



# Full wwPDB X-ray Structure Validation Report ⓘ

Mar 20, 2026 – 09:25 AM UTC

PDB ID : 5ODE / pdb\_00005ode  
Title : Structure of a novel oxidoreductase from *Gloeobacter violaceus*  
Authors : Buey, R.M.; Galindo-Trigo, S.; de Pereda, J.M.; Balsera, M.  
Deposited on : 2017-07-05  
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 : 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

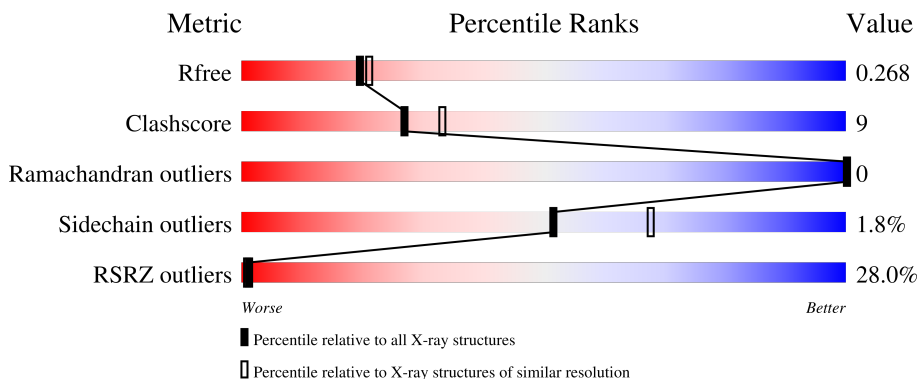
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 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	351	 27% 78% 13% • 8%
1	B	351	 25% 81% 10% • 8%

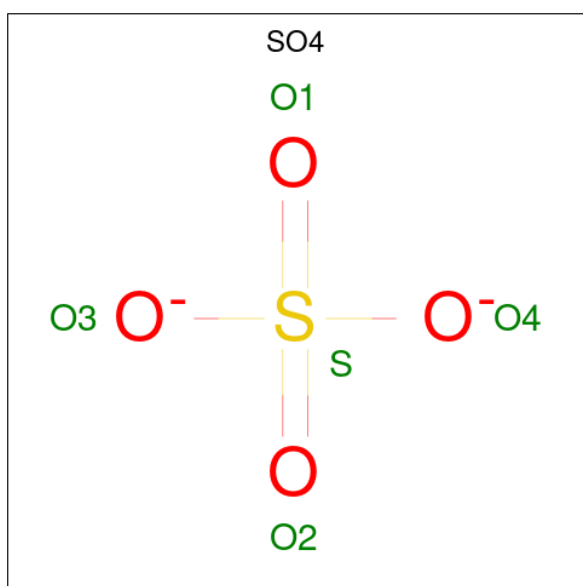
The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
3	SO4	A	405	-	-	X	-
3	SO4	A	406	-	-	-	X
3	SO4	B	402	-	-	X	-
3	SO4	B	405	-	-	X	-



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	
2	A	1	Total	C	H	N	O	P	0	0
			83	27	30	9	15	2		
2	A	1	Total	C	H	N	O	P	0	0
			84	27	31	9	15	2		
2	B	1	Total	C	H	N	O	P	0	0
			83	27	30	9	15	2		
2	B	1	Total	C	H	N	O	P	0	0
			84	27	31	9	15	2		

- Molecule 3 is SULFATE ION (CCD ID: SO4) (formula: O<sub>4</sub>S).



Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	1	Total	O S	0	0
			5	4 1		
3	A	1	Total	O S	0	0
			5	4 1		
3	A	1	Total	O S	0	0
			5	4 1		
3	A	1	Total	O S	0	0
			5	4 1		
3	A	1	Total	O S	0	0
			5	4 1		
3	B	1	Total	O S	0	0
			5	4 1		
3	B	1	Total	O S	0	0
			5	4 1		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	B	1	Total	O	S	0	0
			5	4	1		
3	B	1	Total	O	S	0	0
			5	4	1		
3	B	1	Total	O	S	0	0
			5	4	1		

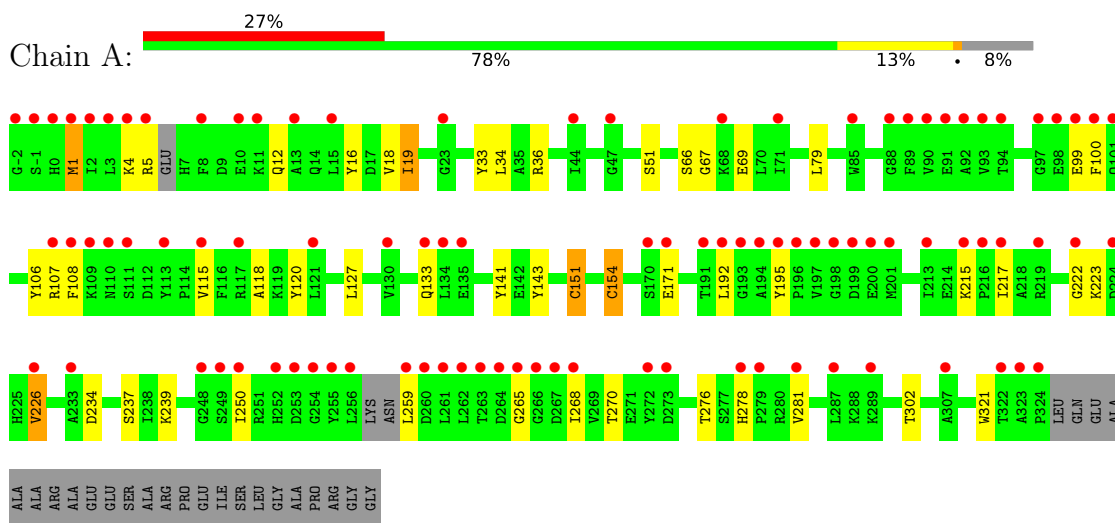
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	146	Total	O	0	0
			146	146		
4	B	116	Total	O	0	0
			116	116		

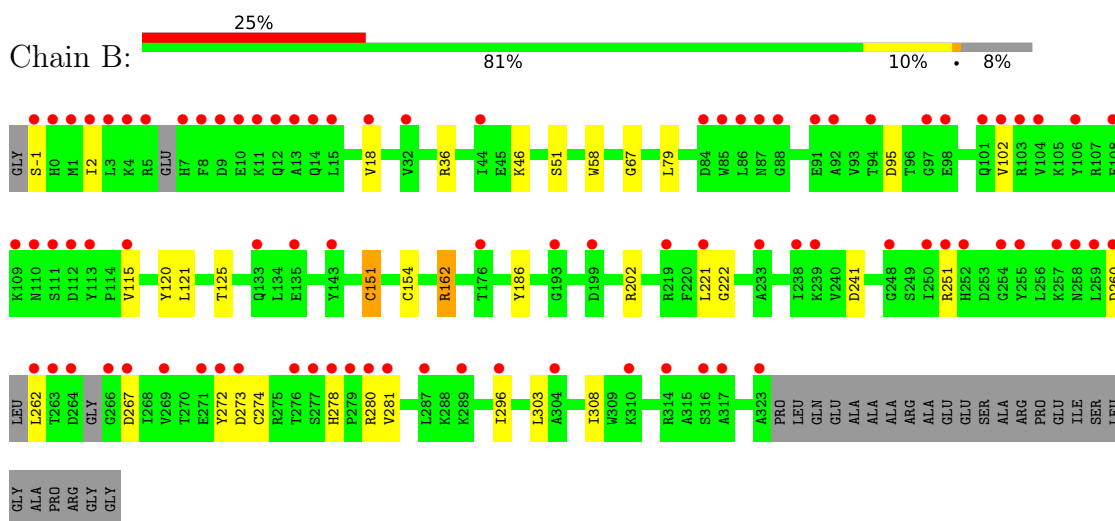
### 3 Residue-property plots [i](#)

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: Gll2934 protein



- Molecule 1: Gll2934 protein



## 4 Data and refinement statistics

Property	Value	Source
Space group	I 2 2 2	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	57.23Å 136.42Å 267.68Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	60.77 – 2.20 60.77 – 2.20	Depositor EDS
% Data completeness (in resolution range)	71.0 (60.77-2.20) 71.1 (60.77-2.20)	Depositor EDS
$R_{merge}$	0.10	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.47 (at 2.20Å)	Xtrriage
Refinement program	PHENIX (1.12rc1_2801: ???)	Depositor
R, $R_{free}$	0.246 , 0.266 0.256 , 0.268	Depositor DCC
$R_{free}$ test set	1974 reflections (3.64%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	33.8	Xtrriage
Anisotropy	0.104	Xtrriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.40 , 49.2	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.33$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
$F_o, F_c$ correlation	0.91	EDS
Total number of atoms	10487	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	54.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.29% 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: SO4, 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	0.46	4/2576 (0.2%)	0.65	4/3490 (0.1%)
1	B	0.13	0/2515	0.32	1/3412 (0.0%)
All	All	0.34	4/5091 (0.1%)	0.51	5/6902 (0.1%)

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	154[A]	CYS	CA-C	7.01	1.61	1.52
1	A	154[B]	CYS	CA-C	7.01	1.61	1.52
1	A	154[A]	CYS	N-CA	5.57	1.53	1.46
1	A	154[B]	CYS	N-CA	5.57	1.53	1.46

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	154[A]	CYS	CA-C-O	6.94	127.90	120.55
1	A	154[B]	CYS	CA-C-O	6.94	127.90	120.55
1	B	2	ILE	N-CA-C	5.60	116.23	108.84
1	A	5	ARG	N-CA-C	5.51	117.28	111.28
1	A	265	GLY	N-CA-C	-5.09	101.12	113.18

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	2514	2462	2483	59	3
1	B	2460	2400	2401	29	0
2	A	106	61	62	5	0
2	B	106	61	62	7	0
3	A	30	0	0	3	0
3	B	25	0	0	5	0
4	A	146	0	0	1	0
4	B	116	0	0	4	0
All	All	5503	4984	5008	94	3

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 9.

All (94) 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:B:18:VAL:HG22	1:B:120:TYR:HB2	1.26	1.18
1:A:1:MET:HE1	1:A:79:LEU:CD1	1.82	1.09
1:A:1:MET:HE1	1:A:79:LEU:HD13	1.27	1.08
1:A:18:VAL:HG21	1:A:34:LEU:HD13	1.35	1.08
1:B:202:ARG:HG2	3:B:402:SO4:O3	1.71	0.91
1:A:18:VAL:HG21	1:A:34:LEU:CD1	2.02	0.89
1:A:4:LYS:HE3	1:A:107:ARG:HH21	1.36	0.88
1:A:100:PHE:HZ	1:A:278:HIS:CE1	1.92	0.87
1:A:141:TYR:OH	3:A:405:SO4:O1	1.95	0.85
1:A:100:PHE:CZ	1:A:278:HIS:HE1	1.95	0.85
1:A:151[B]:CYS:HB3	1:A:154[B]:CYS:SG	2.22	0.80
1:A:18:VAL:CG2	1:A:34:LEU:HD13	2.12	0.79
1:A:223:LYS:O	1:A:226:VAL:HG12	1.83	0.79
1:A:100:PHE:CZ	1:A:278:HIS:CE1	2.72	0.77
2:B:401:FAD:N1	2:B:401:FAD:O4'	2.19	0.76
1:B:202:ARG:CG	3:B:402:SO4:O3	2.34	0.74
1:A:36:ARG:NH1	1:B:58:TRP:HB3	2.03	0.74
3:A:405:SO4:O3	4:A:501:HOH:O	2.08	0.71
1:B:-1:SER:CB	4:B:584:HOH:O	2.40	0.70
1:B:18:VAL:HG21	1:B:308:ILE:HD13	1.72	0.69
1:A:143:TYR:OH	1:A:222:GLY:CA	2.40	0.69
1:A:143:TYR:CZ	1:A:222:GLY:HA3	2.28	0.68
1:A:143:TYR:CE1	1:A:222:GLY:HA3	2.27	0.68
1:B:46:LYS:NZ	2:B:401:FAD:O2A	2.27	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:18:VAL:HG22	1:B:120:TYR:CB	2.16	0.67
1:B:162:ARG:NH1	4:B:504:HOH:O	2.28	0.67
1:A:223:LYS:O	1:A:226:VAL:CG1	2.44	0.65
1:B:222:GLY:O	3:B:405:SO4:O4	2.15	0.64
1:A:66:SER:OG	1:A:69:GLU:HG3	1.98	0.63
1:A:143:TYR:OH	1:A:222:GLY:C	2.42	0.63
1:A:1:MET:HE1	1:A:79:LEU:HD11	1.79	0.62
1:A:108:PHE:CE1	2:A:401:FAD:C5A	2.83	0.62
2:A:401:FAD:H3'	3:A:405:SO4:O2	2.00	0.61
1:A:106:TYR:O	1:A:107:ARG:HB2	1.99	0.60
2:B:401:FAD:HO4'	2:B:401:FAD:C2	2.14	0.59
1:A:151[B]:CYS:SG	1:A:154[B]:CYS:SG	3.00	0.59
1:B:95:ASP:OD2	1:B:278:HIS:NE2	2.35	0.58
1:A:133:GLN:OE1	1:A:133:GLN:HA	2.03	0.58
1:B:251:ARG:NH2	1:B:267:ASP:OD1	2.36	0.58
1:A:151[B]:CYS:CB	1:A:154[B]:CYS:SG	2.92	0.57
1:A:268:ILE:HD12	1:A:268:ILE:H	1.70	0.56
1:A:127:LEU:C	1:A:127:LEU:HD12	2.31	0.56
1:A:278:HIS:ND1	1:A:281:VAL:HG13	2.21	0.56
1:A:192:LEU:HD11	1:A:217:ILE:HD12	1.89	0.53
2:B:401:FAD:N1	2:B:401:FAD:H2'	2.23	0.53
1:B:151[B]:CYS:HB3	1:B:154:CYS:SG	2.49	0.52
1:A:127:LEU:HB2	1:A:250:ILE:O	2.08	0.52
1:A:1:MET:N	1:A:1:MET:CE	2.73	0.52
1:A:19:ILE:HG13	1:A:118:ALA:HB2	1.92	0.52
1:B:-1:SER:CB	1:B:79:LEU:O	2.58	0.52
1:B:280:ARG:NH1	4:B:513:HOH:O	2.44	0.51
1:A:1:MET:N	1:A:1:MET:HE3	2.27	0.49
1:A:108:PHE:HE1	2:A:401:FAD:C5A	2.26	0.49
1:A:192:LEU:HD11	1:A:217:ILE:CD1	2.42	0.49
1:A:151[B]:CYS:CB	1:A:154[B]:CYS:HG	2.25	0.49
1:A:1:MET:CE	1:A:79:LEU:CD1	2.74	0.49
1:A:195:TYR:N	1:A:195:TYR:CD1	2.81	0.48
1:A:143:TYR:CZ	1:A:222:GLY:CA	2.94	0.48
1:A:4:LYS:N	1:A:4:LYS:HD3	2.28	0.48
1:A:33:TYR:CE2	1:A:302:THR:HG23	2.49	0.47
1:B:121:LEU:O	1:B:281:VAL:HA	2.14	0.47
1:B:272:TYR:O	1:B:303:LEU:HD13	2.14	0.47
1:B:18:VAL:HG21	1:B:308:ILE:HG21	1.96	0.47
1:A:16:TYR:O	1:A:118:ALA:HA	2.15	0.47
1:A:18:VAL:HG12	1:A:120:TYR:HB2	1.97	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:102:VAL:C	1:B:115:VAL:HG23	2.39	0.47
1:B:125:THR:HB	2:B:400:FAD:C8A	2.44	0.46
1:A:127:LEU:HD12	1:A:127:LEU:O	2.15	0.46
1:A:12:GLN:HG2	1:A:115:VAL:O	2.16	0.45
1:A:143:TYR:OH	1:A:222:GLY:N	2.49	0.45
1:B:260:ASP:HA	1:B:262:LEU:N	2.32	0.45
2:B:400:FAD:H9	2:B:400:FAD:H1'1	1.83	0.44
1:A:1:MET:HE3	1:A:1:MET:H	1.83	0.44
1:A:192:LEU:HD11	1:A:217:ILE:CG1	2.49	0.43
1:A:192:LEU:HD11	1:A:217:ILE:HG13	1.99	0.43
1:A:270:THR:HG22	1:A:276:THR:HG22	2.01	0.43
1:B:202:ARG:CD	3:B:402:SO4:O3	2.67	0.43
1:A:171:GLU:N	1:A:195:TYR:CE2	2.87	0.42
1:B:51:SER:O	1:B:67:GLY:HA3	2.20	0.42
2:B:401:FAD:H9	2:B:401:FAD:H1'1	1.83	0.42
1:B:18:VAL:CG2	1:B:308:ILE:HG21	2.50	0.42
1:B:221:LEU:HA	3:B:405:SO4:O2	2.19	0.42
1:A:51:SER:O	1:A:67:GLY:HA3	2.20	0.42
1:A:100:PHE:N	1:A:118:ALA:O	2.48	0.42
1:B:273:ASP:O	1:B:274:CYS:HB2	2.20	0.41
2:A:400:FAD:H1'1	2:A:400:FAD:H9	1.81	0.41
1:A:226:VAL:O	1:A:226:VAL:HG13	2.20	0.41
1:A:108:PHE:HE1	2:A:401:FAD:N7A	2.18	0.41
1:A:278:HIS:HB3	1:A:281:VAL:HG22	2.03	0.41
1:A:192:LEU:CD1	1:A:217:ILE:HG13	2.51	0.41
1:A:321:TRP:CE3	1:B:186:TYR:HA	2.56	0.41
1:B:241:ASP:HA	4:B:514:HOH:O	2.21	0.40

All (3) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:215:LYS:NZ	1:A:234:ASP:OD2[3_555]	1.98	0.22
1:A:215:LYS:HZ3	1:A:234:ASP:OD2[3_555]	1.58	0.02
1:A:237:SER:OG	1:A:239:LYS:NZ[3_555]	2.19	0.01

## 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	322/351 (92%)	309 (96%)	13 (4%)	0	100	100
1	B	317/351 (90%)	309 (98%)	8 (2%)	0	100	100
All	All	639/702 (91%)	618 (97%)	21 (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	253/278 (91%)	246 (97%)	7 (3%)	38	52
1	B	240/278 (86%)	236 (98%)	4 (2%)	53	69
All	All	493/556 (89%)	482 (98%)	11 (2%)	51	61

All (11) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	1	MET
1	A	19	ILE
1	A	99	GLU
1	A	151[A]	CYS
1	A	151[B]	CYS
1	A	226	VAL
1	A	259	LEU
1	B	151[A]	CYS

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Mol	Chain	Res	Type
1	B	151[B]	CYS
1	B	162	ARG
1	B	296	ILE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (2) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	110	ASN
1	A	278	HIS

### 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](#)

15 ligands are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
3	SO4	A	402	-	4,4,4	0.40	0	6,6,6	0.15	0
3	SO4	B	403	-	4,4,4	0.23	0	6,6,6	0.06	0
2	FAD	A	400	-	58,58,58	1.42	10 (17%)	85,89,89	1.60	19 (22%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
2	FAD	B	400	-	58,58,58	1.44	10 (17%)	85,89,89	1.60	17 (20%)
3	SO4	A	406	-	4,4,4	0.41	0	6,6,6	0.06	0
2	FAD	A	401	-	58,58,58	1.44	9 (15%)	85,89,89	1.63	19 (22%)
3	SO4	B	404	-	4,4,4	0.37	0	6,6,6	0.08	0
3	SO4	A	403	-	4,4,4	0.23	0	6,6,6	0.08	0
3	SO4	B	402	-	4,4,4	0.40	0	6,6,6	0.13	0
2	FAD	B	401	-	58,58,58	1.43	9 (15%)	85,89,89	1.67	18 (21%)
3	SO4	B	406	-	4,4,4	0.23	0	6,6,6	0.07	0
3	SO4	A	404	-	4,4,4	0.39	0	6,6,6	0.09	0
3	SO4	A	407	-	4,4,4	0.39	0	6,6,6	0.09	0
3	SO4	B	405	-	4,4,4	0.36	0	6,6,6	0.10	0
3	SO4	A	405	-	4,4,4	0.39	0	6,6,6	0.25	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	401	-	-	11/34/50/50	0/6/6/6
2	FAD	A	401	-	-	7/34/50/50	0/6/6/6
2	FAD	A	400	-	-	2/34/50/50	0/6/6/6
2	FAD	B	400	-	-	7/34/50/50	0/6/6/6

All (38) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	400	FAD	C9A-C5X	5.13	1.49	1.41
2	B	401	FAD	C9A-C5X	5.04	1.49	1.41
2	A	400	FAD	C9A-C5X	5.02	1.49	1.41
2	A	401	FAD	C9A-C5X	4.94	1.49	1.41
2	A	401	FAD	C5A-C4A	4.56	1.47	1.39
2	B	401	FAD	C5A-C4A	4.39	1.46	1.39
2	B	400	FAD	C5A-C4A	4.26	1.46	1.39
2	A	400	FAD	C5A-C4A	4.18	1.46	1.39
2	A	401	FAD	C8-C7	3.25	1.48	1.40
2	B	401	FAD	C8-C7	3.19	1.48	1.40
2	A	400	FAD	C8-C7	3.19	1.48	1.40
2	B	400	FAD	C8-C7	3.18	1.48	1.40
2	B	401	FAD	C4-N3	-2.84	1.33	1.38
2	B	400	FAD	C4-N3	-2.79	1.33	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	401	FAD	C5A-C6A	2.75	1.48	1.41
2	A	400	FAD	C4-N3	-2.73	1.33	1.38
2	A	400	FAD	C5A-C6A	2.70	1.48	1.41
2	B	400	FAD	C5A-C6A	2.68	1.48	1.41
2	B	401	FAD	C5A-C6A	2.67	1.48	1.41
2	A	401	FAD	C4-N3	-2.65	1.33	1.38
2	A	401	FAD	C5X-N5	-2.58	1.34	1.39
2	B	400	FAD	C5X-N5	-2.53	1.34	1.39
2	A	401	FAD	C5A-N7A	-2.43	1.34	1.39
2	A	400	FAD	C5X-N5	-2.43	1.35	1.39
2	B	400	FAD	C5A-N7A	-2.40	1.34	1.39
2	B	401	FAD	C5A-N7A	-2.37	1.34	1.39
2	B	401	FAD	C5X-N5	-2.32	1.35	1.39
2	A	401	FAD	C8A-N7A	2.26	1.36	1.31
2	A	400	FAD	C5A-N7A	-2.25	1.35	1.39
2	A	400	FAD	C8A-N7A	2.23	1.36	1.31
2	B	400	FAD	C8A-N7A	2.22	1.35	1.31
2	B	401	FAD	C8A-N7A	2.19	1.35	1.31
2	B	401	FAD	C2-N3	-2.19	1.34	1.39
2	B	400	FAD	C4A-N9A	-2.19	1.33	1.37
2	A	400	FAD	C4A-N9A	-2.10	1.33	1.37
2	A	400	FAD	C2-N3	-2.09	1.34	1.39
2	B	400	FAD	C2-N3	-2.07	1.34	1.39
2	A	401	FAD	C2-N3	-2.01	1.34	1.39

All (73) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	401	FAD	C5A-C4A-N3A	-6.34	117.98	126.72
2	B	401	FAD	C5A-C4A-N3A	-5.93	118.56	126.72
2	A	400	FAD	C5A-C4A-N3A	-5.53	119.10	126.72
2	B	400	FAD	C5A-C4A-N3A	-5.43	119.24	126.72
2	A	401	FAD	N3A-C4A-N9A	4.79	135.31	127.17
2	B	401	FAD	N3A-C4A-N9A	4.66	135.09	127.17
2	A	400	FAD	N3A-C4A-N9A	4.35	134.56	127.17
2	B	400	FAD	N3A-C4A-N9A	4.31	134.50	127.17
2	A	401	FAD	C2A-N3A-C4A	4.06	121.74	111.83
2	B	401	FAD	C2A-N3A-C4A	3.94	121.45	111.83
2	A	400	FAD	C2A-N3A-C4A	3.87	121.28	111.83
2	A	401	FAD	C4A-C5A-N7A	-3.86	106.17	110.58
2	A	400	FAD	N3A-C2A-N1A	-3.85	122.75	128.58
2	B	400	FAD	N3A-C2A-N1A	-3.83	122.79	128.58

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	401	FAD	C4A-C5A-N7A	-3.80	106.23	110.58
2	B	400	FAD	C2A-N3A-C4A	3.80	121.11	111.83
2	B	401	FAD	N3A-C2A-N1A	-3.73	122.93	128.58
2	A	400	FAD	C4A-C5A-N7A	-3.71	106.34	110.58
2	B	400	FAD	C4A-C5A-N7A	-3.66	106.40	110.58
2	A	401	FAD	N3A-C2A-N1A	-3.58	123.17	128.58
2	B	400	FAD	C4A-N9A-C8A	3.28	109.18	105.74
2	A	400	FAD	C4A-N9A-C8A	3.22	109.12	105.74
2	B	401	FAD	C4A-N9A-C8A	3.05	108.94	105.74
2	B	401	FAD	C5A-N7A-C8A	2.95	108.09	103.45
2	B	400	FAD	C5A-N7A-C8A	2.88	107.98	103.45
2	A	401	FAD	C5A-N7A-C8A	2.88	107.97	103.45
2	A	400	FAD	C5A-N7A-C8A	2.84	107.91	103.45
2	B	401	FAD	C4X-C10-N1	-2.75	117.85	124.59
2	B	400	FAD	C4X-C10-N1	-2.74	117.88	124.59
2	A	401	FAD	C4X-C10-N1	-2.72	117.92	124.59
2	A	400	FAD	C4X-C10-N1	-2.68	118.02	124.59
2	B	400	FAD	N9A-C8A-N7A	-2.65	110.18	113.94
2	A	400	FAD	N9A-C8A-N7A	-2.57	110.29	113.94
2	B	400	FAD	C6A-C5A-N7A	2.52	136.95	132.09
2	A	400	FAD	C6A-C5A-N7A	2.51	136.92	132.09
2	B	401	FAD	N9A-C8A-N7A	-2.50	110.39	113.94
2	B	401	FAD	C4-C4X-N5	2.49	121.64	118.21
2	B	401	FAD	C3B-C2B-C1B	2.42	106.05	101.46
2	A	400	FAD	C4-C4X-N5	2.41	121.53	118.21
2	A	400	FAD	C4X-C10-N10	2.36	119.86	116.48
2	A	401	FAD	C3B-C2B-C1B	2.33	105.87	101.46
2	B	401	FAD	C4-N3-C2	-2.32	121.52	125.64
2	A	401	FAD	C4A-N9A-C8A	2.32	108.17	105.74
2	A	400	FAD	C4-N3-C2	-2.31	121.54	125.64
2	B	401	FAD	C6A-C5A-N7A	2.30	136.53	132.09
2	A	401	FAD	C4X-C10-N10	2.30	119.77	116.48
2	B	400	FAD	C4-C4X-N5	2.29	121.37	118.21
2	A	401	FAD	C4-C4X-N5	2.26	121.32	118.21
2	B	401	FAD	C4X-C4-N3	2.26	119.00	113.25
2	B	401	FAD	O4-C4-C4X	-2.25	120.60	126.53
2	A	400	FAD	O4-C4-C4X	-2.25	120.60	126.53
2	A	401	FAD	C4-N3-C2	-2.23	121.68	125.64
2	B	400	FAD	O4-C4-C4X	-2.22	120.66	126.53
2	B	400	FAD	C2A-N1A-C6A	2.21	122.37	118.73
2	A	401	FAD	O4-C4-C4X	-2.21	120.71	126.53
2	B	401	FAD	C10-N1-C2	2.19	121.59	116.85

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	401	FAD	C4X-C10-N10	2.18	119.61	116.48
2	A	401	FAD	C6A-C5A-N7A	2.17	136.26	132.09
2	A	400	FAD	C2A-N1A-C6A	2.16	122.28	118.73
2	B	400	FAD	C4-N3-C2	-2.16	121.81	125.64
2	A	400	FAD	C10-N1-C2	2.15	121.51	116.85
2	B	401	FAD	C2A-N1A-C6A	2.15	122.26	118.73
2	B	400	FAD	C4X-C4-N3	2.14	118.69	113.25
2	B	400	FAD	C10-N1-C2	2.13	121.46	116.85
2	A	400	FAD	C4X-C4-N3	2.11	118.62	113.25
2	A	401	FAD	N9A-C8A-N7A	-2.09	110.97	113.94
2	A	401	FAD	C10-N1-C2	2.08	121.35	116.85
2	A	400	FAD	O2-C2-N1	-2.06	118.37	121.80
2	A	400	FAD	C9A-N10-C10	-2.06	117.61	120.75
2	A	401	FAD	C9A-N10-C10	-2.02	117.67	120.75
2	B	400	FAD	C4X-C10-N10	2.01	119.35	116.48
2	A	401	FAD	O2-C2-N1	-2.01	118.47	121.80
2	A	401	FAD	C4X-C4-N3	2.00	118.35	113.25

There are no chirality outliers.

All (27) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	401	FAD	C3'-C4'-C5'-O5'
2	A	401	FAD	O4'-C4'-C5'-O5'
2	A	401	FAD	C5'-O5'-P-O1P
2	B	400	FAD	O4'-C4'-C5'-O5'
2	B	400	FAD	PA-O3P-P-O5'
2	B	401	FAD	O4B-C4B-C5B-O5B
2	B	401	FAD	C2'-C1'-N10-C10
2	B	401	FAD	N10-C1'-C2'-O2'
2	A	401	FAD	O4B-C4B-C5B-O5B
2	B	400	FAD	O4B-C4B-C5B-O5B
2	B	400	FAD	C3B-C4B-C5B-O5B
2	B	401	FAD	C3B-C4B-C5B-O5B
2	A	400	FAD	O4B-C4B-C5B-O5B
2	A	400	FAD	C3B-C4B-C5B-O5B
2	B	401	FAD	C2'-C3'-C4'-O4'
2	A	401	FAD	C3B-C4B-C5B-O5B
2	B	400	FAD	C3'-C4'-C5'-O5'
2	B	401	FAD	O3'-C3'-C4'-C5'
2	B	401	FAD	C2'-C3'-C4'-C5'
2	A	401	FAD	PA-O3P-P-O2P

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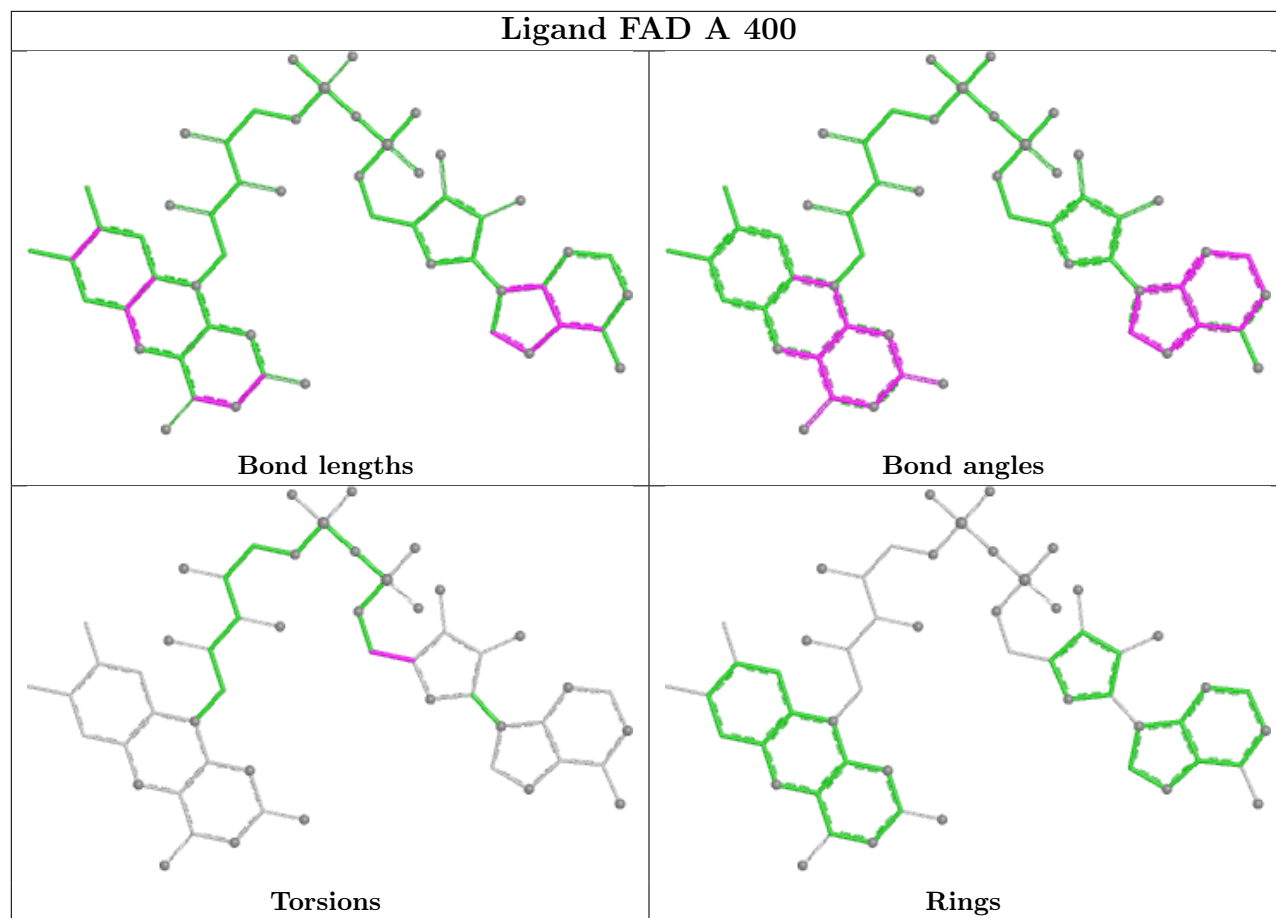
Mol	Chain	Res	Type	Atoms
2	B	401	FAD	PA-O3P-P-O2P
2	B	401	FAD	N10-C1'-C2'-C3'
2	B	401	FAD	O3'-C3'-C4'-O4'
2	B	400	FAD	C5'-O5'-P-O2P
2	B	401	FAD	PA-O3P-P-O1P
2	A	401	FAD	PA-O3P-P-O1P
2	B	400	FAD	P-O3P-PA-O2A

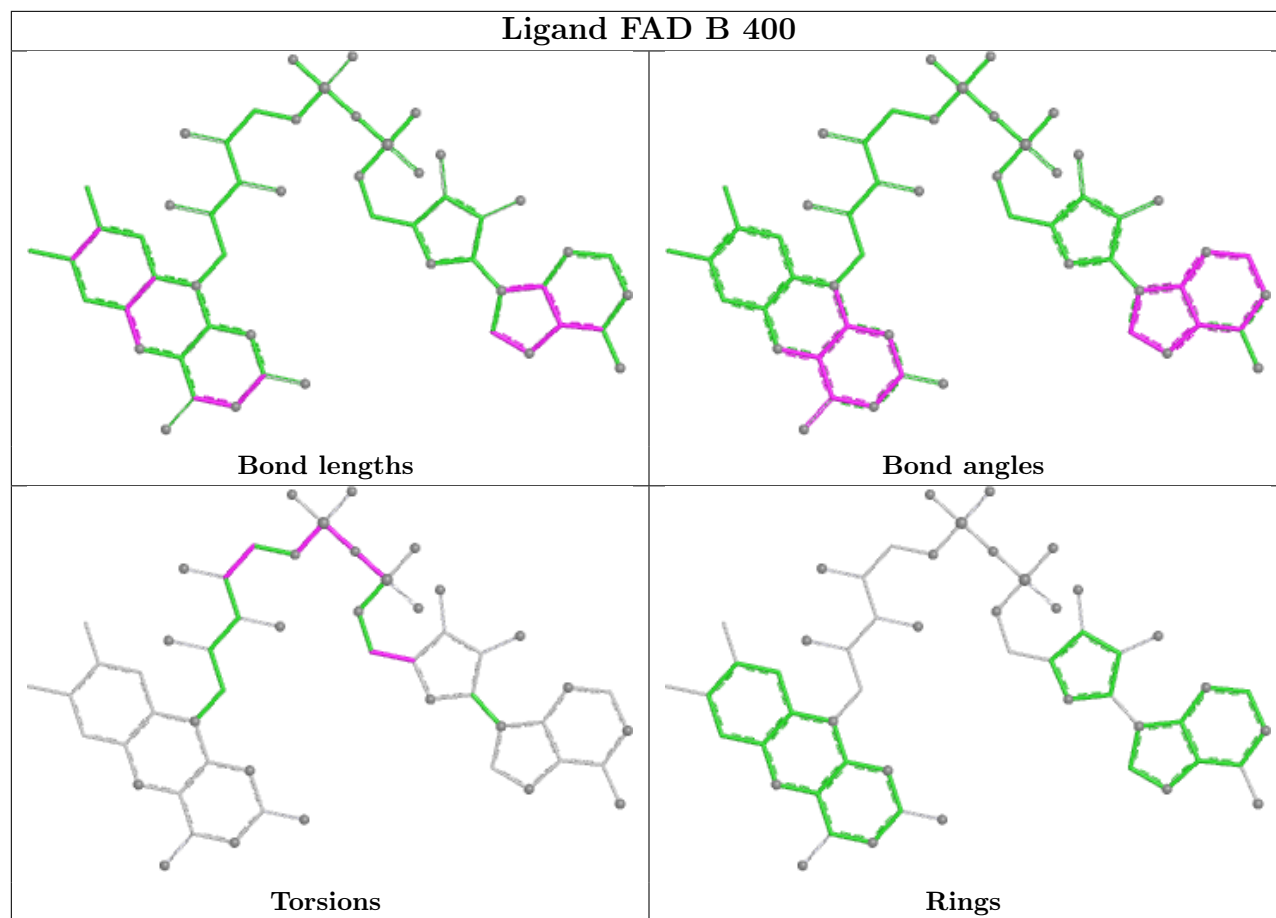
There are no ring outliers.

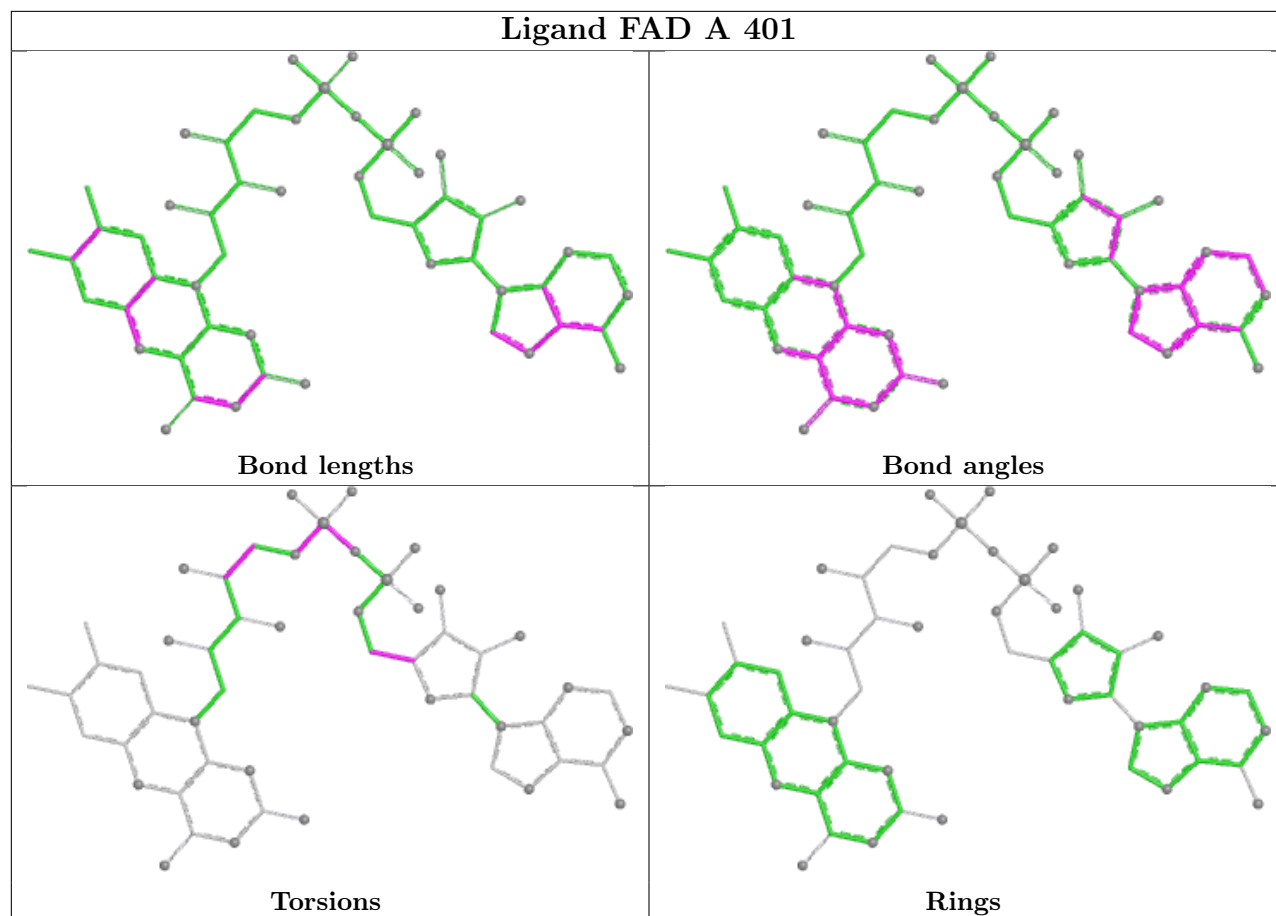
7 monomers are involved in 19 short contacts:

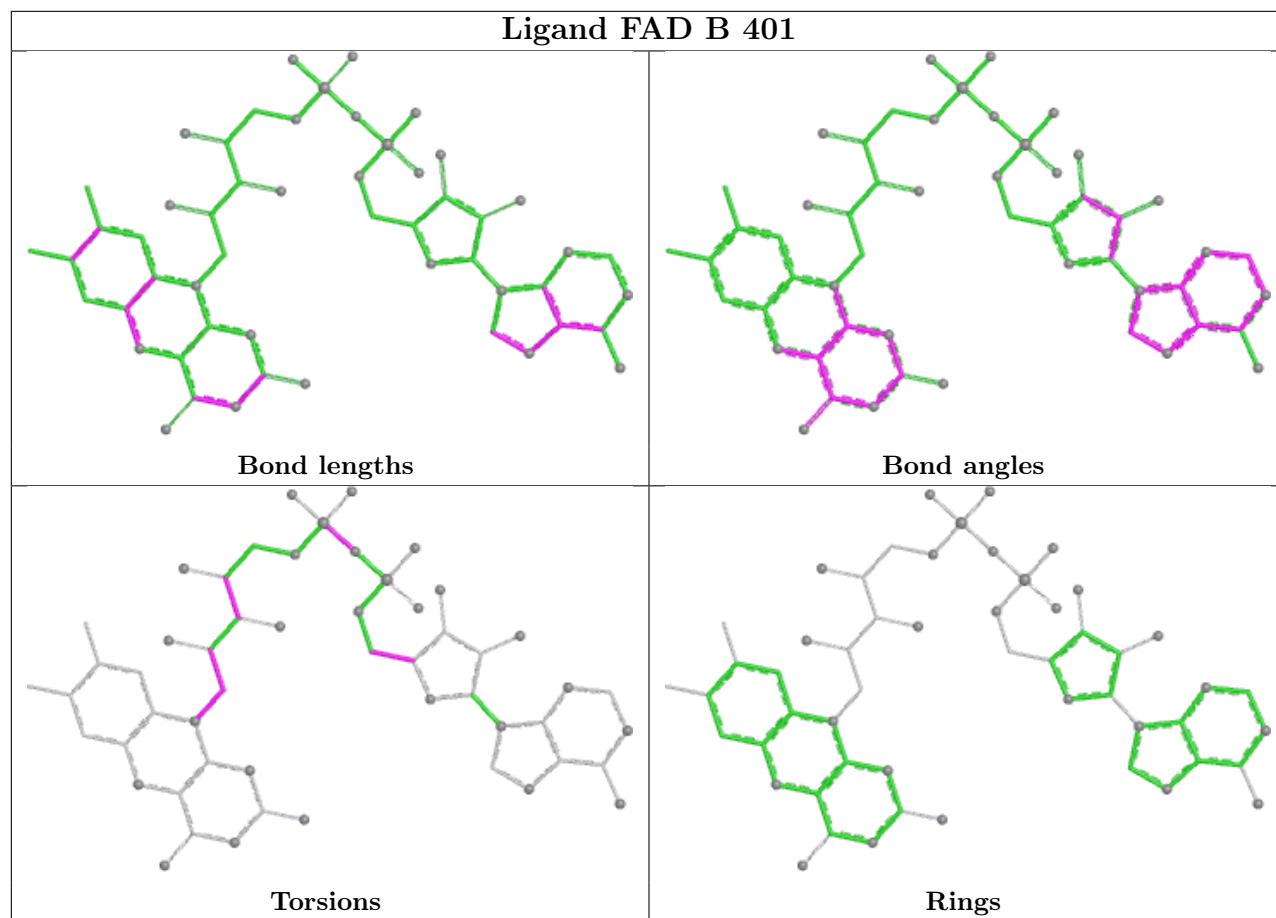
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	400	FAD	1	0
2	B	400	FAD	2	0
2	A	401	FAD	4	0
3	B	402	SO4	3	0
2	B	401	FAD	5	0
3	B	405	SO4	2	0
3	A	405	SO4	3	0

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









## 5.7 Other polymers [i](#)

There are no such residues in this entry.

## 5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

## 6 Fit of model and data

### 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	324/351 (92%)	1.66	95 (29%) <b>1</b> <b>1</b>	28, 50, 90, 123	2 (0%)
1	B	322/351 (91%)	1.48	86 (26%) <b>1</b> <b>1</b>	23, 51, 92, 130	1 (0%)
All	All	646/702 (92%)	1.57	181 (28%) <b>1</b> <b>1</b>	23, 51, 91, 130	3 (0%)

All (181) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	323	ALA	9.2
1	B	1	MET	7.5
1	A	5	ARG	7.4
1	A	261	LEU	7.3
1	A	196	PRO	7.1
1	A	266	GLY	7.0
1	A	260	ASP	6.8
1	A	264	ASP	6.7
1	B	266	GLY	6.6
1	A	263	THR	6.5
1	A	259	LEU	6.4
1	A	323	ALA	5.8
1	A	267	ASP	5.8
1	A	-2	GLY	5.7
1	A	109	LYS	5.6
1	A	1	MET	5.6
1	B	262	LEU	5.4
1	A	256	LEU	5.2
1	B	3	LEU	5.1
1	A	195	TYR	5.0
1	A	262	LEU	5.0
1	B	2	ILE	5.0
1	B	272	TYR	4.9
1	B	0	HIS	4.9

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>	<b>RSRZ</b>
1	B	176	THR	4.8
1	B	273	ASP	4.8
1	B	109	LYS	4.8
1	B	108	PHE	4.8
1	A	0	HIS	4.7
1	B	110	ASN	4.6
1	B	239	LYS	4.6
1	A	108	PHE	4.6
1	A	68	LYS	4.5
1	A	111	SER	4.5
1	A	273	ASP	4.4
1	A	272	TYR	4.3
1	A	268	ILE	4.3
1	B	106	TYR	4.3
1	B	18	VAL	4.3
1	B	98	GLU	4.3
1	A	324	PRO	4.2
1	A	113	TYR	4.2
1	B	264	ASP	4.2
1	B	263	THR	4.1
1	A	98	GLU	4.1
1	B	260	ASP	4.1
1	A	135	GLU	4.1
1	A	192	LEU	3.9
1	A	100	PHE	3.9
1	B	94	THR	3.8
1	A	193	GLY	3.8
1	A	15	LEU	3.8
1	B	7	HIS	3.8
1	B	115	VAL	3.8
1	B	-1	SER	3.7
1	A	-1	SER	3.7
1	B	267	ASP	3.7
1	B	13	ALA	3.7
1	A	121	LEU	3.6
1	A	110	ASN	3.6
1	B	113	TYR	3.6
1	B	85	TRP	3.5
1	A	99	GLU	3.5
1	A	93	VAL	3.5
1	A	233	ALA	3.4
1	B	104	VAL	3.4

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>	<b>RSRZ</b>
1	A	201	MET	3.4
1	B	102	VAL	3.4
1	A	198	GLY	3.4
1	A	2	ILE	3.4
1	A	255	TYR	3.3
1	A	250	ILE	3.3
1	A	89	PHE	3.3
1	B	8	PHE	3.3
1	A	279	PRO	3.3
1	A	4	LYS	3.3
1	A	92	ALA	3.2
1	B	277	SER	3.2
1	B	12	GLN	3.2
1	B	101	GLN	3.2
1	B	112	ASP	3.2
1	B	135	GLU	3.2
1	A	97	GLY	3.2
1	B	269	VAL	3.1
1	A	307	ALA	3.0
1	A	322	THR	3.0
1	A	215	LYS	3.0
1	A	88	GLY	3.0
1	A	265	GLY	3.0
1	B	254	GLY	2.9
1	A	219	ARG	2.9
1	A	222	GLY	2.9
1	A	254	GLY	2.9
1	A	47	GLY	2.9
1	A	3	LEU	2.8
1	B	281	VAL	2.8
1	B	87	ASN	2.8
1	B	9	ASP	2.8
1	A	217	ILE	2.8
1	B	296	ILE	2.8
1	B	271	GLU	2.8
1	A	216	PRO	2.8
1	B	11	LYS	2.7
1	A	171	GLU	2.7
1	A	170	SER	2.7
1	B	280	ARG	2.7
1	B	199	ASP	2.7
1	B	289	LYS	2.7

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>	<b>RSRZ</b>
1	A	133	GLN	2.6
1	B	258	ASN	2.6
1	A	115	VAL	2.6
1	B	238	ILE	2.6
1	A	10	GLU	2.6
1	A	197	VAL	2.6
1	A	248	GLY	2.6
1	B	15	LEU	2.6
1	B	14	GLN	2.5
1	A	71	ILE	2.5
1	A	90	VAL	2.5
1	B	250	ILE	2.5
1	B	10	GLU	2.5
1	B	221	LEU	2.5
1	A	8	PHE	2.5
1	A	278	HIS	2.5
1	A	199	ASP	2.5
1	A	224	ASP	2.5
1	A	94	THR	2.5
1	B	317	ALA	2.4
1	A	101	GLN	2.4
1	A	11	LYS	2.4
1	A	252	HIS	2.4
1	A	107	ARG	2.4
1	B	143	TYR	2.4
1	B	259	LEU	2.4
1	B	248	GLY	2.4
1	B	32	VAL	2.4
1	B	310	LYS	2.4
1	B	251	ARG	2.3
1	B	276	THR	2.3
1	A	226	VAL	2.3
1	A	191	THR	2.3
1	A	287	LEU	2.3
1	A	289	LYS	2.3
1	B	86	LEU	2.3
1	B	278	HIS	2.2
1	B	111	SER	2.2
1	B	44	ILE	2.2
1	A	117	ARG	2.2
1	A	130	VAL	2.2
1	A	281	VAL	2.2

*Continued on next page...*

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Mol	Chain	Res	Type	RSRZ
1	B	4	LYS	2.2
1	B	233	ALA	2.2
1	B	304	ALA	2.2
1	B	255	TYR	2.2
1	B	84	ASP	2.2
1	A	91	GLU	2.2
1	B	314	ARG	2.2
1	B	316	SER	2.2
1	A	85	TRP	2.2
1	B	97	GLY	2.1
1	B	133	GLN	2.1
1	A	13	ALA	2.1
1	A	194	ALA	2.1
1	B	92	ALA	2.1
1	B	219	ARG	2.1
1	A	253	ASP	2.1
1	A	23	GLY	2.1
1	B	88	GLY	2.1
1	A	134	LEU	2.1
1	A	200	GLU	2.1
1	B	279	PRO	2.1
1	B	5	ARG	2.1
1	A	44	ILE	2.1
1	B	257	LYS	2.1
1	B	287	LEU	2.0
1	B	252	HIS	2.0
1	B	193	GLY	2.0
1	A	213	ILE	2.0
1	B	91	GLU	2.0
1	A	249	SER	2.0
1	B	103	ARG	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

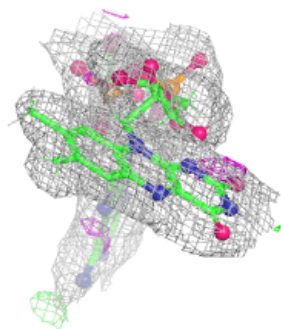
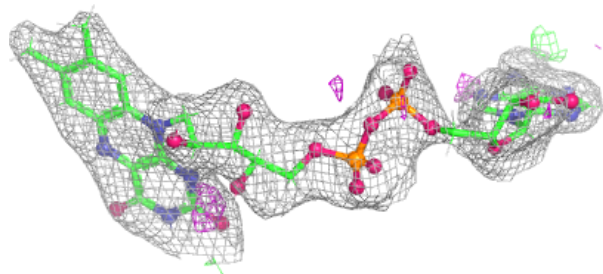
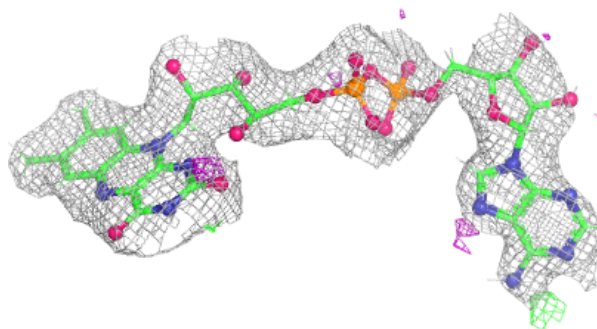
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 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	SO4	A	403	5/5	0.32	0.19	163,167,177,185	0
3	SO4	B	403	5/5	0.62	0.28	196,196,205,209	0
3	SO4	B	406	5/5	0.62	0.17	127,130,135,146	0
3	SO4	A	405	5/5	0.67	0.30	124,149,173,178	0
3	SO4	B	405	5/5	0.73	0.21	134,137,149,158	0
3	SO4	B	402	5/5	0.74	0.24	150,166,180,185	0
3	SO4	A	406	5/5	0.76	0.44	30,30,30,30	0
3	SO4	A	402	5/5	0.79	0.27	144,147,156,165	0
3	SO4	A	404	5/5	0.80	0.13	102,104,118,129	0
3	SO4	B	404	5/5	0.82	0.25	102,115,128,140	0
2	FAD	B	401	53/53	0.83	0.16	27,75,125,143	0
3	SO4	A	407	5/5	0.85	0.42	30,30,30,30	0
2	FAD	A	401	53/53	0.90	0.14	27,53,99,118	0
2	FAD	B	400	53/53	0.92	0.12	27,36,56,64	0
2	FAD	A	400	53/53	0.94	0.10	27,33,47,58	0

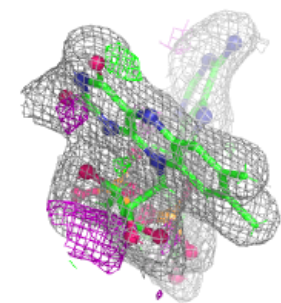
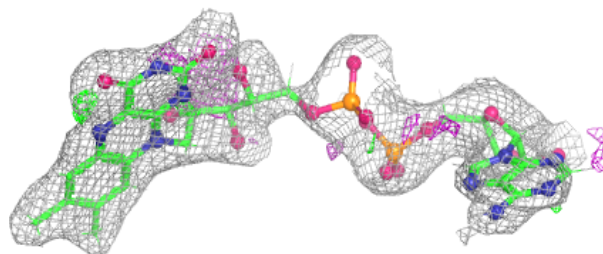
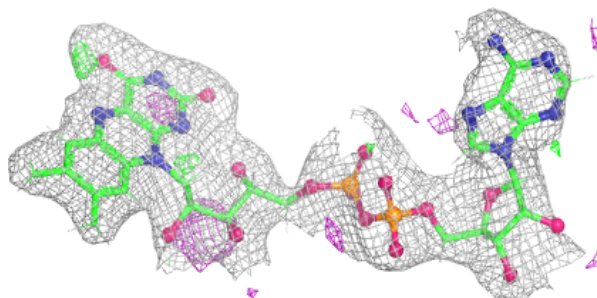
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

**Electron density around FAD B 401:**

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

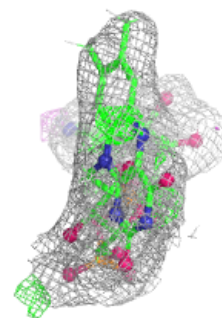
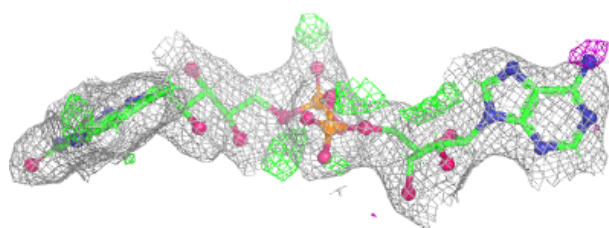
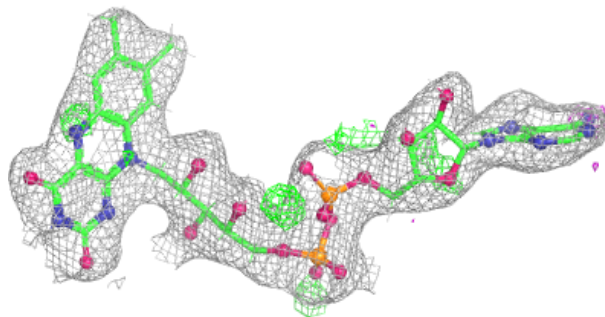
**Electron density around FAD A 401:**

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

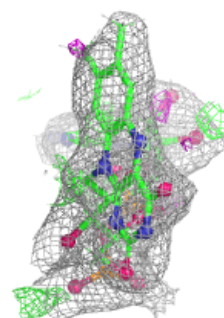
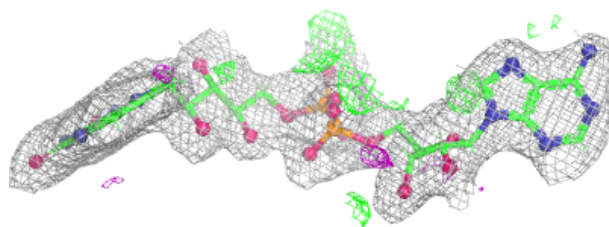
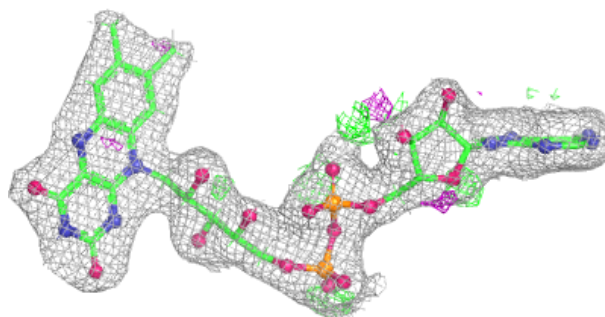


**Electron density around FAD B 400:**

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

**Electron density around FAD A 400:**

$2mF_o-DF_c$  (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.