



# Full wwPDB X-ray Structure Validation Report ⓘ

May 15, 2020 – 04:42 pm BST

PDB ID : 2PGO  
Title : The crystal structure of FAD and ThDP dependent Cyclohexane-1,2-dione Hydrolase (Cdh) from *Azoarcus* sp. strain 22Lin  
Authors : Steinbach, A.K.; Warkentin, E.; Kroneck, P.M.H.; Ermler, U.  
Deposited on : 2007-04-10  
Resolution : 1.26 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

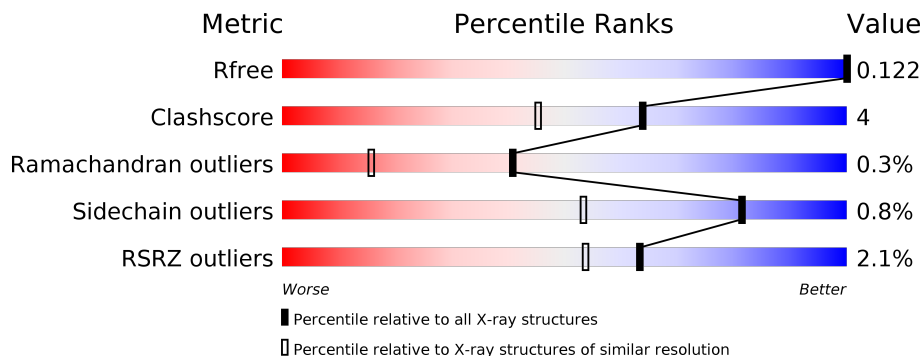
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 1.26 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	1023 (1.28-1.24)
Clashscore	141614	1060 (1.28-1.24)
Ramachandran outliers	138981	1029 (1.28-1.24)
Sidechain outliers	138945	1028 (1.28-1.24)
RSRZ outliers	127900	1004 (1.28-1.24)

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	589	
1	B	589	

## 2 Entry composition [i](#)

There are 8 unique types of molecules in this entry. The entry contains 10640 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 Cyclohexane-1,2-dione Hydrolase (Cdh).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	587	4643	2947	817	855	24	0	46	0
1	B	587	4602	2922	815	843	22	0	39	0

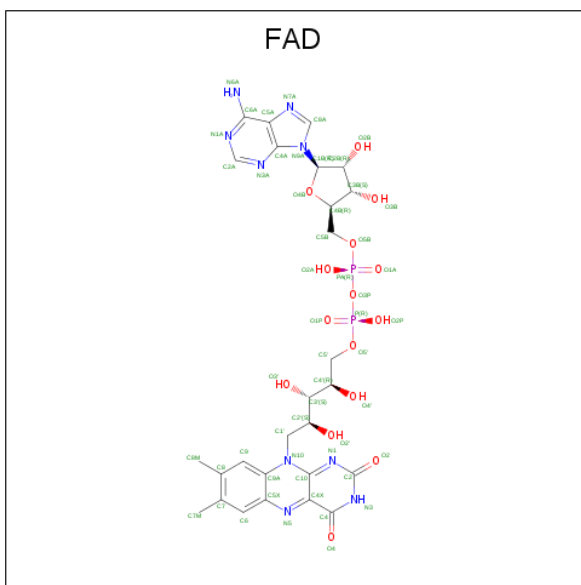
- Molecule 2 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

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

- Molecule 3 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

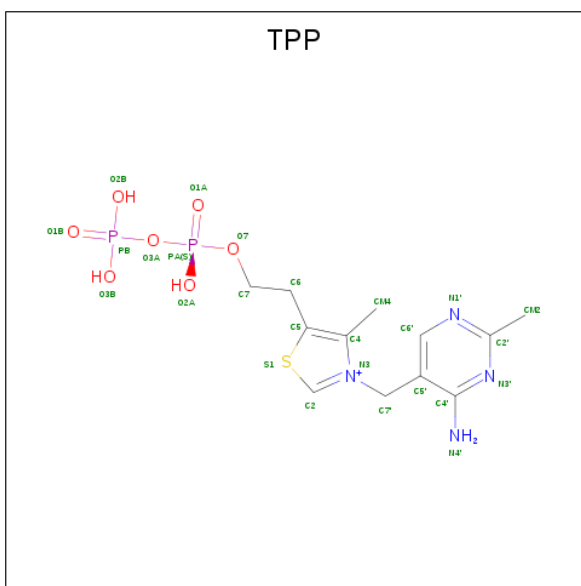
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	B	1	Total	Cl	0	0
			1	1		
3	A	1	Total	Cl	0	0
			1	1		

- Molecule 4 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>).



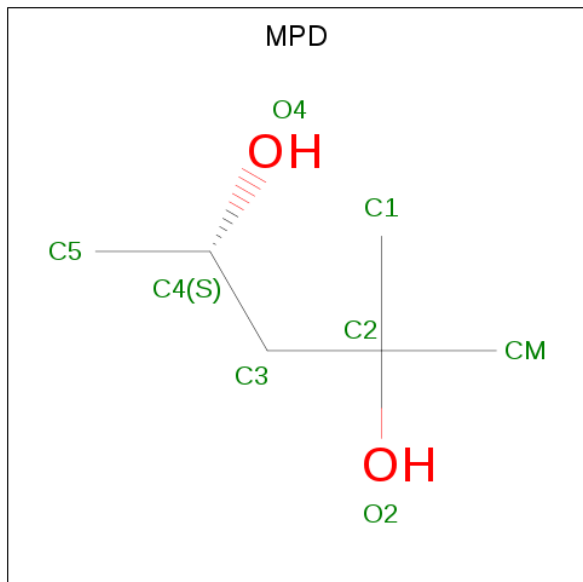
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	
4	A	1	Total	C	N	O	P	0	0
			53	27	9	15	2		
4	B	1	Total	C	N	O	P	0	0
			53	27	9	15	2		

- Molecule 5 is THIAMINE DIPHOSPHATE (three-letter code: TPP) (formula:  $C_{12}H_{19}N_4O_7P_2S$ ).



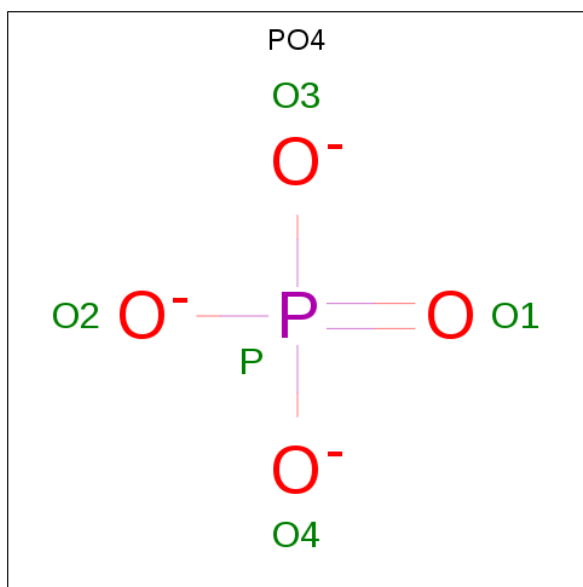
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	
5	A	1	Total	C	N	O	P	S	0	0
			26	12	4	7	2	1		
5	B	1	Total	C	N	O	P	S	0	0
			26	12	4	7	2	1		

- Molecule 6 is (4S)-2-METHYL-2,4-PENTANEDIOL (three-letter code: MPD) (formula:  $C_6H_{14}O_2$ ).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
6	A	1	Total	C	O	0	0
			8	6	2		
6	A	1	Total	C	O	0	0
			8	6	2		

- Molecule 7 is PHOSPHATE ION (three-letter code: PO4) (formula:  $O_4P$ ).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
7	B	1	Total	O	P	0	0
			5	4	1		

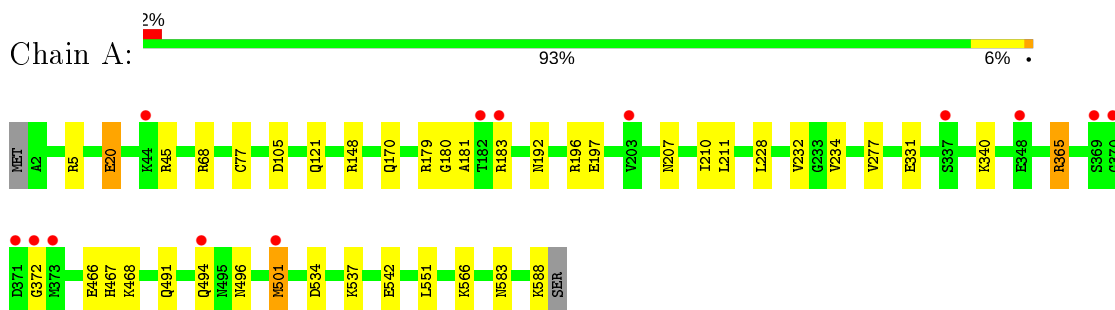
- Molecule 8 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
8	A	588	Total	O	0	0
			588	588		
8	B	624	Total	O	0	1
			624	624		

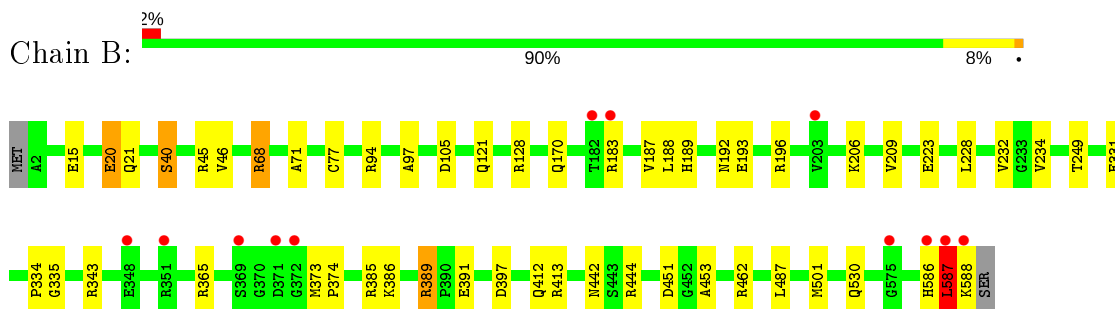
### 3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA and DNA 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: Cyclohexane-1,2-dione Hydrolase (Cdh)



- Molecule 1: Cyclohexane-1,2-dione Hydrolase (Cdh)



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 41 21 2	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	123.60Å 123.60Å 144.30Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	5.00 – 1.26 19.89 – 1.26	Depositor EDS
% Data completeness (in resolution range)	93.2 (5.00-1.26) 93.3 (19.89-1.26)	Depositor EDS
$R_{merge}$	0.06	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	4.86 (at 1.26Å)	Xtrriage
Refinement program	REFMAC 5.2.0005	Depositor
R, $R_{free}$	0.097 , 0.120 0.101 , 0.122	Depositor DCC
$R_{free}$ test set	13765 reflections (4.95%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	7.3	Xtrriage
Anisotropy	0.105	Xtrriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.37 , 57.4	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.32$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
$F_o, F_c$ correlation	0.98	EDS
Total number of atoms	10640	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	9.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.75% 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, CL, PO4, MPD, TPP, 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	0.89	6/4915 (0.1%)	0.93	13/6662 (0.2%)
1	B	0.92	10/4860 (0.2%)	0.96	20/6591 (0.3%)
All	All	0.90	16/9775 (0.2%)	0.94	33/13253 (0.2%)

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
1	B	0	1
All	All	0	2

All (16) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	179	ARG	CG-CD	-7.51	1.33	1.51
1	B	223	GLU	CD-OE2	7.31	1.33	1.25
1	A	20	GLU	CD-OE2	7.21	1.33	1.25
1	B	40[A]	SER	CB-OG	6.50	1.50	1.42
1	B	40[B]	SER	CB-OG	6.50	1.50	1.42
1	B	20	GLU	CB-CG	-6.49	1.39	1.52
1	B	223	GLU	CG-CD	6.24	1.61	1.51
1	B	20	GLU	CD-OE2	6.23	1.32	1.25
1	B	40[A]	SER	CA-CB	6.06	1.62	1.52
1	B	40[B]	SER	CA-CB	6.06	1.62	1.52
1	A	20	GLU	CB-CG	-6.04	1.40	1.52
1	B	386	LYS	CE-NZ	5.86	1.63	1.49
1	A	5	ARG	CB-CG	-5.82	1.36	1.52
1	B	94	ARG	CG-CD	-5.20	1.39	1.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	542	GLU	CG-CD	-5.10	1.44	1.51
1	A	491	GLN	CB-CG	-5.04	1.39	1.52

All (33) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	413	ARG	NE-CZ-NH1	-11.80	114.40	120.30
1	B	68	ARG	NE-CZ-NH1	-9.70	115.45	120.30
1	B	343	ARG	NE-CZ-NH1	9.03	124.81	120.30
1	B	389	ARG	NE-CZ-NH2	-8.69	115.95	120.30
1	B	94	ARG	NE-CZ-NH1	8.43	124.52	120.30
1	B	68	ARG	NE-CZ-NH2	7.57	124.08	120.30
1	A	534	ASP	CB-CG-OD2	-7.51	111.54	118.30
1	A	196[A]	ARG	NE-CZ-NH2	-7.05	116.77	120.30
1	A	196[B]	ARG	NE-CZ-NH2	-7.05	116.77	120.30
1	B	462	ARG	NE-CZ-NH1	-6.89	116.86	120.30
1	B	105	ASP	CB-CG-OD2	-6.58	112.38	118.30
1	A	501[A]	MET	CG-SD-CE	-6.50	89.81	100.20
1	A	501[B]	MET	CG-SD-CE	-6.50	89.81	100.20
1	A	501[C]	MET	CG-SD-CE	-6.50	89.81	100.20
1	B	444	ARG	NE-CZ-NH1	-6.46	117.07	120.30
1	B	343	ARG	NE-CZ-NH2	-6.17	117.22	120.30
1	B	105	ASP	CB-CG-OD1	6.12	123.81	118.30
1	B	385	ARG	NE-CZ-NH1	-5.66	117.47	120.30
1	A	105	ASP	CB-CG-OD1	5.63	123.36	118.30
1	A	588[A]	LYS	CB-CA-C	5.47	121.34	110.40
1	A	588[B]	LYS	CB-CA-C	5.47	121.34	110.40
1	B	365[A]	ARG	NE-CZ-NH2	-5.45	117.58	120.30
1	B	365[B]	ARG	NE-CZ-NH2	-5.45	117.58	120.30
1	A	148	ARG	NE-CZ-NH1	-5.35	117.62	120.30
1	A	534	ASP	CB-CG-OD1	5.30	123.07	118.30
1	B	20	GLU	CG-CD-OE2	5.28	128.86	118.30
1	B	97[A]	ALA	CB-CA-C	-5.14	102.40	110.10
1	B	97[B]	ALA	CB-CA-C	-5.14	102.40	110.10
1	B	209[A]	VAL	CB-CA-C	-5.13	101.64	111.40
1	B	209[B]	VAL	CB-CA-C	-5.13	101.64	111.40
1	B	451	ASP	CB-CG-OD1	-5.09	113.72	118.30
1	A	196[A]	ARG	NE-CZ-NH1	5.04	122.82	120.30
1	A	196[B]	ARG	NE-CZ-NH1	5.04	122.82	120.30

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	372	GLY	Peptide
1	B	587	LEU	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	4643	0	4599	37	2
1	B	4602	0	4582	40	2
2	A	1	0	0	0	0
2	B	1	0	0	0	0
3	A	1	0	0	1	0
3	B	1	0	0	1	0
4	A	53	0	31	0	0
4	B	53	0	31	0	0
5	A	26	0	16	1	0
5	B	26	0	16	1	0
6	A	16	0	28	6	0
7	B	5	0	0	0	0
8	A	588	0	0	16	0
8	B	624	0	0	22	2
All	All	10640	0	9303	79	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 4.

All (79) 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:442[B]:ASN:ND2	8:B:830:HOH:O	1.79	1.04
1:A:331[B]:GLU:OE1	8:A:1169:HOH:O	1.78	1.00
1:B:331[A]:GLU:OE2	8:B:1219:HOH:O	1.79	0.99
1:B:192[A]:ASN:OD1	1:B:196[A]:ARG:NH1	1.96	0.98
1:B:45:ARG:C	8:B:1221:HOH:O	2.04	0.95
6:A:621:MPD:H53	6:A:621:MPD:HM1	1.49	0.95
1:B:334[A]:PRO:O	8:B:1225:HOH:O	1.81	0.95
1:B:20:GLU:OE1	1:B:68:ARG:NH1	2.08	0.87

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:588:LYS:HD3	8:B:1238:HOH:O	1.78	0.83
1:A:232[B]:VAL:HG23	1:A:234[B]:VAL:HG12	1.62	0.82
1:B:15:GLU:OE2	1:B:40[A]:SER:OG	1.99	0.78
1:A:566:LYS:O	8:A:1161:HOH:O	2.03	0.77
1:A:68[B]:ARG:NH1	8:A:1158:HOH:O	2.17	0.77
1:B:442[B]:ASN:ND2	8:B:912:HOH:O	2.15	0.77
1:A:467:HIS:O	1:A:468[A]:LYS:HG2	1.86	0.76
1:A:20:GLU:OE1	8:A:1158:HOH:O	2.03	0.75
1:A:551[B]:LEU:HD23	6:A:620:MPD:HM2	1.72	0.72
1:B:188[B]:LEU:HD11	8:B:1179:HOH:O	1.90	0.71
1:A:551[B]:LEU:CD2	6:A:620:MPD:HM2	2.24	0.68
1:A:192[B]:ASN:ND2	8:A:983:HOH:O	2.27	0.66
1:A:331[A]:GLU:OE1	8:A:1169:HOH:O	2.13	0.65
3:A:611:CL:CL	5:B:615:TPP:H2	2.37	0.62
1:A:494[B]:GLN:HG3	8:A:1036:HOH:O	2.00	0.62
1:B:46:VAL:N	8:B:1221:HOH:O	2.28	0.62
1:A:466[B]:GLU:HG2	1:B:501[B]:MET:HE2	1.82	0.61
1:A:183[B]:ARG:NH1	8:A:867:HOH:O	2.32	0.61
1:A:468[B]:LYS:HE2	1:A:537:LYS:HG2	1.82	0.60
1:A:211[A]:LEU:HD12	1:A:277:VAL:HG13	1.84	0.60
1:B:188[A]:LEU:HD12	1:B:189:HIS:N	2.18	0.59
1:B:232[A]:VAL:HG12	1:B:234:VAL:HG23	1.84	0.58
1:B:588:LYS:CD	8:B:1238:HOH:O	2.44	0.58
6:A:621:MPD:H53	6:A:621:MPD:CM	2.30	0.58
5:A:614:TPP:H2	3:B:610:CL:CL	2.43	0.55
1:B:170[A]:GLN:HG3	8:B:1208:HOH:O	2.05	0.55
1:A:228:LEU:O	1:A:232[B]:VAL:HG22	2.09	0.52
1:A:466[B]:GLU:HG2	1:B:501[B]:MET:CE	2.39	0.52
1:A:232[A]:VAL:HG12	1:A:234[A]:VAL:HG23	1.91	0.51
1:A:232[B]:VAL:HG23	1:A:234[B]:VAL:CG1	2.38	0.51
1:B:128:ARG:HD2	8:B:1223:HOH:O	2.09	0.51
1:B:389:ARG:HD2	8:B:1193:HOH:O	2.10	0.51
1:A:197[A]:GLU:OE1	8:A:880:HOH:O	2.20	0.49
1:B:188[A]:LEU:HD12	1:B:189:HIS:H	1.77	0.49
1:A:365[B]:ARG:NH2	8:A:1111:HOH:O	2.46	0.48
1:A:170[B]:GLN:NE2	8:A:1112:HOH:O	2.46	0.48
1:B:193[A]:GLU:HG3	8:B:1126:HOH:O	2.13	0.47
1:A:207[B]:ASN:ND2	8:A:1038:HOH:O	2.42	0.47
1:B:228:LEU:O	1:B:232[B]:VAL:HG22	2.15	0.47
1:B:187:VAL:O	1:B:189:HIS:CD2	2.67	0.47
1:A:210:ILE:HD11	1:A:234[B]:VAL:HG11	1.97	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:586:HIS:O	1:B:587:LEU:HB2	2.15	0.46
1:A:501[A]:MET:HE2	8:B:825:HOH:O	2.16	0.46
1:A:466[B]:GLU:CG	1:B:501[B]:MET:HE2	2.46	0.45
1:B:192[B]:ASN:ND2	8:B:1075:HOH:O	2.49	0.45
1:B:588:LYS:CE	8:B:1238:HOH:O	2.65	0.44
1:A:181[B]:ALA:HA	8:A:937:HOH:O	2.16	0.44
1:B:391:GLU:OE2	8:B:1155:HOH:O	2.21	0.44
1:A:210:ILE:CD1	1:A:234[B]:VAL:HG11	2.48	0.43
1:A:210:ILE:HD12	1:A:234[B]:VAL:HG13	2.00	0.43
1:B:232[A]:VAL:HG12	1:B:234:VAL:CG2	2.47	0.43
1:A:183[B]:ARG:CZ	8:A:867:HOH:O	2.67	0.42
1:B:232[A]:VAL:HG13	8:B:1050:HOH:O	2.19	0.42
1:B:335[A]:GLY:HA2	8:B:998:HOH:O	2.18	0.42
1:A:551[B]:LEU:CD2	6:A:620:MPD:H31	2.49	0.42
1:B:586:HIS:O	1:B:587:LEU:CB	2.66	0.42
1:B:170[A]:GLN:NE2	8:B:1208:HOH:O	2.51	0.42
1:A:331[B]:GLU:HG2	8:A:1078:HOH:O	2.20	0.41
1:A:551[B]:LEU:HD23	6:A:620:MPD:H31	2.03	0.41
1:B:128:ARG:CD	8:B:1223:HOH:O	2.68	0.41
1:B:397:ASP:CG	1:B:453:ALA:HB1	2.41	0.41
1:B:21:GLN:O	1:B:71:ALA:HA	2.21	0.41
1:A:20:GLU:OE1	1:A:68[A]:ARG:NH1	2.54	0.41
1:B:373:MET:HA	1:B:374:PRO:C	2.42	0.40
1:A:210:ILE:CD1	1:A:234[B]:VAL:CG1	2.99	0.40
1:A:494[A]:GLN:HG3	1:A:496[A]:ASN:ND2	2.36	0.40
1:B:170[A]:GLN:NE2	8:B:1088:HOH:O	2.55	0.40
1:B:249:THR:HG23	1:B:412:GLN:HE22	1.87	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:121:GLN:NE2	1:B:121[A]:GLN:NE2[8_665]	1.59	0.61
1:A:180[B]:GLY:O	8:B:1089:HOH:O[6_455]	1.80	0.40
1:B:442[B]:ASN:OD1	8:B:988:HOH:O[4_554]	2.00	0.20

## 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	631/589 (107%)	621 (98%)	9 (1%)	1 (0%)	47	18
1	B	624/589 (106%)	613 (98%)	9 (1%)	2 (0%)	41	16
All	All	1255/1178 (106%)	1234 (98%)	18 (1%)	3 (0%)	41	18

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	77	CYS
1	B	77	CYS
1	B	587	LEU

### 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	493/453 (109%)	488 (99%)	5 (1%)	76	42
1	B	487/453 (108%)	481 (99%)	6 (1%)	71	35
All	All	980/906 (108%)	969 (99%)	11 (1%)	81	39

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

Mol	Chain	Res	Type
1	A	45	ARG
1	A	340	LYS
1	A	365[A]	ARG

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Mol	Chain	Res	Type
1	A	365[B]	ARG
1	A	583	ASN
1	B	183[A]	ARG
1	B	183[B]	ARG
1	B	206[A]	LYS
1	B	206[B]	LYS
1	B	530[A]	GLN
1	B	530[B]	GLN

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (8) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	116	GLN
1	A	352	GLN
1	A	484	ASN
1	A	583	ASN
1	B	189	HIS
1	B	484	ASN
1	B	491	GLN
1	B	583	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 carbohydrates in this entry.

## 5.6 Ligand geometry [i](#)

Of 11 ligands modelled in this entry, 4 are monoatomic - leaving 7 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	MPD	A	621	-	7,7,7	0.63	0	9,10,10	1.18	1 (11%)
5	TPP	B	615	-	22,27,27	1.46	3 (13%)	29,40,40	1.36	3 (10%)
5	TPP	A	614	-	22,27,27	1.38	5 (22%)	29,40,40	1.56	2 (6%)
7	PO4	B	625	-	4,4,4	0.20	0	6,6,6	0.86	0
6	MPD	A	620	-	7,7,7	0.43	0	9,10,10	0.72	0
4	FAD	A	612	-	51,58,58	1.13	6 (11%)	60,89,89	2.16	5 (8%)
4	FAD	B	613	-	51,58,58	1.12	4 (7%)	60,89,89	1.85	5 (8%)

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	MPD	A	621	-	-	0/5/5/5	-
6	MPD	A	620	-	-	0/5/5/5	-
5	TPP	A	614	-	-	0/16/17/17	0/2/2/2
5	TPP	B	615	-	-	0/16/17/17	0/2/2/2
4	FAD	A	612	-	-	3/30/50/50	0/6/6/6
4	FAD	B	613	-	-	3/30/50/50	0/6/6/6

All (18) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	B	613	FAD	C4X-C10	3.65	1.42	1.38
4	A	612	FAD	C4X-C10	3.61	1.42	1.38
5	B	615	TPP	C4-N3	-3.09	1.37	1.39
5	A	614	TPP	C2-N3	-3.08	1.29	1.36
5	B	615	TPP	C6-C5	-3.02	1.49	1.50
5	B	615	TPP	C4'-N3'	2.85	1.39	1.35
5	A	614	TPP	C6-C5	-2.72	1.49	1.50
4	A	612	FAD	C10-N1	2.55	1.36	1.33
4	B	613	FAD	C9A-N10	2.54	1.41	1.38
5	A	614	TPP	C2'-N1'	2.42	1.38	1.34
4	A	612	FAD	C4-N3	2.31	1.37	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	612	FAD	C2A-N1A	2.24	1.38	1.33
5	A	614	TPP	C4-N3	-2.21	1.37	1.39
4	B	613	FAD	C4-N3	2.19	1.36	1.33
4	A	612	FAD	C5X-N5	2.15	1.38	1.35
4	B	613	FAD	C5X-N5	2.08	1.38	1.35
5	A	614	TPP	C5'-C4'	2.06	1.46	1.42
4	A	612	FAD	O4B-C1B	2.01	1.43	1.41

All (16) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	612	FAD	C4-N3-C2	11.76	125.07	115.14
4	B	613	FAD	C4-N3-C2	10.00	123.59	115.14
4	A	612	FAD	C1'-N10-C9A	7.21	123.97	118.29
4	A	612	FAD	C4X-C4-N3	-6.51	114.52	123.43
5	A	614	TPP	C6-C5-C4	5.81	132.10	127.43
4	B	613	FAD	C4X-C4-N3	-5.42	116.01	123.43
4	B	613	FAD	C1'-N10-C9A	4.41	121.76	118.29
5	B	615	TPP	C6-C5-C4	3.69	130.39	127.43
5	A	614	TPP	C5-C4-N3	3.19	113.95	107.57
5	B	615	TPP	C5-C4-N3	2.84	113.25	107.57
4	A	612	FAD	C5A-C6A-N6A	2.57	124.26	120.35
5	B	615	TPP	CM2-C2'-N1'	2.47	119.86	117.14
4	B	613	FAD	C5X-C9A-N10	2.40	119.45	117.72
6	A	621	MPD	O2-C2-CM	2.35	115.63	108.08
4	B	613	FAD	C4X-N5-C5X	2.31	119.08	116.77
4	A	612	FAD	C1'-N10-C10	-2.28	116.36	118.41

There are no chirality outliers.

All (6) torsion outliers are listed below:

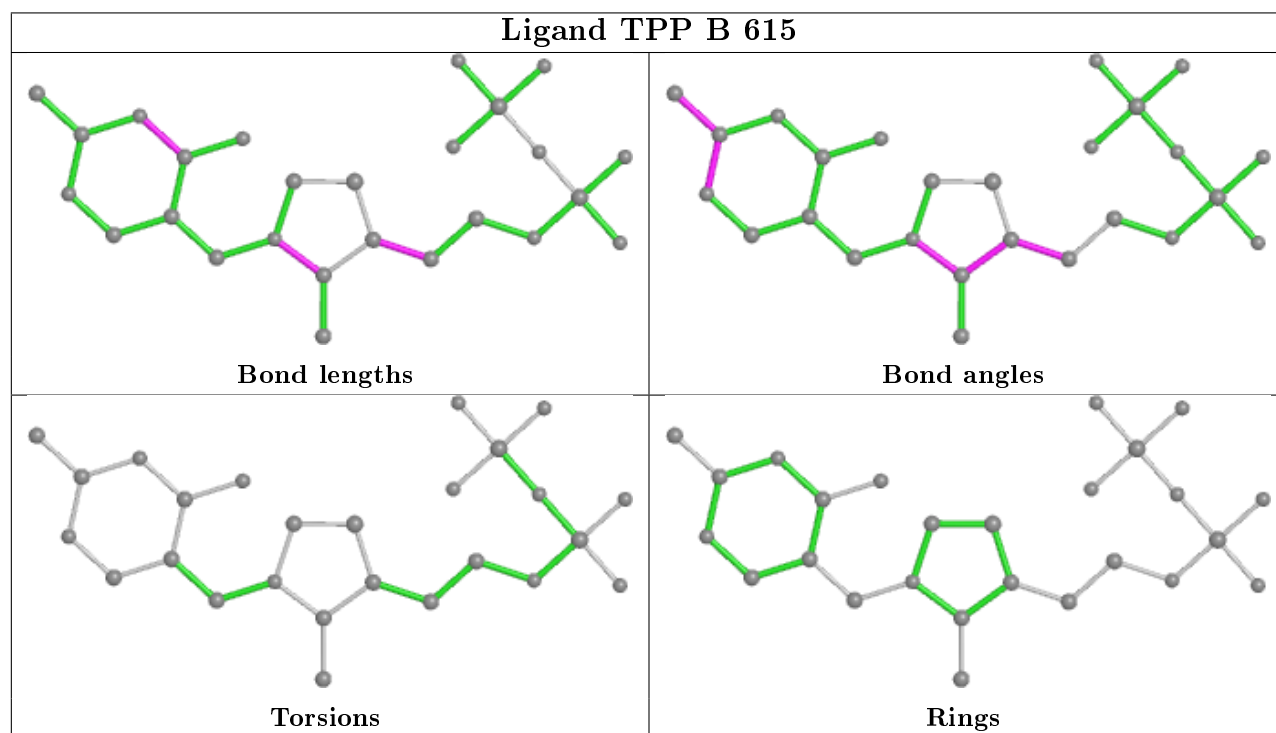
Mol	Chain	Res	Type	Atoms
4	A	612	FAD	PA-O3P-P-O5'
4	B	613	FAD	PA-O3P-P-O5'
4	A	612	FAD	C4B-C5B-O5B-PA
4	B	613	FAD	C4B-C5B-O5B-PA
4	A	612	FAD	O4B-C4B-C5B-O5B
4	B	613	FAD	O4B-C4B-C5B-O5B

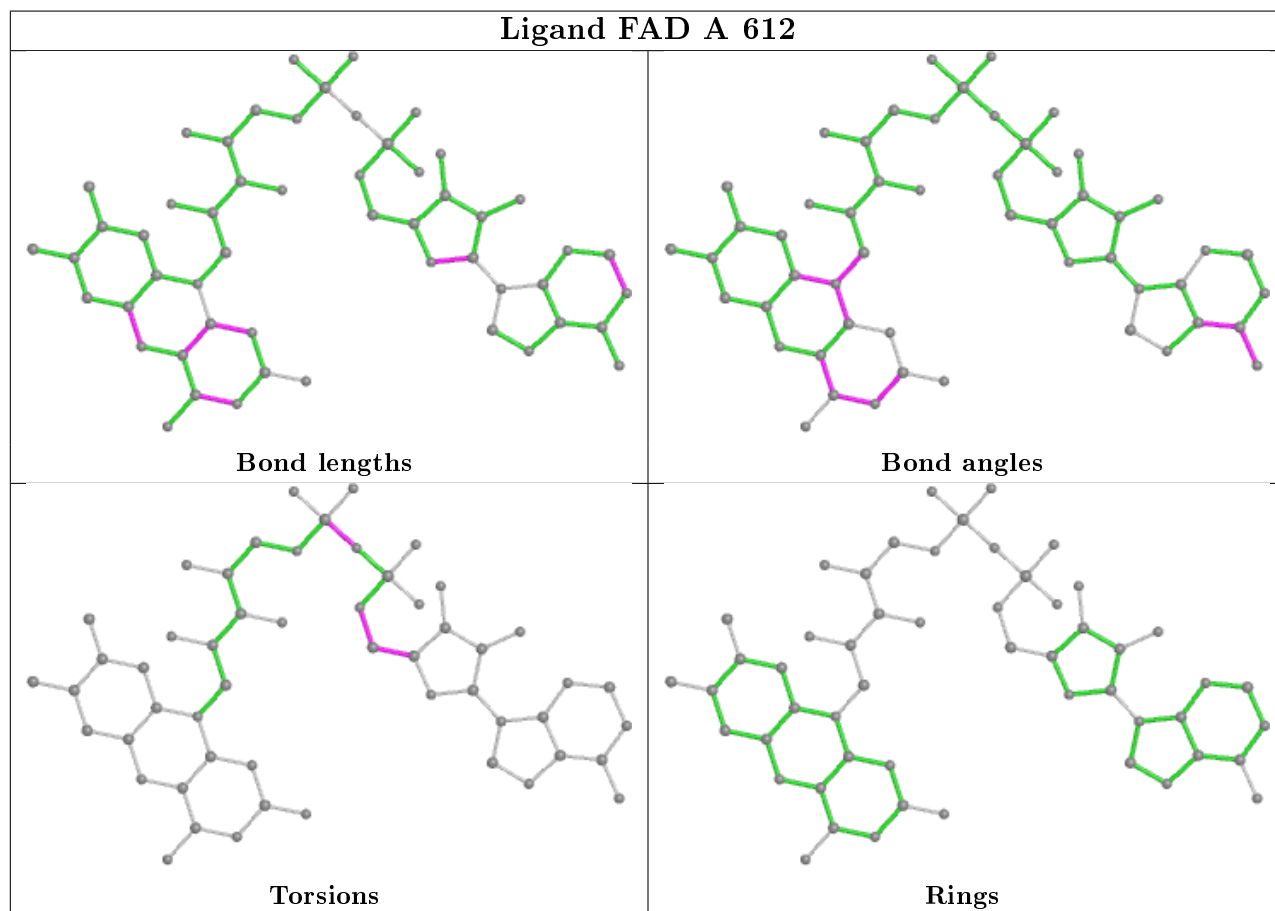
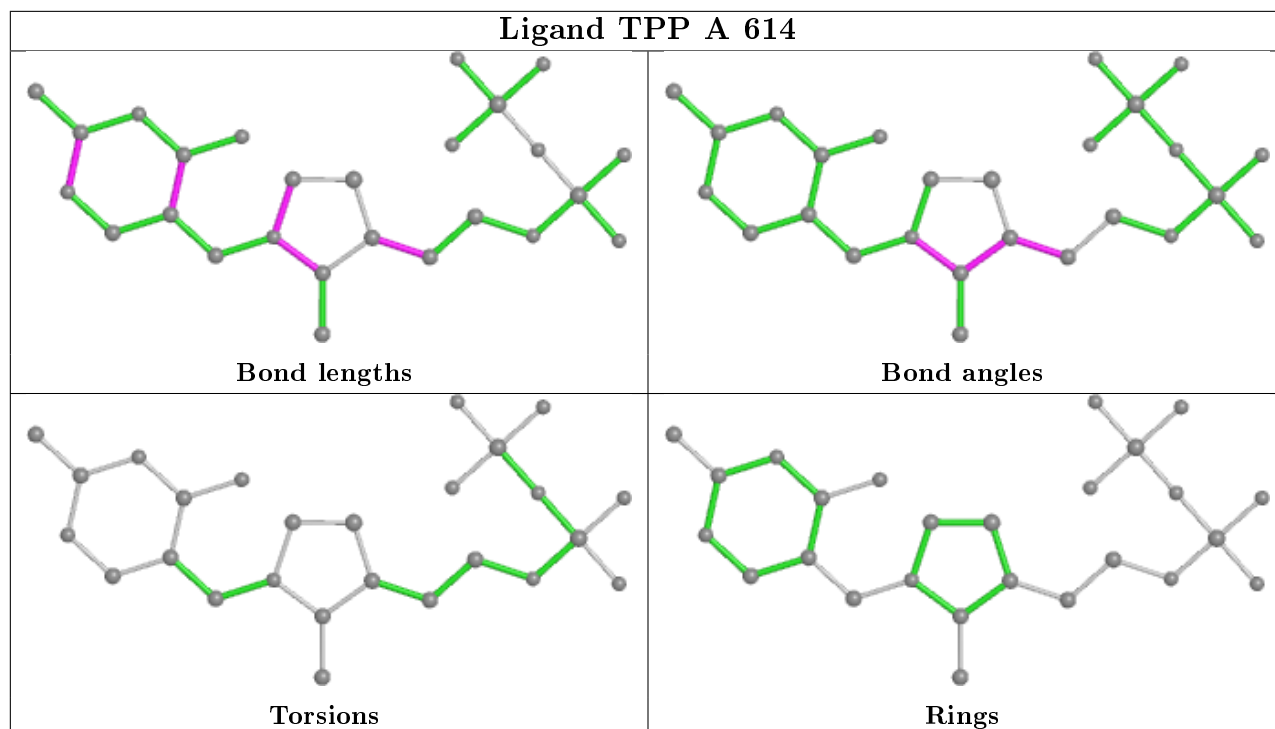
There are no ring outliers.

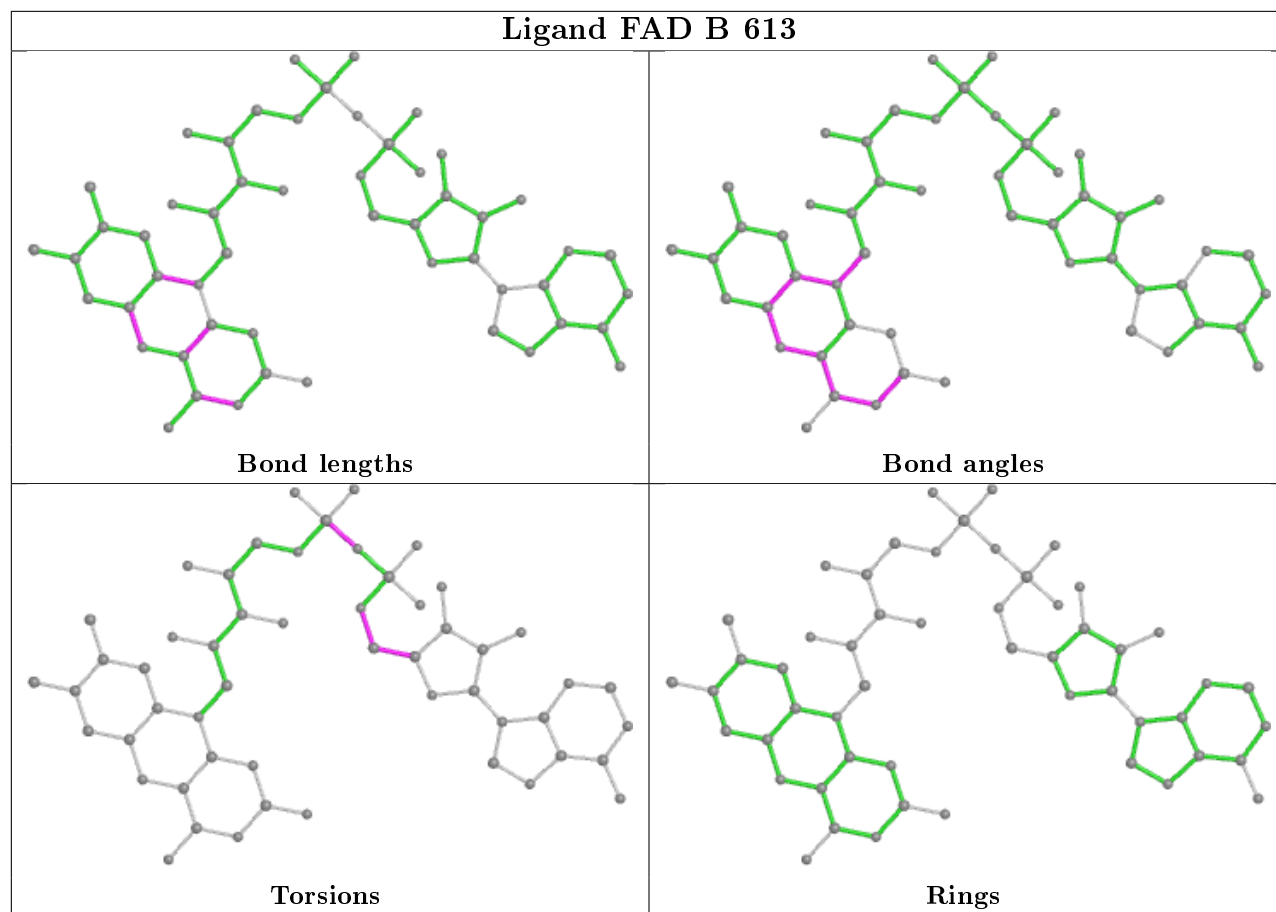
4 monomers are involved in 8 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	A	621	MPD	2	0
5	B	615	TPP	1	0
5	A	614	TPP	1	0
6	A	620	MPD	4	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 [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	587/589 (99%)	-0.52	13 (2%) 62 52	3, 7, 17, 36	2 (0%)
1	B	587/589 (99%)	-0.51	12 (2%) 65 55	4, 7, 17, 44	3 (0%)
All	All	1174/1178 (99%)	-0.52	25 (2%) 63 54	3, 7, 17, 44	5 (0%)

All (25) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	587	LEU	9.4
1	B	588	LYS	8.1
1	A	371	ASP	7.6
1	A	370	GLY	6.0
1	A	369	SER	4.8
1	A	183[A]	ARG	4.8
1	A	372	GLY	4.2
1	A	182[A]	THR	3.8
1	B	183[A]	ARG	3.3
1	A	348	GLU	2.7
1	A	44[A]	LYS	2.7
1	A	501[A]	MET	2.6
1	B	348	GLU	2.6
1	B	372	GLY	2.6
1	B	351	ARG	2.6
1	B	182[A]	THR	2.5
1	B	586	HIS	2.5
1	B	371	ASP	2.5
1	B	575	GLY	2.4
1	A	373	MET	2.4
1	A	203	VAL	2.2
1	A	337	SER	2.1
1	B	203	VAL	2.1
1	A	494[A]	GLN	2.1

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Mol	Chain	Res	Type	RSRZ
1	B	369[A]	SER	2.1

## 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](#)

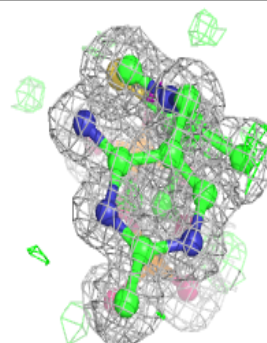
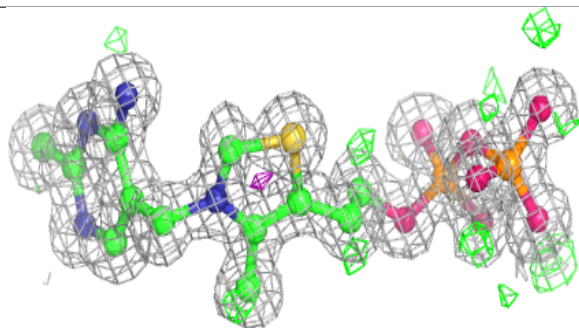
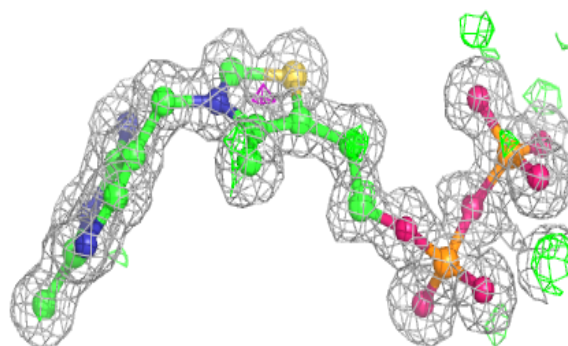
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 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
7	PO4	B	625	5/5	0.85	0.12	13,19,24,24	5
6	MPD	A	621	8/8	0.86	0.17	11,15,22,23	8
6	MPD	A	620	8/8	0.96	0.07	10,14,15,15	0
5	TPP	B	615	26/26	0.99	0.04	3,4,5,8	0
4	FAD	A	612	53/53	0.99	0.04	3,4,5,6	0
5	TPP	A	614	26/26	0.99	0.04	3,4,6,7	0
4	FAD	B	613	53/53	0.99	0.04	3,4,6,6	0
3	CL	A	611	1/1	1.00	0.03	6,6,6,6	0
3	CL	B	610	1/1	1.00	0.01	5,5,5,5	0
2	MG	A	608	1/1	1.00	0.07	3,3,3,3	0
2	MG	B	609	1/1	1.00	0.07	2,2,2,2	0

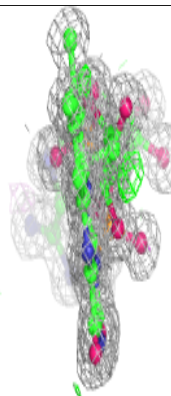
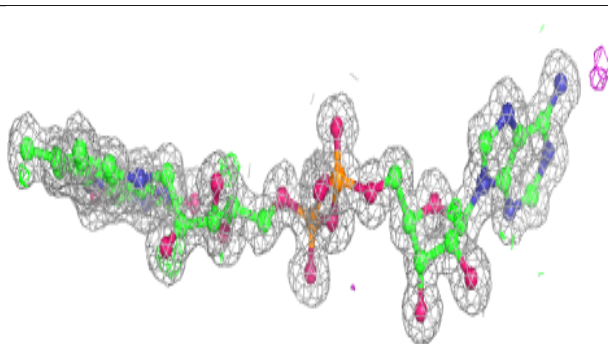
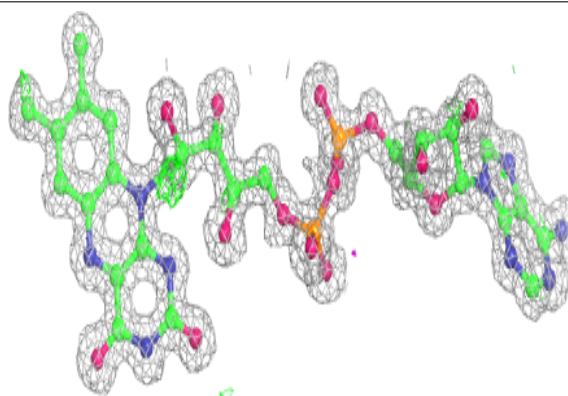
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

**Electron density around TPP B 615:**

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

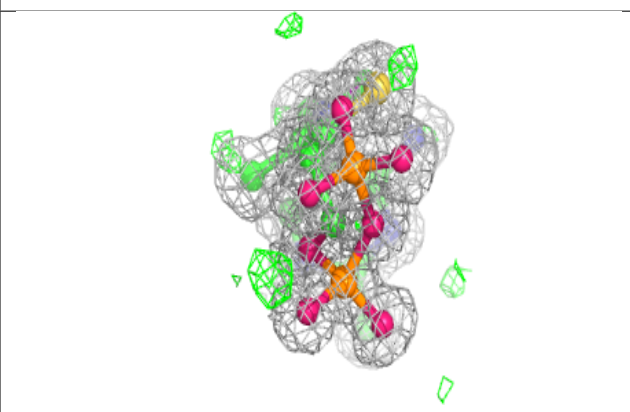
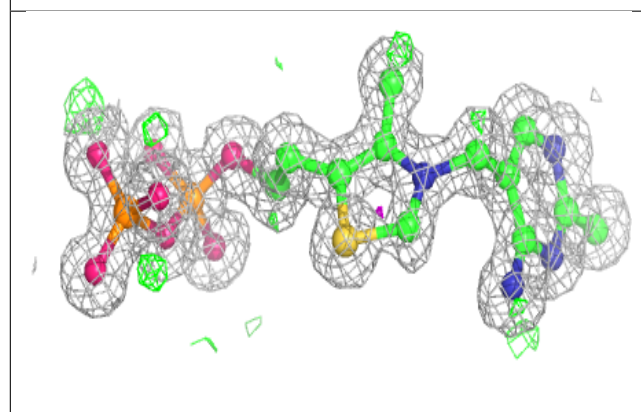
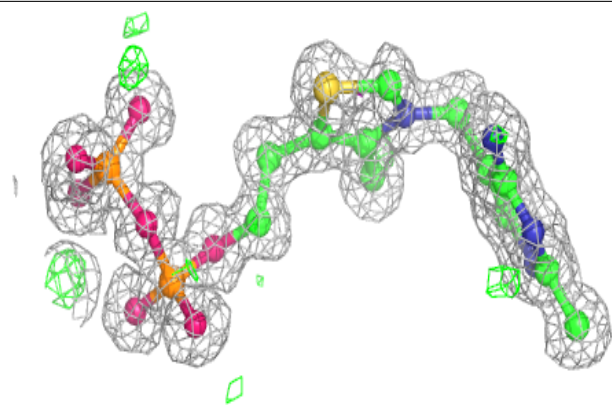
**Electron density around FAD A 612:**

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

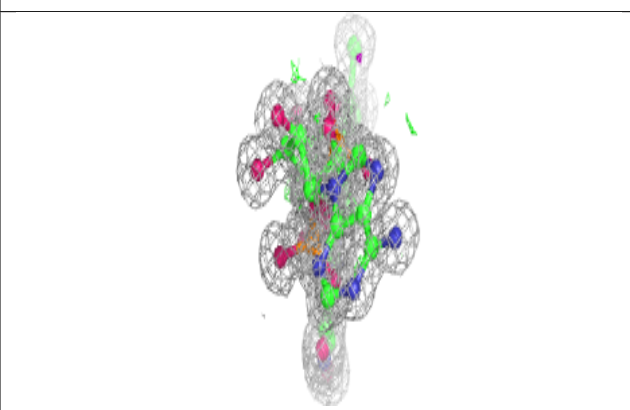
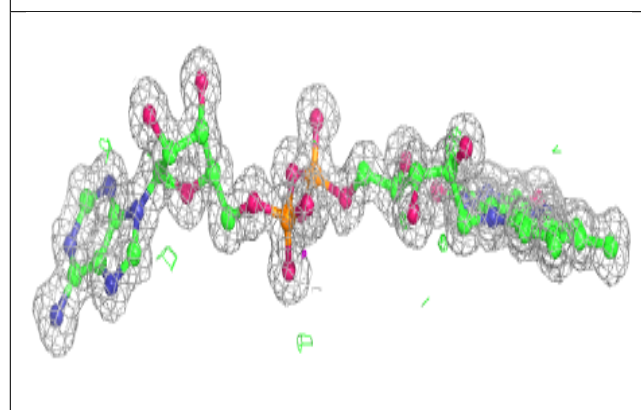
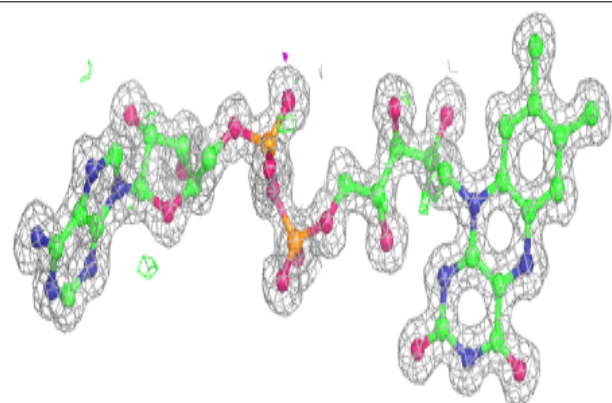


**Electron density around TPP A 614:**

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

**Electron density around FAD B 613:**

$2mF_o-DF_c$  (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.