



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 14, 2026 – 09:48 PM UTC

PDB ID : 1POW / pdb_00001pow
Title : THE REFINED STRUCTURES OF A STABILIZED MUTANT AND OF WILD-TYPE PYRUVATE OXIDASE FROM LACTOBACILLUS PLAN-TARUM
Authors : Muller, Y.A.; Schulz, G.E.
Deposited on : 1993-11-09
Resolution : 2.50 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

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>.

The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

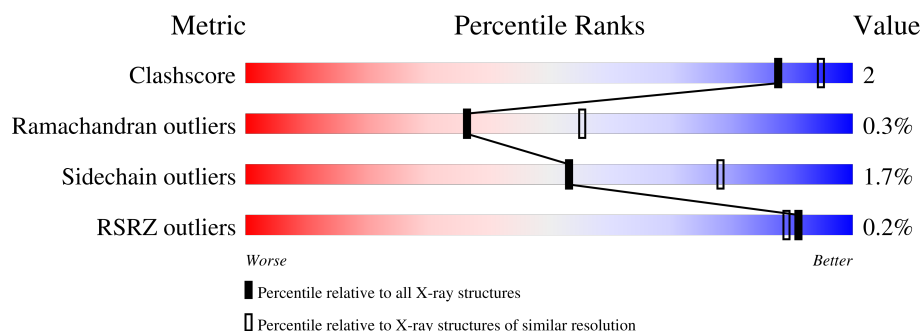
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.50 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))
Clashscore	190562	6492 (2.50-2.50)
Ramachandran outliers	187476	6378 (2.50-2.50)
Sidechain outliers	187428	6380 (2.50-2.50)
RSRZ outliers	180081	5833 (2.50-2.50)

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 ≥ 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	585	 84% 15% .
1	B	585	 85% 14% .

2 Entry composition [i](#)

There are 5 unique types of molecules in this entry. The entry contains 9322 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.

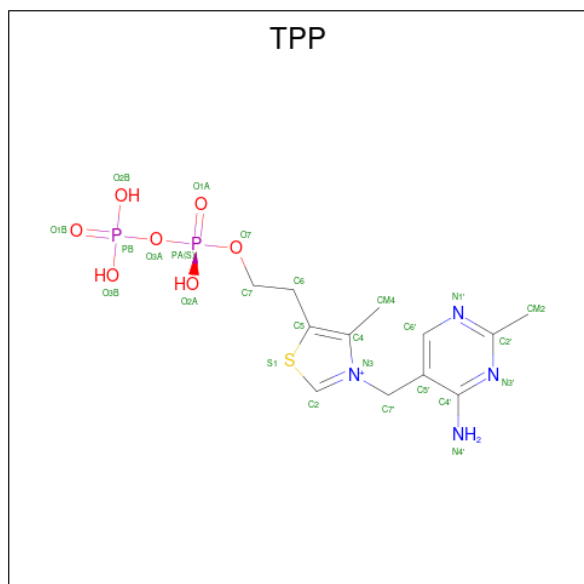
- Molecule 1 is a protein called PYRUVATE OXIDASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	585	Total	C	N	O	S	0	0	0
			4521	2866	779	862	14			
1	B	585	Total	C	N	O	S	0	0	0
			4521	2866	779	862	14			

- Molecule 2 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

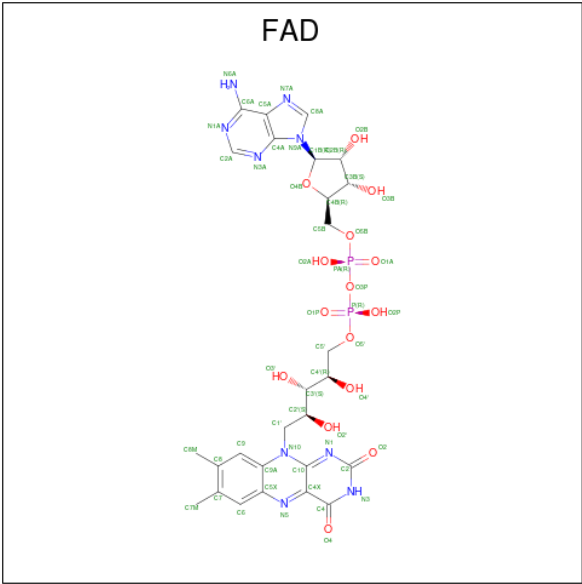
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	1	Total	Mg	0	0
			1	1		
2	B	1	Total	Mg	0	0
			1	1		

- Molecule 3 is THIAMINE DIPHOSPHATE (CCD ID: TPP) (formula: C₁₂H₁₉N₄O₇P₂S).



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

- Molecule 4 is FLAVIN-ADENINE DINUCLEOTIDE (CCD ID: FAD) (formula: C₂₇H₃₃N₉O₁₅P₂).



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		

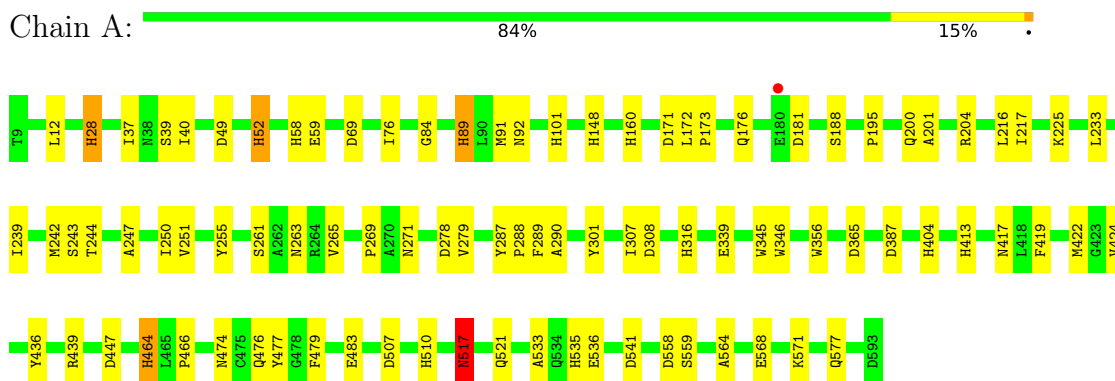
- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	60	Total	O	0	0
			60	60		
5	B	60	Total	O	0	0
			60	60		

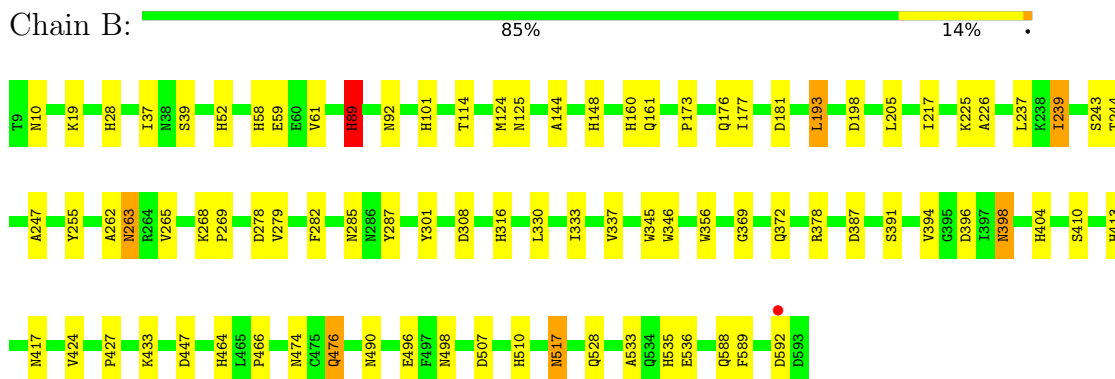
3 Residue-property plots

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: PYRUVATE OXIDASE



• Molecule 1: PYRUVATE OXIDASE



4 Data and refinement statistics

Property	Value	Source
Space group	C 2 2 21	Depositor
Cell constants a, b, c, α , β , γ	121.60Å 155.40Å 167.10Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	10.00 – 2.50 10.00 – 2.50	Depositor EDS
% Data completeness (in resolution range)	(Not available) (10.00-2.50) 90.7 (10.00-2.50)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$	-	Xtriage
Refinement program	X-PLOR	Depositor
R, R_{free}	0.198 , (Not available) 0.177 , (Not available)	Depositor DCC
R_{free} test set	No test flags present.	wwPDB-VP
Wilson B-factor (Å ²)	17.2	Xtriage
Anisotropy	0.137	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.35 , 49.6	EDS
L-test for twinning ¹	$\langle L \rangle = 0.42$, $\langle L^2 \rangle = 0.24$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	9322	wwPDB-VP
Average B, all atoms (Å ²)	12.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.44% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Theoretical 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: TPP, FAD, MG

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	0.82	16/4616 (0.3%)	1.53	49/6284 (0.8%)
1	B	0.82	15/4616 (0.3%)	1.55	61/6284 (1.0%)
All	All	0.82	31/9232 (0.3%)	1.54	110/12568 (0.9%)

All (31) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	89	HIS	CD2-NE2	-7.07	1.30	1.37
1	B	404	HIS	CD2-NE2	-6.97	1.30	1.37
1	B	58	HIS	CD2-NE2	-6.81	1.30	1.37
1	B	89	HIS	CD2-NE2	-6.69	1.30	1.37
1	A	510	HIS	CD2-NE2	-6.68	1.30	1.37
1	B	316	HIS	CD2-NE2	-6.61	1.30	1.37
1	A	58	HIS	CD2-NE2	-6.60	1.30	1.37
1	B	413	HIS	CD2-NE2	-6.59	1.30	1.37
1	B	510	HIS	CD2-NE2	-6.59	1.30	1.37
1	A	52	HIS	CD2-NE2	-6.56	1.30	1.37
1	B	101	HIS	CD2-NE2	-6.51	1.30	1.37
1	A	160	HIS	CD2-NE2	-6.51	1.30	1.37
1	B	52	HIS	CD2-NE2	-6.49	1.30	1.37
1	A	28	HIS	CD2-NE2	-6.42	1.30	1.37
1	B	148	HIS	CD2-NE2	-6.40	1.30	1.37
1	A	404	HIS	CD2-NE2	-6.38	1.30	1.37
1	A	535	HIS	CD2-NE2	-6.27	1.30	1.37
1	B	28	HIS	CD2-NE2	-6.23	1.30	1.37
1	A	101	HIS	CD2-NE2	-6.22	1.31	1.37
1	A	413	HIS	CD2-NE2	-6.21	1.31	1.37
1	B	535	HIS	CD2-NE2	-6.18	1.31	1.37
1	B	464	HIS	CD2-NE2	-6.14	1.31	1.37
1	A	148	HIS	CD2-NE2	-6.12	1.31	1.37
1	A	316	HIS	CD2-NE2	-6.07	1.31	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	464	HIS	CD2-NE2	-6.01	1.31	1.37
1	B	160	HIS	CD2-NE2	-5.85	1.31	1.37
1	B	404	HIS	CG-ND1	-5.51	1.32	1.38
1	A	89	HIS	CG-ND1	-5.47	1.32	1.38
1	B	316	HIS	CG-ND1	-5.19	1.32	1.38
1	A	37	ILE	CA-CB	5.10	1.61	1.54
1	A	404	HIS	CG-ND1	-5.05	1.32	1.38

All (110) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	474	ASN	CA-CB-CG	11.16	123.76	112.60
1	A	474	ASN	CA-CB-CG	10.22	122.82	112.60
1	B	447	ASP	CA-CB-CG	9.27	121.87	112.60
1	A	265	VAL	N-CA-C	-9.09	96.48	106.21
1	A	447	ASP	CA-CB-CG	8.81	121.41	112.60
1	B	278	ASP	CA-CB-CG	8.18	120.78	112.60
1	B	308	ASP	CA-CB-CG	8.00	120.60	112.60
1	A	476	GLN	OE1-CD-NE2	-7.45	115.15	122.60
1	B	198	ASP	CA-CB-CG	7.40	120.00	112.60
1	A	417	ASN	N-CA-C	7.13	120.09	111.82
1	A	517	ASN	OD1-CG-ND2	-7.09	115.51	122.60
1	B	417	ASN	N-CA-C	7.04	118.61	111.07
1	A	92	ASN	OD1-CG-ND2	-6.74	115.86	122.60
1	B	285	ASN	CA-CB-CG	6.69	119.29	112.60
1	B	417	ASN	CA-CB-CG	6.63	119.23	112.60
1	B	92	ASN	OD1-CG-ND2	-6.58	116.02	122.60
1	B	282	PHE	CA-CB-CG	6.51	120.31	113.80
1	B	447	ASP	N-CA-C	6.41	119.09	111.33
1	A	558	ASP	CA-CB-CG	6.34	118.94	112.60
1	B	387	ASP	CA-CB-CG	6.34	118.94	112.60
1	A	510	HIS	CB-CG-CD2	-6.31	123.00	131.20
1	B	476	GLN	OE1-CD-NE2	-6.30	116.30	122.60
1	B	10	ASN	OD1-CG-ND2	-6.21	116.39	122.60
1	B	510	HIS	CB-CG-CD2	-6.17	123.17	131.20
1	A	49	ASP	CA-CB-CG	6.16	118.76	112.60
1	A	308	ASP	CA-CB-CG	6.08	118.68	112.60
1	A	419	PHE	N-CA-C	-5.99	104.33	111.69
1	B	589	PHE	CA-CB-CG	-5.99	107.81	113.80
1	B	101	HIS	CB-CG-CD2	-5.97	123.44	131.20
1	B	490	ASN	OD1-CG-ND2	-5.96	116.64	122.60
1	A	477	TYR	N-CA-C	-5.88	97.59	108.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	365	ASP	N-CA-C	5.88	119.51	112.93
1	B	507	ASP	CA-CB-CG	5.87	118.47	112.60
1	A	251	VAL	N-CA-C	-5.84	100.07	108.48
1	B	372	GLN	OE1-CD-NE2	-5.80	116.80	122.60
1	B	396	ASP	CA-CB-CG	5.79	118.39	112.60
1	A	507	ASP	CA-CB-CG	5.79	118.39	112.60
1	B	346	TRP	CG-CD2-CE3	5.78	139.68	133.90
1	A	290	ALA	N-CA-C	5.78	118.07	111.02
1	B	474	ASN	OD1-CG-ND2	-5.77	116.83	122.60
1	B	424	VAL	N-CA-C	5.71	120.42	113.00
1	A	422	MET	N-CA-C	-5.71	103.00	110.53
1	A	278	ASP	CA-CB-CG	5.67	118.27	112.60
1	B	176	GLN	OE1-CD-NE2	-5.66	116.94	122.60
1	A	521	GLN	OE1-CD-NE2	-5.64	116.96	122.60
1	B	193	LEU	N-CA-C	-5.63	99.35	108.41
1	A	517	ASN	CB-CG-ND2	5.61	124.82	116.40
1	A	200	GLN	OE1-CD-NE2	-5.61	116.99	122.60
1	B	356	TRP	CG-CD2-CE3	5.60	139.50	133.90
1	A	424	VAL	N-CA-C	5.59	119.94	111.89
1	A	271	ASN	OD1-CG-ND2	-5.57	117.03	122.60
1	A	101	HIS	CB-CG-CD2	-5.57	123.96	131.20
1	A	91	MET	N-CA-C	5.55	120.53	111.37
1	A	255	TYR	CA-C-N	5.54	125.90	119.47
1	A	255	TYR	C-N-CA	5.54	125.90	119.47
1	B	265	VAL	N-CA-C	-5.54	97.81	109.34
1	A	58	HIS	CB-CG-CD2	-5.51	124.03	131.20
1	A	171	ASP	CA-CB-CG	5.51	118.11	112.60
1	B	19	LYS	CA-CB-CG	-5.51	103.09	114.10
1	B	592	ASP	CA-CB-CG	5.51	118.11	112.60
1	A	84	GLY	CA-C-N	5.47	125.29	119.28
1	A	84	GLY	C-N-CA	5.47	125.29	119.28
1	B	255	TYR	CA-C-N	5.47	125.14	119.56
1	B	255	TYR	C-N-CA	5.47	125.14	119.56
1	B	308	ASP	CA-C-N	5.45	125.53	119.32
1	B	308	ASP	C-N-CA	5.45	125.53	119.32
1	A	181	ASP	CA-CB-CG	5.41	118.01	112.60
1	B	181	ASP	CA-CB-CG	5.37	117.97	112.60
1	B	125	ASN	OD1-CG-ND2	-5.37	117.23	122.60
1	B	244	THR	N-CA-C	-5.36	103.31	110.55
1	A	52	HIS	CB-CG-CD2	-5.36	124.24	131.20
1	A	541	ASP	CA-CB-CG	5.36	117.96	112.60
1	B	378	ARG	N-CA-C	-5.35	105.53	111.36

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	413	HIS	CA-CB-CG	5.34	119.14	113.80
1	A	346	TRP	CG-CD2-CE3	5.31	139.21	133.90
1	B	262	ALA	CA-C-N	5.30	131.66	121.54
1	B	262	ALA	C-N-CA	5.30	131.66	121.54
1	B	528	GLN	OE1-CD-NE2	-5.30	117.30	122.60
1	B	398	ASN	CB-CG-ND2	5.29	124.33	116.40
1	A	476	GLN	CG-CD-NE2	5.25	124.28	116.40
1	B	346	TRP	CB-CG-CD1	-5.25	119.03	126.90
1	A	239	ILE	CA-C-O	-5.24	116.26	119.51
1	B	517	ASN	OD1-CG-ND2	-5.24	117.36	122.60
1	B	345	TRP	CG-CD2-CE3	5.24	139.14	133.90
1	B	356	TRP	CB-CG-CD1	-5.21	119.08	126.90
1	B	369	GLY	CA-C-N	5.20	125.36	119.90
1	B	369	GLY	C-N-CA	5.20	125.36	119.90
1	B	391	SER	N-CA-C	-5.20	100.26	108.73
1	A	345	TRP	CG-CD2-CE3	5.19	139.09	133.90
1	A	76	ILE	N-CA-C	5.19	116.37	109.37
1	A	217	ILE	N-CA-C	-5.19	100.85	108.11
1	A	40	ILE	N-CA-C	-5.18	105.36	111.00
1	B	10	ASN	CB-CG-ND2	5.14	124.11	116.40
1	B	316	HIS	CB-CG-CD2	-5.14	124.52	131.20
1	A	316	HIS	CB-CG-CD2	-5.12	124.54	131.20
1	B	398	ASN	OD1-CG-ND2	-5.08	117.52	122.60
1	A	356	TRP	CE2-CD2-CG	-5.06	101.12	107.20
1	A	346	TRP	CE2-CD2-CG	-5.06	101.13	107.20
1	B	356	TRP	CE2-CD2-CG	-5.04	101.15	107.20
1	A	69	ASP	CA-CB-CG	5.04	117.64	112.60
1	B	588	GLN	OE1-CD-NE2	-5.04	117.56	122.60
1	B	239	ILE	CA-C-N	5.02	124.95	119.78
1	B	239	ILE	C-N-CA	5.02	124.95	119.78
1	B	161	GLN	OE1-CD-NE2	-5.02	117.58	122.60
1	A	387	ASP	CA-CB-CG	5.02	117.62	112.60
1	B	345	TRP	CE2-CD2-CG	-5.02	101.18	107.20
1	A	181	ASP	N-CA-C	5.01	118.55	112.23
1	A	244	THR	N-CA-C	-5.01	103.79	110.55
1	B	404	HIS	CB-CG-CD2	-5.00	124.69	131.20
1	B	28	HIS	CB-CG-CD2	-5.00	124.70	131.20

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	4521	0	4467	19	0
1	B	4521	0	4467	17	0
2	A	1	0	0	0	0
2	B	1	0	0	0	0
3	A	26	0	16	0	0
3	B	26	0	16	0	0
4	A	53	0	31	0	0
4	B	53	0	31	0	0
5	A	60	0	0	0	0
5	B	60	0	0	0	0
All	All	9322	0	9028	36	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 2.

All (36) 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:205:LEU:HD23	1:B:333:ILE:HD11	1.80	0.63
1:A:436:TYR:HB3	1:A:439:ARG:HG3	1.83	0.59
1:A:39:SER:HB2	1:A:173:PRO:HB2	1.86	0.58
1:A:243:SER:HB2	1:A:247:ALA:HB3	1.86	0.57
1:A:195:PRO:HD2	1:A:307:ILE:HD11	1.90	0.54
1:B:237:LEU:HD21	1:B:337:VAL:HB	1.91	0.53
1:A:12:LEU:HD23	1:A:176:GLN:HG2	1.90	0.52
1:A:216:LEU:HD13	1:A:242:MET:SD	2.49	0.51
1:B:533:ALA:HA	1:B:536:GLU:O	2.11	0.50
1:A:464:HIS:O	1:A:466:PRO:HD3	2.12	0.50
1:B:59:GLU:HB2	1:B:89:HIS:HB3	1.93	0.49
1:B:279:VAL:HG22	1:B:301:TYR:HB2	1.94	0.49
1:A:279:VAL:HG22	1:A:301:TYR:HB2	1.95	0.47
1:B:476:GLN:HG2	1:B:496:GLU:HG2	1.96	0.47
1:B:61:VAL:HG13	1:B:427:PRO:HB3	1.96	0.47
1:B:39:SER:HB2	1:B:173:PRO:HB2	1.96	0.47
1:A:59:GLU:HB2	1:A:89:HIS:HB3	1.96	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:243:SER:HB2	1:B:247:ALA:HB3	1.97	0.46
1:A:564:ALA:O	1:A:568:GLU:HG2	2.16	0.46
1:B:433:LYS:HE2	1:B:466:PRO:HD2	1.99	0.45
1:A:28:HIS:HA	1:A:52:HIS:O	2.17	0.44
1:B:144:ALA:HA	1:B:177:ILE:HG21	1.98	0.44
1:B:268:LYS:HB3	1:B:269:PRO:HD3	1.99	0.44
1:A:571:LYS:HD3	1:A:577:GLN:HA	2.00	0.44
1:A:533:ALA:HA	1:A:536:GLU:O	2.19	0.43
1:A:287:TYR:HA	1:A:288:PRO:HD2	1.95	0.42
1:A:172:LEU:HB2	1:A:173:PRO:HD3	2.01	0.42
1:A:201:ALA:HA	1:A:204:ARG:HH11	1.83	0.42
1:A:247:ALA:HB1	1:A:250:ILE:HD12	2.01	0.42
1:B:226:ALA:HB1	1:B:330:LEU:HD12	2.01	0.42
1:A:479:PHE:O	1:A:483:GLU:HG3	2.20	0.42
1:B:263:ASN:HB2	1:B:287:TYR:OH	2.20	0.41
1:B:394:VAL:HA	1:B:398:ASN:OD1	2.20	0.41
1:B:124:MET:HE2	1:B:124:MET:HB3	1.91	0.41
1:A:287:TYR:CZ	1:A:289:PHE:HB2	2.56	0.40
1:B:217:ILE:HG13	1:B:239:ILE:HG21	2.03	0.40

There are no symmetry-related clashes.

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	583/585 (100%)	568 (97%)	13 (2%)	2 (0%)	36	55
1	B	583/585 (100%)	565 (97%)	17 (3%)	1 (0%)	43	63
All	All	1166/1170 (100%)	1133 (97%)	30 (3%)	3 (0%)	36	55

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	263	ASN
1	A	263	ASN
1	A	517	ASN

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	470/470 (100%)	462 (98%)	8 (2%)	53	78
1	B	470/470 (100%)	462 (98%)	8 (2%)	53	78
All	All	940/940 (100%)	924 (98%)	16 (2%)	53	78

All (16) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	188	SER
1	A	225	LYS
1	A	233	LEU
1	A	261	SER
1	A	269	PRO
1	A	339	GLU
1	A	517	ASN
1	A	559	SER
1	B	37	ILE
1	B	89	HIS
1	B	114	THR
1	B	193	LEU
1	B	225	LYS
1	B	410	SER
1	B	498	ASN
1	B	517	ASN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (21) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	10	ASN
1	A	200	GLN
1	A	267	GLN
1	A	298	ASN
1	A	316	HIS
1	A	336	GLN
1	A	347	GLN
1	A	443	ASN
1	A	460	GLN
1	A	469	ASN
1	A	512	GLN
1	A	517	ASN
1	A	528	GLN
1	B	52	HIS
1	B	175	GLN
1	B	176	GLN
1	B	187	ASN
1	B	336	GLN
1	B	417	ASN
1	B	512	GLN
1	B	517	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 oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 6 ligands modelled in this entry, 2 are monoatomic - leaving 4 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The

Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
3	TPP	B	611	2	26,27,27	1.55	6 (23%)	38,40,40	1.71	5 (13%)
4	FAD	A	612	-	58,58,58	1.03	2 (3%)	85,89,89	1.19	10 (11%)
4	FAD	B	612	-	58,58,58	1.09	4 (6%)	85,89,89	1.25	11 (12%)
3	TPP	A	611	2	26,27,27	1.65	8 (30%)	38,40,40	1.80	6 (15%)

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	TPP	B	611	2	-	2/17/17/17	0/2/2/2
4	FAD	A	612	-	-	2/34/50/50	0/6/6/6
4	FAD	B	612	-	-	2/34/50/50	0/6/6/6
3	TPP	A	611	2	-	3/17/17/17	0/2/2/2

All (20) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	611	TPP	C4-N3	-3.36	1.33	1.39
3	B	611	TPP	C2-S1	2.86	1.77	1.69
3	A	611	TPP	PA-O3A	2.83	1.62	1.59
3	B	611	TPP	C4-N3	-2.82	1.34	1.39
3	A	611	TPP	C2-S1	2.75	1.77	1.69
3	A	611	TPP	PB-O2B	-2.73	1.44	1.54
4	B	612	FAD	PA-O3P	2.71	1.62	1.59
4	B	612	FAD	C5X-N5	-2.60	1.34	1.39
3	B	611	TPP	PB-O3B	-2.58	1.45	1.54
3	B	611	TPP	PB-O2B	-2.56	1.45	1.54
3	B	611	TPP	C7'-C5'	2.37	1.55	1.51
3	A	611	TPP	PB-O3B	-2.34	1.46	1.54
4	A	612	FAD	C5X-N5	-2.23	1.35	1.39
3	A	611	TPP	PA-O2A	-2.21	1.45	1.55
3	A	611	TPP	C7'-C5'	2.20	1.55	1.51
4	A	612	FAD	C5A-C4A	2.13	1.42	1.39
4	B	612	FAD	P-O2P	-2.13	1.45	1.55

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	B	612	FAD	PA-O5B	-2.10	1.51	1.59
3	A	611	TPP	PA-O7	-2.03	1.51	1.59
3	B	611	TPP	PA-O2A	-2.03	1.46	1.55

All (32) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	611	TPP	C2-S1-C5	-7.42	86.30	91.22
3	B	611	TPP	C2-S1-C5	-6.81	86.71	91.22
3	A	611	TPP	C6'-N1'-C2'	3.54	121.89	116.07
3	B	611	TPP	C6'-N1'-C2'	3.54	121.89	116.07
4	A	612	FAD	C5A-C4A-N3A	-3.21	122.30	126.72
3	B	611	TPP	C5'-C6'-N1'	-2.99	118.97	123.83
3	A	611	TPP	N1'-C2'-N3'	-2.98	120.57	125.53
4	B	612	FAD	N3A-C2A-N1A	2.97	133.08	128.58
4	A	612	FAD	O4B-C1B-C2B	-2.90	100.40	106.62
4	B	612	FAD	C1'-C2'-C3'	2.70	116.99	109.66
3	A	611	TPP	C5'-C6'-N1'	-2.64	119.53	123.83
4	A	612	FAD	O2A-PA-O3P	2.64	114.42	107.27
4	B	612	FAD	O4B-C1B-C2B	-2.61	101.03	106.62
4	B	612	FAD	C5A-C4A-N3A	-2.60	123.13	126.72
4	A	612	FAD	O2-C2-N1	-2.59	117.50	121.80
4	B	612	FAD	C4-N3-C2	-2.56	121.10	125.64
3	B	611	TPP	N1'-C2'-N3'	-2.40	121.53	125.53
4	A	612	FAD	C4-N3-C2	-2.35	121.48	125.64
4	B	612	FAD	C6A-C5A-C4A	2.32	120.35	117.18
4	A	612	FAD	C4A-C5A-N7A	-2.31	107.95	110.58
4	B	612	FAD	C4X-C10-N1	-2.29	118.97	124.59
3	A	611	TPP	CM2-C2'-N1'	2.25	119.60	117.20
4	A	612	FAD	N3A-C4A-N9A	2.25	130.99	127.17
4	A	612	FAD	C4X-C10-N10	2.17	119.59	116.48
4	A	612	FAD	N3A-C2A-N1A	2.14	131.82	128.58
4	B	612	FAD	C4X-C10-N10	2.08	119.45	116.48
3	B	611	TPP	CM2-C2'-N3'	2.06	120.21	117.13
4	B	612	FAD	N3A-C4A-N9A	2.05	130.65	127.17
3	A	611	TPP	C2'-N3'-C4'	2.05	121.24	118.10
4	A	612	FAD	C6A-C5A-C4A	2.04	119.97	117.18
4	B	612	FAD	N6A-C6A-N1A	2.03	122.91	118.38
4	B	612	FAD	C4A-C5A-N7A	-2.02	108.28	110.58

There are no chirality outliers.

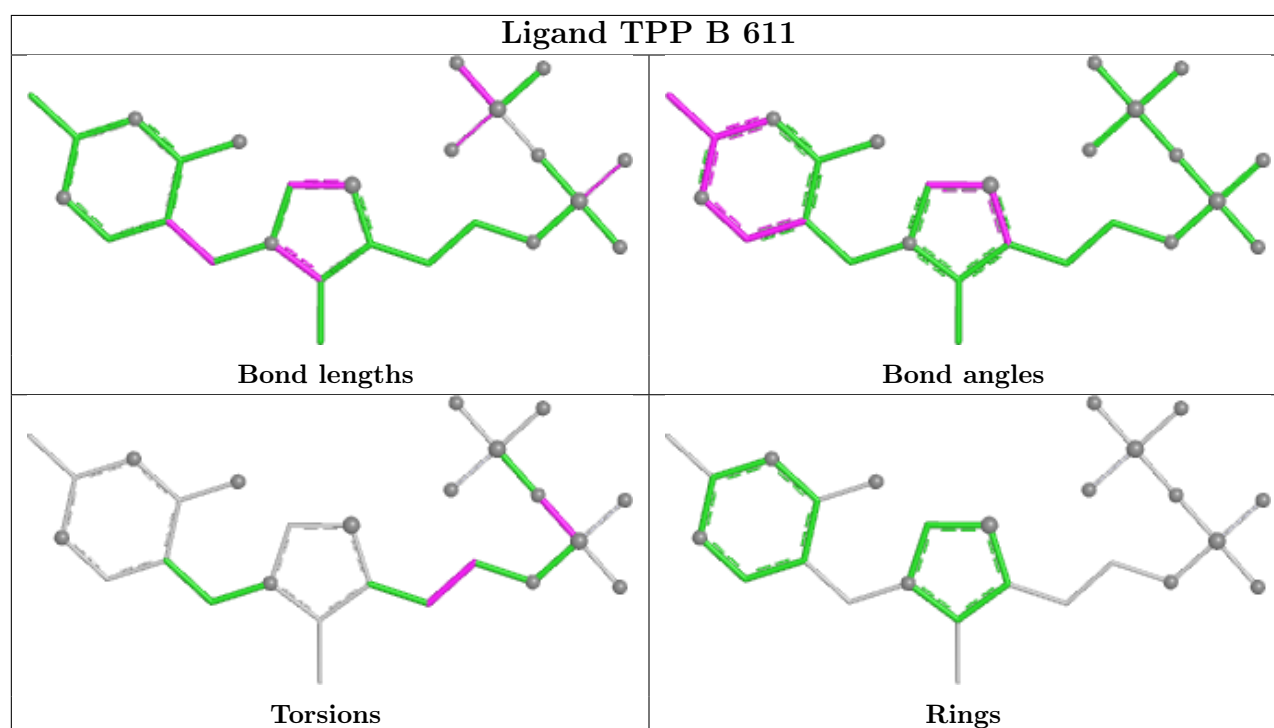
All (9) torsion outliers are listed below:

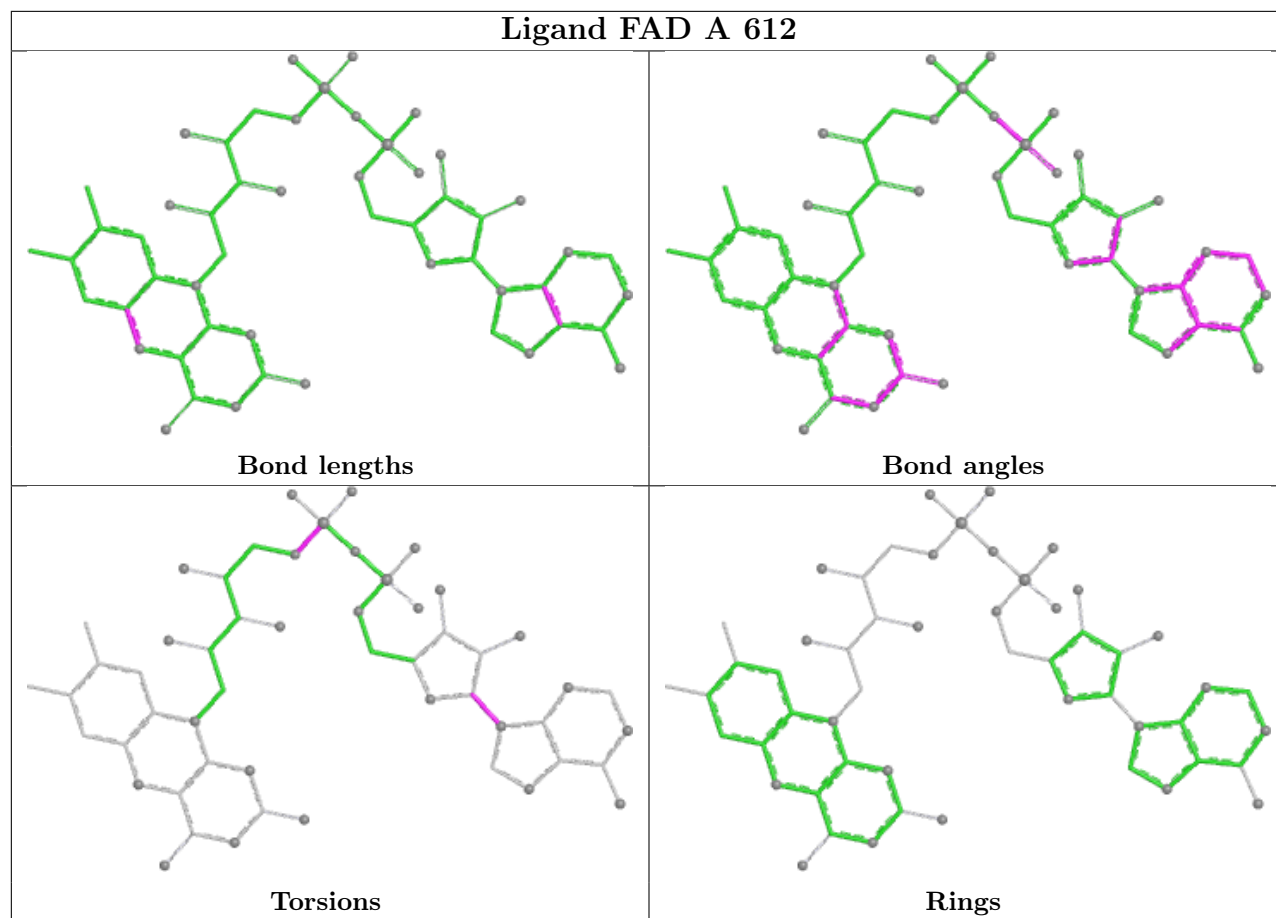
Mol	Chain	Res	Type	Atoms
3	B	611	TPP	PB-O3A-PA-O7
4	A	612	FAD	C5'-O5'-P-O1P
3	A	611	TPP	PA-O3A-PB-O2B
3	A	611	TPP	PA-O3A-PB-O3B
3	A	611	TPP	C5-C6-C7-O7
4	B	612	FAD	C5'-O5'-P-O1P
3	B	611	TPP	C5-C6-C7-O7
4	A	612	FAD	C2B-C1B-N9A-C8A
4	B	612	FAD	O4B-C4B-C5B-O5B

There are no ring outliers.

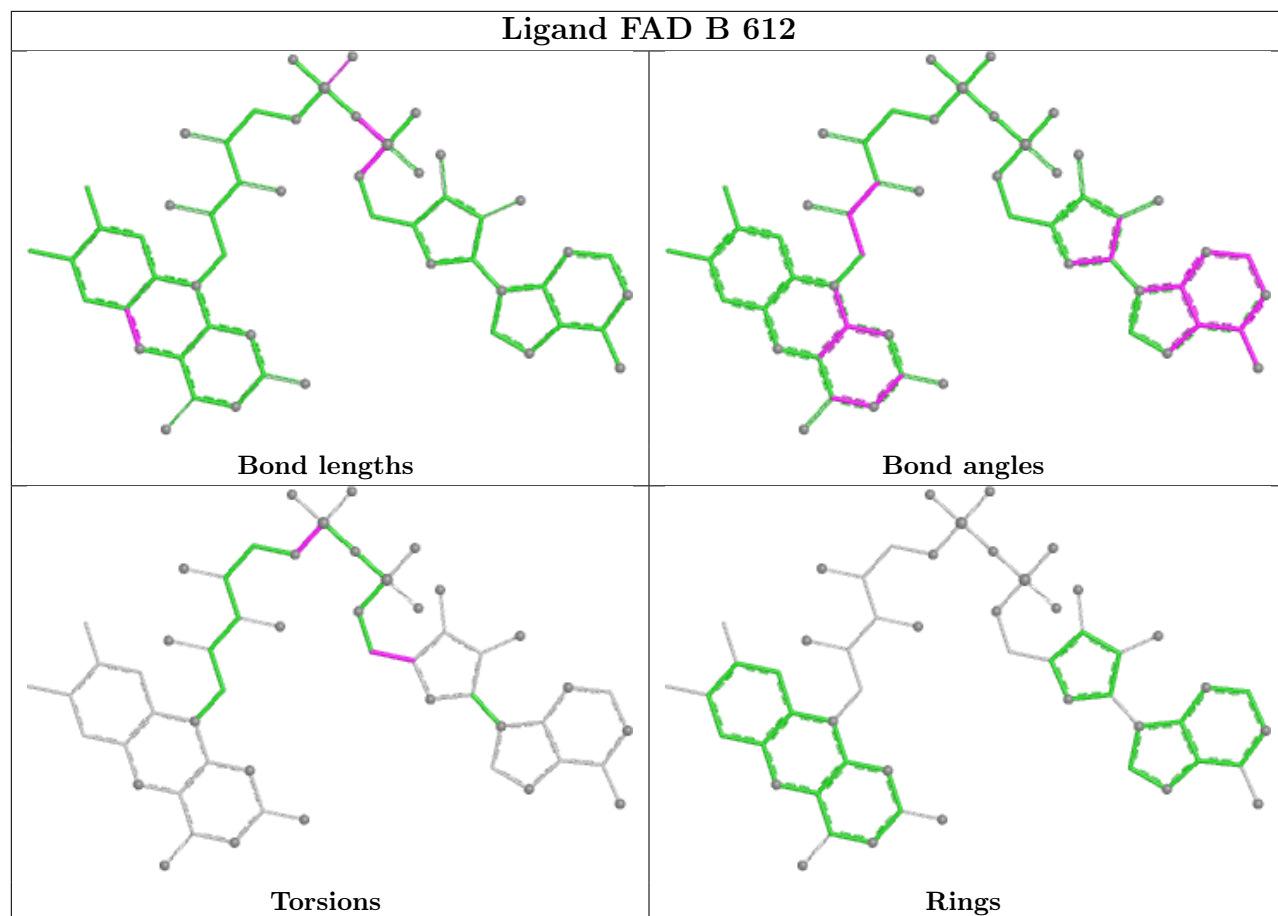
No monomer is involved in short contacts.

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

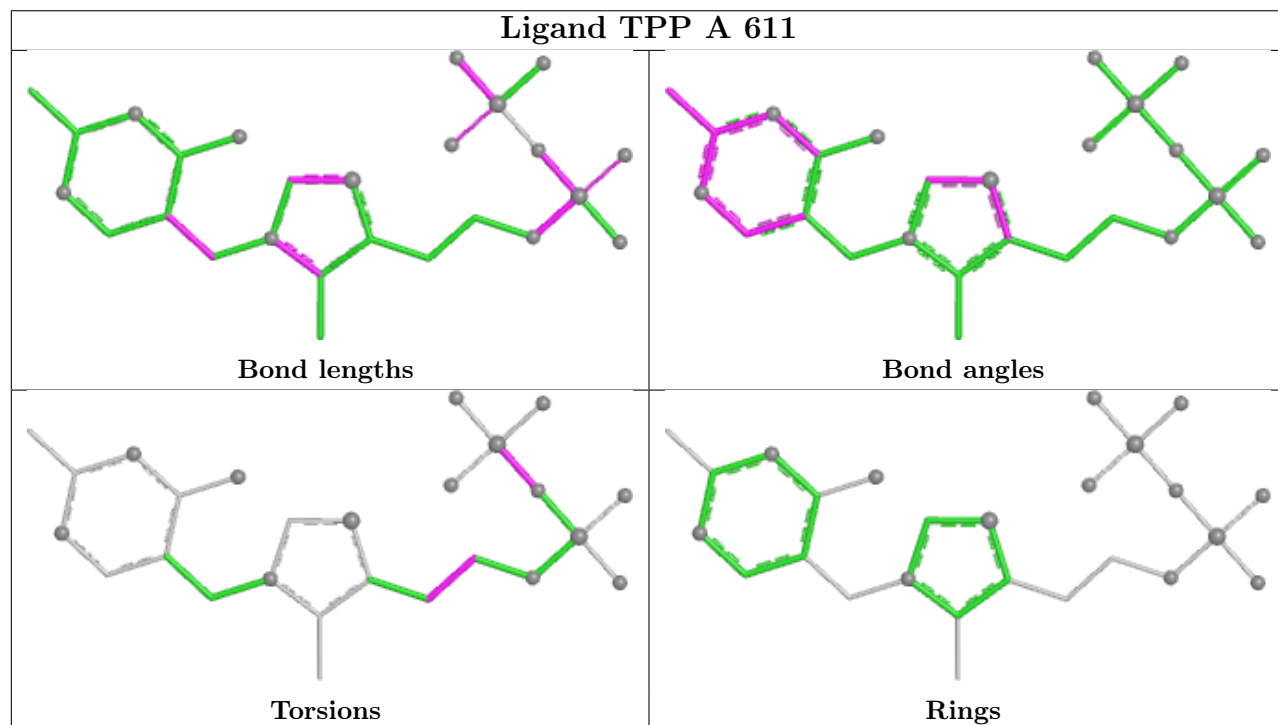




Ligand FAD B 612



Ligand TPP A 611



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 [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, 95th 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 ²)	Q<0.9
1	A	585/585 (100%)	-0.75	1 (0%) 91 89	2, 10, 32, 48	0
1	B	585/585 (100%)	-0.77	1 (0%) 91 89	2, 8, 28, 49	0
All	All	1170/1170 (100%)	-0.76	2 (0%) 91 89	2, 9, 30, 49	0

All (2) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	180	GLU	2.5
1	B	592	ASP	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 oligosaccharides in this entry.

6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th 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 ²)	Q<0.9
2	MG	B	610	1/1	0.96	0.13	2,2,2,2	0
3	TPP	B	611	26/26	0.97	0.06	2,3,6,10	0
4	FAD	A	612	53/53	0.97	0.05	3,8,13,14	0

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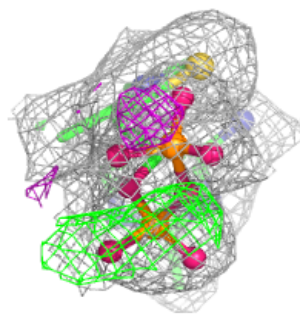
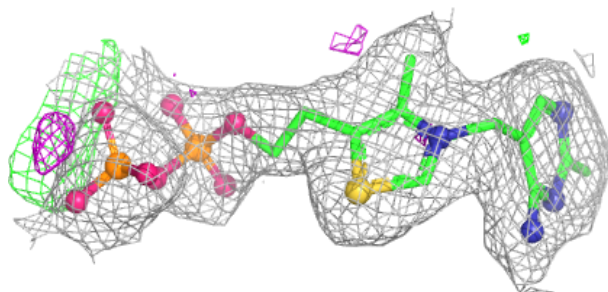
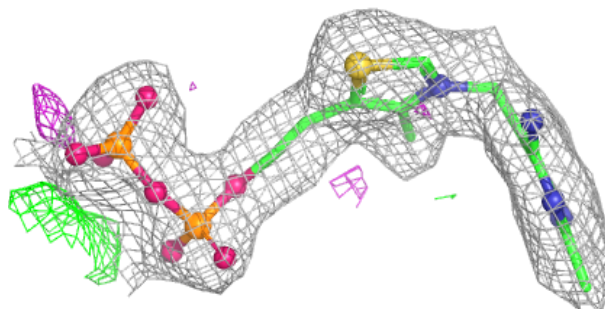
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
2	MG	A	610	1/1	0.98	0.08	2,2,2,2	0
3	TPP	A	611	26/26	0.98	0.05	2,6,10,12	0
4	FAD	B	612	53/53	0.98	0.05	2,8,14,16	0

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.

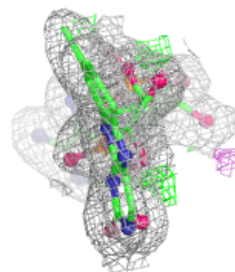
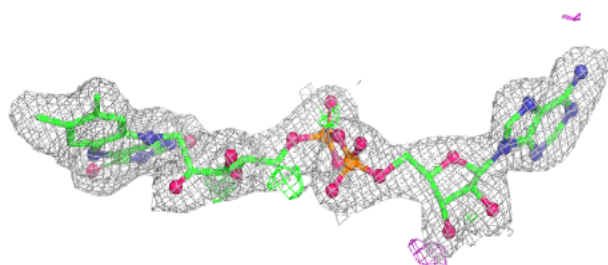
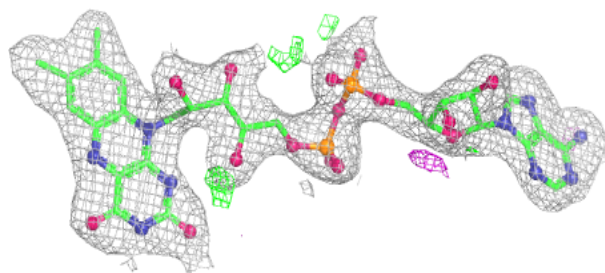
Electron density around TPP B 611:

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

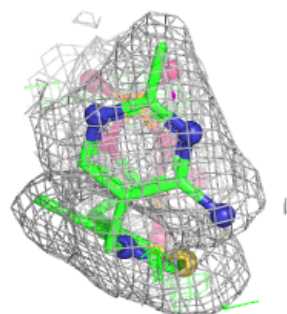
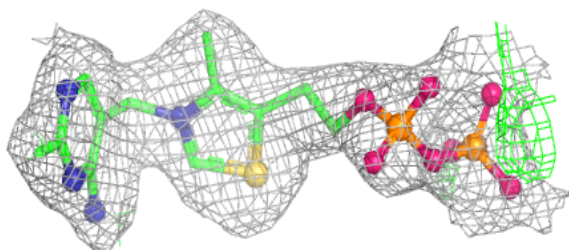
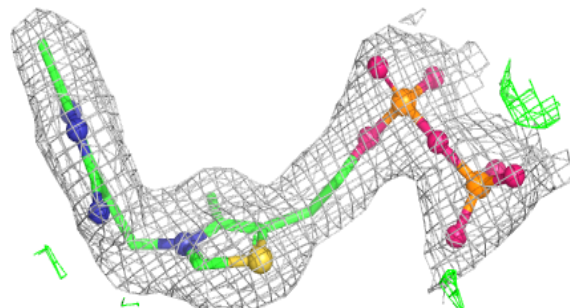


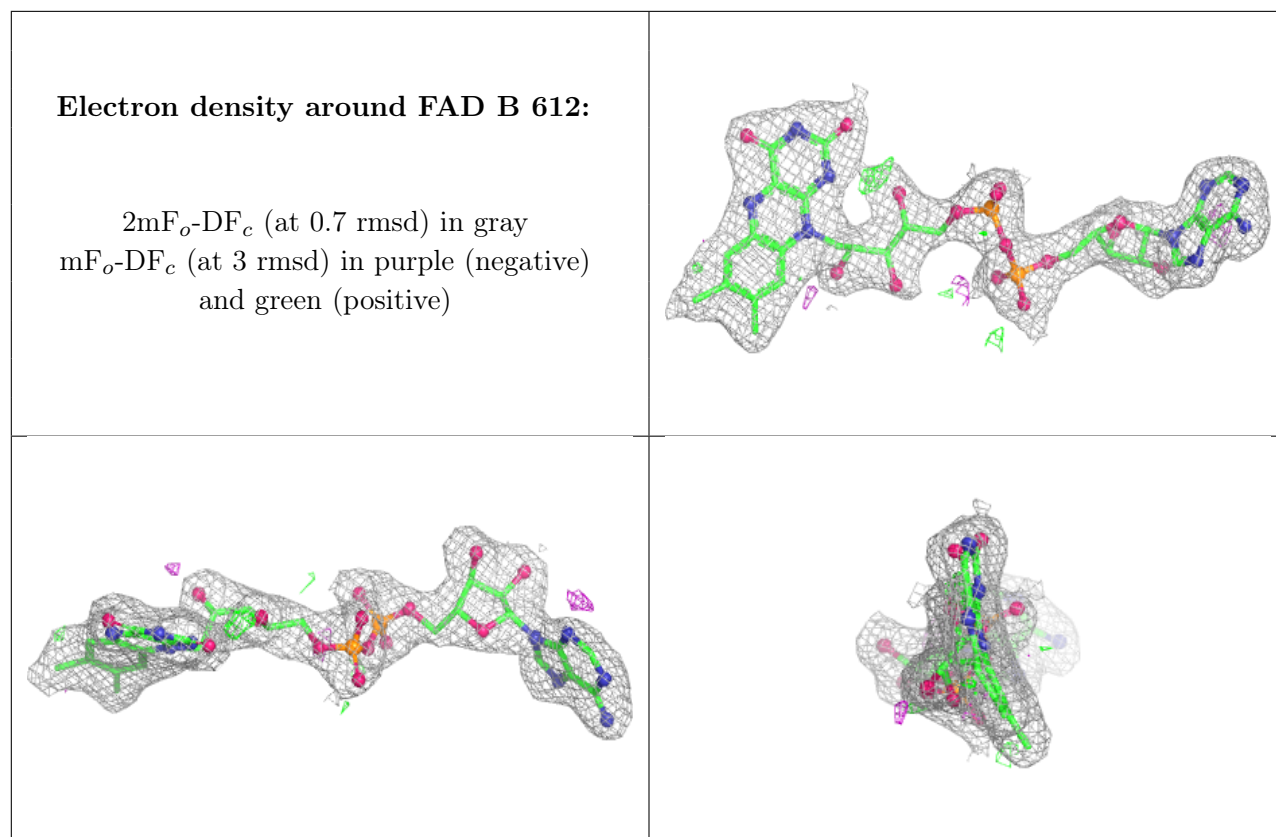
Electron density around FAD A 612:

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

**Electron density around TPP A 611:**

$2mF_o-DF_c$ (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.