



# Full wwPDB X-ray Structure Validation Report ⓘ

Dec 12, 2023 – 01:48 pm GMT

PDB ID : 2Y4G  
Title : Structure of the Tirandamycin-bound FAD-dependent tirandamycin oxidase TamL in P212121 space group  
Authors : Carlson, J.C.; Li, S.; Gunatilleke, S.S.; Anzai, Y.; Burr, D.A.; Podust, L.M.; Sherman, D.H.  
Deposited on : 2011-01-05  
Resolution : 2.03 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 : 4.02b-467  
Mogul : 1.8.4, CSD as541be (2020)  
Xtriage (Phenix) : 1.13  
EDS : 2.36  
buster-report : 1.1.7 (2018)  
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)  
Refmac : 5.8.0158  
CCP4 : 7.0.044 (Gargrove)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.36

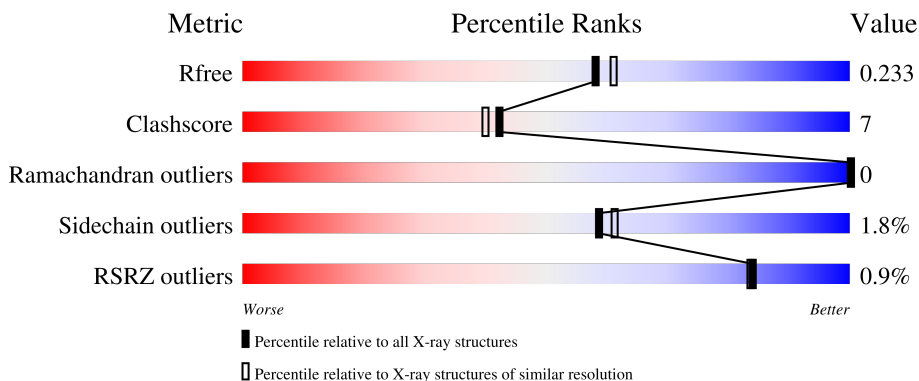
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.03 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))
$R_{free}$	130704	10434 (2.04-2.00)
Clashscore	141614	11643 (2.04-2.00)
Ramachandran outliers	138981	11493 (2.04-2.00)
Sidechain outliers	138945	11492 (2.04-2.00)
RSRZ outliers	127900	10220 (2.04-2.00)

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	530	 82% 11% • 6%
1	B	530	 82% 12% • 6%

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
6	GOL	A	1505	-	-	X	-

## 2 Entry composition [i](#)

There are 7 unique types of molecules in this entry. The entry contains 8921 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 TAML.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	500	3943	2481	714	738	10	0	12	0
1	B	500	4001	2513	732	748	8	0	19	0

There are 60 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-29	MET	-	expression tag	UNP D3Y1I2
A	-28	GLY	-	expression tag	UNP D3Y1I2
A	-27	SER	-	expression tag	UNP D3Y1I2
A	-26	HIS	-	expression tag	UNP D3Y1I2
A	-25	HIS	-	expression tag	UNP D3Y1I2
A	-24	HIS	-	expression tag	UNP D3Y1I2
A	-23	HIS	-	expression tag	UNP D3Y1I2
A	-22	HIS	-	expression tag	UNP D3Y1I2
A	-21	HIS	-	expression tag	UNP D3Y1I2
A	-20	HIS	-	expression tag	UNP D3Y1I2
A	-19	HIS	-	expression tag	UNP D3Y1I2
A	-18	GLY	-	expression tag	UNP D3Y1I2
A	-17	SER	-	expression tag	UNP D3Y1I2
A	-16	ASP	-	expression tag	UNP D3Y1I2
A	-15	TYR	-	expression tag	UNP D3Y1I2
A	-14	ASP	-	expression tag	UNP D3Y1I2
A	-13	ILE	-	expression tag	UNP D3Y1I2
A	-12	PRO	-	expression tag	UNP D3Y1I2
A	-11	THR	-	expression tag	UNP D3Y1I2
A	-10	THR	-	expression tag	UNP D3Y1I2
A	-9	GLU	-	expression tag	UNP D3Y1I2
A	-8	ASN	-	expression tag	UNP D3Y1I2
A	-7	LEU	-	expression tag	UNP D3Y1I2
A	-6	TYR	-	expression tag	UNP D3Y1I2
A	-5	PHE	-	expression tag	UNP D3Y1I2

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Chain	Residue	Modelled	Actual	Comment	Reference
A	-4	GLN	-	expression tag	UNP D3Y1I2
A	-3	GLY	-	expression tag	UNP D3Y1I2
A	-2	SER	-	expression tag	UNP D3Y1I2
A	-1	GLU	-	expression tag	UNP D3Y1I2
A	0	PHE	-	expression tag	UNP D3Y1I2
B	-29	MET	-	expression tag	UNP D3Y1I2
B	-28	GLY	-	expression tag	UNP D3Y1I2
B	-27	SER	-	expression tag	UNP D3Y1I2
B	-26	HIS	-	expression tag	UNP D3Y1I2
B	-25	HIS	-	expression tag	UNP D3Y1I2
B	-24	HIS	-	expression tag	UNP D3Y1I2
B	-23	HIS	-	expression tag	UNP D3Y1I2
B	-22	HIS	-	expression tag	UNP D3Y1I2
B	-21	HIS	-	expression tag	UNP D3Y1I2
B	-20	HIS	-	expression tag	UNP D3Y1I2
B	-19	HIS	-	expression tag	UNP D3Y1I2
B	-18	GLY	-	expression tag	UNP D3Y1I2
B	-17	SER	-	expression tag	UNP D3Y1I2
B	-16	ASP	-	expression tag	UNP D3Y1I2
B	-15	TYR	-	expression tag	UNP D3Y1I2
B	-14	ASP	-	expression tag	UNP D3Y1I2
B	-13	ILE	-	expression tag	UNP D3Y1I2
B	-12	PRO	-	expression tag	UNP D3Y1I2
B	-11	THR	-	expression tag	UNP D3Y1I2
B	-10	THR	-	expression tag	UNP D3Y1I2
B	-9	GLU	-	expression tag	UNP D3Y1I2
B	-8	ASN	-	expression tag	UNP D3Y1I2
B	-7	LEU	-	expression tag	UNP D3Y1I2
B	-6	TYR	-	expression tag	UNP D3Y1I2
B	-5	PHE	-	expression tag	UNP D3Y1I2
B	-4	GLN	-	expression tag	UNP D3Y1I2
B	-3	GLY	-	expression tag	UNP D3Y1I2
B	-2	SER	-	expression tag	UNP D3Y1I2
B	-1	GLU	-	expression tag	UNP D3Y1I2
B	0	PHE	-	expression tag	UNP D3Y1I2

- Molecule 2 is FLAVIN-ADENINE DINUCLEOTIDE (three-letter code: FAD) (formula: C<sub>27</sub>H<sub>33</sub>N<sub>9</sub>O<sub>15</sub>P<sub>2</sub>).

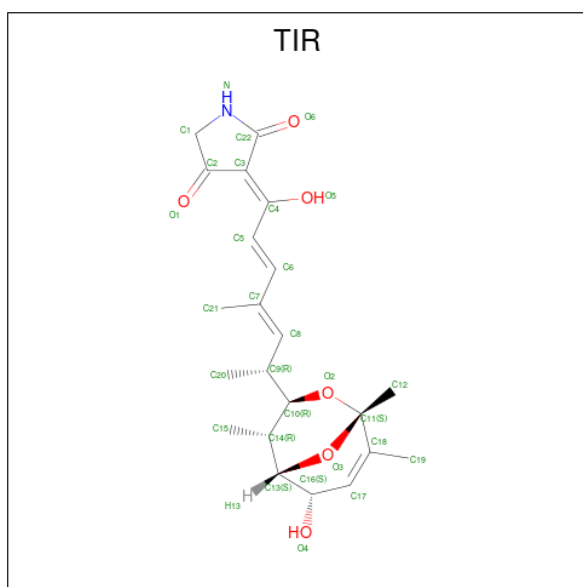


Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	
			Total	C	N	O			P
2	A	1	53	27	9	15	2	0	0
2	B	1	53	27	9	15	2	0	0

- Molecule 3 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	Mg		
3	A	2	2	2	0	0
3	B	2	2	2	0	0

- Molecule 4 is TIRANDAMYCIN E (three-letter code: TIR) (formula: C<sub>22</sub>H<sub>29</sub>NO<sub>6</sub>).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	C	N	O		
4	A	1	29	22	1	6	0	0
4	B	1	29	22	1	6	0	0

- Molecule 5 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	Cl		
5	A	4	4	4	0	0
5	B	1	1	1	0	0

- Molecule 6 is GLYCEROL (three-letter code: GOL) (formula: C<sub>3</sub>H<sub>8</sub>O<sub>3</sub>).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	A	1	Total C O 6 3 3	0	0
6	A	1	Total C O 6 3 3	0	0
6	A	1	Total C O 6 3 3	0	0
6	B	1	Total C O 6 3 3	0	0

- Molecule 7 is water.

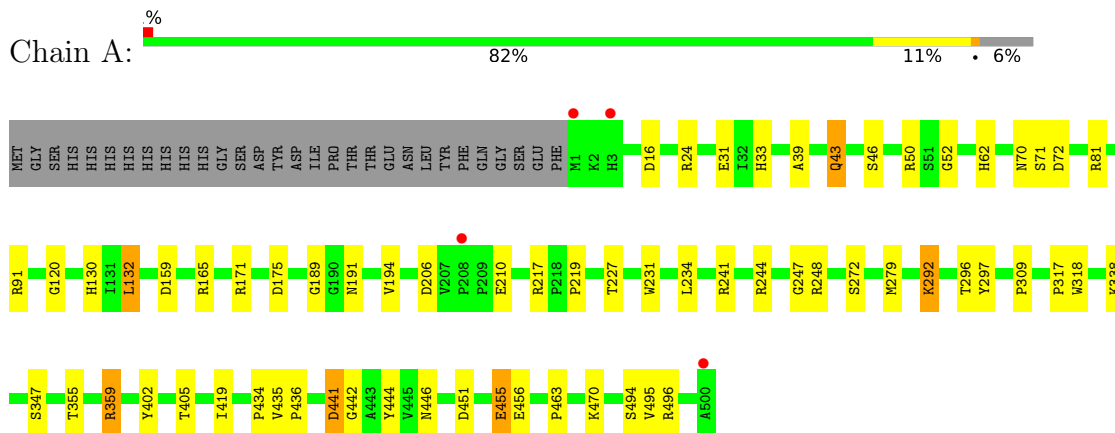
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
7	A	373	Total O 373 373	0	0
7	B	407	Total O 407 407	0	0



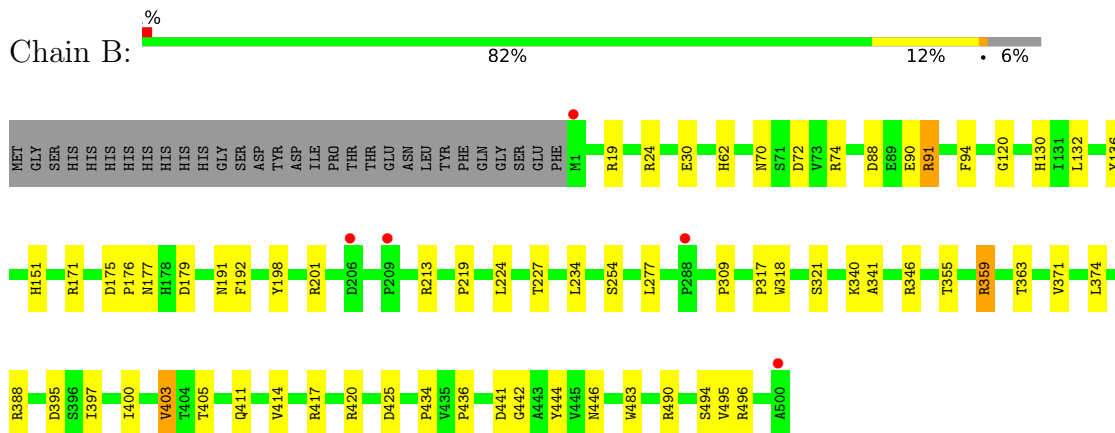
### 3 Residue-property plots

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: TAML



- Molecule 1: TAML



## 4 Data and refinement statistics i

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	64.02Å 130.40Å 134.54Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	134.54 – 2.03 67.27 – 2.03	Depositor EDS
% Data completeness (in resolution range)	91.4 (134.54-2.03) 91.4 (67.27-2.03)	Depositor EDS
$R_{merge}$	0.12	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.68 (at 2.03Å)	Xtrriage
Refinement program	REFMAC 5.5.0109	Depositor
R, $R_{free}$	0.159 , 0.236 0.159 , 0.233	Depositor DCC
$R_{free}$ test set	3397 reflections (5.05%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	22.9	Xtrriage
Anisotropy	0.336	Xtrriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.32 , 41.1	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.32$	Xtrriage
Estimated twinning fraction	0.014 for -h,l,k	Xtrriage
$F_o, F_c$ correlation	0.96	EDS
Total number of atoms	8921	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	22.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.16% 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: MG, TIR, FAD, CL, GOL

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	0.98	1/4046 (0.0%)	0.92	6/5529 (0.1%)
1	B	0.97	3/4106 (0.1%)	0.90	10/5610 (0.2%)
All	All	0.98	4/8152 (0.0%)	0.91	16/11139 (0.1%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	1

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	192	PHE	CE2-CZ	5.91	1.48	1.37
1	B	198	TYR	CD2-CE2	5.18	1.47	1.39
1	B	94	PHE	CE2-CZ	5.08	1.47	1.37
1	A	194	VAL	CB-CG2	5.05	1.63	1.52

All (16) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed( $^{\circ}$ )	Ideal( $^{\circ}$ )
1	A	81	ARG	NE-CZ-NH1	9.50	125.05	120.30
1	A	81	ARG	NE-CZ-NH2	-7.07	116.76	120.30
1	B	91	ARG	NE-CZ-NH2	-6.19	117.21	120.30
1	B	24	ARG	NE-CZ-NH1	6.05	123.32	120.30
1	B	19	ARG	NE-CZ-NH2	-6.01	117.30	120.30
1	A	91	ARG	NE-CZ-NH1	5.94	123.27	120.30
1	B	395	ASP	CB-CG-OD1	5.93	123.64	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	388	ARG	NE-CZ-NH2	-5.77	117.42	120.30
1	B	171	ARG	NE-CZ-NH1	5.53	123.06	120.30
1	A	175	ASP	CB-CG-OD1	5.39	123.15	118.30
1	A	91	ARG	NE-CZ-NH2	-5.34	117.63	120.30
1	B	388	ARG	NE-CZ-NH1	5.33	122.96	120.30
1	B	417	ARG	NE-CZ-NH1	5.21	122.91	120.30
1	B	179	ASP	CB-CG-OD1	5.17	122.95	118.30
1	B	91	ARG	CG-CD-NE	-5.15	100.98	111.80
1	A	441	ASP	CB-CG-OD2	5.12	122.91	118.30

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	206	ASP	Peptide

## 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	3943	0	3800	54	0
1	B	4001	0	3845	43	0
2	A	53	0	29	8	0
2	B	53	0	30	8	0
3	A	2	0	0	0	0
3	B	2	0	0	0	0
4	A	29	0	28	5	0
4	B	29	0	28	8	0
5	A	4	0	0	1	0
5	B	1	0	0	0	0
6	A	18	0	24	10	0
6	B	6	0	8	1	0
7	A	373	0	0	9	0
7	B	407	0	0	10	0
All	All	8921	0	7792	109	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 7.

All (109) 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:62:HIS:ND1	2:B:600:FAD:HM83	0.94	1.26
1:B:62:HIS:CE1	2:B:600:FAD:HM83	1.86	1.09
2:B:600:FAD:N5	4:B:800:TIR:H16	1.67	1.09
2:A:600:FAD:N5	4:A:800:TIR:H16	1.71	1.05
1:A:24:ARG:HH22	6:A:1505:GOL:H31	1.21	1.03
1:B:346[B]:ARG:HD3	7:B:2276:HOH:O	1.61	0.99
1:A:463:PRO:HA	6:A:1507:GOL:H11	1.45	0.95
1:A:62:HIS:CE1	2:A:600:FAD:C8M	2.50	0.94
1:A:62:HIS:ND1	2:A:600:FAD:HM81	1.82	0.94
1:B:496[B]:ARG:HD2	7:B:2393:HOH:O	1.67	0.93
1:A:279[B]:MET:CE	1:A:297:TYR:OH	2.20	0.89
1:A:405[B]:THR:HG22	7:A:2289:HOH:O	1.70	0.89
2:B:600:FAD:C4X	4:B:800:TIR:H16	2.04	0.86
1:A:279[B]:MET:HE2	1:A:297:TYR:OH	1.80	0.82
1:A:463:PRO:HA	6:A:1507:GOL:C1	2.12	0.78
1:B:359:ARG:NH1	1:B:425:ASP:OD2	2.18	0.76
2:A:600:FAD:C4X	4:A:800:TIR:H16	2.19	0.73
1:A:279[B]:MET:HE1	1:A:297:TYR:OH	1.90	0.71
1:A:338:LYS:HZ3	6:A:1505:GOL:H32	1.55	0.69
1:A:130:HIS:HD2	2:A:600:FAD:O2'	1.76	0.68
1:A:496:ARG:HD3	5:A:1504:CL:CL	2.32	0.67
1:B:444:TYR:CZ	1:B:446:ASN:HB2	2.30	0.67
1:A:435[A]:VAL:HG13	7:A:2309:HOH:O	1.96	0.65
1:B:411:GLN:O	1:B:414:VAL:HG12	1.97	0.64
1:A:52:GLY:O	6:A:1506:GOL:H31	1.98	0.63
1:A:292:LYS:O	1:A:296:THR:HG23	1.98	0.63
1:A:70:ASN:ND2	1:A:72:ASP:HB2	2.13	0.63
1:A:191:ASN:HD21	1:A:494:SER:HA	1.64	0.62
1:A:444:TYR:CZ	1:A:446:ASN:HB2	2.35	0.61
1:B:227:THR:HG23	1:B:309:PRO:HB2	1.83	0.61
1:A:317:PRO:HD3	7:A:2192:HOH:O	1.99	0.61
1:B:120:GLY:H	1:B:130:HIS:CE1	2.19	0.60
1:A:46[A]:SER:O	1:A:50:ARG:HG3	2.02	0.59
1:A:24:ARG:NH2	6:A:1505:GOL:H31	2.05	0.59
1:B:340:LYS:HE3	1:B:420:ARG:HA	1.85	0.58
1:A:231:TRP:CD1	1:A:272:SER:HA	2.38	0.58
1:A:171:ARG:HD2	7:A:2163:HOH:O	2.04	0.58
1:A:39:ALA:O	1:A:43[A]:GLN:HG2	2.03	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:62:HIS:ND1	2:A:600:FAD:C8	2.60	0.57
1:A:338:LYS:NZ	6:A:1505:GOL:H32	2.19	0.57
1:B:62:HIS:ND1	2:B:600:FAD:C8	2.65	0.57
1:B:88:ASP:OD1	1:B:90:GLU:HB2	2.04	0.57
1:B:496[B]:ARG:NH2	7:B:2395:HOH:O	2.29	0.57
4:A:800:TIR:H121	4:A:800:TIR:H315	1.86	0.56
1:A:210[B]:GLU:HG2	7:A:2184:HOH:O	2.04	0.56
1:B:219:PRO:O	1:B:318:TRP:HB2	2.05	0.56
1:A:338:LYS:HE2	6:A:1505:GOL:O1	2.07	0.55
1:A:71:SER:HB3	7:A:2037:HOH:O	2.05	0.55
1:A:347:SER:HB2	7:A:2261:HOH:O	2.06	0.55
1:A:159:ASP:HB3	1:A:165[A]:ARG:NH1	2.22	0.55
1:A:455:GLU:HG2	1:A:456:GLU:N	2.23	0.54
1:B:363:THR:HA	7:B:2295:HOH:O	2.07	0.53
1:B:191:ASN:HD21	1:B:494:SER:HA	1.74	0.52
1:B:224:LEU:HD11	1:B:321:SER:HB2	1.91	0.52
1:A:120:GLY:H	1:A:130:HIS:CE1	2.28	0.52
1:A:191:ASN:ND2	1:A:495:VAL:H	2.07	0.51
1:B:405[A]:THR:HG22	7:B:2322:HOH:O	2.09	0.51
2:A:600:FAD:N5	4:A:800:TIR:C16	2.61	0.50
1:B:346[B]:ARG:HD2	7:B:2213:HOH:O	2.12	0.50
2:B:600:FAD:C4X	4:B:800:TIR:C16	2.86	0.50
1:B:371[B]:VAL:HG23	1:B:403:VAL:HG13	1.92	0.50
1:A:463:PRO:CA	6:A:1507:GOL:H11	2.31	0.49
1:B:374:LEU:HD12	1:B:374:LEU:N	2.29	0.48
1:A:219:PRO:O	1:A:318:TRP:HB2	2.13	0.48
1:A:234:LEU:O	7:A:2195:HOH:O	2.20	0.48
1:B:30:GLU:OE2	1:B:74:ARG:HD3	2.13	0.48
1:A:231:TRP:CG	1:A:272:SER:HA	2.49	0.48
4:B:800:TIR:C21	4:B:800:TIR:H14	2.44	0.48
1:B:130:HIS:HD2	2:B:600:FAD:O2'	1.98	0.47
1:A:434:PRO:O	1:A:442:GLY:HA2	2.14	0.46
1:A:451:ASP:OD1	6:A:1505:GOL:H12	2.14	0.46
1:A:355:THR:O	1:A:359:ARG:HG3	2.15	0.46
1:B:72:ASP:HB3	7:B:2066:HOH:O	2.15	0.46
4:B:800:TIR:H14	4:B:800:TIR:H121	1.98	0.45
1:A:402:TYR:HB3	1:A:419[A]:ILE:HD11	1.98	0.45
1:A:241:ARG:HA	1:A:241:ARG:HD2	1.82	0.45
1:A:70:ASN:HD21	1:A:72:ASP:HB2	1.81	0.45
1:A:159:ASP:HB3	1:A:165[A]:ARG:HH12	1.82	0.45
4:B:800:TIR:C15	4:B:800:TIR:O4	2.64	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:436:PRO:HA	1:B:441:ASP:HA	1.99	0.44
2:A:600:FAD:C4X	4:A:800:TIR:C16	2.91	0.44
1:B:234:LEU:HD21	1:B:277[A]:LEU:HD11	1.98	0.44
1:B:346[B]:ARG:NH1	7:B:2275:HOH:O	2.49	0.44
1:B:91:ARG:HD3	7:B:2113:HOH:O	2.17	0.43
1:B:151:HIS:CD2	1:B:201[B]:ARG:HD3	2.52	0.43
1:B:191:ASN:ND2	1:B:495:VAL:H	2.16	0.43
1:B:490:ARG:HH12	6:B:1502:GOL:HO2	1.65	0.43
4:B:800:TIR:O4	4:B:800:TIR:H215	2.17	0.43
1:A:16:ASP:OD1	1:B:317:PRO:HB2	2.19	0.43
1:A:132:LEU:HD13	1:A:189:GLY:HA2	2.00	0.43
1:B:177:ASN:ND2	1:B:483:TRP:HH2	2.16	0.43
1:B:175:ASP:OD1	1:B:176:PRO:HD2	2.17	0.43
1:A:444:TYR:CE2	1:A:446:ASN:HB2	2.52	0.43
1:B:62:HIS:CG	2:B:600:FAD:C8M	2.87	0.43
1:A:70:ASN:ND2	1:A:72:ASP:H	2.17	0.43
1:B:434:PRO:O	1:B:442:GLY:HA2	2.19	0.42
1:B:177:ASN:ND2	1:B:483:TRP:CH2	2.88	0.42
1:B:355:THR:O	1:B:359:ARG:HB2	2.19	0.42
1:B:254:SER:HB2	1:B:397:ILE:HG22	2.02	0.41
1:A:436:PRO:HA	1:A:441:ASP:HA	2.02	0.41
1:B:201[B]:ARG:HE	1:B:201[B]:ARG:HB2	1.64	0.41
1:A:31:GLU:OE1	1:A:33:HIS:HE1	2.03	0.41
1:A:227:THR:HG23	1:A:309:PRO:HB2	2.02	0.41
1:B:234:LEU:CD2	1:B:277[A]:LEU:HD11	2.51	0.41
1:B:341:ALA:HB3	7:B:2341:HOH:O	2.21	0.41
4:B:800:TIR:H121	4:B:800:TIR:H9	1.92	0.41
1:A:247:GLY:HA3	1:A:347:SER:CB	2.51	0.40
1:A:470:LYS:NZ	7:A:2332:HOH:O	2.53	0.40
1:B:120:GLY:HA2	1:B:136:TYR:O	2.22	0.40

There are no symmetry-related clashes.

## 5.3 Torsion angles [i](#)

### 5.3.1 Protein backbone [i](#)

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	510/530 (96%)	498 (98%)	12 (2%)	0	100	100
1	B	517/530 (98%)	503 (97%)	14 (3%)	0	100	100
All	All	1027/1060 (97%)	1001 (98%)	26 (2%)	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	401/421 (95%)	392 (98%)	9 (2%)	52	53
1	B	407/421 (97%)	401 (98%)	6 (2%)	65	68
All	All	808/842 (96%)	793 (98%)	15 (2%)	59	59

All (15) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	43[A]	GLN
1	A	43[B]	GLN
1	A	132	LEU
1	A	217	ARG
1	A	244	ARG
1	A	248	ARG
1	A	292	LYS
1	A	359	ARG
1	A	455	GLU
1	B	70	ASN
1	B	132	LEU
1	B	213	ARG
1	B	359	ARG
1	B	400	ILE
1	B	403	VAL



Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (10) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	33	HIS
1	A	70	ASN
1	A	130	HIS
1	A	191	ASN
1	A	225	ASN
1	B	130	HIS
1	B	151	HIS
1	B	177	ASN
1	B	191	ASN
1	B	225	ASN

### 5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

## 5.4 Non-standard residues in protein, DNA, RNA chains [i](#)

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

## 5.5 Carbohydrates [i](#)

There are no monosaccharides in this entry.

## 5.6 Ligand geometry [i](#)

Of 17 ligands modelled in this entry, 9 are monoatomic - leaving 8 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	$\# Z  > 2$
6	GOL	A	1505	-	5,5,5	0.74	0	5,5,5	0.89	0
6	GOL	B	1502	-	5,5,5	0.48	0	5,5,5	1.36	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
4	TIR	B	800	3	30,31,31	1.82	8 (26%)	36,47,47	4.38	12 (33%)
2	FAD	A	600	1	53,58,58	1.00	2 (3%)	68,89,89	1.57	16 (23%)
4	TIR	A	800	3	30,31,31	1.70	7 (23%)	36,47,47	4.00	13 (36%)
2	FAD	B	600	1	53,58,58	1.28	5 (9%)	68,89,89	1.74	18 (26%)
6	GOL	A	1507	-	5,5,5	0.65	0	5,5,5	1.12	0
6	GOL	A	1506	-	5,5,5	0.97	0	5,5,5	1.15	1 (20%)

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
6	GOL	A	1505	-	-	4/4/4/4	-
6	GOL	B	1502	-	-	2/4/4/4	-
4	TIR	B	800	3	-	4/17/62/62	0/3/3/3
2	FAD	A	600	1	-	6/30/50/50	0/6/6/6
4	TIR	A	800	3	-	2/17/62/62	0/3/3/3
2	FAD	B	600	1	-	6/30/50/50	0/6/6/6
6	GOL	A	1507	-	-	2/4/4/4	-
6	GOL	A	1506	-	-	2/4/4/4	-

All (22) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	800	TIR	O1-C2	4.56	1.32	1.23
2	B	600	FAD	C4X-N5	4.33	1.39	1.30
4	B	800	TIR	C3-C4	3.81	1.51	1.40
4	B	800	TIR	O1-C2	3.75	1.30	1.23
2	B	600	FAD	C4-N3	-3.62	1.32	1.38
4	A	800	TIR	O6-C22	3.59	1.30	1.23
4	B	800	TIR	C5-C4	3.44	1.50	1.45
4	B	800	TIR	O6-C22	3.20	1.29	1.23
4	A	800	TIR	C5-C4	3.04	1.49	1.45
4	B	800	TIR	C17-C18	2.89	1.37	1.33
2	A	600	FAD	C4X-N5	2.89	1.36	1.30
4	B	800	TIR	C1-N	2.87	1.49	1.44
4	A	800	TIR	C3-C4	2.84	1.48	1.40
4	B	800	TIR	C16-C17	2.82	1.54	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	800	TIR	C1-N	2.68	1.49	1.44
2	B	600	FAD	C9-C8	2.50	1.43	1.39
2	B	600	FAD	C9A-N10	-2.43	1.36	1.41
2	B	600	FAD	C1'-C2'	-2.24	1.49	1.52
4	B	800	TIR	C22-N	2.17	1.37	1.34
2	A	600	FAD	O4B-C1B	2.08	1.44	1.41
4	A	800	TIR	C16-C17	2.05	1.53	1.50
4	A	800	TIR	C22-N	2.02	1.37	1.34

All (60) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	B	800	TIR	C1-C2-C3	15.32	115.08	106.82
4	B	800	TIR	C3-C22-N	14.47	116.88	107.26
4	A	800	TIR	C1-C2-C3	13.80	114.26	106.82
4	A	800	TIR	C3-C22-N	12.53	115.59	107.26
4	B	800	TIR	C22-C3-C2	-11.13	97.95	107.53
4	A	800	TIR	C22-C3-C2	-9.47	99.38	107.53
2	B	600	FAD	N3A-C2A-N1A	-5.10	120.71	128.68
4	A	800	TIR	C5-C4-C3	-5.00	119.40	124.51
4	B	800	TIR	O2-C11-O3	-4.69	106.00	110.91
4	B	800	TIR	C5-C4-C3	-4.66	119.75	124.51
4	A	800	TIR	O1-C2-C3	-4.47	121.34	128.74
2	B	600	FAD	C4X-C10-N10	4.14	122.53	116.48
4	A	800	TIR	O2-C11-O3	-4.11	106.60	110.91
2	B	600	FAD	C4-C4X-N5	4.00	123.93	118.23
2	A	600	FAD	C4-N3-C2	-3.74	118.73	125.64
4	B	800	TIR	O1-C2-C3	-3.72	122.58	128.74
2	A	600	FAD	N3A-C2A-N1A	-3.59	123.07	128.68
4	B	800	TIR	C5-C6-C7	-3.44	121.03	126.23
2	B	600	FAD	C4-N3-C2	-3.41	119.34	125.64
4	A	800	TIR	O5-C4-C5	3.31	120.37	115.75
2	B	600	FAD	C10-C4X-N5	-3.25	117.96	124.86
2	A	600	FAD	C10-C4X-N5	-3.11	118.26	124.86
2	A	600	FAD	C4-C4X-N5	3.05	122.58	118.23
4	B	800	TIR	O4-C16-C17	2.91	115.85	109.31
4	A	800	TIR	O4-C16-C17	2.90	115.85	109.31
2	A	600	FAD	C4'-C3'-C2'	-2.88	107.37	113.36
2	B	600	FAD	O3'-C3'-C2'	-2.87	101.87	108.81
4	A	800	TIR	O2-C10-C14	2.87	114.74	109.58
2	A	600	FAD	C4X-C10-N1	-2.86	118.09	124.73
2	B	600	FAD	C7M-C7-C8	2.85	126.57	120.74

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	600	FAD	O4-C4-N3	-2.82	114.72	120.12
2	B	600	FAD	C4X-C4-N3	2.80	120.30	113.19
2	A	600	FAD	C4X-C10-N10	2.79	120.56	116.48
2	A	600	FAD	C4X-C4-N3	2.73	120.12	113.19
4	B	800	TIR	O5-C4-C5	2.72	119.54	115.75
2	A	600	FAD	C10-N1-C2	2.66	122.22	116.90
2	B	600	FAD	C4X-C10-N1	-2.57	118.78	124.73
2	B	600	FAD	C4'-C3'-C2'	-2.55	108.06	113.36
2	A	600	FAD	C9-C9A-N10	2.55	125.28	121.84
4	B	800	TIR	O6-C22-C3	-2.54	120.97	129.10
2	B	600	FAD	O3B-C3B-C2B	-2.51	103.69	111.82
2	A	600	FAD	C1'-C2'-C3'	-2.39	103.10	109.79
2	B	600	FAD	C2A-N1A-C6A	2.39	122.84	118.75
2	A	600	FAD	C5A-C6A-N6A	2.37	123.96	120.35
4	A	800	TIR	O6-C22-C3	-2.34	121.61	129.10
6	A	1506	GOL	C3-C2-C1	2.34	120.81	111.70
2	A	600	FAD	O4-C4-C4X	-2.29	120.52	126.60
2	B	600	FAD	C6-C7-C8	-2.26	116.43	119.67
2	B	600	FAD	O4B-C1B-C2B	-2.23	103.67	106.93
2	A	600	FAD	C4A-C5A-N7A	-2.21	107.09	109.40
2	B	600	FAD	C5A-C6A-N6A	2.21	123.71	120.35
2	B	600	FAD	C5X-C6-C7	2.21	124.76	120.71
4	B	800	TIR	C11-O2-C10	2.15	119.49	114.18
2	B	600	FAD	O4'-C4'-C5'	-2.13	105.12	109.92
2	A	600	FAD	C5X-N5-C4X	2.05	121.48	118.07
4	B	800	TIR	O6-C22-N	-2.04	122.15	125.51
4	A	800	TIR	C11-O2-C10	2.04	119.22	114.18
4	A	800	TIR	C9-C10-C14	-2.02	112.23	115.55
4	A	800	TIR	C16-C17-C18	-2.01	118.60	123.78
2	A	600	FAD	O2-C2-N1	-2.01	118.50	121.83

There are no chirality outliers.

All (28) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	600	FAD	O3'-C3'-C4'-C5'
2	B	600	FAD	O3'-C3'-C4'-C5'
4	A	800	TIR	C5-C6-C7-C21
4	B	800	TIR	C5-C6-C7-C21
6	A	1505	GOL	C1-C2-C3-O3
6	A	1506	GOL	O1-C1-C2-O2
6	A	1506	GOL	O1-C1-C2-C3

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Mol	Chain	Res	Type	Atoms
6	B	1502	GOL	O1-C1-C2-C3
6	A	1505	GOL	O2-C2-C3-O3
2	A	600	FAD	C2'-C3'-C4'-C5'
2	A	600	FAD	O3'-C3'-C4'-O4'
2	B	600	FAD	O3'-C3'-C4'-O4'
6	A	1505	GOL	O1-C1-C2-C3
6	A	1507	GOL	C1-C2-C3-O3
4	A	800	TIR	C5-C6-C7-C8
2	B	600	FAD	C2'-C3'-C4'-C5'
6	A	1507	GOL	O2-C2-C3-O3
2	A	600	FAD	C2'-C3'-C4'-O4'
2	B	600	FAD	C2'-C3'-C4'-O4'
6	B	1502	GOL	O1-C1-C2-O2
4	B	800	TIR	C5-C6-C7-C8
6	A	1505	GOL	O1-C1-C2-O2
4	B	800	TIR	C14-C10-C9-C8
2	A	600	FAD	PA-O3P-P-O2P
4	B	800	TIR	C14-C10-C9-C20
2	B	600	FAD	PA-O3P-P-O2P
2	A	600	FAD	PA-O3P-P-O1P
2	B	600	FAD	PA-O3P-P-O1P

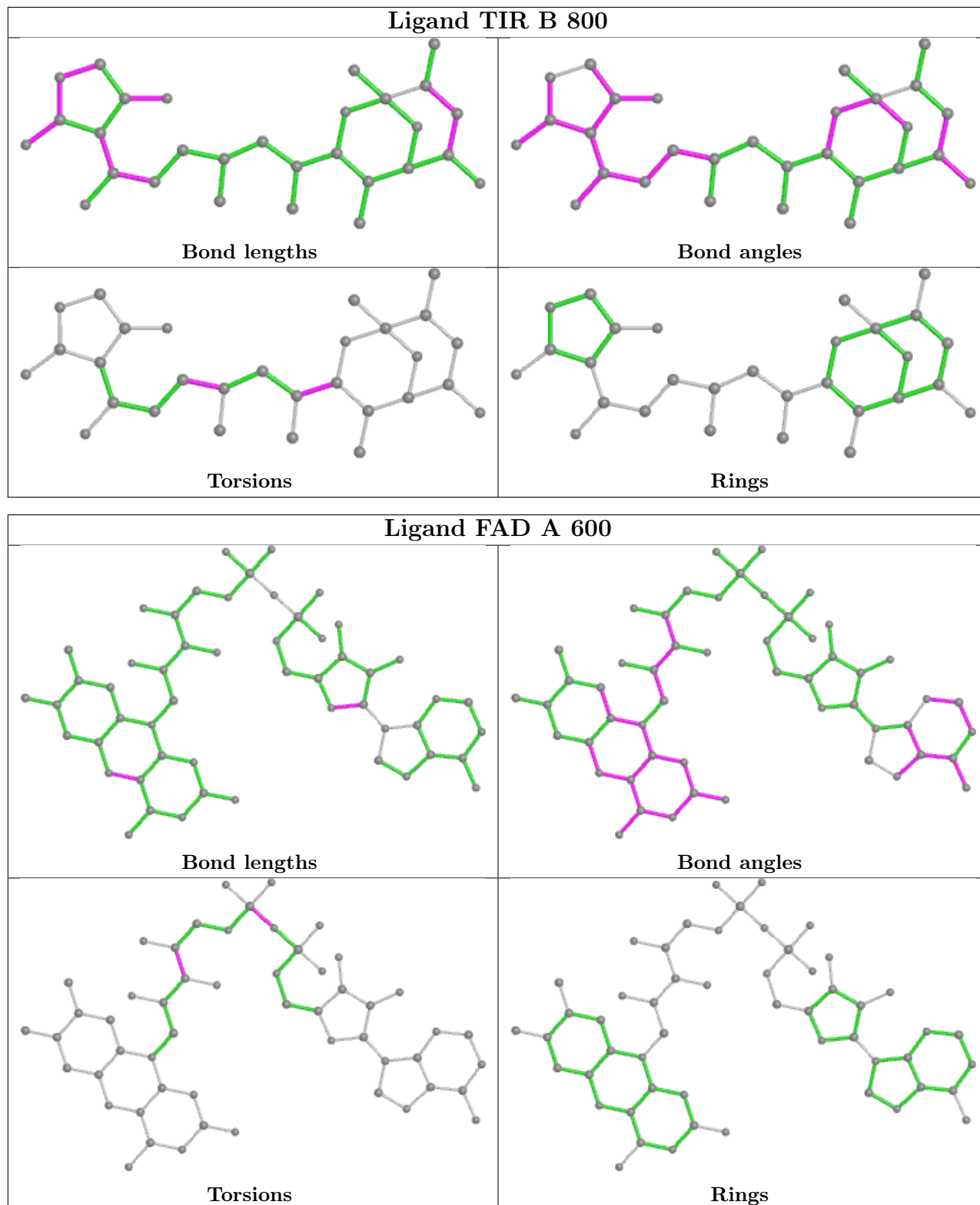
There are no ring outliers.

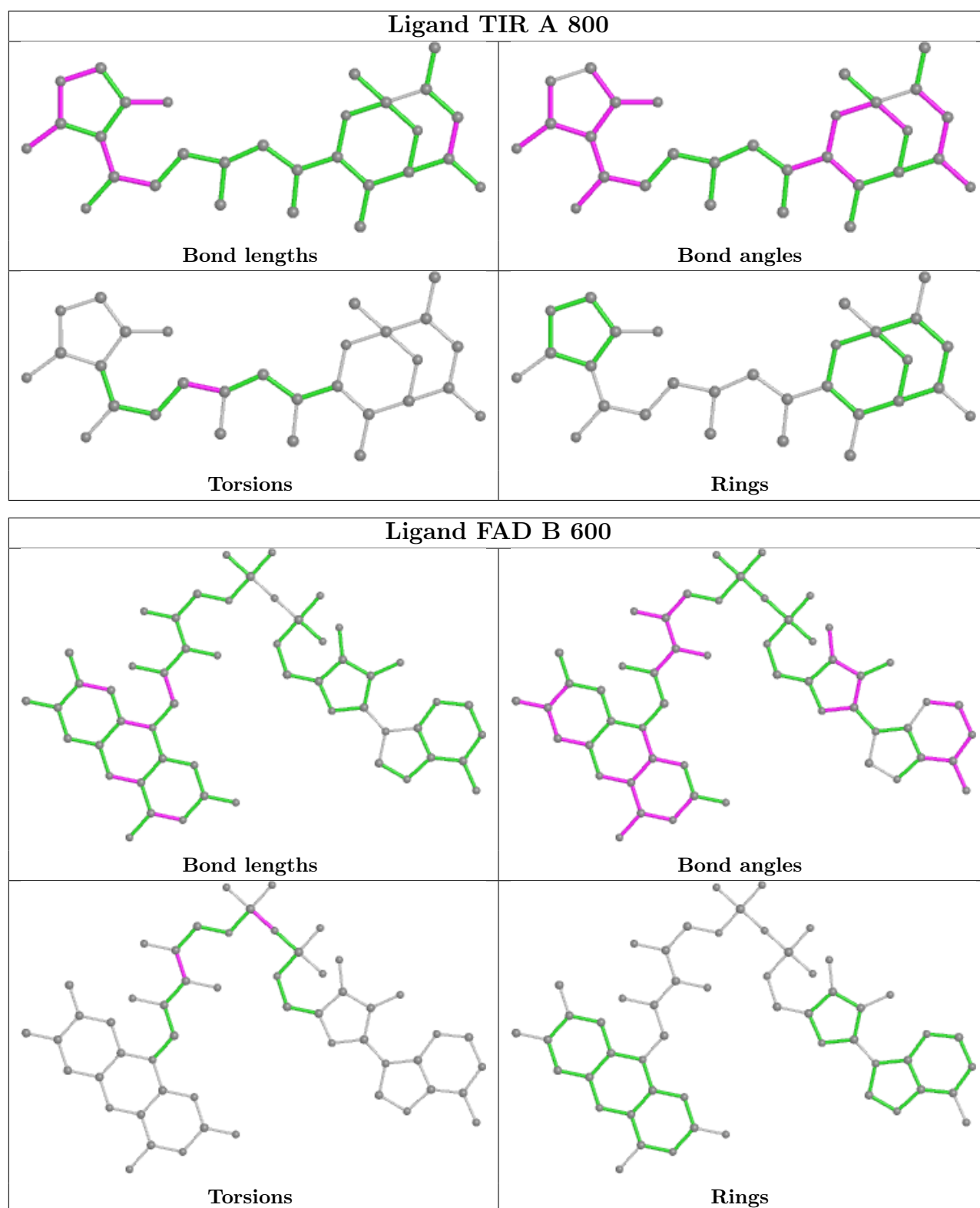
8 monomers are involved in 33 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	A	1505	GOL	6	0
6	B	1502	GOL	1	0
4	B	800	TIR	8	0
2	A	600	FAD	8	0
4	A	800	TIR	5	0
2	B	600	FAD	8	0
6	A	1507	GOL	3	0
6	A	1506	GOL	1	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring

in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.





## 5.7 Other polymers [i](#)

There are no such residues in this entry.

## 5.8 Polymer linkage issues

There are no chain breaks in this entry.



## 6 Fit of model and data [i](#)

### 6.1 Protein, DNA and RNA chains [i](#)

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	500/530 (94%)	-0.20	4 (0%) 86 85	11, 19, 37, 48	0
1	B	500/530 (94%)	-0.20	5 (1%) 82 82	12, 19, 38, 49	0
All	All	1000/1060 (94%)	-0.20	9 (0%) 84 83	11, 19, 37, 49	0

All (9) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	500	ALA	5.4
1	A	500	ALA	3.7
1	A	208	PRO	2.9
1	A	1	MET	2.9
1	B	206	ASP	2.9
1	B	1	MET	2.7
1	B	288	PRO	2.7
1	A	3	HIS	2.7
1	B	209	PRO	2.6

### 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 monosaccharides in this entry.

### 6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum,

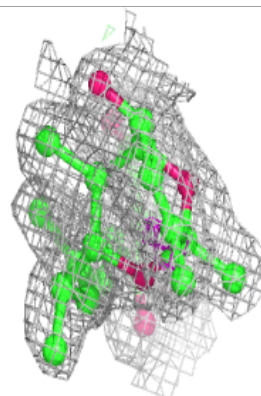
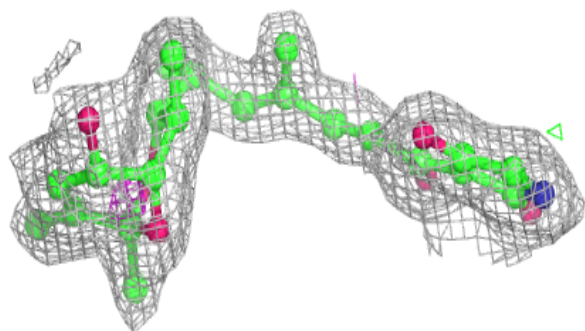
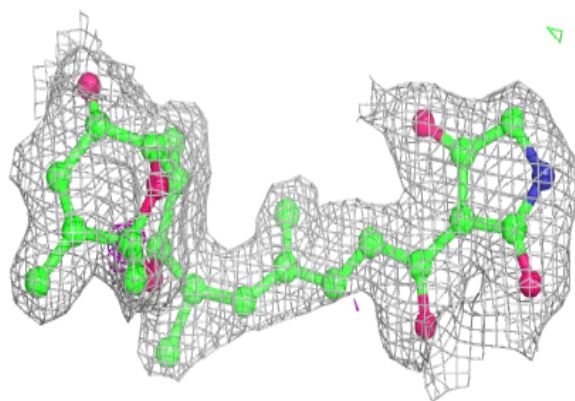
median, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
6	GOL	A	1505	6/6	0.87	0.20	34,36,37,42	0
5	CL	B	1501	1/1	0.88	0.10	68,68,68,68	0
6	GOL	B	1502	6/6	0.89	0.24	39,46,47,50	0
6	GOL	A	1506	6/6	0.90	0.23	34,41,42,42	0
4	TIR	A	800	29/29	0.91	0.15	25,31,33,35	0
4	TIR	B	800	29/29	0.91	0.17	21,27,30,32	0
5	CL	A	1504	1/1	0.93	0.07	48,48,48,48	0
6	GOL	A	1507	6/6	0.96	0.20	19,34,37,38	0
3	MG	A	900	1/1	0.97	0.07	27,27,27,27	0
3	MG	B	900	1/1	0.97	0.07	33,33,33,33	0
2	FAD	A	600	53/53	0.98	0.11	8,13,16,19	0
2	FAD	B	600	53/53	0.98	0.10	8,13,16,17	0
5	CL	A	1503	1/1	0.98	0.10	53,53,53,53	0
3	MG	A	700	1/1	0.99	0.07	24,24,24,24	0
5	CL	A	1501	1/1	0.99	0.06	43,43,43,43	0
3	MG	B	700	1/1	0.99	0.13	28,28,28,28	0
5	CL	A	1502	1/1	1.00	0.11	38,38,38,38	0

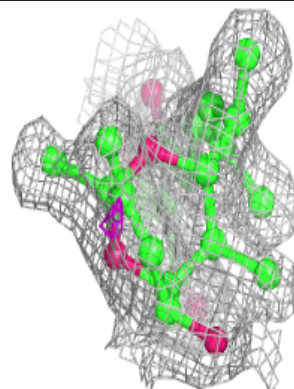
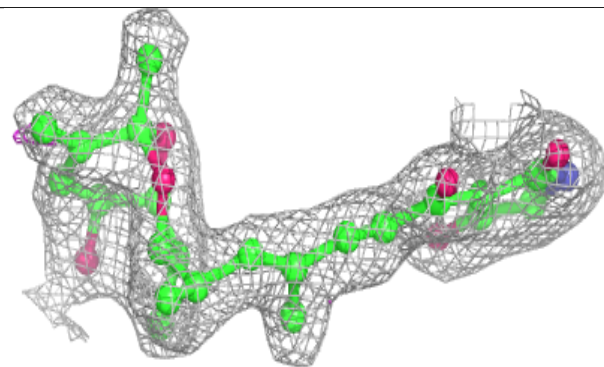
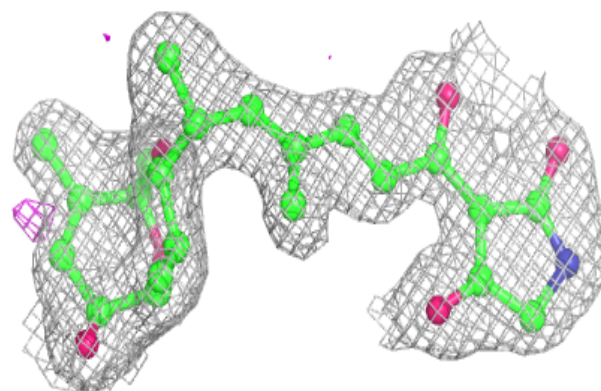
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

**Electron density around TIR A 800:**

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

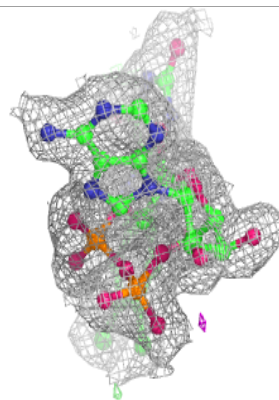
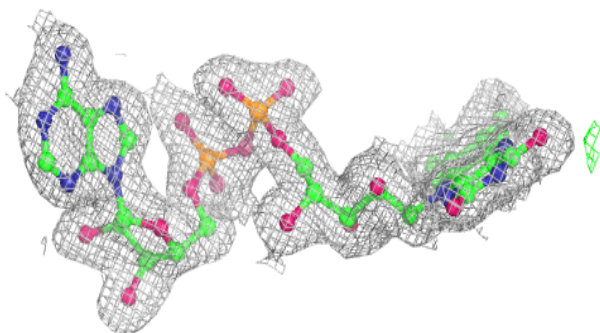
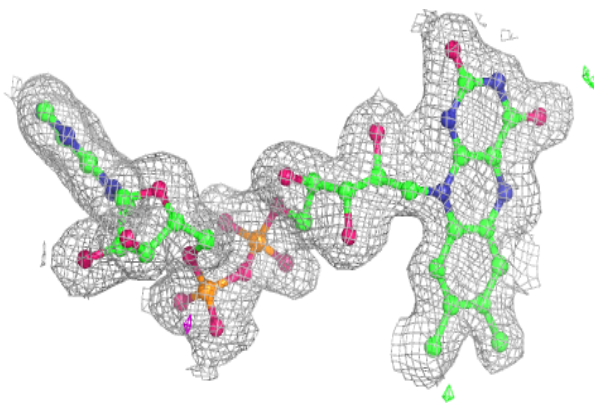
**Electron density around TIR B 800:**

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

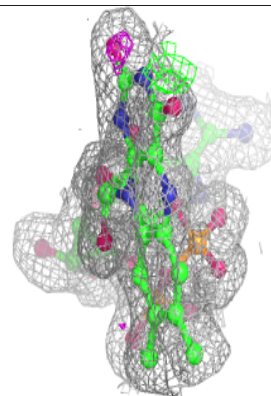
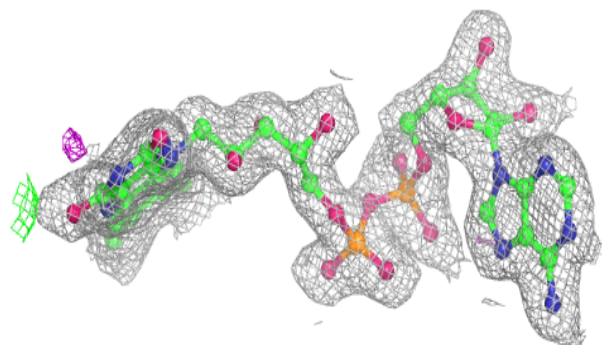
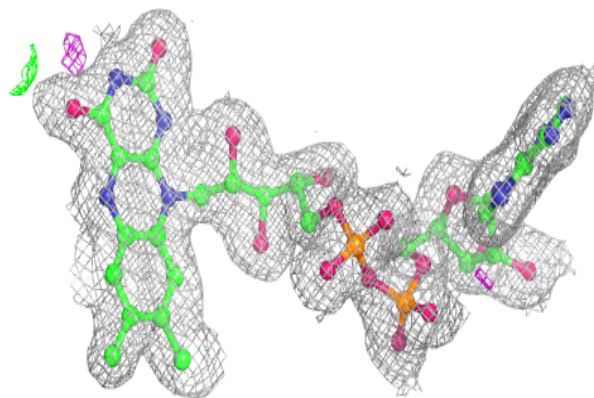


**Electron density around FAD A 600:**

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

**Electron density around FAD B 600:**

$2mF_o-DF_c$  (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.