharides in this entry.

## 5.6 Ligand geometry [i](#)

Of 20 ligands modelled in this entry, 6 are monoatomic - leaving 14 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	D	501	-	58,58,58	0.94	2 (3%)	85,89,89	0.90	4 (4%)
3	IMD	B	502	-	5,5,5	0.32	0	5,5,5	0.85	0
4	PEG	C	503	-	6,6,6	0.25	0	5,5,5	0.29	0



Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
4	PEG	A	503	-	6,6,6	0.27	0	5,5,5	0.23	0
2	FAD	B	501	-	58,58,58	0.88	1 (1%)	85,89,89	0.88	4 (4%)
3	IMD	A	502	-	5,5,5	0.30	0	5,5,5	0.85	0
3	IMD	C	505	-	5,5,5	0.32	0	5,5,5	0.96	0
3	IMD	D	502	-	5,5,5	0.37	0	5,5,5	0.73	0
4	PEG	D	503	-	6,6,6	0.22	0	5,5,5	0.28	0
5	A1BE9	A	504	-	17,17,17	0.73	0	22,25,25	1.92	6 (27%)
2	FAD	A	501	-	58,58,58	0.88	2 (3%)	85,89,89	1.00	7 (8%)
2	FAD	C	501	-	58,58,58	0.96	2 (3%)	85,89,89	0.82	1 (1%)
4	PEG	C	504	-	6,6,6	0.25	0	5,5,5	0.21	0
3	IMD	C	502	-	5,5,5	0.31	0	5,5,5	0.83	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	D	501	-	-	5/34/50/50	0/6/6/6
3	IMD	B	502	-	-	-	0/1/1/1
4	PEG	C	503	-	-	3/4/4/4	-
4	PEG	A	503	-	-	4/4/4/4	-
2	FAD	B	501	-	-	4/34/50/50	0/6/6/6
3	IMD	A	502	-	-	-	0/1/1/1
3	IMD	C	505	-	-	-	0/1/1/1
5	A1BE9	A	504	-	-	4/4/25/25	0/3/3/3
4	PEG	D	503	-	-	2/4/4/4	-
3	IMD	D	502	-	-	-	0/1/1/1
2	FAD	A	501	-	-	4/34/50/50	0/6/6/6
2	FAD	C	501	-	-	6/34/50/50	0/6/6/6
4	PEG	C	504	-	-	2/4/4/4	-
3	IMD	C	502	-	-	-	0/1/1/1

All (7) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	501	FAD	P-O3P	4.11	1.63	1.59
2	C	501	FAD	P-O3P	4.01	1.63	1.59
2	A	501	FAD	P-O3P	3.55	1.63	1.59

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	501	FAD	PA-O3P	3.17	1.62	1.59
2	B	501	FAD	P-O3P	3.02	1.62	1.59
2	D	501	FAD	PA-O3P	2.34	1.62	1.59
2	C	501	FAD	PA-O3P	2.13	1.61	1.59

All (22) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	A	504	A1BE9	C10-C09-N04	-4.23	106.02	111.19
2	C	501	FAD	O2P-P-O1P	3.30	127.81	112.44
5	A	504	A1BE9	C08-C09-C10	-3.30	106.54	112.15
5	A	504	A1BE9	C11-C10-C09	3.24	127.86	120.24
5	A	504	A1BE9	C09-N04-C02	2.79	125.35	119.17
5	A	504	A1BE9	C08-C07-C06	-2.58	105.86	110.61
2	A	501	FAD	C2B-C1B-N9A	2.51	119.55	113.30
2	B	501	FAD	O3P-PA-O1A	-2.47	103.28	110.70
2	A	501	FAD	O3P-PA-O1A	-2.42	103.41	110.70
2	D	501	FAD	O2P-P-O3P	-2.39	100.82	107.27
2	A	501	FAD	O2P-P-O1P	2.33	123.28	112.44
2	B	501	FAD	O2P-P-O1P	2.31	123.20	112.44
2	D	501	FAD	O2A-PA-O1A	2.29	123.10	112.44
2	D	501	FAD	C2B-C1B-N9A	2.19	118.75	113.30
2	D	501	FAD	O2P-P-O1P	2.16	122.48	112.44
2	A	501	FAD	C9A-C5X-N5	-2.14	120.18	122.45
2	B	501	FAD	O4B-C1B-C2B	-2.14	102.04	106.62
2	A	501	FAD	O2A-PA-O3P	2.11	112.98	107.27
2	A	501	FAD	O4B-C1B-N9A	-2.07	104.11	108.09
2	B	501	FAD	O4B-C1B-N9A	-2.06	104.13	108.09
5	A	504	A1BE9	C07-C06-C15	-2.02	105.27	109.79
2	A	501	FAD	O2A-PA-O1A	2.00	121.77	112.44

There are no chirality outliers.

All (34) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	A	504	A1BE9	O03-C02-N04-C05
4	C	503	PEG	O1-C1-C2-O2
4	C	503	PEG	O2-C3-C4-O4
4	C	504	PEG	O2-C3-C4-O4
4	A	503	PEG	C1-C2-O2-C3
4	A	503	PEG	O2-C3-C4-O4
4	C	504	PEG	O1-C1-C2-O2

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Mol	Chain	Res	Type	Atoms
5	A	504	A1BE9	C01-C02-N04-C05
5	A	504	A1BE9	O03-C02-N04-C09
2	A	501	FAD	PA-O3P-P-O5'
2	C	501	FAD	PA-O3P-P-O5'
2	D	501	FAD	PA-O3P-P-O5'
2	C	501	FAD	O4B-C4B-C5B-O5B
2	A	501	FAD	P-O3P-PA-O2A
2	D	501	FAD	P-O3P-PA-O2A
4	D	503	PEG	O2-C3-C4-O4
2	B	501	FAD	P-O3P-PA-O2A
2	C	501	FAD	P-O3P-PA-O2A
2	D	501	FAD	O4B-C4B-C5B-O5B
5	A	504	A1BE9	C01-C02-N04-C09
2	A	501	FAD	O4B-C4B-C5B-O5B
2	B	501	FAD	PA-O3P-P-O5'
4	D	503	PEG	C1-C2-O2-C3
4	A	503	PEG	O1-C1-C2-O2
2	A	501	FAD	P-O3P-PA-O1A
2	C	501	FAD	P-O3P-PA-O1A
2	D	501	FAD	P-O3P-PA-O1A
4	C	503	PEG	C1-C2-O2-C3
4	A	503	PEG	C4-C3-O2-C2
2	C	501	FAD	C3B-C4B-C5B-O5B
2	D	501	FAD	C3B-C4B-C5B-O5B
2	B	501	FAD	PA-O3P-P-O2P
2	C	501	FAD	PA-O3P-P-O2P
2	B	501	FAD	O4B-C4B-C5B-O5B

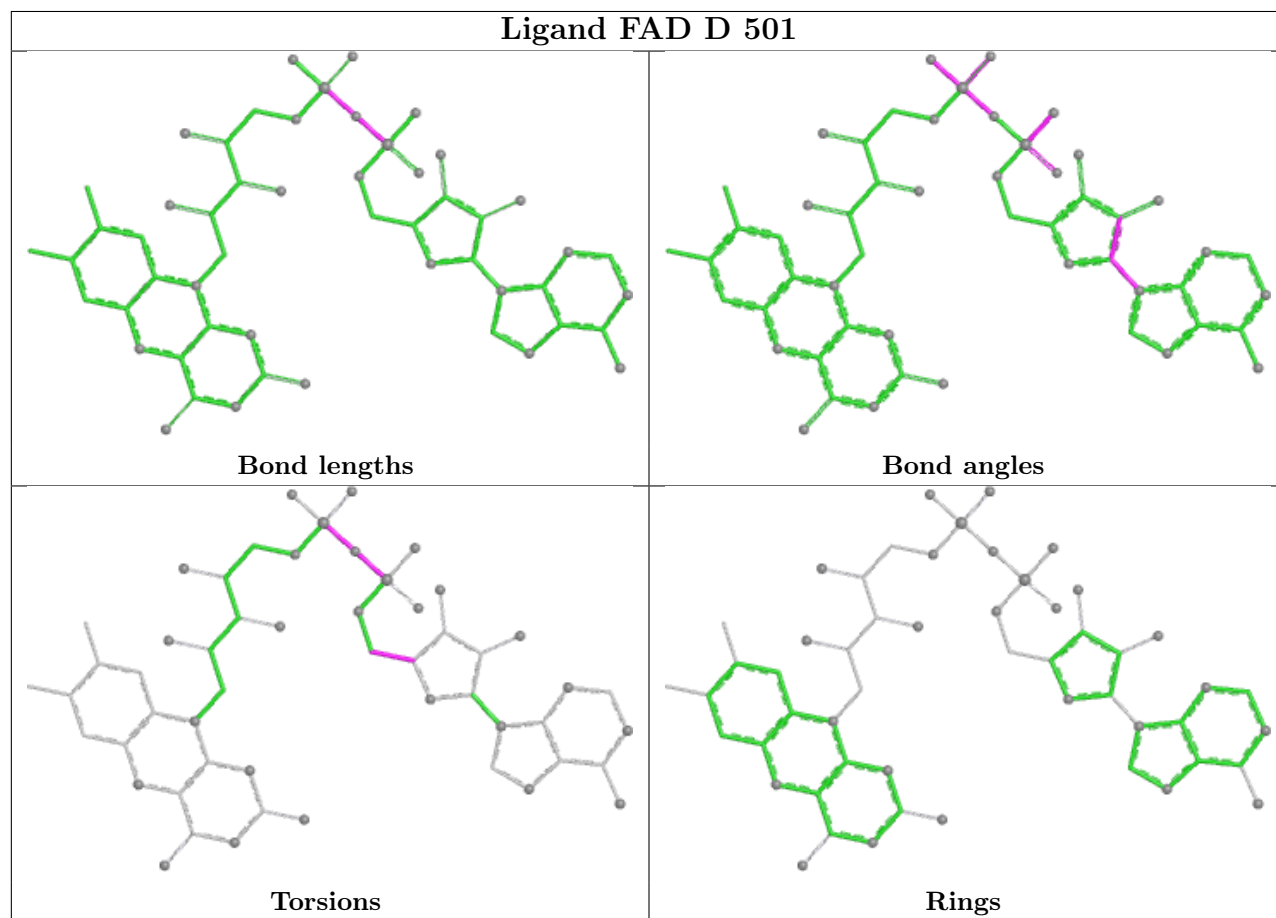
There are no ring outliers.

4 monomers are involved in 5 short contacts:

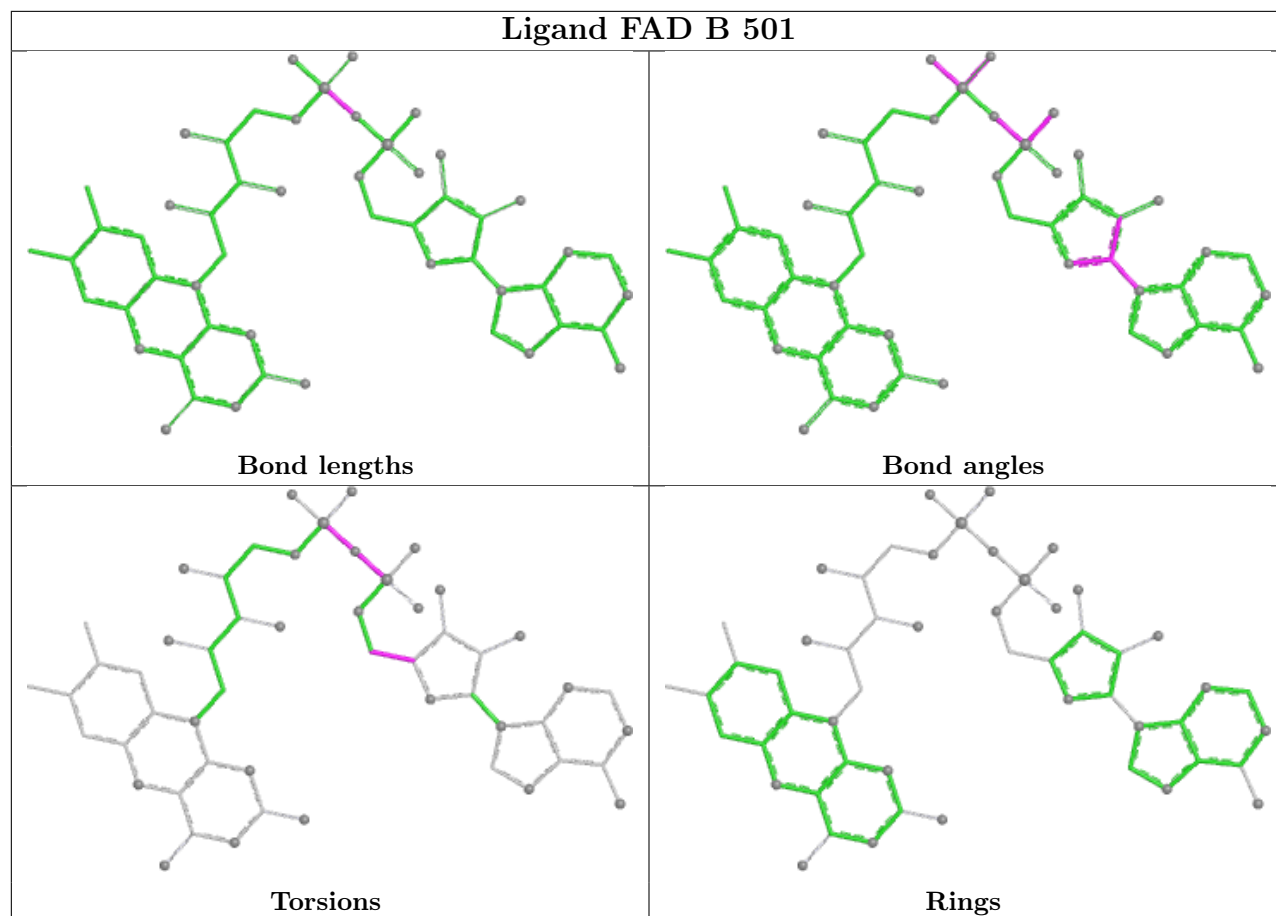
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	D	501	FAD	1	0
3	C	505	IMD	2	0
2	A	501	FAD	1	0
2	C	501	FAD	1	0

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.

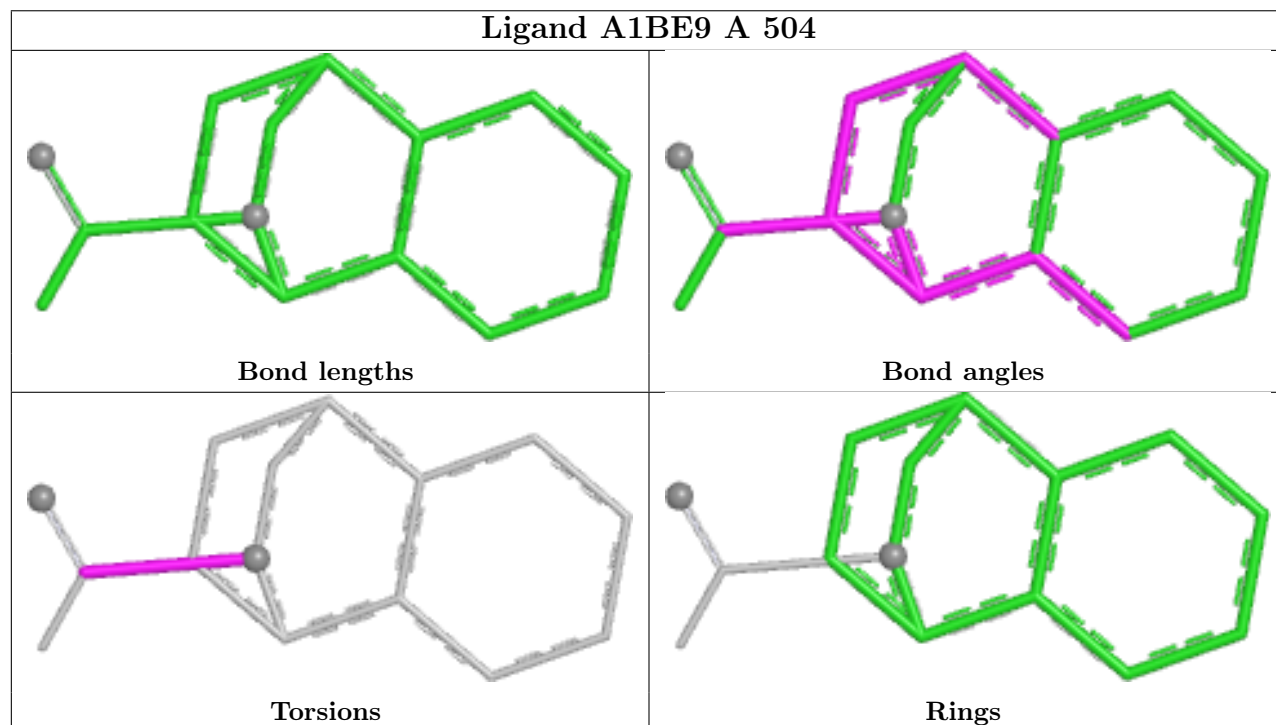
Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD 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.

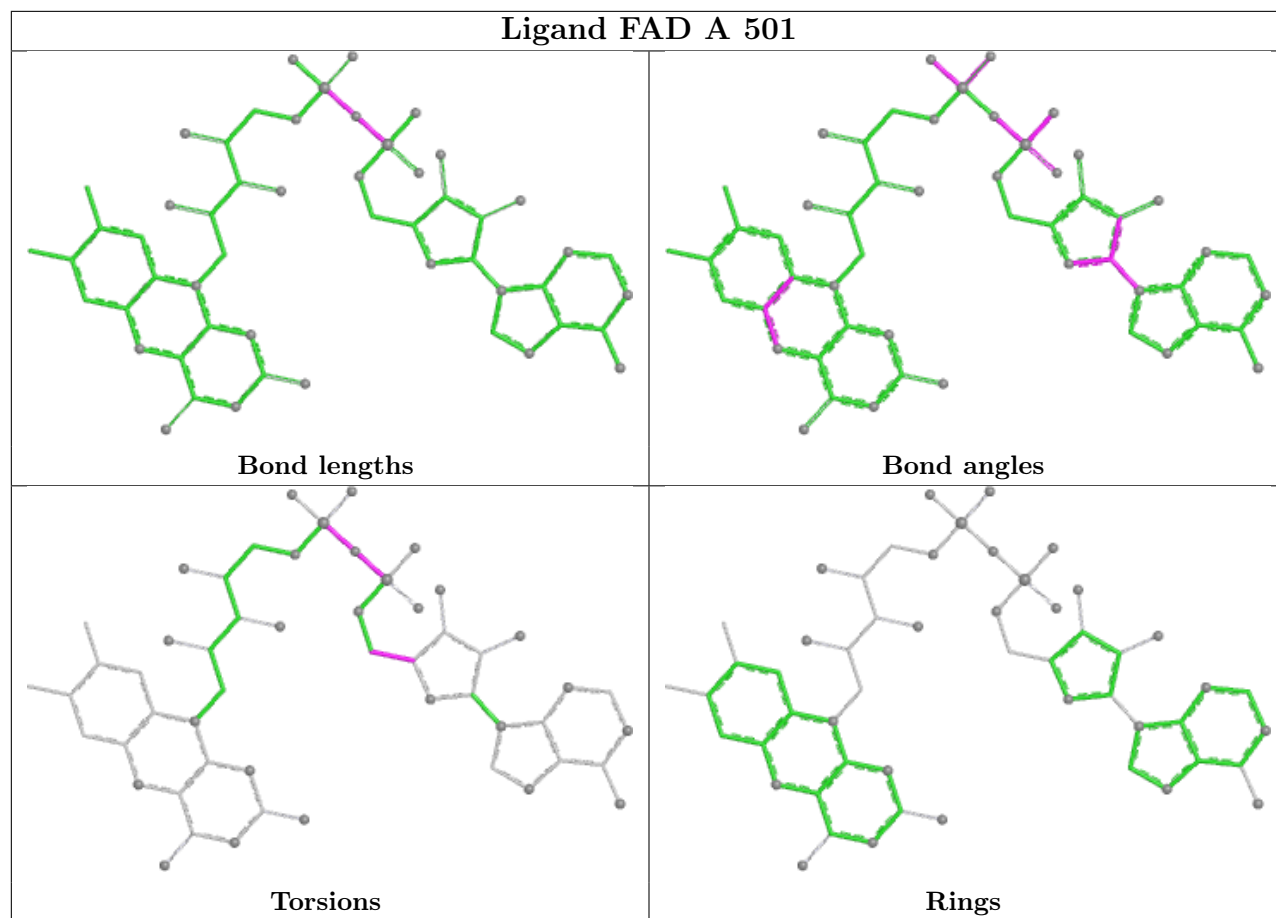


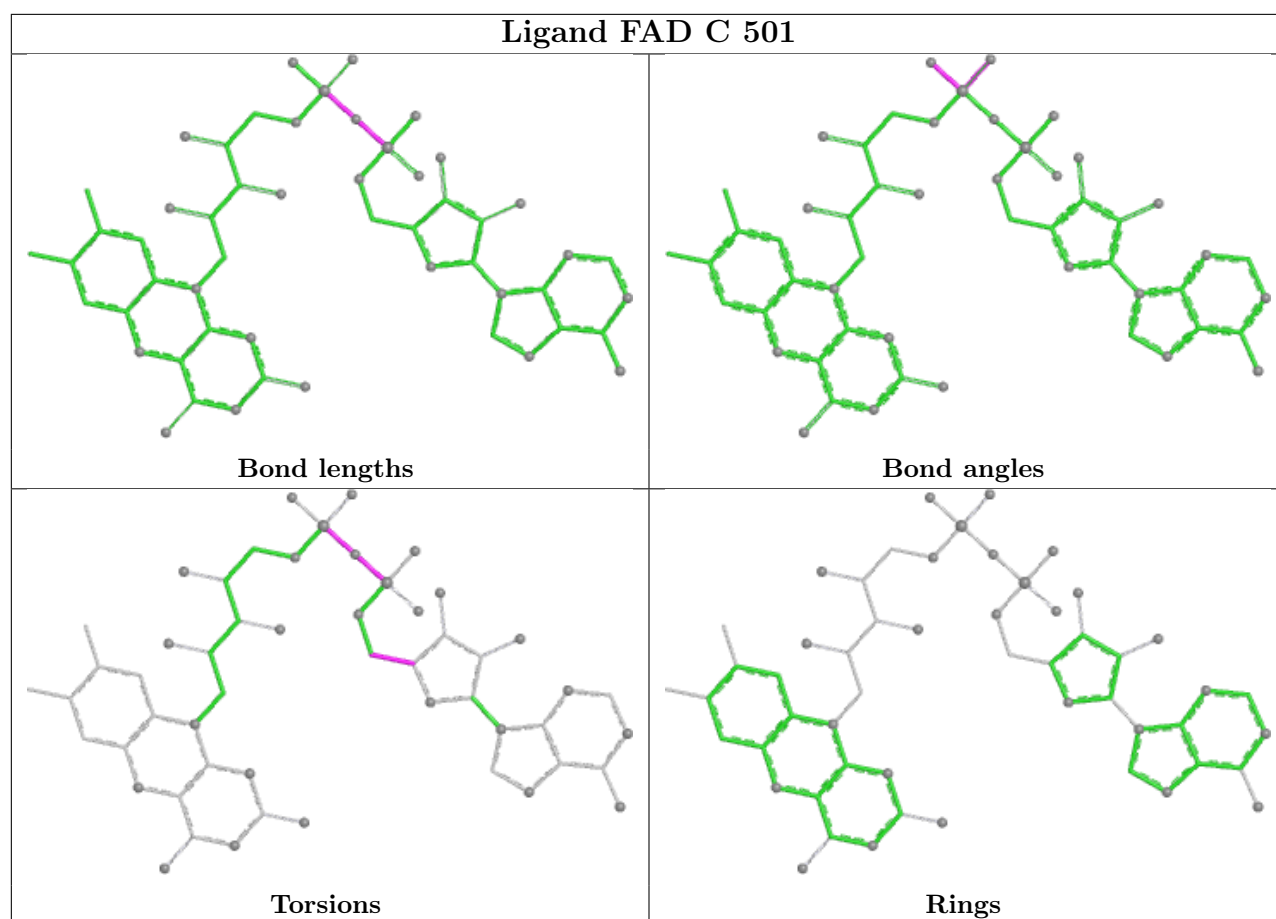
## Ligand FAD B 501



## Ligand A1BE9 A 504







## 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%)	0.07	9 (1%) 67 72	15, 27, 41, 57	1 (0%)
1	B	487/495 (98%)	0.42	24 (4%) 35 37	21, 31, 49, 75	0
1	C	486/495 (98%)	0.60	45 (9%) 14 15	9, 33, 59, 83	1 (0%)
1	D	489/495 (98%)	0.23	9 (1%) 67 72	19, 30, 44, 60	1 (0%)
All	All	1951/1980 (98%)	0.33	87 (4%) 38 41	9, 30, 52, 83	3 (0%)

All (87) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	455	TYR	4.8
1	D	331[C]	ARG	3.7
1	C	305	PRO	3.7
1	C	354	PRO	3.6
1	B	353	LYS	3.5
1	C	455	TYR	3.5
1	C	396	PHE	3.5
1	A	352	ASN	3.5
1	C	488	PRO	3.4
1	B	4	ALA	3.3
1	C	319	VAL	3.3
1	B	352	ASN	3.3
1	A	396	PHE	3.3
1	C	147	VAL	3.3
1	D	455	TYR	3.2
1	B	396	PHE	3.2
1	C	350	PHE	3.2
1	C	299	VAL	3.1
1	C	26	LEU	3.1
1	A	488	PRO	3.0
1	C	343	ALA	3.0

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Mol	Chain	Res	Type	RSRZ
1	B	2	SER	2.9
1	A	228[A]	ARG	2.9
1	C	346	VAL	2.9
1	B	351	GLY	2.9
1	B	448	ASN	2.8
1	A	0	HIS	2.8
1	C	134	VAL	2.8
1	B	146	ALA	2.8
1	C	4	ALA	2.8
1	B	354	PRO	2.8
1	C	31	VAL	2.7
1	C	136	VAL	2.7
1	C	146	ALA	2.7
1	B	488	PRO	2.6
1	C	320	PRO	2.6
1	C	5	PHE	2.6
1	B	147	VAL	2.6
1	C	123	PHE	2.6
1	D	305	PRO	2.6
1	C	348	THR	2.5
1	C	24	ALA	2.5
1	C	135	VAL	2.5
1	B	321	ASN	2.5
1	C	151	LEU	2.5
1	B	32	ALA	2.5
1	C	3	LYS	2.4
1	C	332	LEU	2.4
1	D	213	PRO	2.4
1	B	153	ALA	2.4
1	B	320	PRO	2.4
1	C	353	LYS	2.4
1	B	319	VAL	2.4
1	A	455	TYR	2.3
1	C	23	ALA	2.3
1	C	314	PHE	2.3
1	C	352	ASN	2.3
1	C	355	ARG	2.3
1	C	154	ASP	2.3
1	B	124	LEU	2.3
1	B	134	VAL	2.3
1	B	299	VAL	2.3
1	D	479	VAL	2.3

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Mol	Chain	Res	Type	RSRZ
1	C	345	LEU	2.2
1	C	21	TRP	2.2
1	C	321	ASN	2.2
1	A	480	LYS	2.2
1	C	27	TYR	2.2
1	D	214	GLY	2.1
1	A	115	ASN	2.1
1	D	486	LYS	2.1
1	B	305	PRO	2.1
1	C	152	GLN	2.1
1	A	472	ARG	2.1
1	C	351	GLY	2.1
1	B	8	VAL	2.1
1	B	472	ARG	2.1
1	C	472	ARG	2.1
1	C	487	LEU	2.1
1	C	117	THR	2.1
1	D	411	PHE	2.1
1	C	300	GLY	2.0
1	D	485	GLU	2.0
1	B	349	VAL	2.0
1	C	129	LEU	2.0
1	C	322	ILE	2.0
1	C	145	SER	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](#)

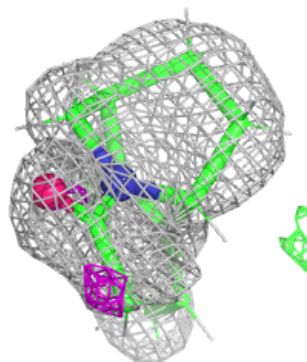
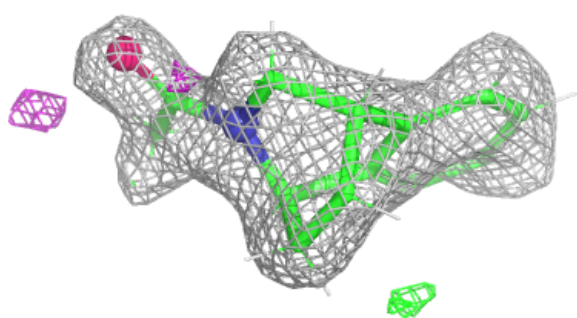
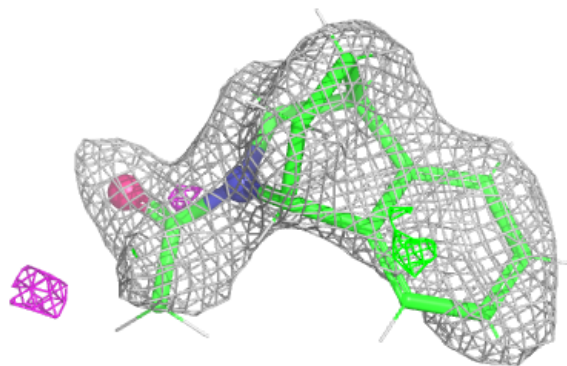
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled 'Q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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
3	IMD	C	505	5/5	0.60	0.22	42,46,49,56	0
3	IMD	A	502	5/5	0.67	0.20	40,51,55,57	0
3	IMD	D	502	5/5	0.68	0.24	45,52,58,62	0
3	IMD	B	502	5/5	0.75	0.18	39,44,51,51	0
3	IMD	C	502	5/5	0.76	0.18	38,45,48,49	0
4	PEG	C	504	7/7	0.77	0.17	54,57,61,63	0
4	PEG	A	503	7/7	0.80	0.16	46,48,54,56	0
4	PEG	C	503	7/7	0.82	0.16	41,49,69,70	0
4	PEG	D	503	7/7	0.82	0.17	45,48,56,58	0
5	A1BE9	A	504	15/15	0.86	0.15	33,42,51,55	30
6	BR	A	505	1/1	0.88	0.26	93,93,93,93	0
6	BR	D	504	1/1	0.90	0.12	113,113,113,113	0
6	BR	B	503	1/1	0.92	0.15	80,80,80,80	0
6	BR	A	506	1/1	0.92	0.12	94,94,94,94	0
2	FAD	C	501	53/53	0.96	0.07	23,29,37,39	0
6	BR	B	504	1/1	0.97	0.21	65,65,65,65	0
2	FAD	B	501	53/53	0.97	0.06	20,25,33,35	0
2	FAD	D	501	53/53	0.98	0.05	20,22,25,26	0
2	FAD	A	501	53/53	0.98	0.05	17,20,23,24	0
6	BR	D	505	1/1	0.99	0.16	56,56,56,56	0

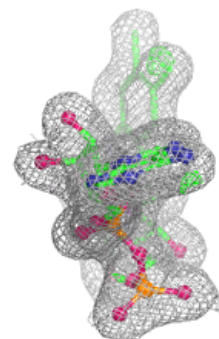
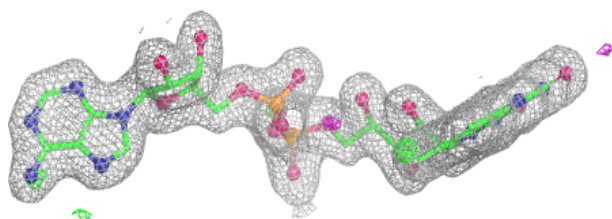
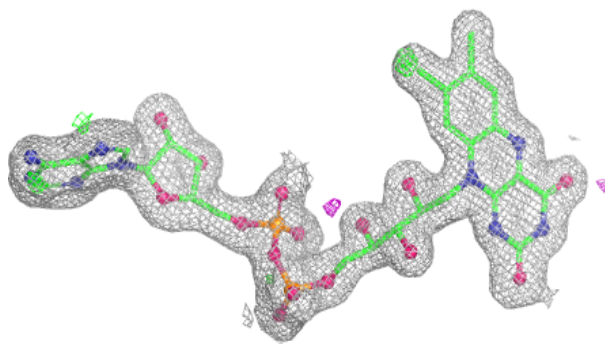
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

**Electron density around A1BE9 A 504:**

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

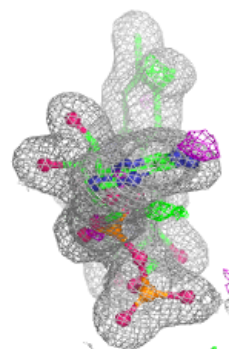
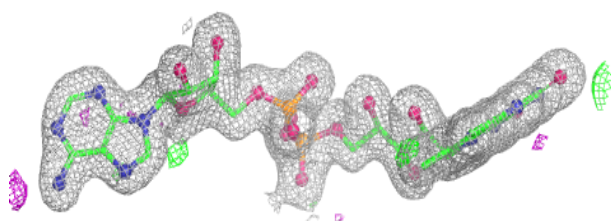
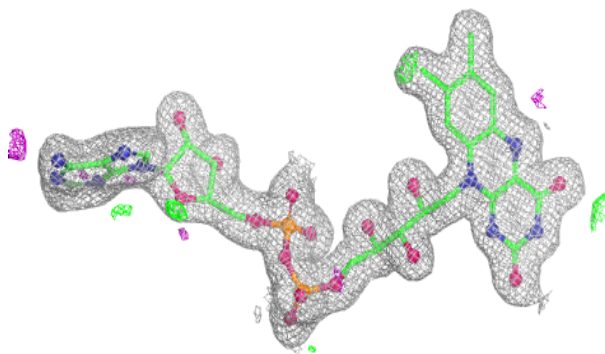
**Electron density around FAD C 501:**

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

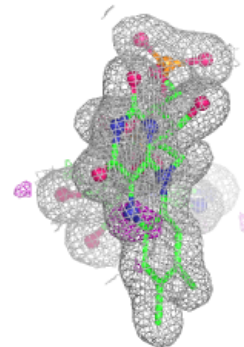
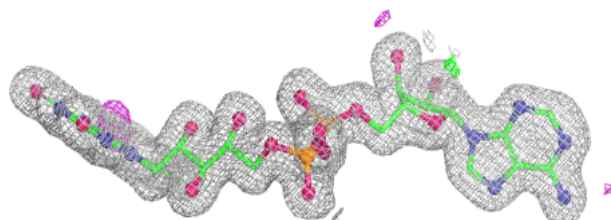
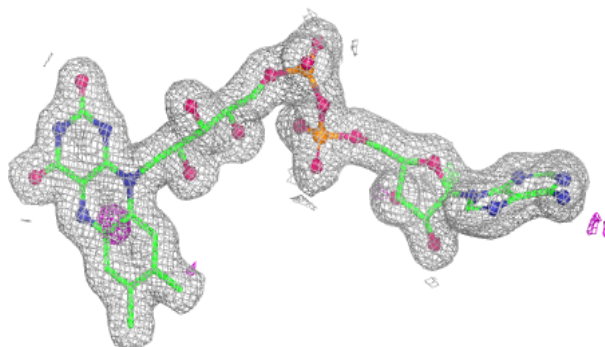


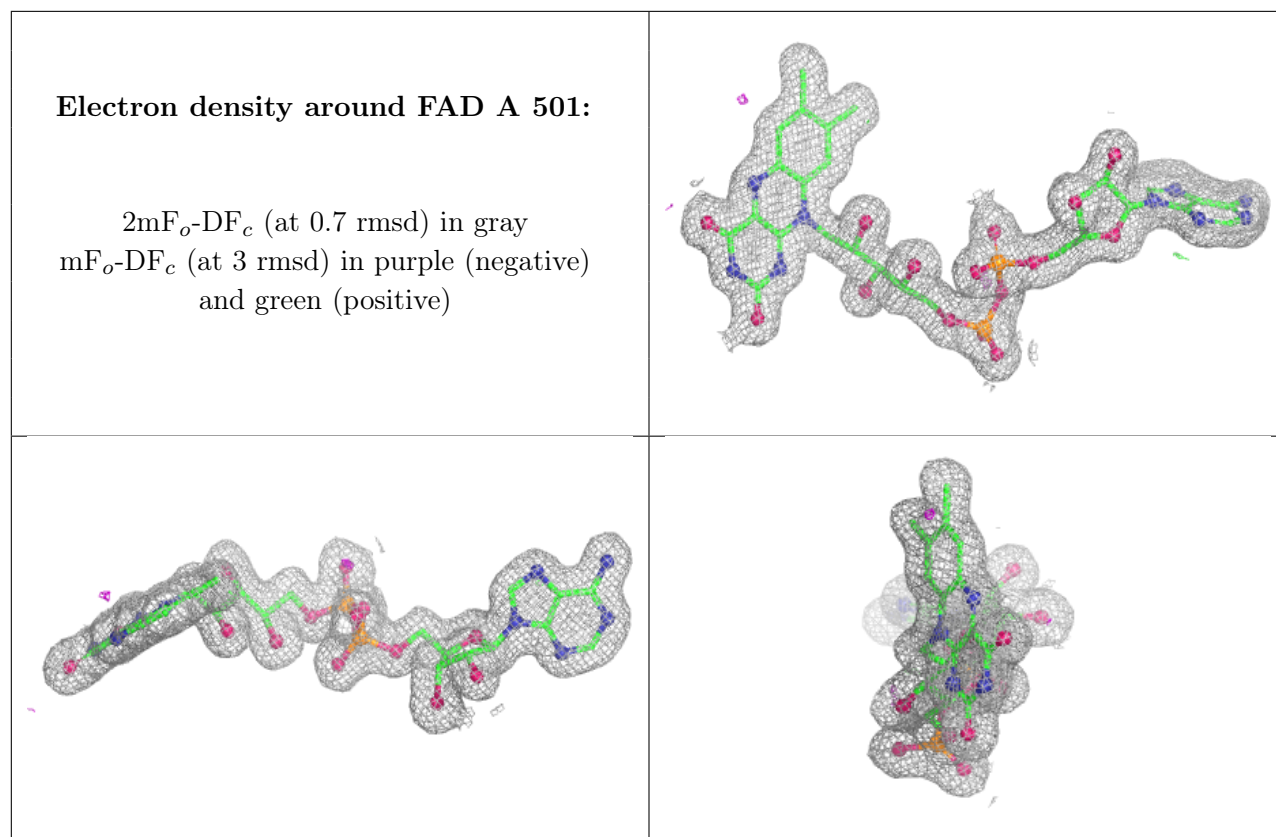
**Electron density around FAD B 501:**

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

**Electron density around FAD 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)





## 6.5 Other polymers [i](#)

There are no such residues in this entry.