



# Full wwPDB X-ray Structure Validation Report ⓘ

May 26, 2026 – 07:19 pm BST

PDB ID : 9RO3 / pdb\_00009ro3  
Title : Crystal structure of Cryptosporidium parvum Thioredoxin Reductase in complex with the auranofin analogue AuP(OCH<sub>3</sub>)<sub>3</sub>Cl  
Authors : Gabriele, F.; Palmera, M.; Ardini, M.; Bogard, J.; Williams, D.L.; Ippoliti, R.; Angelucci, F.  
Deposited on : 2025-06-20  
Resolution : 2.20 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	:	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

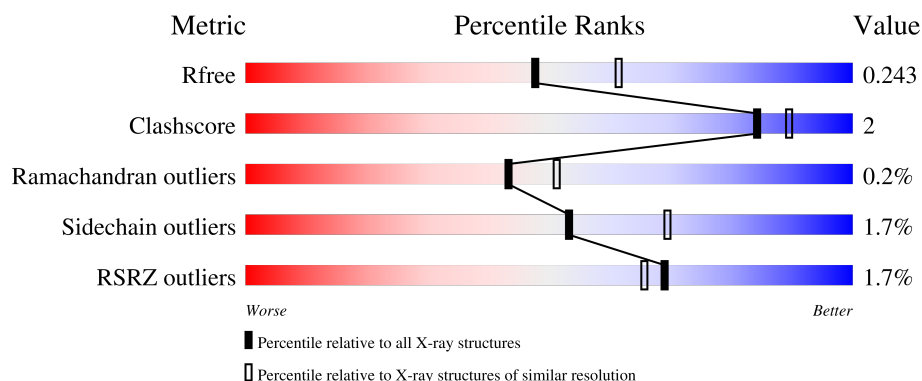
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 2.20 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	6164 (2.20-2.20)
Clashscore	190562	6851 (2.20-2.20)
Ramachandran outliers	187476	6768 (2.20-2.20)
Sidechain outliers	187428	6769 (2.20-2.20)
RSRZ outliers	180081	6166 (2.20-2.20)

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	521	<div> <div>87%</div> <div>7% • 6%</div> </div>
1	B	521	<div> <div>90%</div> <div>• • 5%</div> </div>
1	C	521	<div> <div>88%</div> <div>5% • 7%</div> </div>
1	D	521	<div> <div>88%</div> <div>5% 7%</div> </div>

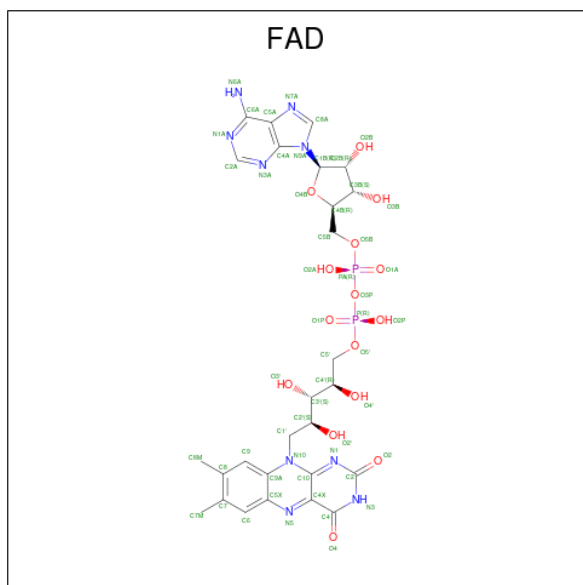


In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called Thioredoxin reductase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	490	Total 3762	C 2400	N 627	O 722	S 13	0	7	0
1	B	493	Total 3751	C 2393	N 622	O 722	S 14	0	4	0
1	C	487	Total 3732	C 2383	N 618	O 718	S 13	0	5	0
1	D	487	Total 3734	C 2386	N 619	O 715	S 14	0	6	0

- Molecule 2 is FLAVIN-ADENINE DINUCLEOTIDE (CCD ID: FAD) (formula:  $C_{27}H_{33}N_9O_{15}P_2$ ) (labeled as "Ligand of Interest" by depositor).



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

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
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 GOLD ION (CCD ID: AU) (formula: Au).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	1	Total	Au	0	0
			1	1		
3	B	1	Total	Au	0	0
			1	1		
3	C	1	Total	Au	0	0
			1	1		

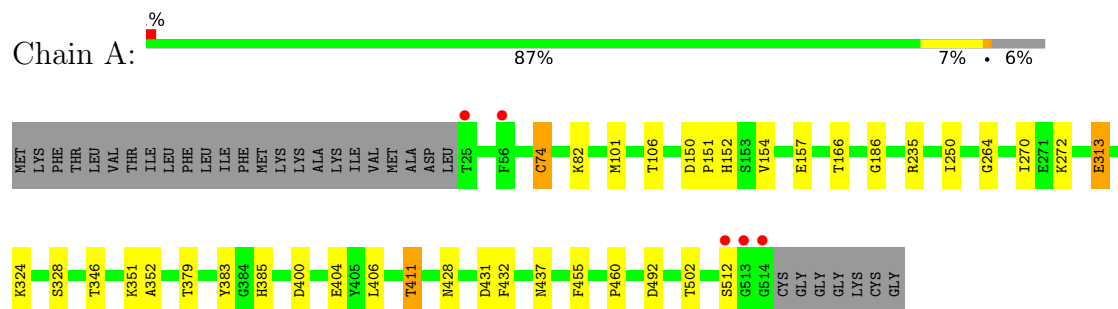
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	83	Total	O	0	0
			83	83		
4	B	93	Total	O	0	0
			93	93		
4	C	46	Total	O	0	0
			46	46		
4	D	38	Total	O	0	0
			38	38		

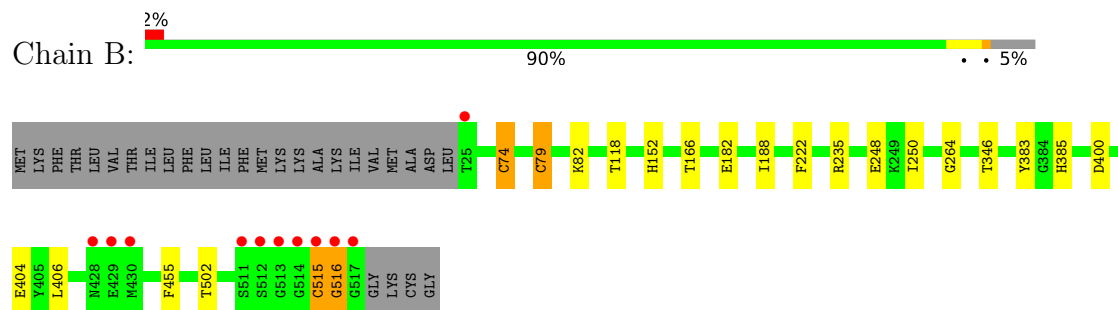
### 3 Residue-property plots

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.

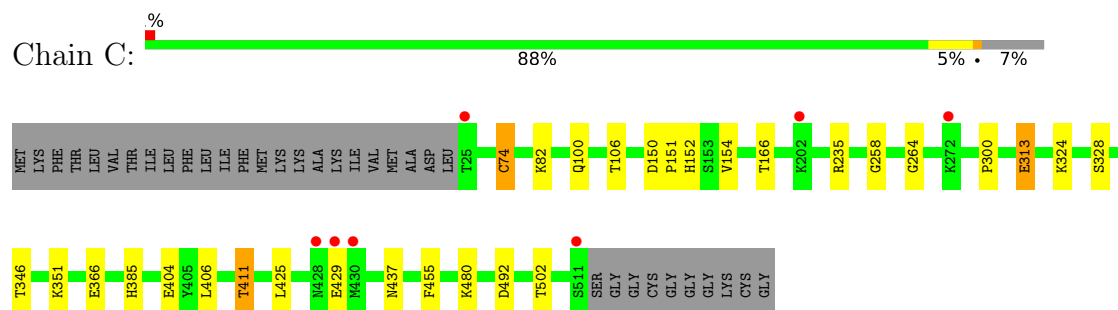
#### • Molecule 1: Thioredoxin reductase



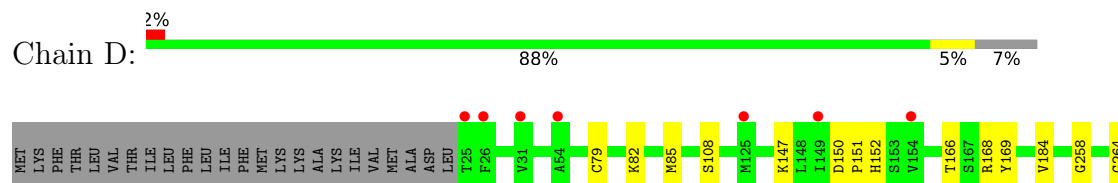
#### • Molecule 1: Thioredoxin reductase

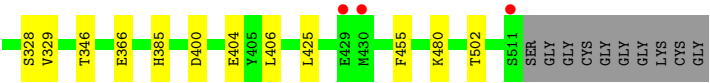


#### • Molecule 1: Thioredoxin reductase



#### • Molecule 1: Thioredoxin reductase





## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	74.30Å 73.25Å 189.52Å 90.00° 90.59° 90.00°	Depositor
Resolution (Å)	45.50 – 2.20 45.50 – 2.20	Depositor EDS
% Data completeness (in resolution range)	98.7 (45.50-2.20) 98.7 (45.50-2.20)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.74 (at 2.20Å)	Xtriage
Refinement program	REFMAC 5.8.0267	Depositor
R, $R_{free}$	0.204 , 0.241 0.208 , 0.243	Depositor DCC
$R_{free}$ test set	5056 reflections (4.87%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	39.5	Xtriage
Anisotropy	0.111	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.29 , 13.8	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.48$ , $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	0.046 for k,h,-l 0.119 for -k,-h,-l 0.086 for h,-k,-l	Xtriage
$F_o, F_c$ correlation	0.95	EDS
Total number of atoms	15454	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	47.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.68% 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: AU, FAD

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	1.10	0/3852	1.35	3/5209 (0.1%)
1	B	1.11	0/3838	1.36	2/5191 (0.0%)
1	C	1.07	1/3816 (0.0%)	1.33	0/5163
1	D	1.09	2/3827 (0.1%)	1.34	2/5177 (0.0%)
All	All	1.09	3/15333 (0.0%)	1.35	7/20740 (0.0%)

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	184	VAL	N-CA	5.19	1.50	1.46
1	C	300	PRO	C-O	-5.07	1.17	1.23
1	D	329	VAL	N-CA	5.00	1.50	1.46

All (7) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	106	THR	CA-CB-OG1	-6.71	99.54	109.60
1	D	328	SER	CA-C-N	5.94	126.87	122.59
1	D	328	SER	C-N-CA	5.94	126.87	122.59
1	B	248	GLU	CB-CG-CD	5.61	122.14	112.60
1	A	352	ALA	CA-C-N	5.11	125.61	119.94
1	A	352	ALA	C-N-CA	5.11	125.61	119.94
1	B	222	PHE	CA-CB-CG	5.04	118.84	113.80

There are no chirality outliers.

There are no planarity outliers.



## 5.2 Too-close contacts ⓘ

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3762	0	3778	25	0
1	B	3751	0	3759	13	0
1	C	3732	0	3741	26	0
1	D	3734	0	3752	12	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	1	0	0	0	0
3	B	1	0	0	0	0
3	C	1	0	0	0	0
4	A	83	0	0	3	0
4	B	93	0	0	2	0
4	C	46	0	0	3	0
4	D	38	0	0	1	0
All	All	15454	0	15154	69	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 (69) 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:74:CYS:SG	4:D:724:HOH:O	2.18	0.99
1:A:411:THR:CG2	1:A:437:ASN:HD21	1.77	0.97
1:C:411:THR:CG2	1:C:437:ASN:HD21	1.79	0.95
1:C:429:GLU:HG2	4:C:746:HOH:O	1.72	0.89
4:A:705:HOH:O	1:B:74:CYS:SG	2.27	0.88
1:A:411:THR:HG23	1:A:437:ASN:HD21	1.42	0.84
1:C:411:THR:HG23	1:C:437:ASN:HD21	1.47	0.79
1:C:429:GLU:CG	4:C:746:HOH:O	2.30	0.78
1:C:366:GLU:OE2	1:D:480:LYS:NZ	2.19	0.75
1:C:480:LYS:NZ	1:D:366:GLU:OE1	2.31	0.63
1:B:515:CYS:O	1:B:516:GLY:O	2.24	0.56
1:C:411:THR:HB	1:C:492:ASP:OD1	2.06	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:411:THR:HB	1:A:492:ASP:OD1	2.07	0.54
1:A:432:PHE:CZ	1:C:235:ARG:CZ	2.91	0.53
1:A:411:THR:HG23	1:A:437:ASN:ND2	2.18	0.52
1:A:74:CYS:SG	4:B:718:HOH:O	2.58	0.51
1:A:385:HIS:HD2	4:A:732:HOH:O	1.92	0.51
1:B:182:GLU:HG2	1:B:188:ILE:HD11	1.93	0.51
1:C:235:ARG:O	1:C:264:GLY:HA2	2.11	0.51
1:A:428:ASN:OD1	1:A:431:ASP:HB2	2.11	0.50
1:B:235:ARG:O	1:B:264:GLY:HA2	2.12	0.49
1:C:411:THR:HG23	1:C:437:ASN:ND2	2.23	0.48
1:A:235:ARG:O	1:A:264:GLY:HA2	2.13	0.48
1:C:429:GLU:HG3	4:C:746:HOH:O	2.06	0.48
1:B:385:HIS:HD2	4:B:743:HOH:O	1.97	0.48
1:C:106:THR:HG22	1:D:108[B]:SER:OG	2.15	0.47
1:A:400:ASP:HB2	4:A:756:HOH:O	2.15	0.47
1:A:150:ASP:HB2	1:A:151:PRO:HD2	1.97	0.46
1:A:432:PHE:CE1	1:C:235:ARG:CZ	2.99	0.45
1:A:101:MET:O	1:B:118:THR:OG1	2.31	0.45
1:C:82:LYS:HD2	1:C:82:LYS:C	2.42	0.45
1:D:385:HIS:HA	1:D:455:PHE:O	2.18	0.44
1:A:404:GLU:O	1:A:502:THR:HA	2.18	0.44
1:C:411:THR:HB	1:C:492:ASP:CG	2.43	0.44
1:C:150:ASP:HB2	1:C:151:PRO:HD2	2.00	0.43
1:A:82:LYS:HD2	1:A:82:LYS:C	2.43	0.43
1:B:74:CYS:HB2	1:B:79:CYS:SG	2.57	0.43
1:C:404:GLU:O	1:C:502:THR:HA	2.18	0.43
1:C:411:THR:CG2	1:C:437:ASN:ND2	2.63	0.42
1:A:411:THR:CG2	1:A:437:ASN:ND2	2.62	0.42
1:B:82:LYS:HD2	1:B:82:LYS:C	2.44	0.42
1:B:404:GLU:O	1:B:502:THR:HA	2.19	0.42
1:D:404:GLU:O	1:D:502:THR:HA	2.18	0.42
1:A:385:HIS:HA	1:A:455:PHE:O	2.20	0.42
1:A:313:GLU:HB2	1:A:328[A]:SER:OG	2.20	0.42
1:C:152:HIS:O	1:C:166:THR:HA	2.20	0.42
1:A:411:THR:HG21	1:A:460:PRO:HG2	2.01	0.42
1:D:150:ASP:HB2	1:D:151:PRO:HD2	2.01	0.42
1:D:258:GLY:HA2	1:D:425:LEU:HD11	2.02	0.42
1:A:152:HIS:O	1:A:166:THR:HA	2.19	0.42
1:C:406:LEU:HD23	1:C:406:LEU:N	2.35	0.42
1:D:82:LYS:C	1:D:82:LYS:HD2	2.44	0.42
1:B:152:HIS:O	1:B:166:THR:HA	2.19	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:411:THR:HB	1:C:492:ASP:OD2	2.21	0.41
1:C:258:GLY:HA2	1:C:425:LEU:HD11	2.01	0.41
1:A:250:ILE:HD11	1:A:383:TYR:HB2	2.03	0.41
1:A:411:THR:HB	1:A:492:ASP:CG	2.46	0.41
1:D:152:HIS:O	1:D:166:THR:HA	2.20	0.41
1:A:406:LEU:N	1:A:406:LEU:HD23	2.35	0.41
1:B:385:HIS:HA	1:B:455:PHE:O	2.21	0.41
1:A:432:PHE:CE1	1:C:235:ARG:NE	2.89	0.41
1:B:406:LEU:N	1:B:406:LEU:HD23	2.36	0.41
1:C:313:GLU:HB2	1:C:328[A]:SER:OG	2.21	0.41
1:C:385:HIS:HA	1:C:455:PHE:O	2.21	0.41
1:D:168:ARG:HD3	1:D:169:TYR:CE2	2.55	0.41
1:D:406:LEU:N	1:D:406:LEU:HD23	2.36	0.40
1:A:186:GLY:HA3	1:A:270:ILE:O	2.22	0.40
1:B:250:ILE:HD11	1:B:383:TYR:HB2	2.03	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	495/521 (95%)	476 (96%)	18 (4%)	1 (0%)	43	51
1	B	495/521 (95%)	474 (96%)	19 (4%)	2 (0%)	30	34
1	C	490/521 (94%)	471 (96%)	19 (4%)	0	100	100
1	D	491/521 (94%)	472 (96%)	19 (4%)	0	100	100
All	All	1971/2084 (95%)	1893 (96%)	75 (4%)	3 (0%)	43	51

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	512	SER
1	B	515	CYS
1	B	516	GLY

### 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	409/427 (96%)	399 (98%)	10 (2%)	43	58
1	B	407/427 (95%)	403 (99%)	4 (1%)	68	81
1	C	406/427 (95%)	398 (98%)	8 (2%)	48	64
1	D	407/427 (95%)	402 (99%)	5 (1%)	63	78
All	All	1629/1708 (95%)	1602 (98%)	27 (2%)	53	69

All (27) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	74	CYS
1	A	154	VAL
1	A	157	GLU
1	A	272	LYS
1	A	313	GLU
1	A	324	LYS
1	A	346	THR
1	A	351	LYS
1	A	379	THR
1	A	411	THR
1	B	74	CYS
1	B	79	CYS
1	B	346	THR
1	B	400	ASP
1	C	74	CYS
1	C	100	GLN
1	C	154	VAL
1	C	313	GLU
1	C	324	LYS

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Mol	Chain	Res	Type
1	C	346	THR
1	C	351	LYS
1	C	411	THR
1	D	79	CYS
1	D	85	MET
1	D	147	LYS
1	D	346	THR
1	D	400	ASP

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	104	HIS
1	A	143	ASN
1	A	152	HIS
1	A	269	ASN
1	A	274	ASN
1	A	276	ASN
1	A	299	ASN
1	A	385	HIS
1	A	418	HIS
1	B	143	ASN
1	B	269	ASN
1	B	274	ASN
1	B	276	ASN
1	B	299	ASN
1	B	385	HIS
1	C	143	ASN
1	C	152	HIS
1	C	274	ASN
1	C	276	ASN
1	C	299	ASN
1	D	76	ASN
1	D	127	ASN
1	D	274	ASN
1	D	276	ASN
1	D	299	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 7 ligands modelled in this entry, 3 are monoatomic - leaving 4 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	C	601	-	56,58,58	0.87	3 (5%)	81,89,89	0.77	2 (2%)
2	FAD	A	601	-	56,58,58	0.70	0	81,89,89	0.91	4 (4%)
2	FAD	D	601	-	56,58,58	0.75	2 (3%)	81,89,89	0.74	0
2	FAD	B	601	-	56,58,58	0.58	0	81,89,89	0.75	1 (1%)

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	C	601	-	-	5/34/50/50	0/6/6/6
2	FAD	A	601	-	-	5/34/50/50	0/6/6/6
2	FAD	D	601	-	-	8/34/50/50	0/6/6/6
2	FAD	B	601	-	-	5/34/50/50	0/6/6/6

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	601	FAD	C2-N3	-2.50	1.33	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	601	FAD	C9-C8	-2.50	1.35	1.39
2	C	601	FAD	C1'-C2'	-2.30	1.49	1.52
2	D	601	FAD	C1'-C2'	-2.07	1.49	1.52
2	C	601	FAD	O2-C2	-2.03	1.20	1.24

All (7) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	601	FAD	P-O3P-PA	3.02	143.18	132.83
2	A	601	FAD	O2'-C2'-C1'	2.58	116.03	109.80
2	A	601	FAD	C2B-C1B-N9A	2.39	119.35	113.30
2	A	601	FAD	C5'-C4'-C3'	-2.23	107.90	112.20
2	C	601	FAD	C2B-C1B-N9A	2.14	118.72	113.30
2	C	601	FAD	O2P-P-O1P	2.13	122.75	112.24
2	B	601	FAD	C2B-C1B-N9A	2.07	118.55	113.30

There are no chirality outliers.

All (23) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	B	601	FAD	O4B-C4B-C5B-O5B
2	D	601	FAD	C5'-O5'-P-O2P
2	D	601	FAD	O4B-C4B-C5B-O5B
2	B	601	FAD	C3B-C4B-C5B-O5B
2	D	601	FAD	C3B-C4B-C5B-O5B
2	A	601	FAD	PA-O3P-P-O5'
2	B	601	FAD	PA-O3P-P-O5'
2	C	601	FAD	PA-O3P-P-O5'
2	D	601	FAD	PA-O3P-P-O5'
2	D	601	FAD	C5'-O5'-P-O3P
2	C	601	FAD	O4B-C4B-C5B-O5B
2	A	601	FAD	P-O3P-PA-O2A
2	B	601	FAD	P-O3P-PA-O2A
2	C	601	FAD	P-O3P-PA-O2A
2	D	601	FAD	P-O3P-PA-O2A
2	A	601	FAD	O4B-C4B-C5B-O5B
2	B	601	FAD	P-O3P-PA-O1A
2	C	601	FAD	P-O3P-PA-O1A
2	C	601	FAD	C3B-C4B-C5B-O5B
2	A	601	FAD	P-O3P-PA-O1A
2	D	601	FAD	P-O3P-PA-O1A
2	D	601	FAD	C5'-O5'-P-O1P

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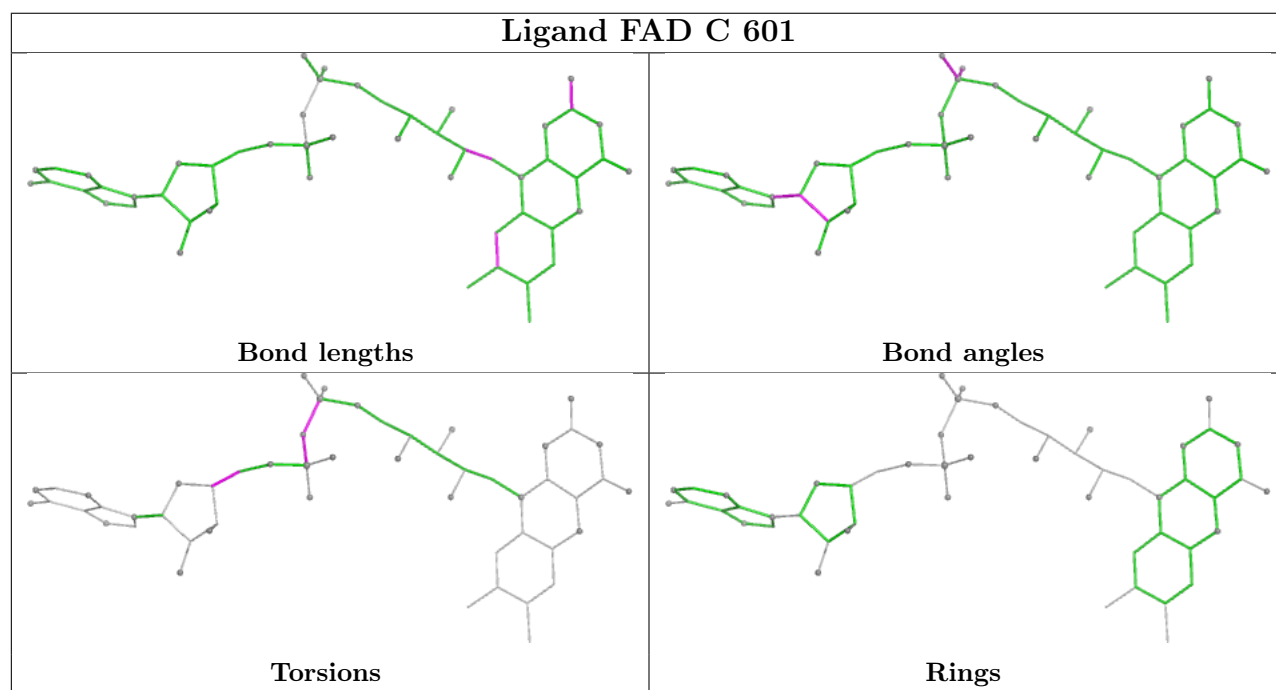
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Mol	Chain	Res	Type	Atoms
2	A	601	FAD	C3B-C4B-C5B-O5B

There are no ring outliers.

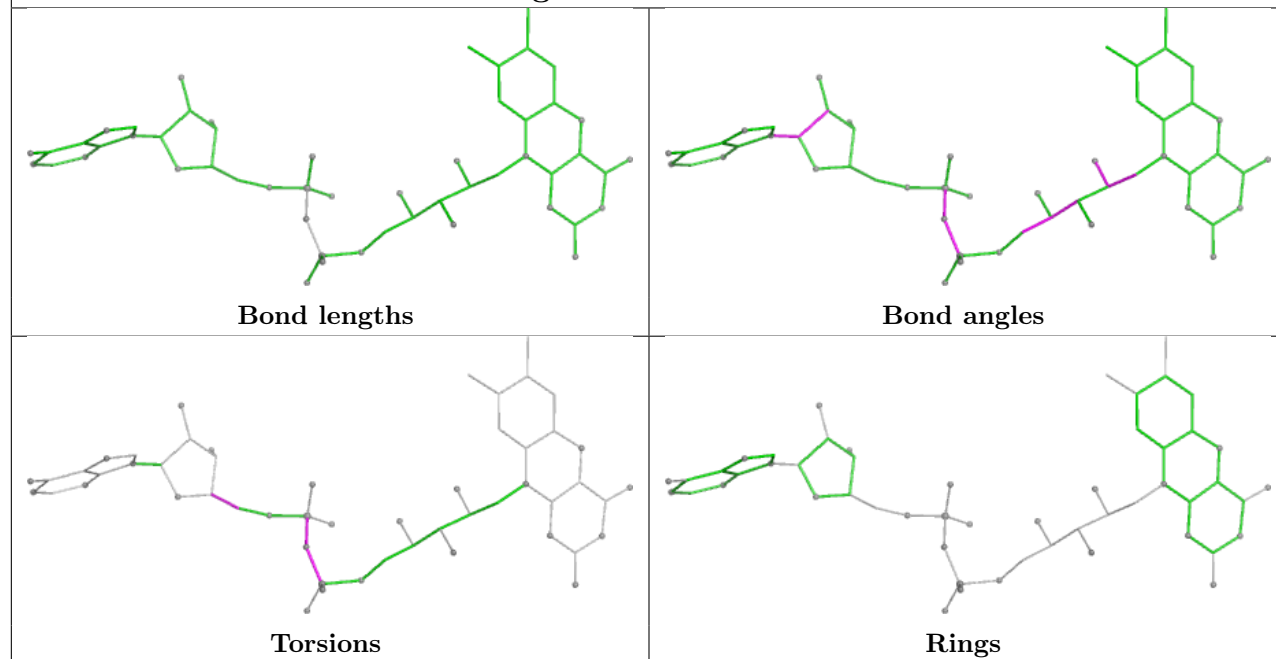
No monomer is involved in short contacts.

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.

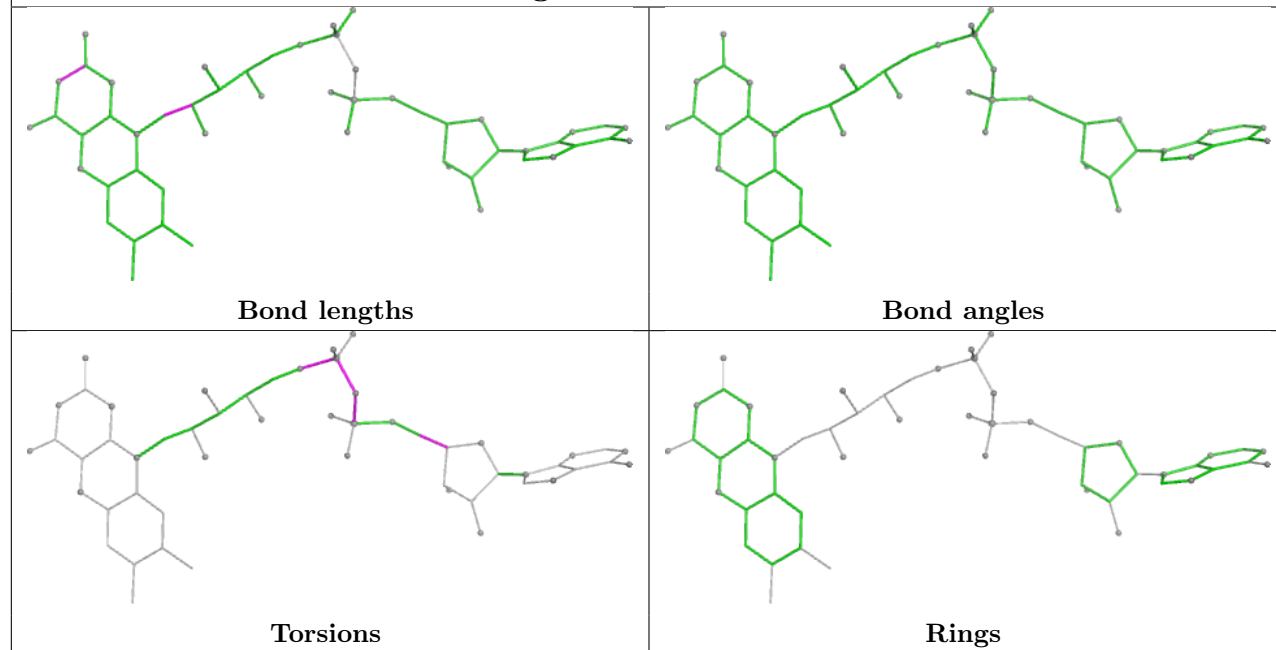


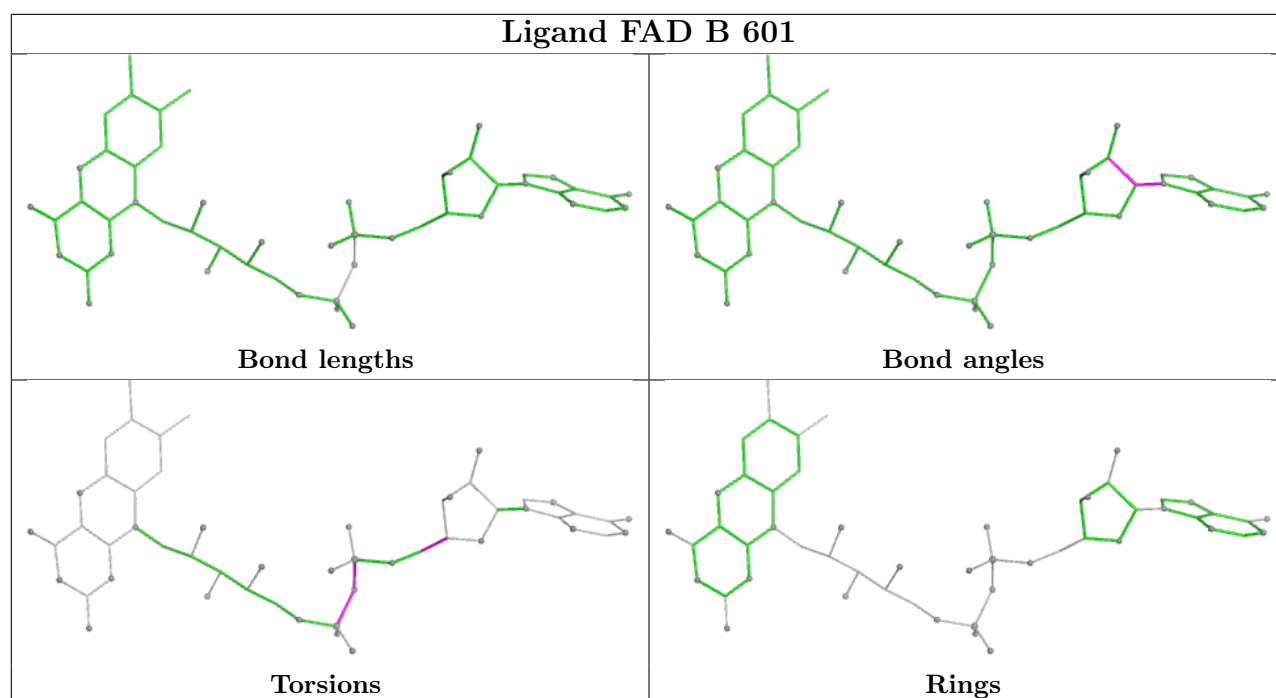


## Ligand FAD A 601



## Ligand FAD D 601





## 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	490/521 (94%)	0.00	5 (1%) 79 77	15, 40, 71, 105	7 (1%)
1	B	493/521 (94%)	-0.09	11 (2%) 62 59	21, 38, 68, 118	4 (0%)
1	C	487/521 (93%)	0.13	7 (1%) 73 71	19, 46, 74, 113	5 (1%)
1	D	487/521 (93%)	0.25	10 (2%) 63 60	25, 50, 81, 112	6 (1%)
All	All	1957/2084 (93%)	0.07	33 (1%) 69 66	15, 44, 76, 118	22 (1%)

All (33) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	517	GLY	5.2
1	B	515	CYS	5.0
1	B	516	GLY	4.7
1	C	25	THR	4.6
1	B	429	GLU	4.6
1	A	25	THR	4.3
1	D	25	THR	4.3
1	B	25	THR	3.9
1	A	513	GLY	3.8
1	A	514	GLY	3.5
1	C	429	GLU	3.2
1	D	149	ILE	3.1
1	B	513	GLY	3.0
1	D	125	MET	2.9
1	A	512	SER	2.7
1	B	512	SER	2.7
1	D	154	VAL	2.6
1	C	430	MET	2.5
1	C	202	LYS	2.4
1	B	514	GLY	2.4
1	C	272	LYS	2.4

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Mol	Chain	Res	Type	RSRZ
1	B	428	ASN	2.3
1	C	511	SER	2.3
1	D	511	SER	2.3
1	B	430	MET	2.3
1	D	54	ALA	2.3
1	D	430	MET	2.2
1	D	26	PHE	2.1
1	D	429	GLU	2.1
1	D	31	VAL	2.1
1	B	511	SER	2.1
1	C	428	ASN	2.0
1	A	56	PHE	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](#)

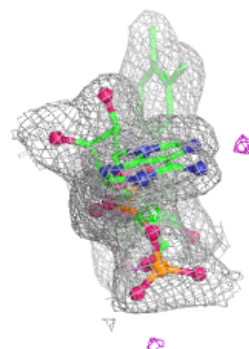
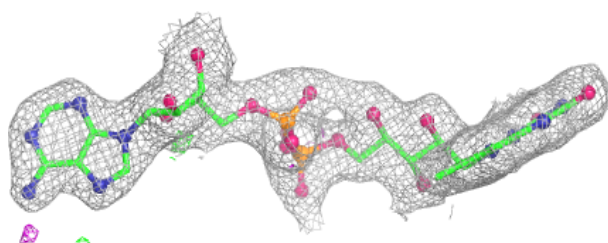
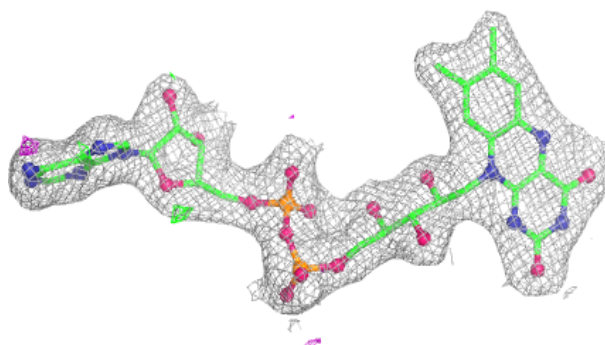
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 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
2	FAD	A	601	53/53	0.96	0.06	26,32,44,48	0
2	FAD	C	601	53/53	0.96	0.06	30,35,46,47	0
2	FAD	D	601	53/53	0.96	0.06	35,41,50,52	0
2	FAD	B	601	53/53	0.97	0.05	23,30,37,38	0
3	AU	B	602	1/1	0.98	0.04	42,42,42,42	1
3	AU	C	602	1/1	0.98	0.04	49,49,49,49	1
3	AU	A	602	1/1	0.99	0.05	47,47,47,47	1

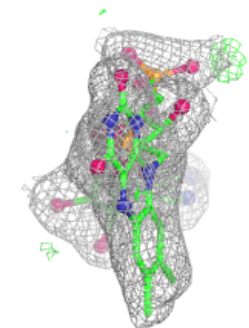
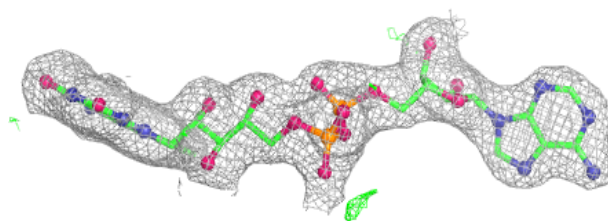
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

**Electron density around FAD A 601:**

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

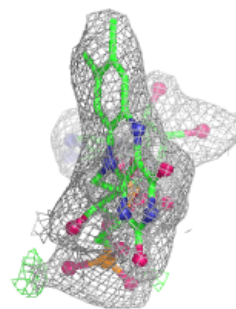
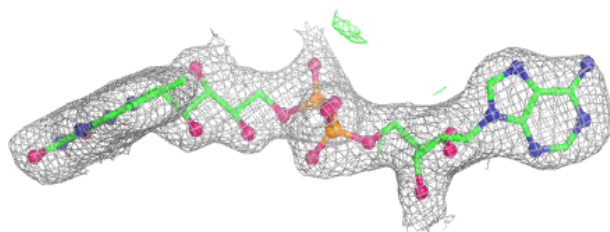
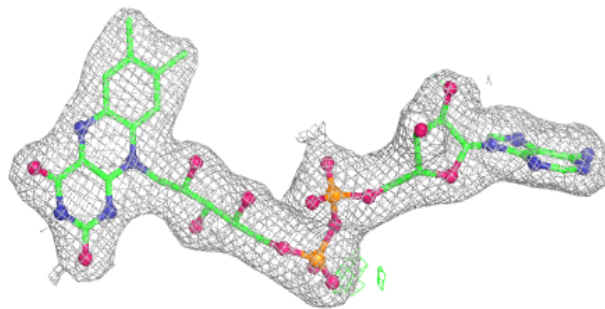
**Electron density around FAD C 601:**

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

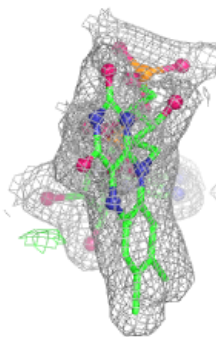
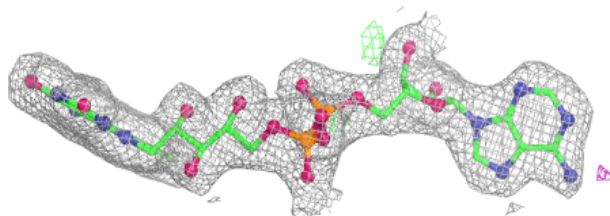
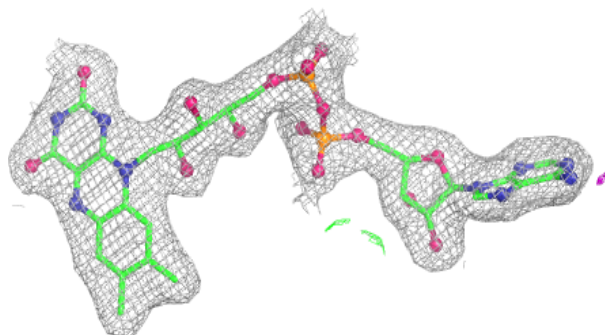


**Electron density around FAD D 601:**

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

**Electron density around FAD B 601:**

$2mF_o-DF_c$  (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.