



# Full wwPDB X-ray Structure Validation Report ⓘ

Nov 3, 2025 – 04:08 pm GMT

PDB ID : 9IFE / pdb\_00009ife  
Title : PANDDA analysis - Crystal structure of Trypanosoma brucei trypanothione reductase in complex with Z943693514  
Authors : Exertier, C.; Antonelli, L.; Ilari, A.; Fiorillo, A.  
Deposited on : 2025-02-18  
Resolution : 1.68 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 : 1.8.4, CSD as541be (2020)  
Xtriage (Phenix) : 2.0  
EDS : 3.0  
buster-report : 1.1.7 (2018)  
Percentile statistics : 20231227.v01 (using entries in the PDB archive December 27th 2023)  
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) : 2.46

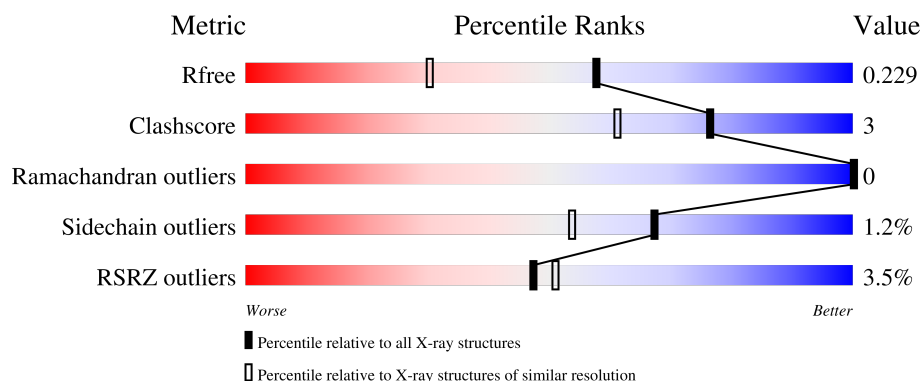
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 1.68 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))
$R_{free}$	164625	8422 (1.70-1.66)
Clashscore	180529	1005 (1.68-1.68)
Ramachandran outliers	177936	9065 (1.70-1.66)
Sidechain outliers	177891	9064 (1.70-1.66)
RSRZ outliers	164620	8421 (1.70-1.66)

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>%</div> <div>92% 7% .</div> </div>
1	B	495	<div> <div>5%</div> <div>91% 7% .</div> </div>
1	C	495	<div> <div>7%</div> <div>90% 8% .</div> </div>
1	D	495	<div> <div>%</div> <div>94% 5% .</div> </div>

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard

residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
4	PEG	C	505	-	-	X	-

## 2 Entry composition

There are 9 unique types of molecules in this entry. The entry contains 16369 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	2	0
			3738	2376	640	702	20			
1	B	487	Total	C	N	O	S	0	4	0
			3772	2400	647	706	19			
1	C	485	Total	C	N	O	S	0	3	0
			3742	2377	638	708	19			
1	D	491	Total	C	N	O	S	0	5	0
			3812	2420	651	721	20			

There are 12 discrepancies between the modelled and reference sequences:

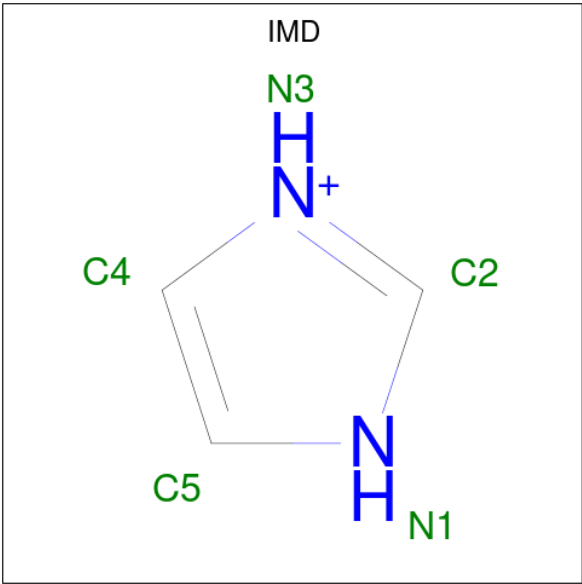
Chain	Residue	Modelled	Actual	Comment	Reference
A	-2	GLY	-	expression tag	UNP Q389T8
A	-1	SER	-	expression tag	UNP Q389T8
A	0	HIS	-	expression tag	UNP Q389T8
B	-2	GLY	-	expression tag	UNP Q389T8
B	-1	SER	-	expression tag	UNP Q389T8
B	0	HIS	-	expression tag	UNP Q389T8
C	-2	GLY	-	expression tag	UNP Q389T8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



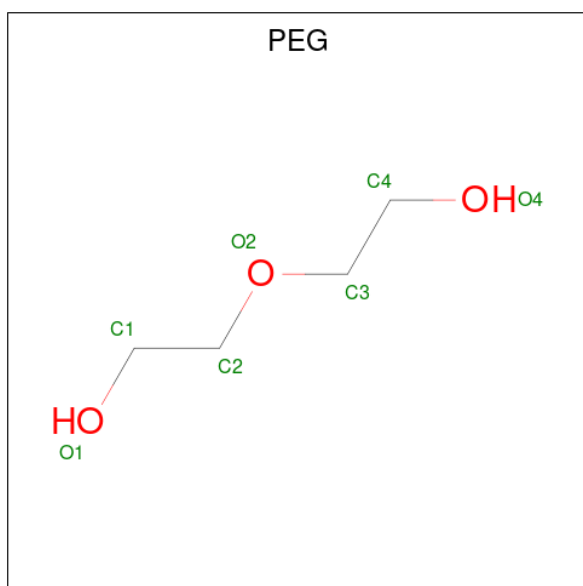
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total 53	C 27	N 9	O 15	P 2	0	0
2	B	1	Total 53	C 27	N 9	O 15	P 2	0	0
2	C	1	Total 53	C 27	N 9	O 15	P 2	0	0
2	D	1	Total 53	C 27	N 9	O 15	P 2	0	0

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



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	1	Total C N 5 3 2	0	0
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	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:  $C_4H_{10}O_3$ ).



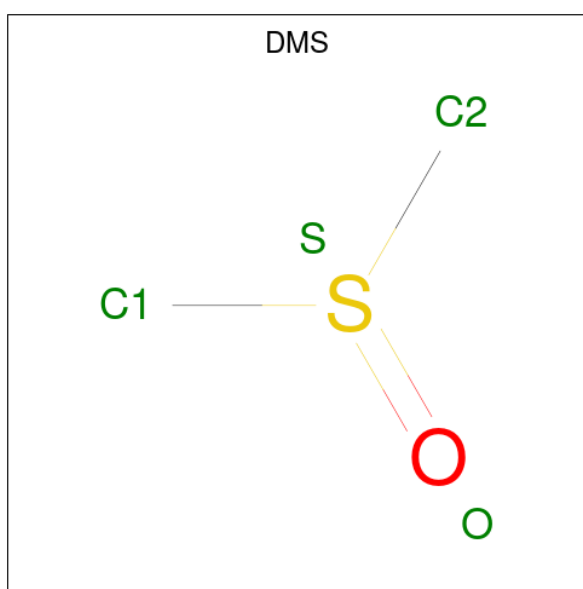
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	1	Total C O 7 4 3	0	0
4	A	1	Total C O 7 4 3	0	0
4	B	1	Total C O 7 4 3	0	0
4	B	1	Total C O 7 4 3	0	0
4	C	1	Total C O 7 4 3	0	0

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	C	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 DIMETHYL SULFOXIDE (CCD ID: DMS) (formula:  $C_2H_6OS$ ).



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

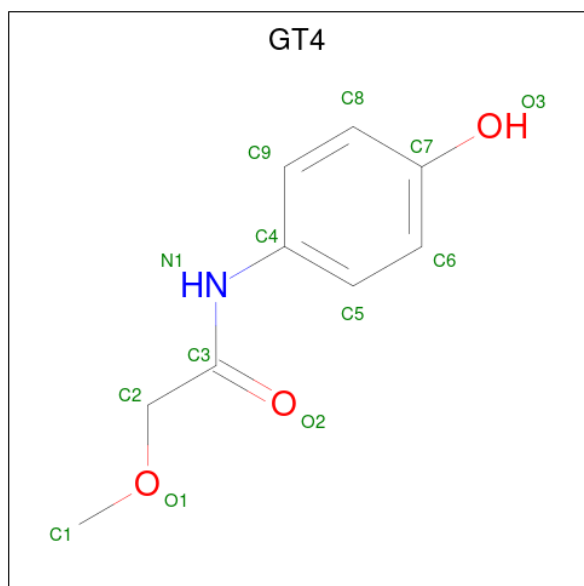
- Molecule 6 is BROMIDE ION (CCD ID: BR) (formula: Br).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	2	Total	Br	0	0
			2	2		
6	B	1	Total	Br	0	0
			1	1		
6	D	2	Total	Br	0	0
			2	2		

- Molecule 7 is SODIUM ION (CCD ID: NA) (formula: Na).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	B	1	Total	Na	0	0
			1	1		

- Molecule 8 is {N}-(4-hydroxyphenyl)-2-methoxy-ethanamide (CCD ID: GT4) (formula: C<sub>9</sub>H<sub>11</sub>NO<sub>3</sub>) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
8	D	1	Total	C	N	O	0	0
			13	9	1	3		

- Molecule 9 is water.

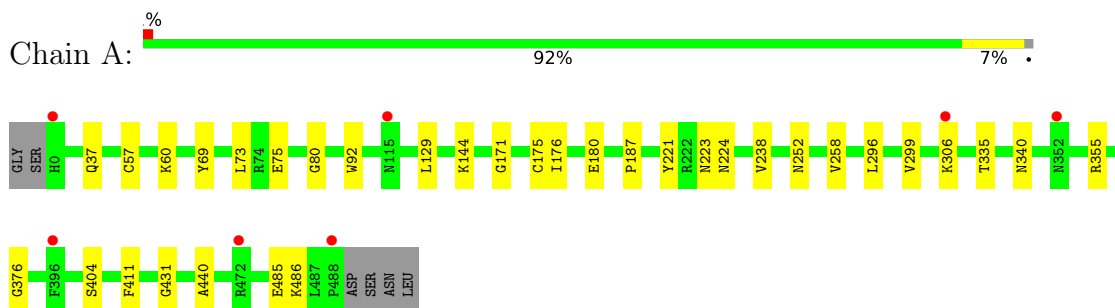
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
9	A	284	Total	O	0	0
			284	284		
9	B	203	Total	O	0	0
			203	203		
9	C	219	Total	O	0	0
			219	219		
9	D	266	Total	O	0	0
			266	266		



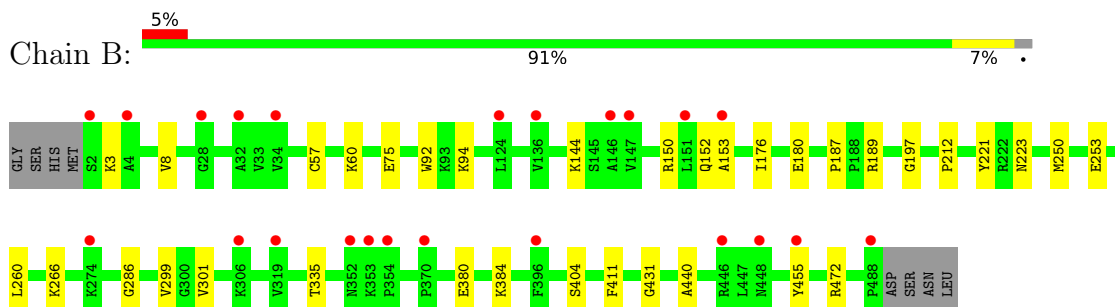
### 3 Residue-property plots [i](#)

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.

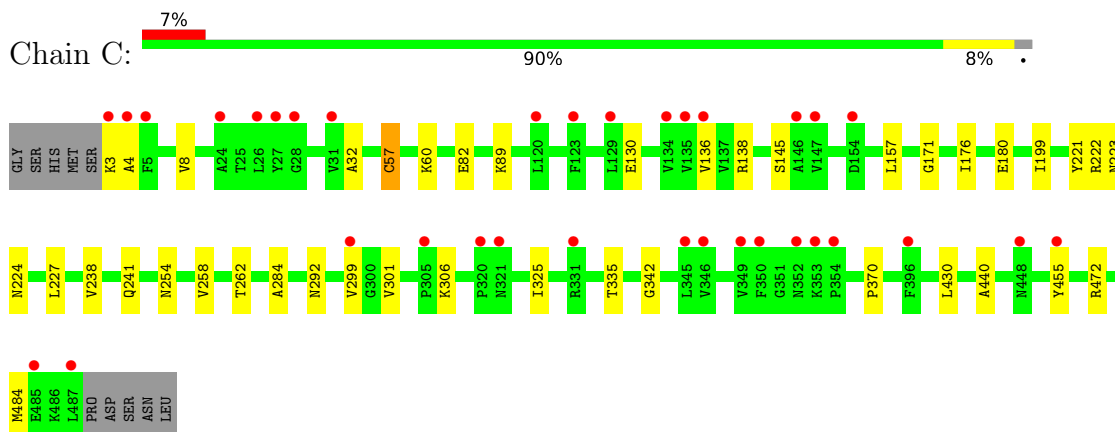
- Molecule 1: Trypanothione reductase



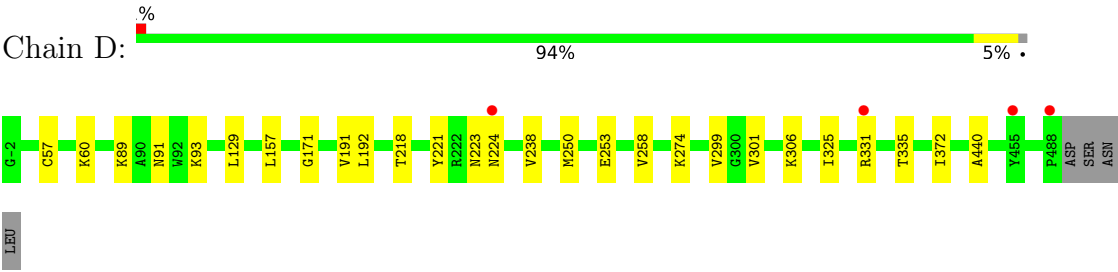
- Molecule 1: Trypanothione reductase



- 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, $\alpha$ , $\beta$ , $\gamma$	101.26Å 63.53Å 169.44Å 90.00° 97.83° 90.00°	Depositor
Resolution (Å)	49.96 – 1.68 49.96 – 1.68	Depositor EDS
% Data completeness (in resolution range)	99.6 (49.96-1.68) 99.6 (49.96-1.68)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.04 (at 1.68Å)	Xtriage
Refinement program	PHENIX 1.21.2	Depositor
R, $R_{free}$	0.196 , 0.229 0.196 , 0.229	Depositor DCC
$R_{free}$ test set	12089 reflections (4.97%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	27.7	Xtriage
Anisotropy	0.066	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.33 , 37.0	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	16369	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	34.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 9.39% 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: DMS, IMD, FAD, NA, GT4, BR, PEG

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	0.31	0/3817	0.50	0/5176
1	B	0.27	0/3857	0.47	0/5227
1	C	0.27	0/3823	0.49	0/5187
1	D	0.28	0/3898	0.48	0/5286
All	All	0.28	0/15395	0.48	0/20876

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	3738	0	3751	22	0
1	B	3772	0	3799	22	0
1	C	3742	0	3739	30	0
1	D	3812	0	3812	13	0
2	A	53	0	31	0	0
2	B	53	0	31	0	0
2	C	53	0	31	1	0
2	D	53	0	31	0	0
3	A	10	0	10	3	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	15	0	15	1	0
3	D	5	0	5	0	0
4	A	14	0	20	1	0
4	B	14	0	20	4	0
4	C	28	0	40	8	0
4	D	7	0	10	0	0
5	A	4	0	6	2	0
6	A	2	0	0	0	0
6	B	1	0	0	0	0
6	D	2	0	0	0	0
7	B	1	0	0	0	0
8	D	13	0	0	0	0
9	A	284	0	0	3	0
9	B	203	0	0	0	0
9	C	219	0	0	1	0
9	D	266	0	0	1	0
All	All	16369	0	15356	86	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 (86) 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:A:224:ASN:HD22	1:A:252:ASN:HD21	1.35	0.73
1:A:37:GLN:HG2	5:A:506:DMS:H22	1.73	0.71
1:B:286:GLY:H	4:B:503:PEG:H32	1.59	0.67
1:A:485:GLU:HG2	1:A:486:LYS:HG2	1.79	0.64
1:C:199:ILE:HD12	4:C:505:PEG:H31	1.80	0.64
1:C:130:GLU:HB2	1:C:136:VAL:CG2	2.30	0.61
1:C:82:GLU:OE1	1:D:89:LYS:HE3	2.00	0.60
1:D:221:TYR:CE2	1:D:223:ASN:HB2	2.38	0.58
1:A:376:GLY:H	3:A:505:IMD:C2	2.16	0.58
1:C:370:PRO:HG2	1:C:430:LEU:HD11	1.87	0.57
1:D:157:LEU:HD11	1:D:325:ILE:HG12	1.87	0.57
1:B:189:ARG:HA	1:B:212:PRO:HD2	1.88	0.56
1:A:129:LEU:HD23	1:A:299:VAL:HG21	1.88	0.56
1:C:292:ASN:H	3:C:507:IMD:HN3	1.54	0.56
1:A:221:TYR:CE2	1:A:223:ASN:HB2	2.42	0.55
1:C:222:ARG:H	4:C:506:PEG:H21	1.72	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:455[A]:TYR:CE1	1:B:472:ARG:HG3	2.42	0.55
1:C:89:LYS:HA	1:C:89:LYS:HE2	1.89	0.55
1:B:286:GLY:N	4:B:503:PEG:H32	2.22	0.54
1:B:299:VAL:HG23	1:B:301:VAL:HG23	1.89	0.54
1:A:355:ARG:NH2	9:A:602:HOH:O	2.41	0.53
1:C:157:LEU:HD11	1:C:325:ILE:HG12	1.90	0.53
1:D:250:MET:HE2	1:D:253:GLU:HG3	1.91	0.52
1:D:238:VAL:HG21	1:D:372:ILE:HD11	1.91	0.51
1:C:254:ASN:OD1	4:C:506:PEG:H12	2.10	0.51
4:C:503:PEG:H12	9:C:602:HOH:O	2.09	0.50
1:B:197:GLY:N	4:B:504:PEG:H31	2.25	0.50
1:A:176:ILE:HB	1:A:180:GLU:HB2	1.94	0.50
1:C:8:VAL:HG22	1:C:32:ALA:HB3	1.94	0.50
1:B:75:GLU:HB3	1:B:404:SER:HB2	1.95	0.49
3:A:505:IMD:H2	9:A:642:HOH:O	2.13	0.49
1:C:130:GLU:HB2	1:C:136:VAL:HG23	1.94	0.49
1:A:75:GLU:HB3	1:A:404:SER:HB2	1.94	0.48
1:A:80:GLY:HA2	1:B:94:LYS:HG2	1.95	0.48
1:A:92:TRP:HB3	1:A:187:PRO:HD3	1.95	0.48
1:C:241:GLN:OE1	1:C:370:PRO:HG3	2.13	0.48
1:B:250:MET:HE2	1:B:253:GLU:HG3	1.96	0.48
1:B:221:TYR:CE2	1:B:223:ASN:HB2	2.49	0.47
1:A:440:ALA:HB3	1:B:440:ALA:HB3	1.95	0.47
1:C:284:ALA:HA	4:C:505:PEG:H21	1.96	0.47
1:A:376:GLY:H	3:A:505:IMD:H2	1.79	0.47
1:C:227:LEU:HD12	1:C:238:VAL:HG11	1.98	0.46
1:D:299:VAL:HG23	1:D:301:VAL:HG23	1.97	0.46
1:C:440:ALA:HB3	1:D:440:ALA:HB3	1.97	0.46
1:C:171:GLY:HA3	1:C:258:VAL:O	2.15	0.46
1:B:197:GLY:H	4:B:504:PEG:H31	1.82	0.45
1:A:411:PHE:CD2	1:A:431:GLY:HA3	2.50	0.45
1:B:266:LYS:HD2	1:B:266:LYS:N	2.31	0.45
1:C:3:LYS:HB2	1:C:3:LYS:HE3	1.73	0.45
1:D:129:LEU:HD23	1:D:299:VAL:HG21	1.98	0.45
1:A:37:GLN:CG	5:A:506:DMS:H22	2.45	0.45
1:C:221:TYR:CE2	1:C:223:ASN:HB2	2.52	0.44
1:D:274:LYS:HE2	9:D:822:HOH:O	2.15	0.44
1:D:91:ASN:OD1	1:D:93:LYS:HE2	2.18	0.44
1:A:340:ASN:HA	9:A:602:HOH:O	2.18	0.44
1:C:3:LYS:HG2	1:C:4:ALA:H	1.83	0.43
1:B:411:PHE:CD2	1:B:431:GLY:HA3	2.53	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:57:CYS:HB3	2:C:501:FAD:C4	2.48	0.43
1:C:455[A]:TYR:CZ	1:C:472:ARG:HD3	2.53	0.43
1:B:92:TRP:HB3	1:B:187:PRO:HD3	2.01	0.43
1:C:325:ILE:HD13	1:C:342:GLY:HA2	2.01	0.43
1:B:8:VAL:HG23	1:B:153:ALA:HB2	2.01	0.43
1:B:150:ARG:HH11	1:B:150:ARG:HB2	1.84	0.43
1:C:199:ILE:CD1	4:C:505:PEG:H22	2.49	0.43
1:B:455[A]:TYR:CZ	1:B:472:ARG:HG3	2.54	0.43
1:A:171:GLY:HA3	1:A:258:VAL:O	2.19	0.42
1:D:171:GLY:HA3	1:D:258:VAL:O	2.19	0.42
1:C:299:VAL:HG23	1:C:301:VAL:HG23	2.02	0.42
1:D:306:LYS:HE2	1:D:306:LYS:HB3	1.63	0.42
1:C:306:LYS:HE2	1:C:306:LYS:HB2	1.87	0.42
1:C:484:MET:HE2	1:C:484:MET:HB3	1.75	0.42
1:B:176:ILE:HB	1:B:180:GLU:HB2	2.02	0.42
1:A:306:LYS:HD2	1:A:306:LYS:HA	1.91	0.42
1:C:138:ARG:HB3	1:C:145:SER:OG	2.20	0.42
1:C:199:ILE:HD12	4:C:505:PEG:H22	2.02	0.41
1:C:325:ILE:HD13	1:C:342:GLY:CA	2.50	0.41
1:A:175:CYS:O	4:A:503:PEG:H11	2.19	0.41
1:C:176:ILE:HB	1:C:180:GLU:HB2	2.01	0.41
1:B:380:GLU:O	1:B:384:LYS:HD2	2.20	0.41
1:A:144:LYS:HB2	1:A:144:LYS:HE2	1.77	0.41
1:B:150:ARG:HB2	1:B:150:ARG:NH1	2.36	0.41
1:A:69:TYR:O	1:A:73:LEU:HG	2.21	0.41
1:A:129:LEU:HD22	1:A:296:LEU:HD23	2.02	0.40
1:B:3:LYS:O	1:B:152:GLN:HG2	2.21	0.40
1:D:192:LEU:HA	1:D:218:THR:O	2.21	0.40
4:C:503:PEG:H11	4:C:503:PEG:H31	1.93	0.40

There are no symmetry-related clashes.

## 5.3 Torsion angles ⓘ

### 5.3.1 Protein backbone ⓘ

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	489/495 (99%)	475 (97%)	14 (3%)	0	100	100
1	B	493/495 (100%)	481 (98%)	12 (2%)	0	100	100
1	C	490/495 (99%)	481 (98%)	9 (2%)	0	100	100
1	D	499/495 (101%)	486 (97%)	13 (3%)	0	100	100
All	All	1971/1980 (100%)	1923 (98%)	48 (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	404/407 (99%)	400 (99%)	4 (1%)	73	62
1	B	408/407 (100%)	403 (99%)	5 (1%)	67	54
1	C	405/407 (100%)	397 (98%)	8 (2%)	50	32
1	D	413/407 (102%)	402 (97%)	11 (3%)	40	20
All	All	1630/1628 (100%)	1602 (98%)	28 (2%)	67	39

All (28) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	57	CYS
1	A	60	LYS
1	A	238	VAL
1	A	335	THR
1	B	57	CYS
1	B	60	LYS
1	B	144	LYS
1	B	260	LEU
1	B	335	THR
1	C	57	CYS
1	C	60	LYS
1	C	224[A]	ASN
1	C	224[B]	ASN

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Mol	Chain	Res	Type
1	C	224[C]	ASN
1	C	224[D]	ASN
1	C	262	THR
1	C	335	THR
1	D	57	CYS
1	D	60	LYS
1	D	191	VAL
1	D	224[A]	ASN
1	D	224[B]	ASN
1	D	224[C]	ASN
1	D	224[D]	ASN
1	D	331[A]	ARG
1	D	331[B]	ARG
1	D	331[D]	ARG
1	D	335	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (15) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	107	ASN
1	A	115	ASN
1	A	152	GLN
1	A	223	ASN
1	A	252	ASN
1	B	107	ASN
1	B	174	HIS
1	B	223	ASN
1	B	224	ASN
1	B	252	ASN
1	C	223	ASN
1	C	252	ASN
1	D	152	GLN
1	D	321	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 [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 28 ligands modelled in this entry, 6 are monoatomic - leaving 22 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	-	53,58,58	0.87	1 (1%)	68,89,89	0.92	4 (5%)
2	FAD	D	501	-	53,58,58	0.78	0	68,89,89	0.98	4 (5%)
4	PEG	B	503	-	6,6,6	0.68	0	5,5,5	0.62	0
2	FAD	C	501	-	53,58,58	0.82	1 (1%)	68,89,89	0.87	4 (5%)
2	FAD	A	501	-	53,58,58	0.76	1 (1%)	68,89,89	1.06	2 (2%)
3	IMD	C	508	-	3,5,5	0.18	0	4,5,5	1.06	0
8	GT4	D	504	-	13,13,13	0.18	0	16,16,16	0.82	1 (6%)
4	PEG	A	503	-	6,6,6	0.25	0	5,5,5	0.30	0
3	IMD	C	502	-	3,5,5	0.20	0	4,5,5	1.02	0
3	IMD	A	502	-	3,5,5	0.14	0	4,5,5	0.97	0
4	PEG	C	505	-	6,6,6	0.49	0	5,5,5	1.07	0
4	PEG	D	503	-	6,6,6	0.22	0	5,5,5	0.37	0
3	IMD	C	507	-	3,5,5	0.13	0	4,5,5	1.03	0
4	PEG	C	503	-	6,6,6	0.22	0	5,5,5	0.32	0
3	IMD	D	502	-	3,5,5	0.13	0	4,5,5	0.95	0
4	PEG	C	504	-	6,6,6	0.23	0	5,5,5	0.24	0
4	PEG	A	504	-	6,6,6	0.23	0	5,5,5	0.21	0
4	PEG	C	506	-	6,6,6	0.32	0	5,5,5	0.56	0
3	IMD	B	502	-	3,5,5	0.14	0	4,5,5	0.96	0
4	PEG	B	504	7	6,6,6	0.29	0	5,5,5	0.69	0
3	IMD	A	505	-	3,5,5	0.18	0	4,5,5	0.89	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
5	DMS	A	506	-	3,3,3	0.54	0	3,3,3	0.31	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	-	-	3/30/50/50	0/6/6/6
2	FAD	D	501	-	-	5/30/50/50	0/6/6/6
4	PEG	B	503	-	-	3/4/4/4	-
2	FAD	C	501	-	-	4/30/50/50	0/6/6/6
2	FAD	A	501	-	-	4/30/50/50	0/6/6/6
3	IMD	C	508	-	-	-	0/1/1/1
8	GT4	D	504	-	-	0/7/7/7	0/1/1/1
4	PEG	A	503	-	-	3/4/4/4	-
3	IMD	C	502	-	-	-	0/1/1/1
3	IMD	A	502	-	-	-	0/1/1/1
4	PEG	C	505	-	-	4/4/4/4	-
4	PEG	D	503	-	-	2/4/4/4	-
3	IMD	C	507	-	-	-	0/1/1/1
4	PEG	C	503	-	-	3/4/4/4	-
3	IMD	D	502	-	-	-	0/1/1/1
4	PEG	C	504	-	-	3/4/4/4	-
4	PEG	A	504	-	-	4/4/4/4	-
4	PEG	C	506	-	-	2/4/4/4	-
3	IMD	B	502	-	-	-	0/1/1/1
4	PEG	B	504	7	-	4/4/4/4	-
3	IMD	A	505	-	-	-	0/1/1/1

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	501	FAD	C8A-N7A	-2.47	1.30	1.34
2	C	501	FAD	C8A-N7A	-2.28	1.30	1.34
2	B	501	FAD	C8A-N7A	-2.12	1.30	1.34

All (15) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
8	D	504	GT4	O1-C2-C3	-3.16	106.60	111.96
2	A	501	FAD	O2P-P-O1P	2.95	126.83	112.24
2	B	501	FAD	O4B-C1B-C2B	-2.68	103.01	106.93
2	C	501	FAD	O2P-P-O1P	2.54	124.82	112.24
2	D	501	FAD	O2P-P-O1P	2.47	124.44	112.24
2	D	501	FAD	O4B-C1B-C2B	-2.32	103.53	106.93
2	B	501	FAD	C5'-C4'-C3'	-2.26	107.84	112.20
2	B	501	FAD	C5A-C6A-N6A	2.24	123.75	120.35
2	D	501	FAD	C5A-C6A-N6A	2.19	123.68	120.35
2	D	501	FAD	O2A-PA-O1A	2.14	122.80	112.24
2	A	501	FAD	O2A-PA-O1A	2.12	122.74	112.24
2	C	501	FAD	O4B-C1B-C2B	-2.09	103.87	106.93
2	C	501	FAD	O2A-PA-O1A	2.08	122.52	112.24
2	B	501	FAD	O2A-PA-O1A	2.07	122.49	112.24
2	C	501	FAD	C10-N1-C2	2.02	120.94	116.90

There are no chirality outliers.

All (44) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	B	504	PEG	O1-C1-C2-O2
4	C	505	PEG	O2-C3-C4-O4
4	C	503	PEG	C1-C2-O2-C3
4	A	504	PEG	O1-C1-C2-O2
4	A	504	PEG	O2-C3-C4-O4
4	B	503	PEG	O1-C1-C2-O2
4	B	503	PEG	O2-C3-C4-O4
4	C	506	PEG	O2-C3-C4-O4
4	B	504	PEG	C4-C3-O2-C2
4	C	505	PEG	O1-C1-C2-O2
4	C	504	PEG	O2-C3-C4-O4
4	B	504	PEG	O2-C3-C4-O4
4	A	503	PEG	O2-C3-C4-O4
4	C	503	PEG	O1-C1-C2-O2
4	C	504	PEG	O1-C1-C2-O2
4	A	504	PEG	C1-C2-O2-C3
4	D	503	PEG	O2-C3-C4-O4
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
4	C	505	PEG	C1-C2-O2-C3
4	A	503	PEG	C1-C2-O2-C3

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Mol	Chain	Res	Type	Atoms
4	C	506	PEG	C4-C3-O2-C2
2	A	501	FAD	O4B-C4B-C5B-O5B
2	A	501	FAD	P-O3P-PA-O2A
4	A	504	PEG	C4-C3-O2-C2
4	B	503	PEG	C1-C2-O2-C3
4	C	505	PEG	C4-C3-O2-C2
4	B	504	PEG	C1-C2-O2-C3
4	D	503	PEG	C4-C3-O2-C2
2	C	501	FAD	P-O3P-PA-O2A
2	D	501	FAD	P-O3P-PA-O2A
2	D	501	FAD	O4B-C4B-C5B-O5B
4	A	503	PEG	O1-C1-C2-O2
4	C	503	PEG	C4-C3-O2-C2
2	B	501	FAD	P-O3P-PA-O2A
2	B	501	FAD	PA-O3P-P-O5'
2	B	501	FAD	O4B-C4B-C5B-O5B
2	C	501	FAD	C3B-C4B-C5B-O5B
2	A	501	FAD	P-O3P-PA-O1A
2	D	501	FAD	P-O3P-PA-O1A
2	D	501	FAD	C3B-C4B-C5B-O5B
4	C	504	PEG	C4-C3-O2-C2

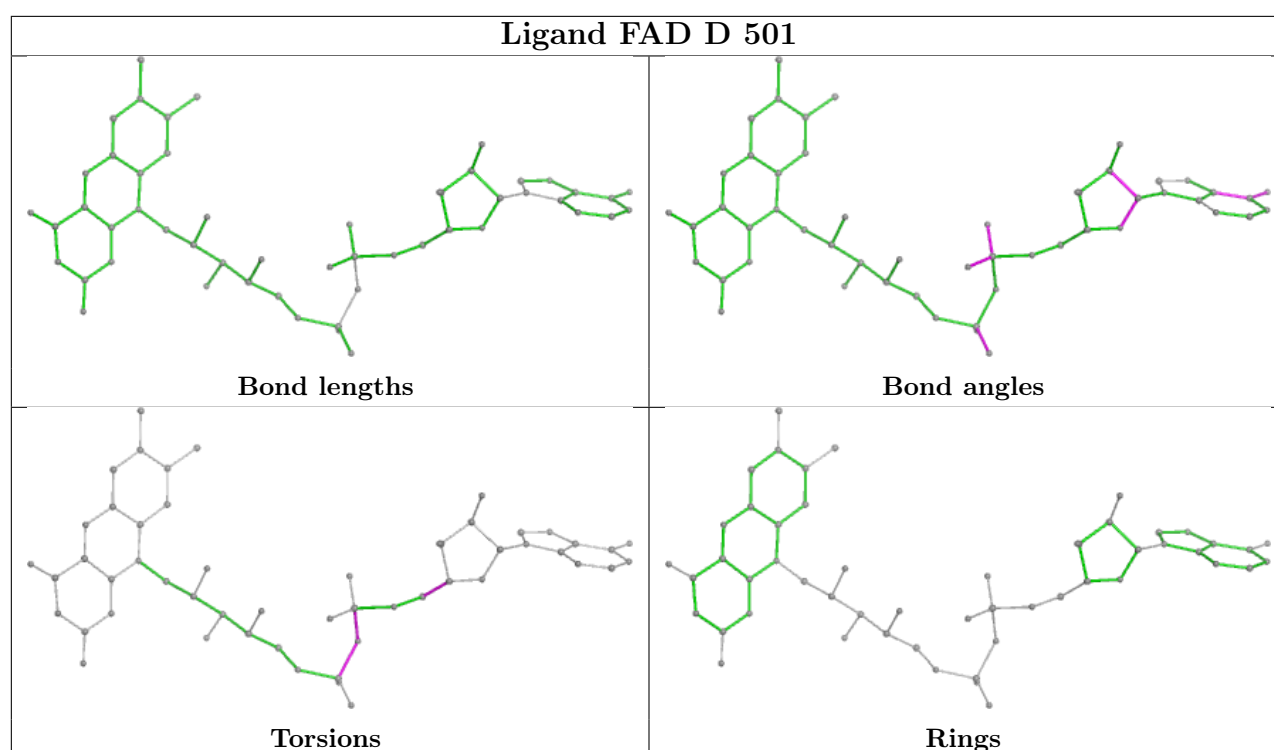
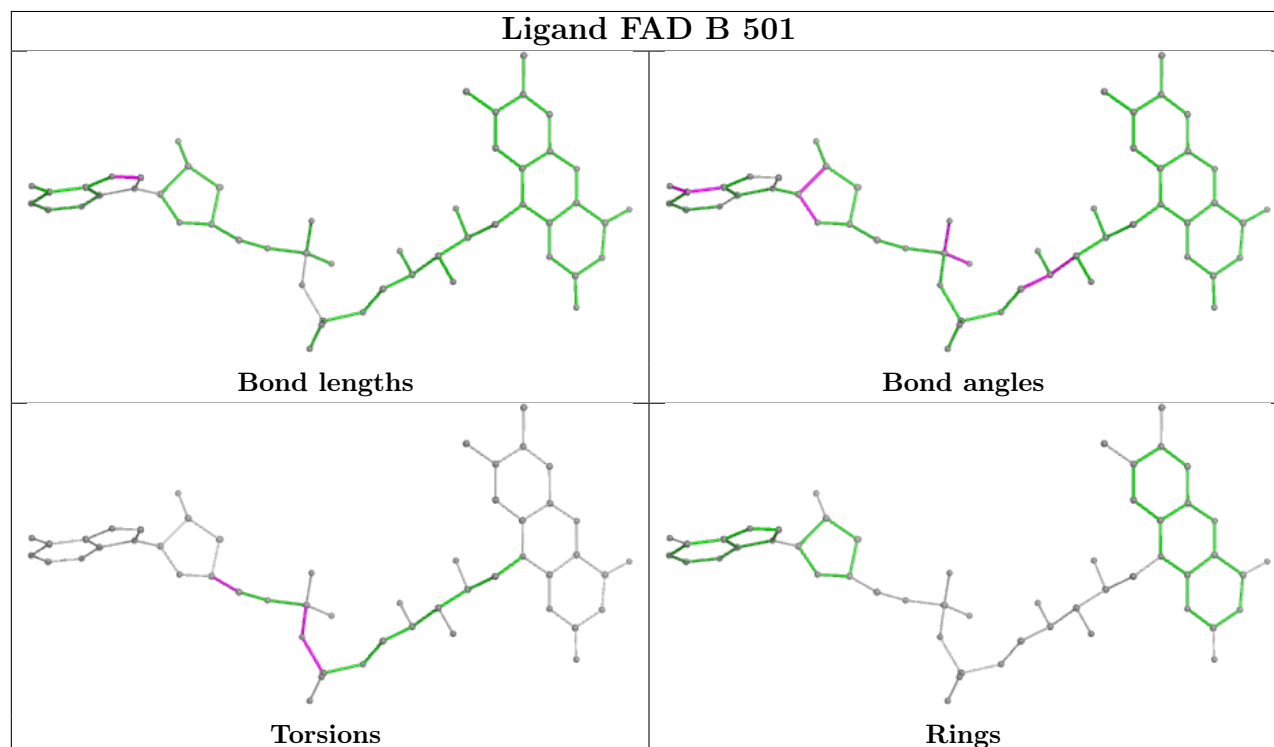
There are no ring outliers.

10 monomers are involved in 20 short contacts:

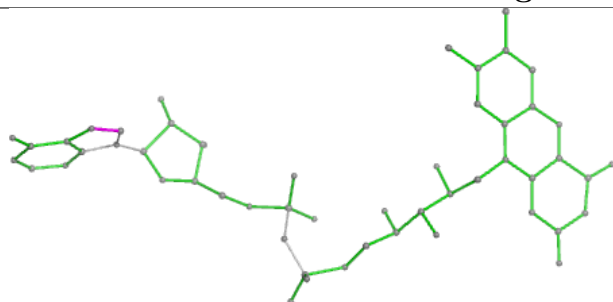
Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	B	503	PEG	2	0
2	C	501	FAD	1	0
4	A	503	PEG	1	0
4	C	505	PEG	4	0
3	C	507	IMD	1	0
4	C	503	PEG	2	0
4	C	506	PEG	2	0
4	B	504	PEG	2	0
3	A	505	IMD	3	0
5	A	506	DMS	2	0

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.

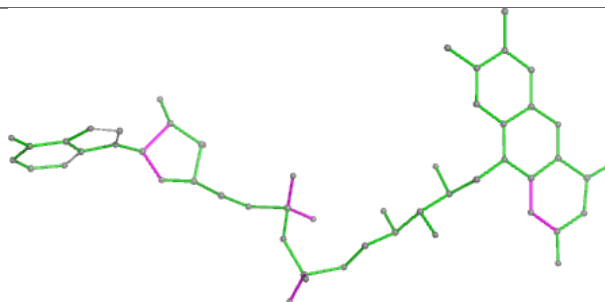
Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD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



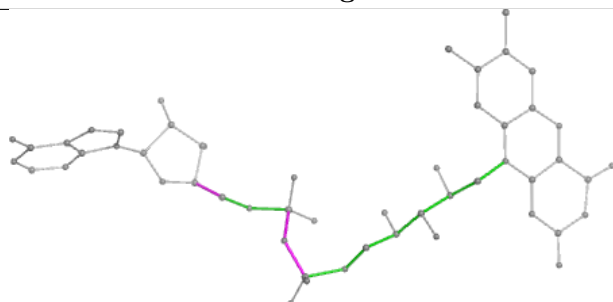
## Ligand FAD C 501



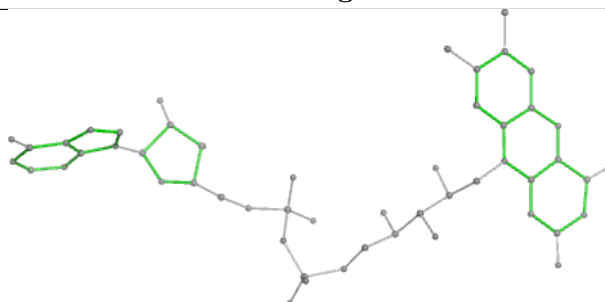
Bond lengths



Bond angles

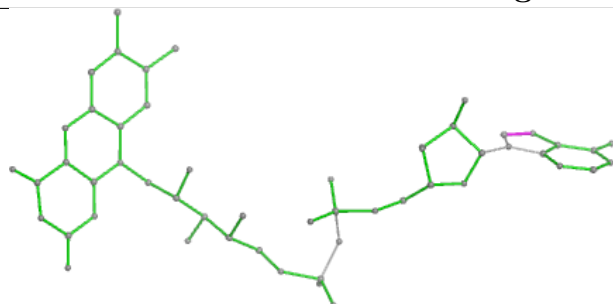


Torsions

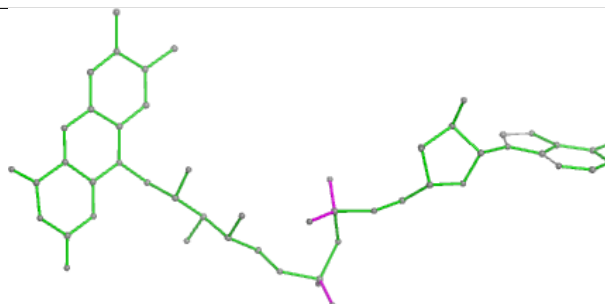


Rings

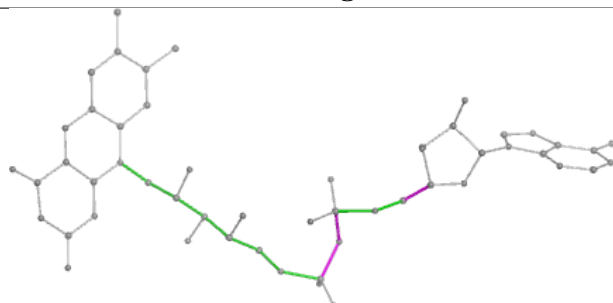
## Ligand FAD A 501



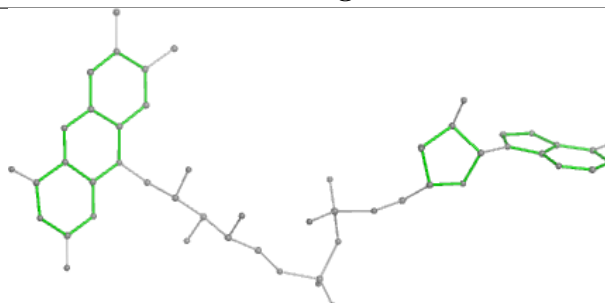
Bond lengths



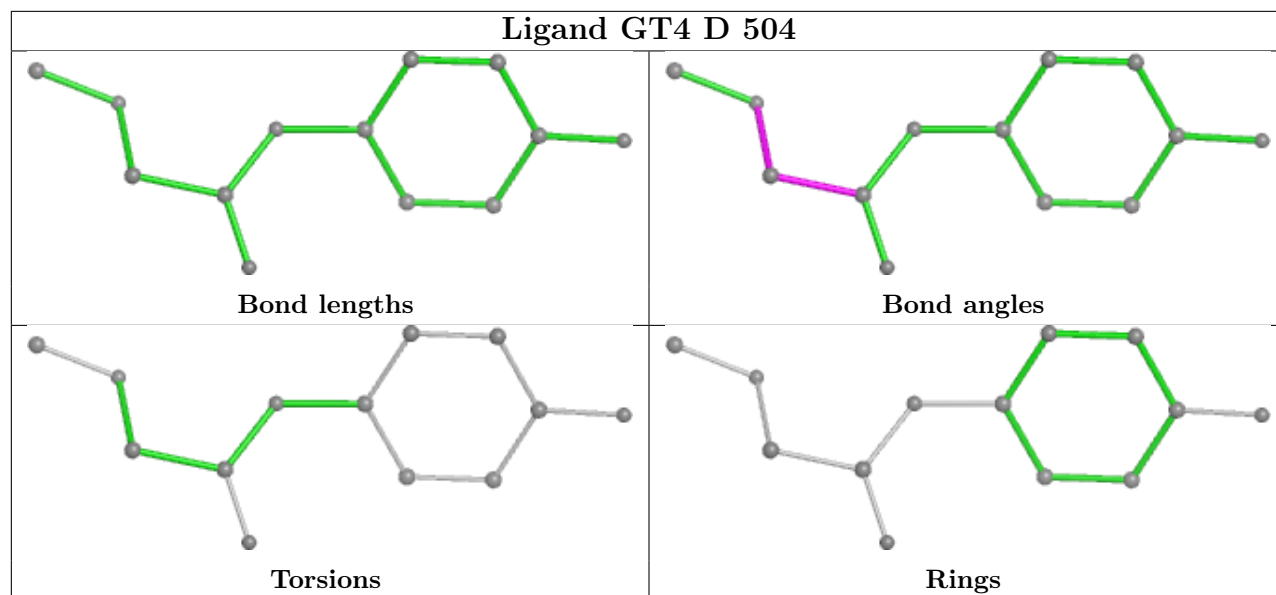
Bond angles



Torsions



Rings



## 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%)	-0.06	7 (1%) 73 76	17, 28, 44, 70	2 (0%)
1	B	487/495 (98%)	0.36	23 (4%) 37 40	8, 33, 53, 88	4 (0%)
1	C	485/495 (97%)	0.43	34 (7%) 24 25	9, 34, 60, 91	3 (0%)
1	D	491/495 (99%)	0.06	4 (0%) 82 85	9, 30, 47, 71	5 (1%)
All	All	1952/1980 (98%)	0.20	68 (3%) 47 51	8, 31, 54, 91	14 (0%)

All (68) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	487	LEU	4.7
1	B	455[A]	TYR	3.8
1	B	488	PRO	3.7
1	C	396	PHE	3.4
1	B	353	LYS	3.3
1	C	331	ARG	3.2
1	C	4	ALA	3.2
1	B	352	ASN	3.1
1	A	0	HIS	3.1
1	B	274[A]	LYS	3.1
1	D	488	PRO	3.0
1	C	353	LYS	3.0
1	D	331[A]	ARG	3.0
1	C	321[A]	ASN	3.0
1	D	455[A]	TYR	3.0
1	B	4	ALA	3.0
1	C	354	PRO	2.9
1	B	446[A]	ARG	2.9
1	B	2	SER	2.9
1	A	115	ASN	2.9
1	B	354	PRO	2.9

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Mol	Chain	Res	Type	RSRZ
1	C	350	PHE	2.8
1	B	147	VAL	2.7
1	B	146	ALA	2.7
1	C	5	PHE	2.6
1	A	472	ARG	2.6
1	D	224[A]	ASN	2.6
1	B	124	LEU	2.5
1	B	448	ASN	2.5
1	A	488	PRO	2.5
1	B	396	PHE	2.5
1	C	24	ALA	2.5
1	C	135	VAL	2.5
1	C	147	VAL	2.5
1	C	136	VAL	2.5
1	C	346	VAL	2.4
1	B	34	VAL	2.4
1	A	396	PHE	2.3
1	C	320	PRO	2.3
1	B	153	ALA	2.3
1	C	134	VAL	2.3
1	B	151	LEU	2.3
1	B	32	ALA	2.3
1	B	319	VAL	2.3
1	B	136	VAL	2.2
1	C	455[A]	TYR	2.2
1	A	352	ASN	2.2
1	C	448	ASN	2.2
1	C	305	PRO	2.2
1	C	352	ASN	2.2
1	C	485	GLU	2.2
1	C	299	VAL	2.2
1	B	28	GLY	2.2
1	B	306	LYS	2.1
1	C	120	LEU	2.1
1	C	349	VAL	2.1
1	C	3	LYS	2.1
1	C	26	LEU	2.1
1	C	27	TYR	2.1
1	C	31	VAL	2.1
1	C	129	LEU	2.1
1	C	345	LEU	2.1
1	C	154	ASP	2.1

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Mol	Chain	Res	Type	RSRZ
1	C	146	ALA	2.0
1	C	123	PHE	2.0
1	A	306	LYS	2.0
1	C	28	GLY	2.0
1	B	370	PRO	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	D	502	5/5	0.70	0.23	57,58,70,74	0
4	PEG	B	504	7/7	0.71	0.25	27,34,42,46	7
3	IMD	C	507	5/5	0.72	0.18	48,51,56,57	0
4	PEG	A	503	7/7	0.73	0.19	52,57,64,66	0
3	IMD	A	502	5/5	0.73	0.18	55,57,64,67	0
3	IMD	A	505	5/5	0.75	0.18	32,43,48,50	0
4	PEG	C	503	7/7	0.78	0.19	40,53,75,81	0
8	GT4	D	504	13/13	0.78	0.16	35,41,47,48	13
5	DMS	A	506	4/4	0.79	0.16	44,45,58,82	0
4	PEG	C	504	7/7	0.80	0.13	65,67,75,76	0
4	PEG	D	503	7/7	0.81	0.18	51,61,73,76	0
4	PEG	A	504	7/7	0.83	0.14	42,48,61,63	0
3	IMD	C	502	5/5	0.83	0.15	41,47,52,56	0
4	PEG	C	505	7/7	0.83	0.23	9,31,38,41	7
3	IMD	B	502	5/5	0.85	0.13	38,39,53,56	0
6	BR	D	505	1/1	0.87	0.14	113,113,113,113	0
4	PEG	C	506	7/7	0.87	0.18	12,40,51,54	0
3	IMD	C	508	5/5	0.88	0.13	39,43,51,54	0

*Continued on next page...*

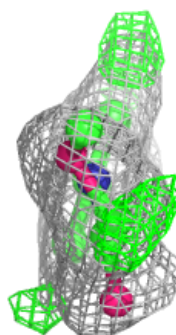
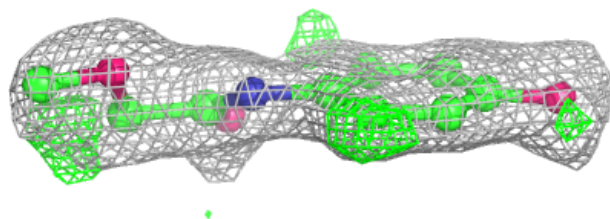
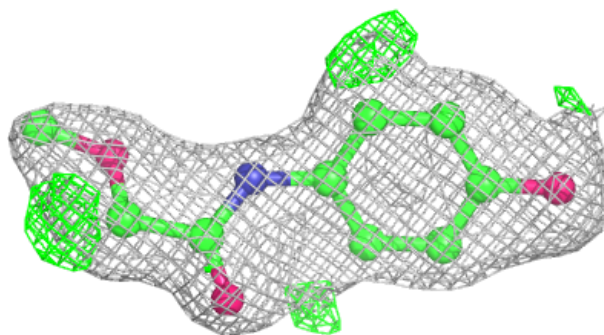
*Continued from previous page...*

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
6	BR	A	508	1/1	0.91	0.12	105,105,105,105	0
4	PEG	B	503	7/7	0.94	0.14	15,29,31,31	7
6	BR	B	505	1/1	0.95	0.16	77,77,77,77	0
6	BR	A	507	1/1	0.96	0.21	64,64,64,64	0
2	FAD	B	501	53/53	0.97	0.07	20,28,37,45	0
2	FAD	C	501	53/53	0.97	0.06	22,30,39,42	0
2	FAD	A	501	53/53	0.98	0.05	16,21,24,25	0
6	BR	D	506	1/1	0.98	0.19	53,53,53,53	0
7	NA	B	506	1/1	0.98	0.14	25,25,25,25	0
2	FAD	D	501	53/53	0.98	0.05	18,23,26,27	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.

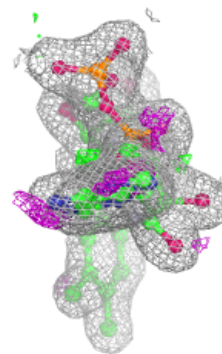
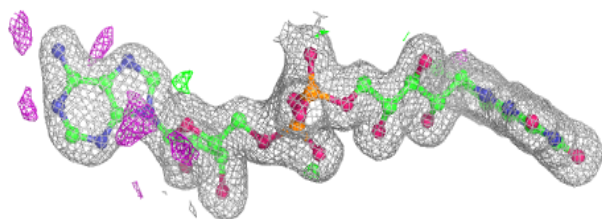
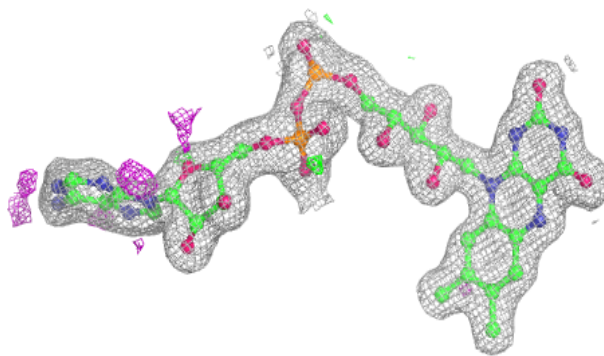
**Electron density around GT4 D 504:**

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)

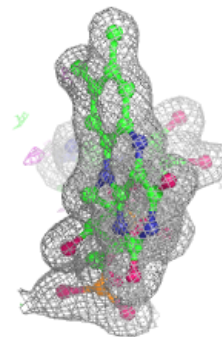
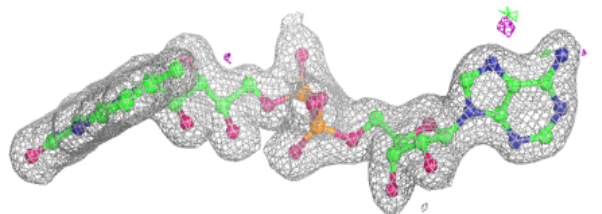
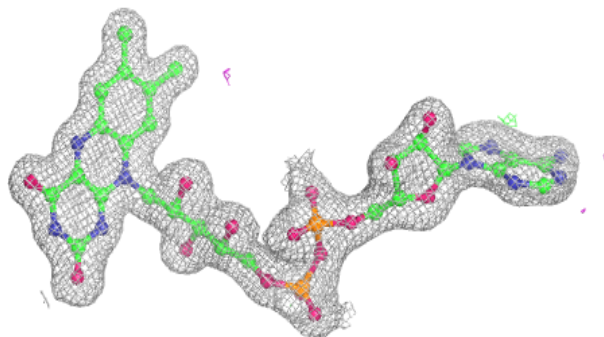


**Electron density around FAD B 501:**

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

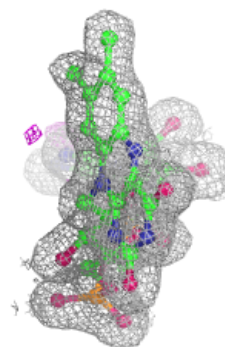
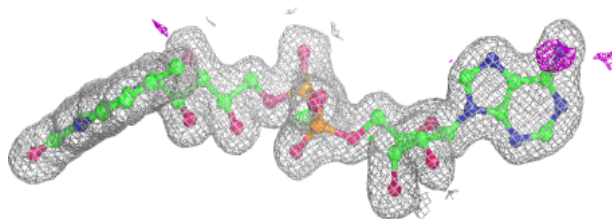
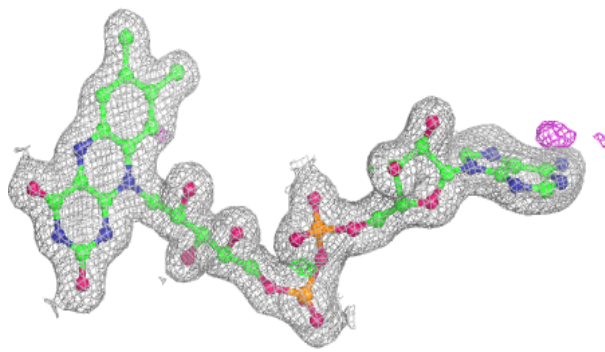
**Electron density around FAD C 501:**

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

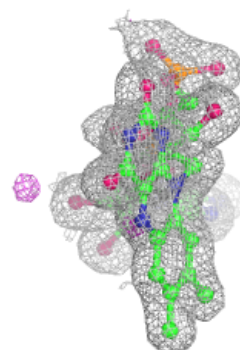
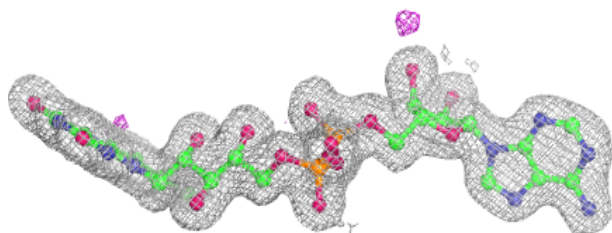
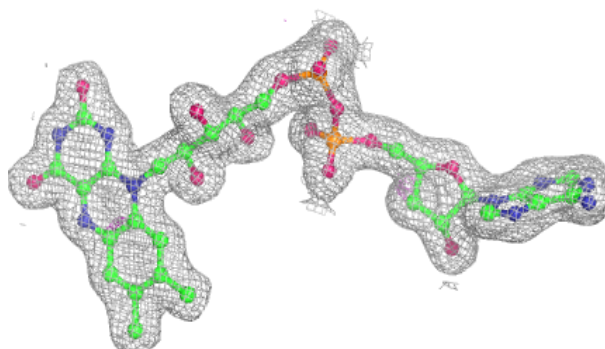


**Electron density around FAD A 501:**

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

**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.