



# Full wwPDB X-ray Structure Validation Report ⓘ

May 25, 2020 – 01:56 pm BST

PDB ID : 2Y3S  
Title : Structure of the tirandamycine-bound FAD-dependent tirandamycin oxidase TamL in C2 space group  
Authors : Carlson, J.C.; Li, S.; Gunatilleke, S.S.; Anzai, Y.; Burr, D.A.; Podust, L.M.; Sherman, D.H.  
Deposited on : 2010-12-23  
Resolution : 1.67 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.

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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 : 1.8.5 (274361), CSD as541be (2020)  
Xtriage (Phenix) : 1.13  
EDS : 2.11  
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) : 2.11



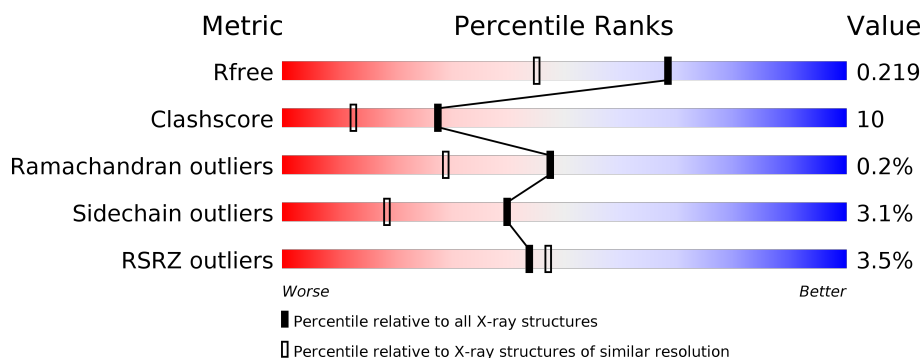
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 1.67 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	6780 (1.70-1.66)
Clashscore	141614	7310 (1.70-1.66)
Ramachandran outliers	138981	7173 (1.70-1.66)
Sidechain outliers	138945	7172 (1.70-1.66)
RSRZ outliers	127900	6661 (1.70-1.66)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on 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	<div> <div>3%</div> <div> <div></div> <div>75%</div> <div>16%</div> <div>• 6%</div> </div> </div>
1	B	530	<div> <div>3%</div> <div> <div></div> <div>76%</div> <div>15%</div> <div>• 7%</div> </div> </div>

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



Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
5	GOL	A	1501	-	-	X	-
5	GOL	A	1502	-	-	X	-
5	GOL	A	1503	-	X	X	-
5	GOL	B	1503	-	-	X	-



## 2 Entry composition

There are 7 unique types of molecules in this entry. The entry contains 8851 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
1	A	497	Total	C	N	O	S	0	23	0
			3943	2489	698	746	10			
1	B	493	Total	C	N	O	S	0	7	0
			3819	2410	687	713	9			

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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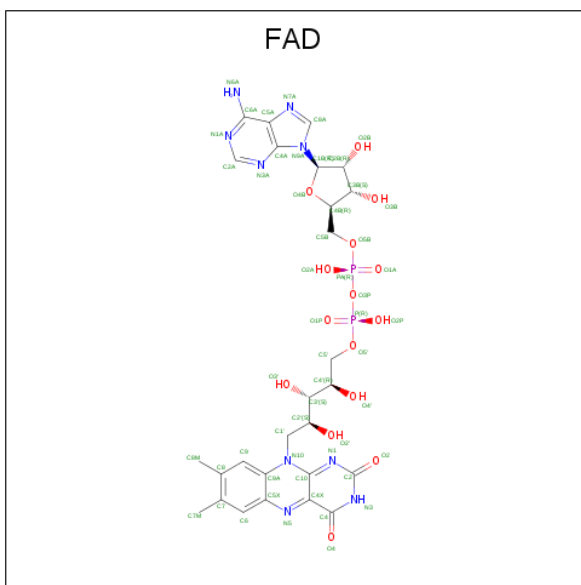


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Chain	Residue	Modelled	Actual	Comment	Reference
A	-4	GLN	-	expression tag	UNP D3Y1I2
A	-3	GLY	-	expression tag	UNP D3Y1I2
A	-2	SER	-	expression tag	UNP D3Y1I2
A	-1	GLU	-	expression tag	UNP D3Y1I2
A	0	PHE	-	expression tag	UNP D3Y1I2
B	-29	MET	-	expression 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

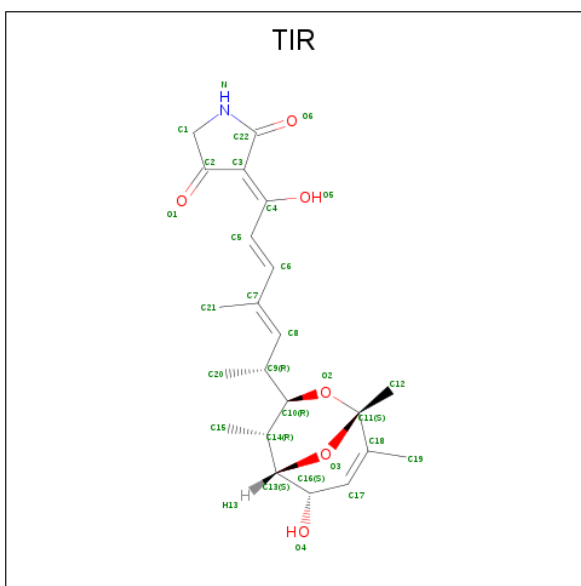
- Molecule 2 is FLAVIN-ADENINE DINUCLEOTIDE (three-letter code: FAD) (formula: C<sub>27</sub>H<sub>33</sub>N<sub>9</sub>O<sub>15</sub>P<sub>2</sub>).





Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
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

- Molecule 3 is TIRANDAMYCIN E (three-letter code: TIR) (formula:  $C_{22}H_{29}NO_6$ ).



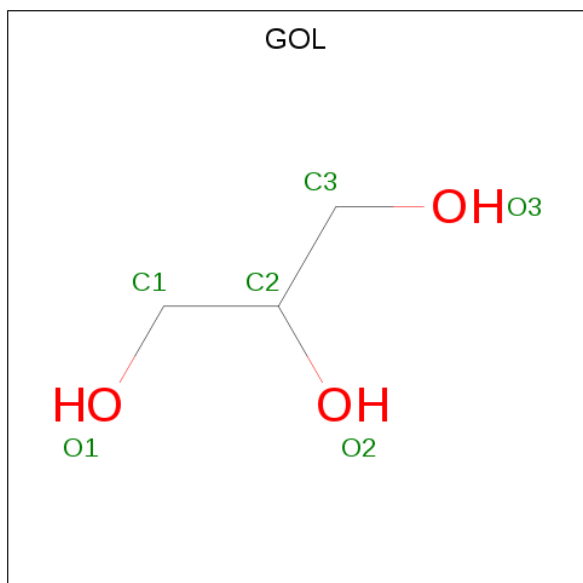
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	A	1	Total 29	C 22	N 1	O 6	0	0
3	B	1	Total 29	C 22	N 1	O 6	0	0



- Molecule 4 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

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

- Molecule 5 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
5	A	1	Total C O 6 3 3	0	0
5	A	1	Total C O 6 3 3	0	0
5	A	1	Total C O 6 3 3	0	0
5	B	1	Total C O 6 3 3	0	0
5	B	1	Total C O 6 3 3	0	0

- Molecule 6 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

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



- Molecule 7 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	A	456	Total 456	O 456	0	0
7	B	432	Total 432	O 432	0	0





- Molecule 1: TAML





## 4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	162.05Å 105.79Å 70.97Å 90.00° 110.67° 90.00°	Depositor
Resolution (Å)	86.76 – 1.67 66.40 – 1.67	Depositor EDS
% Data completeness (in resolution range)	92.8 (86.76-1.67) 92.8 (66.40-1.67)	Depositor EDS
$R_{merge}$	0.11	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.65 (at 1.67Å)	Xtriage
Refinement program	REFMAC 5.5.0109	Depositor
R, $R_{free}$	0.161 , 0.220 0.160 , 0.219	Depositor DCC
$R_{free}$ test set	6026 reflections (5.01%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	16.8	Xtriage
Anisotropy	0.195	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.34 , 54.2	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.48$ , $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.96	EDS
Total number of atoms	8851	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	18.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 10.55% 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 ⓘ

### 5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: GOL, MG, FAD, TIR, CL

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	1.26	12/4089 (0.3%)	1.07	24/5587 (0.4%)
1	B	1.27	11/3940 (0.3%)	1.07	25/5380 (0.5%)
All	All	1.26	23/8029 (0.3%)	1.07	49/10967 (0.4%)

All (23) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	198	TYR	CD2-CE2	7.09	1.50	1.39
1	B	427	TYR	CD1-CE1	7.04	1.50	1.39
1	B	286	THR	CB-CG2	-6.74	1.30	1.52
1	A	468	TYR	CE2-CZ	6.53	1.47	1.38
1	A	447	TYR	CD1-CE1	6.18	1.48	1.39
1	A	64	TYR	CD2-CE2	6.15	1.48	1.39
1	A	377	TYR	CE1-CZ	6.06	1.46	1.38
1	B	428	ALA	CA-CB	5.96	1.65	1.52
1	A	73	VAL	CB-CG1	5.80	1.65	1.52
1	A	67	PHE	CE2-CZ	5.71	1.48	1.37
1	B	14	TYR	CE2-CZ	5.70	1.46	1.38
1	B	181	TRP	CE3-CZ3	5.70	1.48	1.38
1	A	469	TYR	CE2-CZ	5.60	1.45	1.38
1	B	196	VAL	CB-CG2	5.57	1.64	1.52
1	A	473	TYR	CE1-CZ	5.50	1.45	1.38
1	B	15	GLU	CB-CG	5.35	1.62	1.52
1	B	469	TYR	CE2-CZ	5.28	1.45	1.38
1	B	250	PHE	CD2-CE2	5.25	1.49	1.39
1	A	89	GLU	CG-CD	-5.19	1.44	1.51
1	A	240	ALA	CA-CB	5.12	1.63	1.52
1	B	396	SER	CB-OG	5.08	1.48	1.42
1	A	444	TYR	CD2-CE2	5.06	1.47	1.39
1	A	464	TRP	CG-CD1	5.05	1.43	1.36



All (49) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	74	ARG	NE-CZ-NH2	-11.75	114.43	120.30
1	A	351	ARG	NE-CZ-NH2	-11.45	114.58	120.30
1	B	74	ARG	NE-CZ-NH1	10.63	125.61	120.30
1	A	351	ARG	NE-CZ-NH1	9.80	125.20	120.30
1	B	312	ASP	CB-CG-OD1	7.90	125.41	118.30
1	A	54	ARG	NE-CZ-NH2	-7.04	116.78	120.30
1	A	163	ASP	CB-CG-OD1	6.91	124.52	118.30
1	A	217	ARG	NE-CZ-NH2	-6.89	116.85	120.30
1	A	50	ARG	NE-CZ-NH1	6.85	123.72	120.30
1	B	359	ARG	NE-CZ-NH2	-6.74	116.93	120.30
1	A	395	ASP	CB-CG-OD1	6.69	124.32	118.30
1	B	323	ARG	NE-CZ-NH2	-6.55	117.03	120.30
1	B	58	ARG	NE-CZ-NH1	6.46	123.53	120.30
1	B	403	VAL	CG1-CB-CG2	6.44	121.20	110.90
1	A	425	ASP	CB-CG-OD1	6.31	123.98	118.30
1	B	471	ASP	CB-CG-OD1	6.26	123.93	118.30
1	A	54	ARG	NE-CZ-NH1	6.23	123.41	120.30
1	B	316	LEU	CA-CB-CG	6.16	129.47	115.30
1	B	323	ARG	NE-CZ-NH1	6.15	123.38	120.30
1	B	47	ARG	NE-CZ-NH1	6.09	123.35	120.30
1	A	471	ASP	CB-CG-OD1	6.04	123.74	118.30
1	A	271	ARG	NE-CZ-NH2	-6.01	117.29	120.30
1	A	277	LEU	CA-CB-CG	5.97	129.04	115.30
1	B	387	ASP	CB-CG-OD1	5.70	123.43	118.30
1	B	449	ASP	CB-CG-OD2	-5.57	113.29	118.30
1	B	312	ASP	CB-CG-OD2	-5.55	113.30	118.30
1	A	271	ARG	NE-CZ-NH1	5.49	123.04	120.30
1	A	336	ARG	NE-CZ-NH1	-5.48	117.56	120.30
1	B	441	ASP	CB-CG-OD2	5.46	123.22	118.30
1	A	235	ASP	CB-CG-OD1	5.44	123.19	118.30
1	B	175	ASP	CB-CG-OD1	5.41	123.17	118.30
1	B	315	ARG	NE-CZ-NH2	-5.40	117.60	120.30
1	B	66	ASP	CB-CG-OD1	5.38	123.14	118.30
1	A	323	ARG	NE-CZ-NH2	-5.37	117.61	120.30
1	B	471	ASP	CB-CG-OD2	-5.33	113.50	118.30
1	B	179	ASP	CB-CG-OD1	5.31	123.08	118.30
1	B	370	GLY	N-CA-C	-5.31	99.83	113.10
1	B	284	ASP	CB-CG-OD2	-5.30	113.53	118.30
1	B	449	ASP	CB-CG-OD1	5.15	122.94	118.30
1	A	58	ARG	NE-CZ-NH2	-5.14	117.73	120.30
1	A	109	LEU	CB-CG-CD1	-5.12	102.30	111.00
1	A	197	ARG	NE-CZ-NH1	5.08	122.84	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	244	ARG	NE-CZ-NH1	5.07	122.83	120.30
1	B	122	CYS	N-CA-CB	-5.06	101.49	110.60
1	A	111	ARG	NE-CZ-NH2	-5.04	117.78	120.30
1	A	388	ARG	NE-CZ-NH2	-5.04	117.78	120.30
1	A	425	ASP	CB-CG-OD2	-5.02	113.78	118.30
1	A	412	ASP	CB-CG-OD1	5.02	122.82	118.30
1	A	122	CYS	N-CA-CB	-5.01	101.57	110.60

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	3943	0	3801	80	0
1	B	3819	0	3700	68	0
2	A	53	0	29	5	0
2	B	53	0	29	9	0
3	A	29	0	28	5	0
3	B	29	0	28	4	0
4	A	1	0	0	0	0
4	B	1	0	0	0	0
5	A	18	0	23	16	0
5	B	12	0	16	8	0
6	A	2	0	0	0	0
6	B	3	0	0	0	0
7	A	456	0	0	20	0
7	B	432	0	0	5	0
All	All	8851	0	7654	156	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 10.

All (156) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.



Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:273:GLN:NE2	1:A:368:PRO:HA	1.48	1.27
1:A:273:GLN:NE2	1:A:368:PRO:CA	2.11	1.13
2:A:600:FAD:N5	3:A:700:TIR:H16	1.65	1.12
1:B:367:ASN:N	1:B:367:ASN:HD22	1.51	1.07
1:A:366:ASP:O	1:A:368:PRO:HD3	1.52	1.06
1:B:366:ASP:C	1:B:367:ASN:HD22	1.57	1.05
1:B:273:GLN:HE22	1:B:368:PRO:N	1.55	1.03
2:B:600:FAD:N5	3:B:700:TIR:H16	1.73	1.02
1:A:273:GLN:HE22	1:A:368:PRO:CA	1.71	1.01
1:B:202[B]:THR:HG21	7:B:2186:HOH:O	1.60	1.00
1:A:201:ARG:NH1	1:A:202:THR:O	1.97	0.98
1:A:273:GLN:HE21	1:A:368:PRO:HA	1.17	0.90
1:A:414[A]:VAL:HG23	7:A:2361:HOH:O	1.72	0.88
1:B:273:GLN:NE2	1:B:368:PRO:HA	1.86	0.88
1:B:273:GLN:NE2	1:B:368:PRO:CA	2.39	0.85
1:A:244:ARG:HG2	7:A:2128:HOH:O	1.79	0.83
1:B:91:ARG:HG2	1:B:91:ARG:HH11	1.42	0.83
1:B:273:GLN:HG3	7:B:2221:HOH:O	1.77	0.83
1:B:284:ASP:OD1	1:B:286:THR:HG22	1.78	0.82
1:B:367:ASN:N	1:B:367:ASN:ND2	2.24	0.82
1:A:50:ARG:HG3	7:A:2161:HOH:O	1.80	0.81
2:A:600:FAD:C4X	3:A:700:TIR:H16	2.11	0.81
1:A:273:GLN:HG3	7:A:2236:HOH:O	1.80	0.80
1:B:75:VAL:CG1	5:B:1503:GOL:H32	2.11	0.80
1:A:366:ASP:O	1:A:368:PRO:CD	2.30	0.79
1:A:323:ARG:HG3	5:A:1501:GOL:H31	1.66	0.78
1:B:273:GLN:NE2	1:B:368:PRO:N	2.32	0.78
1:A:273:GLN:NE2	1:A:368:PRO:CB	2.46	0.78
1:B:62:HIS:CE1	2:B:600:FAD:C8M	2.67	0.77
1:A:151:HIS:HD2	7:A:2149:HOH:O	1.68	0.76
1:B:273:GLN:HE21	1:B:368:PRO:HA	1.49	0.76
1:B:75:VAL:HG13	5:B:1503:GOL:H32	1.66	0.76
1:A:273:GLN:NE2	1:A:368:PRO:HB3	2.02	0.74
1:A:111:ARG:HH21	5:A:1501:GOL:H11	1.52	0.74
1:B:62:HIS:ND1	2:B:600:FAD:HM81	1.96	0.74
1:B:363:THR:C	1:B:365:TYR:H	1.92	0.72
1:A:71[B]:SER:HB3	7:A:2080:HOH:O	1.90	0.72
1:A:273:GLN:HE22	1:A:368:PRO:CB	2.03	0.71
1:A:234:LEU:HD12	1:A:307:VAL:HG21	1.72	0.71
1:B:366:ASP:CA	1:B:367:ASN:HD22	2.04	0.71
1:A:236[B]:GLU:OE2	7:A:2214:HOH:O	2.09	0.70
1:B:366:ASP:C	1:B:367:ASN:ND2	2.40	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:600:FAD:C4X	3:B:700:TIR:H16	2.23	0.68
1:B:223[B]:LEU:HD22	1:B:285:ALA:HB2	1.76	0.67
1:A:111:ARG:NH2	5:A:1501:GOL:H11	2.10	0.66
1:B:273:GLN:HE22	1:B:367:ASN:C	1.99	0.66
1:B:284:ASP:OD1	1:B:286:THR:CG2	2.44	0.65
1:A:155[B]:VAL:HG21	1:A:180:LEU:HD21	1.77	0.65
1:B:411:GLN:O	1:B:415:HIS:HD2	1.80	0.63
1:A:59[B]:SER:OG	2:A:600:FAD:O2P	2.16	0.63
1:B:351:ARG:NH2	7:B:2288:HOH:O	2.27	0.63
1:B:62:HIS:CG	2:B:600:FAD:C8M	2.74	0.63
1:B:91:ARG:CG	1:B:91:ARG:HH11	2.10	0.63
1:A:359:ARG:NH2	1:A:425:ASP:OD2	2.30	0.62
1:A:86:GLY:HA3	5:A:1502:GOL:C3	2.30	0.61
1:A:273:GLN:HE22	1:A:368:PRO:N	1.99	0.61
1:B:273:GLN:HE22	1:B:368:PRO:CA	2.07	0.61
1:A:421[A]:GLU:HG3	1:A:424:ARG:NH2	2.16	0.60
1:B:33:HIS:HE1	5:B:1503:GOL:O3	1.84	0.60
1:A:142[A]:MET:CE	5:A:1503:GOL:O2	2.50	0.60
1:B:62:HIS:ND1	2:B:600:FAD:C8	2.62	0.59
1:B:444:TYR:CZ	1:B:446:ASN:HB2	2.37	0.59
1:B:33:HIS:CE1	5:B:1503:GOL:H11	2.38	0.58
1:B:227:THR:HG23	1:B:309:PRO:HB2	1.83	0.58
1:A:33:HIS:HE1	7:A:2039:HOH:O	1.85	0.58
1:A:415:HIS:HE1	7:A:2324:HOH:O	1.87	0.58
1:A:273:GLN:CG	7:A:2236:HOH:O	2.47	0.58
1:A:33:HIS:HD2	7:A:2002:HOH:O	1.87	0.57
1:A:122:CYS:HB2	1:A:125:VAL:HG23	1.88	0.56
1:A:74:ARG:HD3	7:A:2030:HOH:O	2.05	0.56
1:A:142[A]:MET:HE3	1:A:262:ASP:HA	1.88	0.55
1:A:359:ARG:HD2	7:A:2321:HOH:O	2.05	0.55
1:A:86:GLY:HA3	5:A:1502:GOL:H31	1.89	0.55
1:A:120:GLY:H	1:A:130:HIS:CE1	2.26	0.54
1:A:155[B]:VAL:HG23	1:A:157:VAL:HG13	1.89	0.54
1:A:142[A]:MET:HE3	5:A:1503:GOL:O2	2.08	0.54
5:A:1501:GOL:H2	7:B:2017:HOH:O	2.08	0.53
1:A:319:LEU:HG	5:A:1501:GOL:H12	1.91	0.53
1:B:44:VAL:HG13	5:B:1503:GOL:H2	1.89	0.53
1:A:142[B]:MET:SD	5:A:1503:GOL:O2	2.66	0.52
1:A:86:GLY:CA	5:A:1502:GOL:H31	2.40	0.52
1:B:366:ASP:CA	1:B:367:ASN:ND2	2.72	0.52
1:A:351:ARG:NE	7:A:2317:HOH:O	2.43	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:351:ARG:HH11	1:B:351:ARG:HB3	1.75	0.52
1:A:234:LEU:CD1	1:A:307:VAL:HG21	2.40	0.52
1:B:91:ARG:CG	1:B:91:ARG:NH1	2.72	0.52
1:B:384:VAL:HG13	1:B:388:ARG:HD2	1.91	0.51
1:B:75:VAL:HG11	5:B:1503:GOL:H32	1.92	0.51
1:B:120:GLY:HA2	1:B:136:TYR:O	2.10	0.51
1:B:436:PRO:HD3	1:B:467:LEU:HD23	1.92	0.51
1:B:363:THR:C	1:B:365:TYR:N	2.60	0.51
1:A:142[A]:MET:HE1	5:A:1503:GOL:O2	2.12	0.50
1:A:191:ASN:HD21	1:A:494:SER:HA	1.77	0.50
1:A:86:GLY:HA3	5:A:1502:GOL:H32	1.92	0.50
1:A:434:PRO:O	1:A:442:GLY:HA2	2.11	0.50
3:B:700:TIR:H121	3:B:700:TIR:H315	1.94	0.50
1:A:142[A]:MET:CE	5:A:1503:GOL:HO2	2.23	0.50
1:A:244:ARG:CG	7:A:2128:HOH:O	2.47	0.49
1:A:480:LYS:HD2	1:A:484:ASP:HB3	1.93	0.49
1:B:223[B]:LEU:HD22	1:B:285:ALA:CB	2.42	0.49
1:A:179[B]:ASP:OD2	7:A:2189:HOH:O	2.19	0.49
2:A:600:FAD:C4X	3:A:700:TIR:C16	2.88	0.49
1:A:71[A]:SER:HB2	7:A:2080:HOH:O	2.13	0.49
1:A:130:HIS:HD2	2:A:600:FAD:O2'	1.96	0.49
1:A:261:CYS:O	5:A:1503:GOL:H12	2.13	0.48
1:A:273:GLN:HE21	1:A:368:PRO:CA	1.97	0.47
1:B:33:HIS:HE1	5:B:1503:GOL:C3	2.26	0.47
1:B:149:TYR:HE2	1:B:202[B]:THR:HG22	1.78	0.47
1:B:191:ASN:HD21	1:B:494:SER:HA	1.78	0.47
1:B:247:GLY:O	1:B:251:GLU:HG3	2.15	0.47
1:A:365[A]:TYR:CD1	1:A:418:TRP:HD1	2.33	0.47
1:A:132:LEU:HD13	1:A:189:GLY:HA2	1.95	0.47
1:A:496:ARG:NE	7:A:2438:HOH:O	2.48	0.47
1:A:227:THR:HG23	1:A:309:PRO:HB2	1.97	0.47
1:A:224:LEU:CD1	1:A:316:LEU:HD12	2.45	0.46
2:B:600:FAD:C4X	3:B:700:TIR:C16	2.93	0.46
1:A:91:ARG:HD2	1:A:199:TRP:CE2	2.51	0.46
1:A:411:GLN:O	1:A:415:HIS:HD2	1.99	0.45
1:B:50:ARG:NH2	7:B:2050:HOH:O	2.49	0.45
1:A:444:TYR:CZ	1:A:446:ASN:HB2	2.52	0.45
1:B:130:HIS:HD2	2:B:600:FAD:O2'	1.99	0.45
1:B:273:GLN:HB2	1:B:273:GLN:HE21	1.50	0.45
1:A:447:TYR:HH	3:A:700:TIR:HO4	1.62	0.45
1:B:273:GLN:HE21	1:B:368:PRO:CA	2.17	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:224:LEU:HD12	1:B:316:LEU:HD22	2.00	0.44
1:B:120:GLY:H	1:B:130:HIS:CE1	2.36	0.44
1:A:151:HIS:CD2	7:A:2149:HOH:O	2.54	0.44
1:B:231:TRP:CD1	1:B:272:SER:HA	2.51	0.44
1:A:351:ARG:NH2	7:A:2313:HOH:O	2.49	0.44
1:B:340:LYS:HE3	1:B:420:ARG:HA	1.99	0.43
1:B:367:ASN:HA	1:B:368:PRO:HD2	1.79	0.43
1:A:159[B]:ASP:HB3	1:A:165:ARG:NH1	2.33	0.43
1:A:231:TRP:CD1	1:A:272:SER:HA	2.54	0.43
1:A:221:GLU:HG2	1:A:317:PRO:HA	2.01	0.43
1:A:421[A]:GLU:OE2	1:A:424:ARG:CZ	2.66	0.43
1:B:33:HIS:NE2	5:B:1503:GOL:H11	2.33	0.43
1:A:421[A]:GLU:OE2	1:A:424:ARG:NH2	2.52	0.42
1:B:62:HIS:HB3	2:B:600:FAD:HM81	2.01	0.42
3:A:700:TIR:H315	3:A:700:TIR:H121	2.01	0.42
1:B:210:GLU:HA	1:B:211:PRO:HD2	1.95	0.42
1:A:224:LEU:HD12	1:A:316:LEU:HD12	2.01	0.41
1:B:269:LEU:HA	1:B:277:LEU:HD22	2.02	0.41
1:B:202[B]:THR:HG23	1:B:215:LEU:HA	2.02	0.41
1:A:242:LEU:C	1:A:242:LEU:HD23	2.41	0.41
1:B:122:CYS:HB2	1:B:125:VAL:HG23	2.01	0.41
1:B:149:TYR:O	1:B:200:LEU:HA	2.21	0.41
1:B:240:ALA:HA	1:B:353:ILE:HG21	2.03	0.41
1:A:7:VAL:HG21	1:A:17:LEU:HD12	2.03	0.41
1:B:355:THR:O	1:B:359:ARG:HG3	2.21	0.41
1:A:421[A]:GLU:OE2	1:A:424:ARG:NH1	2.54	0.40
1:A:111:ARG:HH21	5:A:1501:GOL:C1	2.29	0.40
1:A:23:LEU:HD11	1:B:316:LEU:HD11	2.03	0.40
1:A:9:PRO:HG3	1:A:14:TYR:CZ	2.57	0.40
1:B:149:TYR:CE2	1:B:202[B]:THR:HG22	2.57	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	518/530 (98%)	504 (97%)	12 (2%)	2 (0%)	34	17
1	B	496/530 (94%)	486 (98%)	10 (2%)	0	100	100
All	All	1014/1060 (96%)	990 (98%)	22 (2%)	2 (0%)	47	29

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	367	ASN
1	A	366	ASP

### 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	408/421 (97%)	396 (97%)	12 (3%)	42	21
1	B	390/421 (93%)	375 (96%)	15 (4%)	33	12
All	All	798/842 (95%)	771 (97%)	27 (3%)	40	15

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

Mol	Chain	Res	Type
1	A	6[A]	SER
1	A	6[B]	SER
1	A	89	GLU
1	A	132	LEU
1	A	159[A]	ASP
1	A	159[B]	ASP
1	A	207	VAL
1	A	273	GLN
1	A	277	LEU
1	A	387[A]	ASP
1	A	387[B]	ASP

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Mol	Chain	Res	Type
1	A	456	GLU
1	B	4	ILE
1	B	6	SER
1	B	9	PRO
1	B	54	ARG
1	B	91	ARG
1	B	132	LEU
1	B	213	ARG
1	B	217	ARG
1	B	286	THR
1	B	316	LEU
1	B	365	TYR
1	B	366	ASP
1	B	367	ASN
1	B	403	VAL
1	B	425	ASP

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (16) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	33	HIS
1	A	43	GLN
1	A	130	HIS
1	A	151	HIS
1	A	191	ASN
1	A	225	ASN
1	A	273	GLN
1	A	415	HIS
1	B	33	HIS
1	B	130	HIS
1	B	177	ASN
1	B	191	ASN
1	B	225	ASN
1	B	273	GLN
1	B	367	ASN
1	B	415	HIS

### 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 carbohydrates in this entry.

## 5.6 Ligand geometry [i](#)

Of 16 ligands modelled in this entry, 7 are monoatomic - leaving 9 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	$\# Z  > 2$
3	TIR	B	700	4	30,31,31	1.68	8 (26%)	36,47,47	4.06	12 (33%)
2	FAD	A	600	1	51,58,58	1.52	9 (17%)	60,89,89	2.60	17 (28%)
5	GOL	B	1503	-	5,5,5	0.76	0	5,5,5	0.89	0
5	GOL	A	1503	-	5,5,5	0.66	0	5,5,5	2.45	4 (80%)
5	GOL	A	1501	-	5,5,5	0.45	0	5,5,5	0.68	0
5	GOL	A	1502	-	5,5,5	0.29	0	5,5,5	0.44	0
5	GOL	B	1501	-	5,5,5	0.83	0	5,5,5	1.36	1 (20%)
2	FAD	B	600	1	51,58,58	1.34	6 (11%)	60,89,89	2.03	10 (16%)
3	TIR	A	700	4	30,31,31	1.84	9 (30%)	36,47,47	4.10	14 (38%)

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
3	TIR	B	700	4	-	2/17/62/62	0/3/3/3
2	FAD	A	600	1	-	5/30/50/50	0/6/6/6
5	GOL	B	1503	-	-	2/4/4/4	-
5	GOL	A	1503	-	-	3/4/4/4	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	GOL	A	1501	-	-	0/4/4/4	-
5	GOL	A	1502	-	-	2/4/4/4	-
5	GOL	B	1501	-	-	0/4/4/4	-
2	FAD	B	600	1	-	5/30/50/50	0/6/6/6
3	TIR	A	700	4	-	0/17/62/62	0/3/3/3

All (32) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	600	FAD	C1'-N10	4.77	1.53	1.48
3	A	700	TIR	O1-C2	4.16	1.31	1.23
2	B	600	FAD	C4X-C10	4.10	1.42	1.38
3	B	700	TIR	O1-C2	3.67	1.30	1.23
3	A	700	TIR	O6-C22	3.62	1.30	1.23
2	B	600	FAD	C2-N3	-3.61	1.31	1.38
2	A	600	FAD	C4X-N5	3.55	1.38	1.33
3	B	700	TIR	C1-C2	-3.49	1.48	1.52
2	A	600	FAD	C6-C5X	-3.44	1.36	1.41
3	A	700	TIR	C17-C18	3.29	1.38	1.33
3	A	700	TIR	C13-C16	3.28	1.57	1.51
2	B	600	FAD	C2A-N3A	3.24	1.37	1.32
2	A	600	FAD	C4X-C10	3.22	1.42	1.38
3	B	700	TIR	C17-C18	3.18	1.38	1.33
3	A	700	TIR	C1-N	3.02	1.49	1.44
3	B	700	TIR	O6-C22	2.94	1.29	1.23
3	B	700	TIR	C22-N	2.63	1.38	1.34
2	A	600	FAD	C7M-C7	2.62	1.56	1.51
3	B	700	TIR	O4-C16	-2.57	1.38	1.43
3	A	700	TIR	O2-C11	2.56	1.46	1.42
2	B	600	FAD	O4-C4	2.53	1.30	1.24
3	A	700	TIR	C3-C4	2.50	1.47	1.40
2	B	600	FAD	C2-N1	-2.47	1.33	1.38
2	A	600	FAD	C4-N3	2.45	1.37	1.33
2	A	600	FAD	O3B-C3B	2.40	1.48	1.43
3	A	700	TIR	C1-C2	-2.24	1.50	1.52
2	A	600	FAD	O4'-C4'	2.22	1.48	1.43
3	A	700	TIR	O3-C11	2.21	1.45	1.42
3	B	700	TIR	C5-C4	2.17	1.48	1.45
3	B	700	TIR	C3-C4	2.13	1.46	1.40
2	A	600	FAD	C9A-N10	-2.10	1.35	1.38
2	B	600	FAD	C2B-C1B	2.08	1.56	1.53



All (58) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	700	TIR	C1-C2-C3	14.47	114.62	106.82
3	B	700	TIR	C1-C2-C3	14.40	114.58	106.82
3	A	700	TIR	C3-C22-N	12.70	115.70	107.26
3	B	700	TIR	C3-C22-N	12.16	115.35	107.26
3	B	700	TIR	C22-C3-C2	-10.74	98.28	107.53
2	A	600	FAD	C10-C4X-N5	-9.88	114.43	121.26
3	A	700	TIR	C22-C3-C2	-9.43	99.42	107.53
2	B	600	FAD	C4-N3-C2	7.43	121.42	115.14
2	A	600	FAD	C4-N3-C2	7.42	121.40	115.14
2	A	600	FAD	C4-C4X-N5	7.32	126.96	118.60
2	A	600	FAD	C4X-N5-C5X	7.23	123.99	116.77
2	B	600	FAD	C10-C4X-N5	-5.76	117.28	121.26
2	B	600	FAD	C4X-N5-C5X	5.30	122.06	116.77
3	A	700	TIR	C5-C4-C3	-5.24	119.15	124.51
3	A	700	TIR	O3-C11-O2	-4.92	105.76	110.91
2	B	600	FAD	C1'-N10-C9A	4.65	121.95	118.29
3	A	700	TIR	O1-C2-C3	-4.42	121.43	128.74
2	B	600	FAD	C4A-C5A-N7A	-4.39	104.82	109.40
3	B	700	TIR	O3-C11-O2	-4.39	106.32	110.91
3	B	700	TIR	O5-C4-C5	4.36	121.84	115.75
2	B	600	FAD	C4-C4X-N5	3.99	123.15	118.60
2	A	600	FAD	C7-C6-C5X	3.80	126.59	121.22
3	A	700	TIR	O5-C4-C5	3.74	120.97	115.75
2	A	600	FAD	C4X-C4-N3	-3.64	118.46	123.43
2	B	600	FAD	C4X-C4-N3	-3.64	118.46	123.43
2	A	600	FAD	N3A-C2A-N1A	-3.57	123.09	128.68
3	B	700	TIR	O1-C2-C3	-3.54	122.88	128.74
2	A	600	FAD	C5X-C9A-N10	-3.46	115.21	117.72
5	A	1503	GOL	C3-C2-C1	3.45	125.10	111.70
2	A	600	FAD	C4'-C3'-C2'	-3.42	106.26	113.36
3	B	700	TIR	C16-C17-C18	-3.13	115.72	123.78
3	B	700	TIR	C20-C9-C10	2.91	116.50	111.11
2	B	600	FAD	N3A-C2A-N1A	-2.84	124.24	128.68
3	A	700	TIR	C9-C10-C14	-2.81	110.93	115.55
3	A	700	TIR	O6-C22-C3	-2.79	120.18	129.10
2	A	600	FAD	C6-C5X-N5	2.78	122.11	119.05
3	B	700	TIR	C5-C4-C3	-2.77	121.68	124.51
3	B	700	TIR	C5-C6-C7	-2.65	122.23	126.23
5	B	1501	GOL	C3-C2-C1	2.56	121.67	111.70
5	A	1503	GOL	O2-C2-C3	-2.51	98.06	109.12
3	B	700	TIR	C13-C16-C17	2.51	117.22	111.08
2	A	600	FAD	C6-C7-C8	-2.39	115.88	119.91

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	700	TIR	C5-C6-C7	-2.38	122.64	126.23
2	A	600	FAD	O2B-C2B-C3B	2.36	119.44	111.82
2	A	600	FAD	C7M-C7-C8	2.30	125.46	120.74
2	B	600	FAD	O2'-C2'-C1'	-2.29	104.08	109.59
5	A	1503	GOL	O1-C1-C2	-2.23	99.50	110.20
2	A	600	FAD	C9A-N10-C10	2.22	124.82	121.91
3	A	700	TIR	C19-C18-C17	-2.19	116.66	121.54
2	A	600	FAD	O3B-C3B-C4B	-2.19	104.73	111.05
3	A	700	TIR	C16-C17-C18	-2.18	118.17	123.78
3	B	700	TIR	O6-C22-C3	-2.17	122.15	129.10
2	A	600	FAD	O3B-C3B-C2B	-2.14	104.89	111.82
2	A	600	FAD	C4-C4X-C10	-2.14	118.54	119.95
3	A	700	TIR	C13-C16-C17	2.12	116.26	111.08
3	A	700	TIR	O2-C11-C12	2.10	112.25	107.62
2	B	600	FAD	C5'-C4'-C3'	-2.08	108.18	112.20
5	A	1503	GOL	O3-C3-C2	-2.01	100.57	110.20

There are no chirality outliers.

All (19) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	600	FAD	O3'-C3'-C4'-C5'
5	B	1503	GOL	C1-C2-C3-O3
5	B	1503	GOL	O2-C2-C3-O3
5	A	1502	GOL	C1-C2-C3-O3
5	A	1503	GOL	O1-C1-C2-C3
3	B	700	TIR	C5-C6-C7-C21
2	A	600	FAD	O3'-C3'-C4'-O4'
2	B	600	FAD	O3'-C3'-C4'-O4'
2	A	600	FAD	C2'-C3'-C4'-O4'
2	A	600	FAD	C2'-C3'-C4'-C5'
5	A	1502	GOL	O2-C2-C3-O3
5	A	1503	GOL	O1-C1-C2-O2
2	B	600	FAD	C2'-C3'-C4'-O4'
3	B	700	TIR	C5-C6-C7-C8
2	B	600	FAD	O3'-C3'-C4'-C5'
2	B	600	FAD	C2'-C3'-C4'-C5'
5	A	1503	GOL	O2-C2-C3-O3
2	A	600	FAD	PA-O3P-P-O2P
2	B	600	FAD	PA-O3P-P-O2P

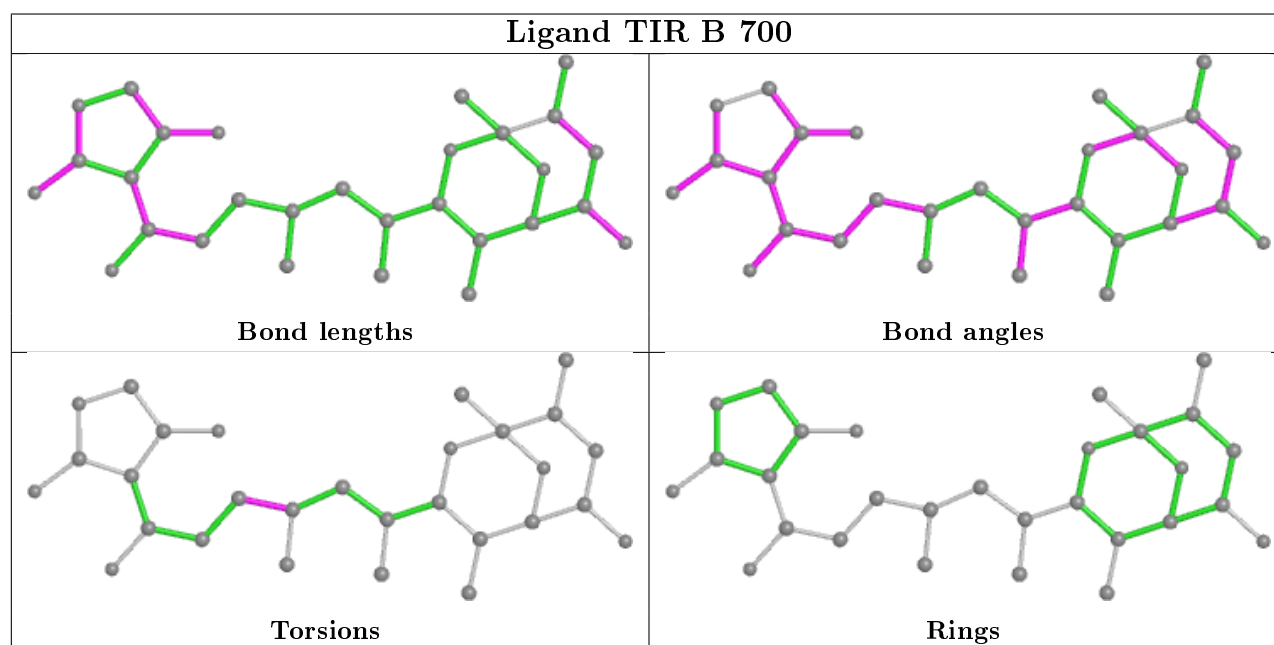
There are no ring outliers.



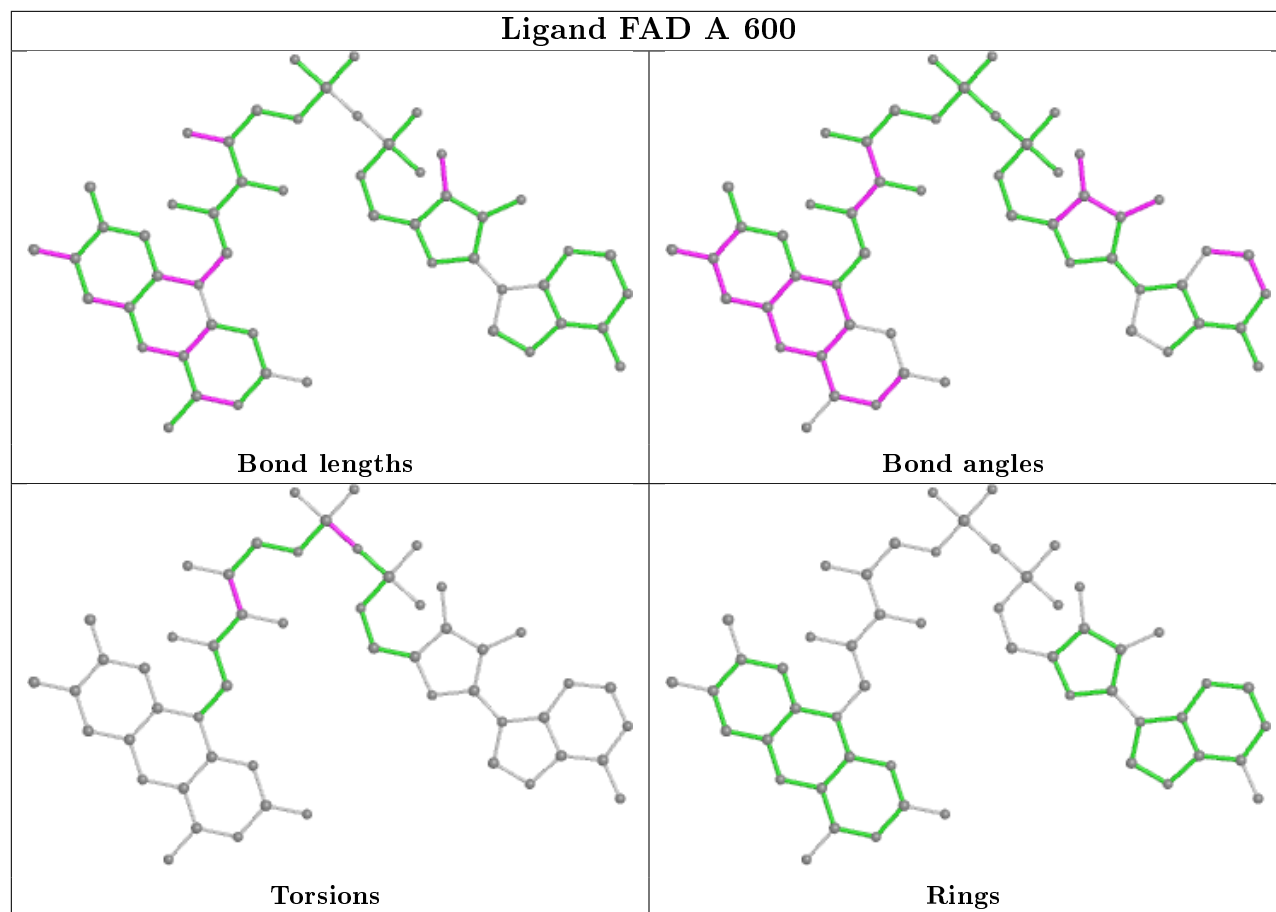
8 monomers are involved in 41 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	B	700	TIR	4	0
2	A	600	FAD	5	0
5	B	1503	GOL	8	0
5	A	1503	GOL	6	0
5	A	1501	GOL	6	0
5	A	1502	GOL	4	0
2	B	600	FAD	9	0
3	A	700	TIR	5	0

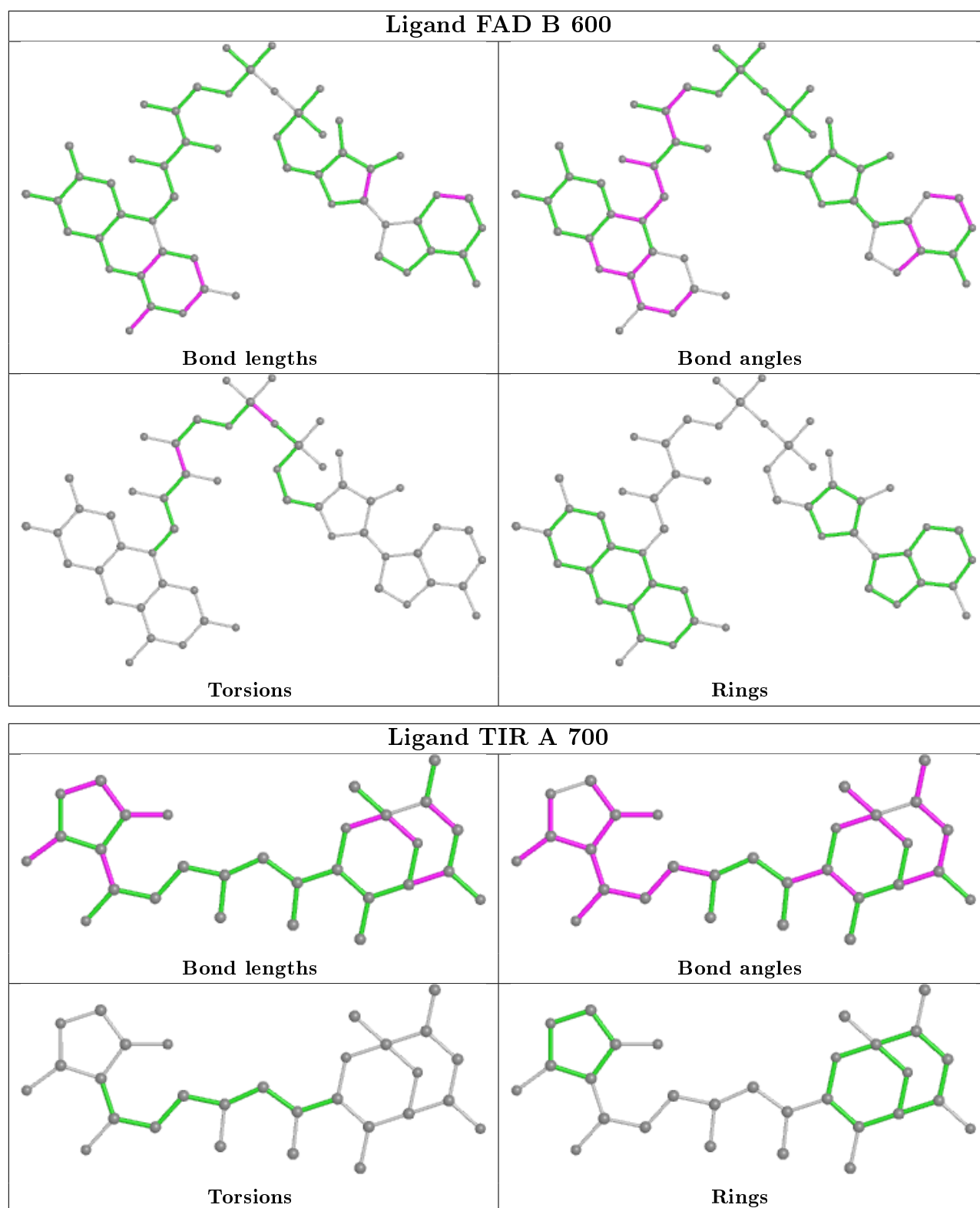
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. 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 ⓘ

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

### 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	497/530 (93%)	0.08	17 (3%) 45 48	9, 14, 30, 45	0
1	B	493/530 (93%)	0.02	18 (3%) 41 44	9, 14, 30, 47	0
All	All	990/1060 (93%)	0.05	35 (3%) 44 47	9, 14, 30, 47	0

All (35) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	365[A]	TYR	7.7
1	B	364	ASP	7.6
1	A	500	ALA	7.6
1	A	206	ASP	7.5
1	A	368	PRO	7.3
1	A	205	ALA	6.9
1	B	500	ALA	6.7
1	B	365	TYR	5.4
1	B	369	ALA	5.2
1	A	233	GLY	5.1
1	A	369	ALA	5.1
1	B	363	THR	4.6
1	B	203	ALA	4.2
1	B	233	GLY	4.1
1	B	368	PRO	4.0
1	A	207	VAL	4.0
1	A	364	ASP	3.9
1	A	363	THR	3.8
1	B	210	GLU	3.7
1	B	212	GLY	3.2
1	B	213	ARG	3.0
1	A	366	ASP	3.0
1	B	366	ASP	3.0
1	A	161[A]	SER	2.9

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Mol	Chain	Res	Type	RSRZ
1	A	50	ARG	2.7
1	B	4	ILE	2.5
1	B	211	PRO	2.5
1	B	176	PRO	2.4
1	A	310	HIS	2.4
1	A	232	GLU	2.4
1	B	310	HIS	2.3
1	A	273	GLN	2.2
1	B	161	SER	2.1
1	A	173	PRO	2.1
1	B	232	GLU	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 carbohydrates 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
5	GOL	B	1501	6/6	0.87	0.13	20,20,24,31	0
5	GOL	B	1503	6/6	0.88	0.21	25,30,30,36	0
5	GOL	A	1502	6/6	0.89	0.23	35,38,40,42	0
3	TIR	B	700	29/29	0.90	0.11	13,17,19,22	0
5	GOL	A	1503	6/6	0.90	0.13	17,25,28,33	0
3	TIR	A	700	29/29	0.90	0.11	14,16,19,20	0
5	GOL	A	1501	6/6	0.94	0.15	26,34,35,36	0
6	CL	B	1504	1/1	0.96	0.14	60,60,60,60	0
2	FAD	B	600	53/53	0.97	0.09	8,10,12,14	0
2	FAD	A	600	53/53	0.97	0.08	7,10,12,15	0
6	CL	B	1502	1/1	0.97	0.04	47,47,47,47	0
4	MG	B	800	1/1	1.00	0.05	18,18,18,18	0

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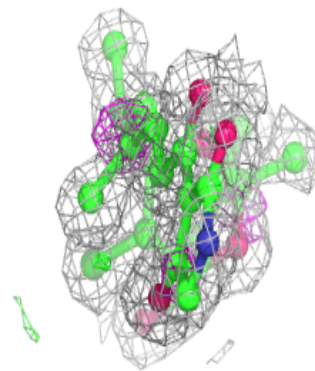
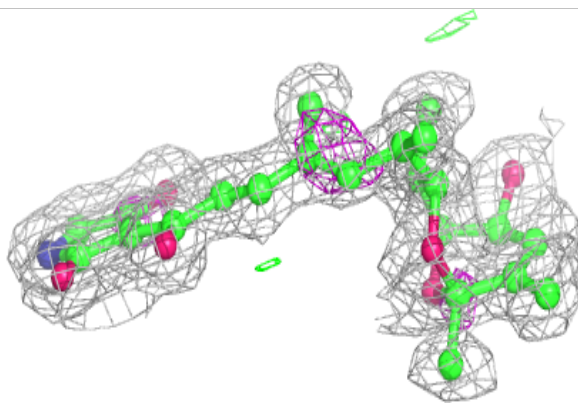
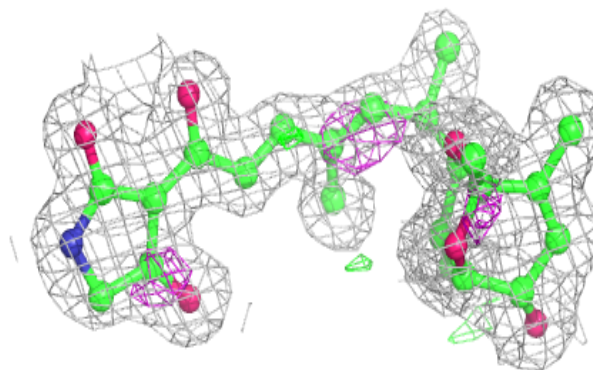
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
6	CL	A	1505	1/1	1.00	0.07	17,17,17,17	0
6	CL	B	1505	1/1	1.00	0.09	19,19,19,19	0
6	CL	A	1504	1/1	1.00	0.04	31,31,31,31	0
4	MG	A	800	1/1	1.00	0.06	18,18,18,18	0

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 B 700:**

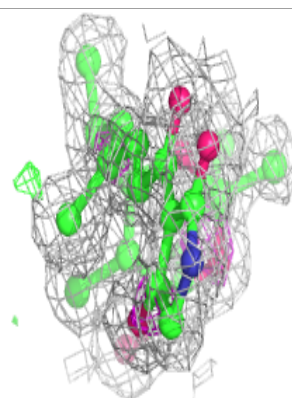
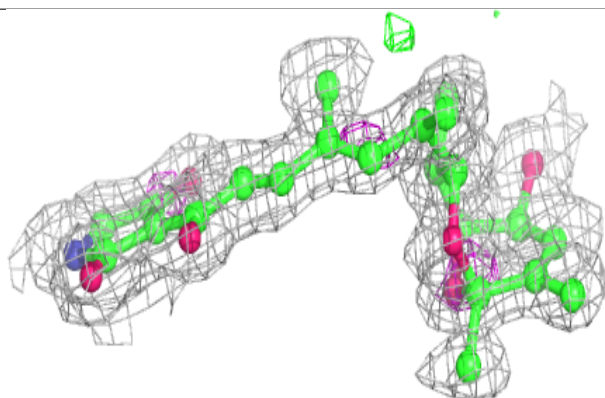
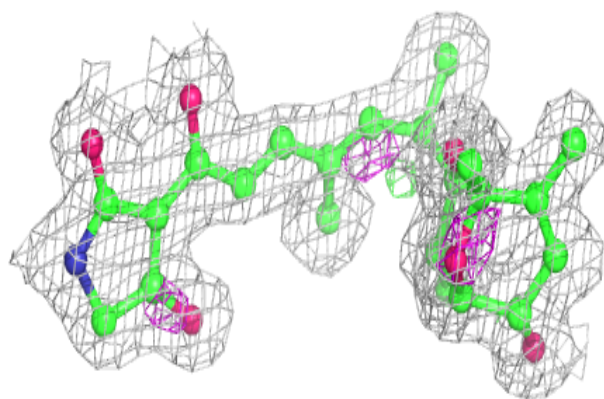
2mF<sub>o</sub>-DF<sub>c</sub> (at 0.7 rmsd) in gray  
mF<sub>o</sub>-DF<sub>c</sub> (at 3 rmsd) in purple (negative)  
and green (positive)



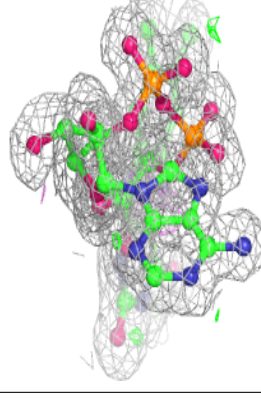
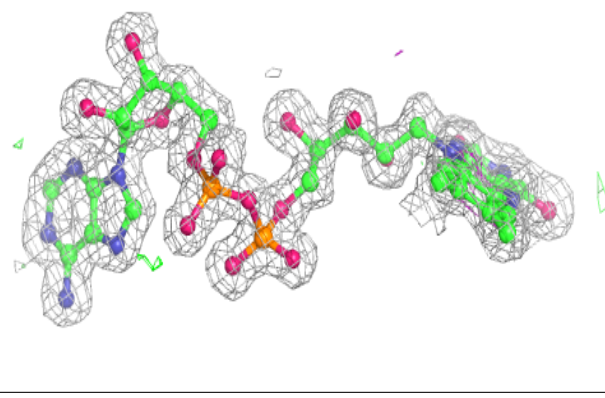
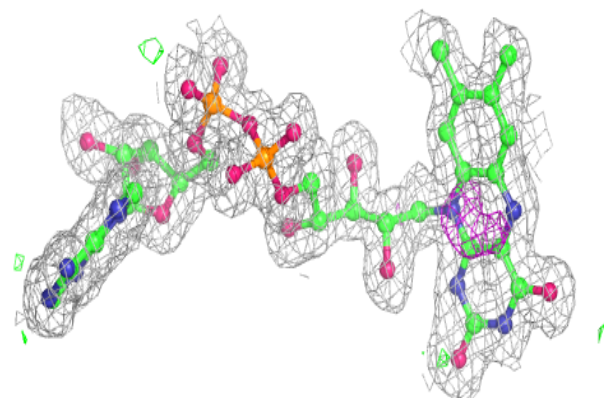


**Electron density around TIR A 700:**

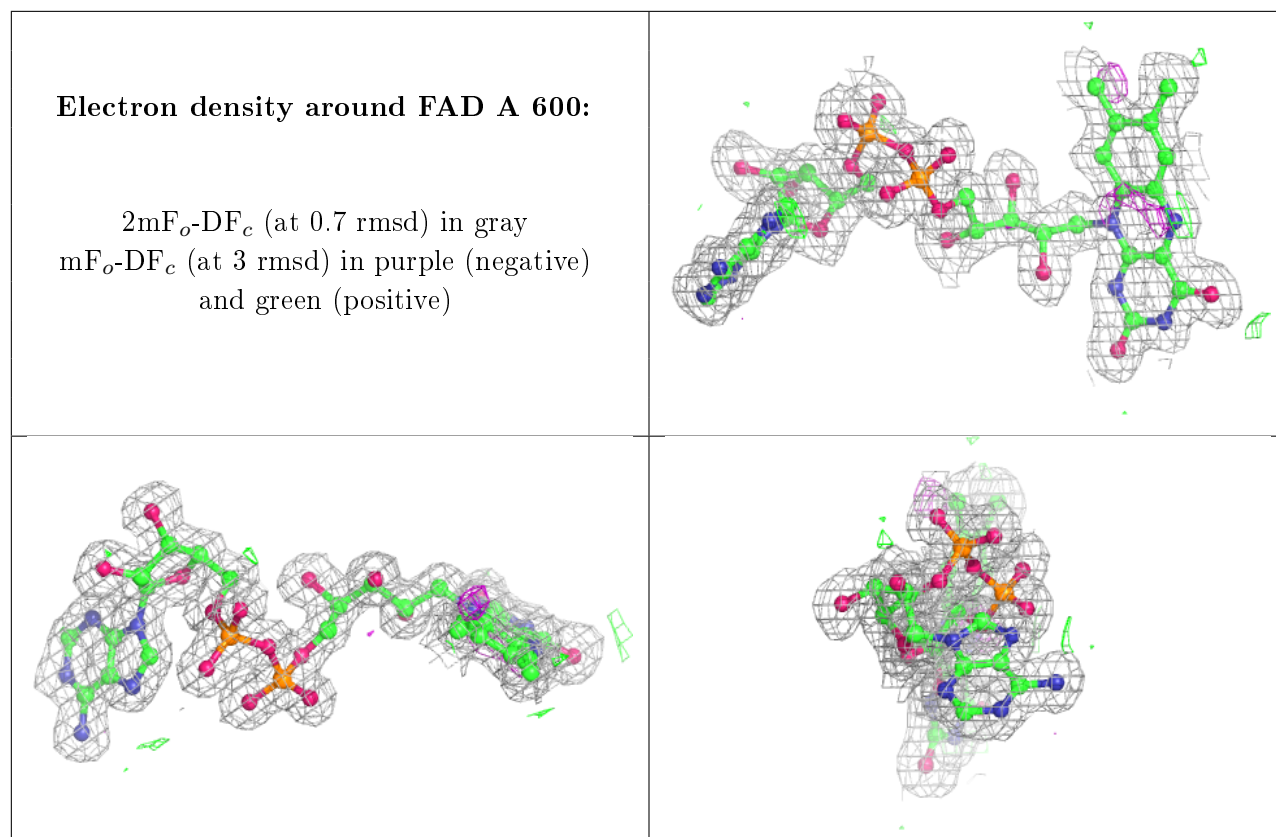
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)

**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 ⓘ

There are no such residues in this entry.