



Full wwPDB X-ray Structure Validation Report ⓘ

Aug 9, 2021 – 06:02 AM EDT

PDB ID : 3EY9
Title : Structural basis for membrane binding and catalytic activation of the peripheral membrane enzyme pyruvate oxidase from Escherichia coli
Authors : Neumann, P.; Weidner, A.; Pech, A.; Stubbs, M.T.; Tittmann, K.
Deposited on : 2008-10-20
Resolution : 2.90 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 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 : 2.23.1
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) : 2.23.1

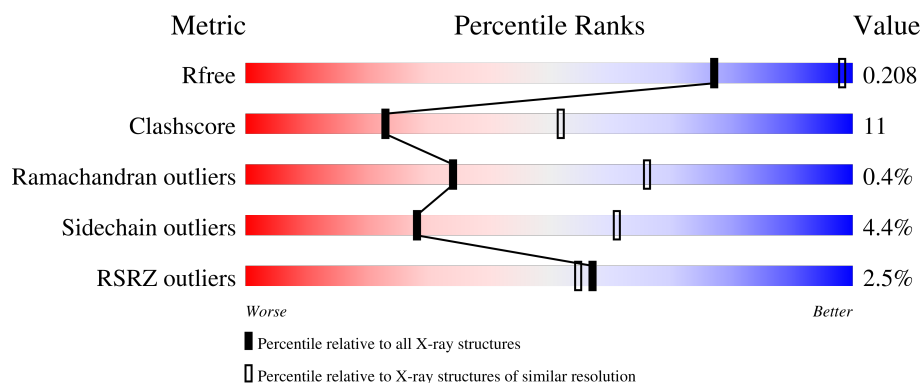
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.90 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	1957 (2.90-2.90)
Clashscore	141614	2172 (2.90-2.90)
Ramachandran outliers	138981	2115 (2.90-2.90)
Sidechain outliers	138945	2117 (2.90-2.90)
RSRZ outliers	127900	1906 (2.90-2.90)

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	572	<div> <div>3%</div> <div> <div></div> <div>77%</div> <div>22%</div> <div>.</div> </div> </div>
1	B	572	<div> <div>2%</div> <div> <div></div> <div>76%</div> <div>22%</div> <div>.</div> </div> </div>

2 Entry composition [i](#)

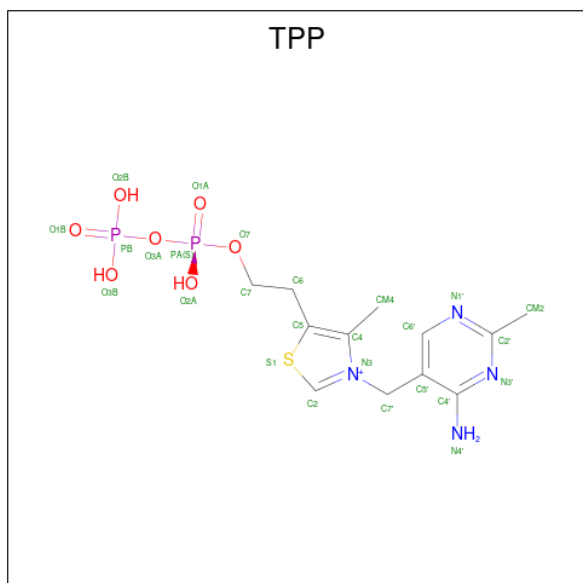
There are 5 unique types of molecules in this entry. The entry contains 8854 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 dehydrogenase [cytochrome].

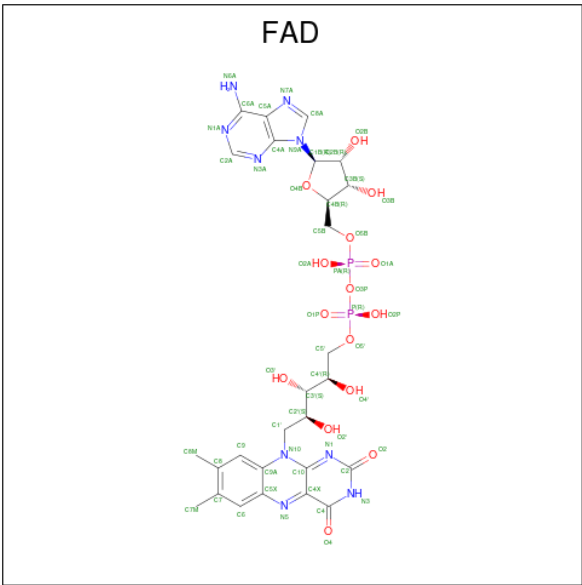
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	571	Total	C	N	O	S	0	0	0
			4342	2750	753	810	29			
1	B	571	Total	C	N	O	S	0	0	0
			4342	2750	753	810	29			

- Molecule 2 is THIAMINE DIPHOSPHATE (three-letter code: TPP) (formula: $C_{12}H_{19}N_4O_7P_2S$).



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

- Molecule 3 is FLAVIN-ADENINE DINUCLEOTIDE (three-letter code: FAD) (formula: $C_{27}H_{33}N_9O_{15}P_2$).



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

- Molecule 4 is SULFATE ION (three-letter code: SO4) (formula: O₄S).



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

- Molecule 5 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

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

- Molecule 1: Pyruvate dehydrogenase [cytochrome]





4 Data and refinement statistics

Property	Value	Source
Space group	P 43 21 2	Depositor
Cell constants a, b, c, α , β , γ	151.37Å 151.37Å 153.74Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	29.97 – 2.90 29.97 – 2.90	Depositor EDS
% Data completeness (in resolution range)	98.8 (29.97-2.90) 98.8 (29.97-2.90)	Depositor EDS
R_{merge}	0.01	Depositor
R_{sym}	0.01	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.75 (at 2.90Å)	Xtriage
Refinement program	PHENIX	Depositor
R, R_{free}	0.182 , 0.216 0.178 , 0.208	Depositor DCC
R_{free} test set	1983 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å ²)	73.5	Xtriage
Anisotropy	0.427	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.29 , 40.7	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	0.010 for -h,l,k 0.000 for -l,-k,-h	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	8854	wwPDB-VP
Average B, all atoms (Å ²)	80.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.77% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical 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: SO4, MG, FAD, TPP

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	0.37	0/4430	0.54	0/6001
1	B	0.36	0/4430	0.54	0/6001
All	All	0.37	0/8860	0.54	0/12002

There are no bond length outliers.

There are no bond angle outliers.

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	4342	0	4348	101	0
1	B	4342	0	4348	110	0
2	A	26	0	16	5	0
2	B	26	0	16	6	0
3	A	53	0	31	2	0
3	B	53	0	31	3	0
4	A	5	0	0	1	0
4	B	5	0	0	1	0
5	A	1	0	0	0	0
5	B	1	0	0	0	0
All	All	8854	0	8790	201	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 11.

All (201) 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:466:VAL:HG21	1:A:529:LYS:HB3	1.45	0.98
1:B:466:VAL:HG21	1:B:529:LYS:HB3	1.45	0.94
1:B:547:SER:H	1:B:550:MET:HE3	1.35	0.91
1:A:371:ALA:H	1:A:426:GLN:NE2	1.69	0.89
1:A:371:ALA:H	1:A:426:GLN:HE22	1.19	0.87
1:A:123:GLU:OE2	1:B:116:HIS:HD2	1.57	0.86
1:B:371:ALA:H	1:B:426:GLN:NE2	1.73	0.86
1:B:371:ALA:H	1:B:426:GLN:HE22	1.27	0.82
1:B:330:LYS:HZ3	1:B:572:ARG:HD3	1.45	0.81
1:A:116:HIS:HD2	1:B:123:GLU:OE2	1.63	0.80
1:A:539:LYS:HA	1:A:542:GLN:HE21	1.48	0.79
1:A:227:LYS:HG2	1:A:329:ARG:HB3	1.64	0.79
1:B:118:GLN:HG2	1:B:130:LEU:HB2	1.66	0.77
1:A:445:SER:HB3	1:A:449:MET:HE3	1.66	0.77
1:B:445:SER:HB3	1:B:449:MET:HE3	1.66	0.77
1:B:227:LYS:HG2	1:B:329:ARG:HB3	1.66	0.76
1:B:330:LYS:HZ3	1:B:572:ARG:HB3	1.50	0.76
1:A:118:GLN:HG2	1:A:130:LEU:HB2	1.66	0.75
1:A:483:HIS:H	1:B:448:GLN:NE2	1.85	0.74
1:B:539:LYS:HA	1:B:542:GLN:HE21	1.51	0.73
1:B:136:GLN:HA	1:B:139:GLN:HE21	1.53	0.73
1:A:136:GLN:HA	1:A:139:GLN:HE21	1.54	0.72
1:B:445:SER:HB3	1:B:449:MET:CE	2.20	0.71
1:A:448:GLN:NE2	1:B:483:HIS:H	1.89	0.71
1:B:141:LEU:HG	1:B:145:MET:HE1	1.73	0.70
1:A:141:LEU:HG	1:A:145:MET:HE2	1.74	0.69
1:A:445:SER:HB3	1:A:449:MET:CE	2.21	0.69
1:A:225:LYS:HG3	1:A:325:GLU:HG2	1.73	0.69
1:A:123:GLU:OE2	1:B:116:HIS:CD2	2.44	0.69
1:B:382:THR:HG23	2:B:611:TPP:O2B	1.94	0.68
1:B:330:LYS:NZ	1:B:572:ARG:HD3	2.09	0.67
1:A:443:PHE:HE2	1:A:491:ALA:HA	1.62	0.65
1:B:237:LYS:HE3	1:B:388:ALA:HA	1.78	0.65
1:A:237:LYS:HE3	1:A:388:ALA:HA	1.79	0.64
1:A:133:SER:O	1:A:136:GLN:HG2	1.97	0.64
1:A:304:VAL:HG11	1:A:307:ALA:HB2	1.79	0.64
1:A:371:ALA:N	1:A:426:GLN:HE22	1.95	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:184:VAL:HG11	1:A:293:ILE:HD11	1.80	0.63
1:B:443:PHE:HE2	1:B:491:ALA:HA	1.62	0.63
1:B:52:VAL:HG13	1:B:413:PRO:HB3	1.80	0.62
1:B:330:LYS:NZ	1:B:572:ARG:HB3	2.15	0.62
1:B:133:SER:O	1:B:136:GLN:HG2	1.99	0.61
1:B:184:VAL:HG11	1:B:293:ILE:HD11	1.81	0.61
2:A:611:TPP:HM43	1:B:25:THR:O	2.00	0.61
1:A:137:ILE:HG22	1:A:138:PRO:HD3	1.82	0.61
1:A:52:VAL:HG13	1:A:413:PRO:HB3	1.83	0.61
1:A:312:ILE:HG12	3:A:612:FAD:C2A	2.31	0.60
1:A:116:HIS:CD2	1:B:123:GLU:OE2	2.51	0.60
1:A:383:PRO:HD3	2:A:611:TPP:O3B	2.01	0.60
1:A:352:PRO:HD3	1:A:361:TYR:CE1	2.37	0.59
1:B:63:LEU:HD12	1:B:418:ALA:HA	1.84	0.59
1:B:304:VAL:HG11	1:B:307:ALA:HB2	1.84	0.59
1:A:447:VAL:HG23	1:A:496:ILE:HD11	1.85	0.58
1:B:371:ALA:N	1:B:426:GLN:HE22	2.00	0.58
1:B:547:SER:N	1:B:550:MET:HE3	2.15	0.58
1:B:3:GLN:HE22	1:B:8:TYR:HA	1.68	0.58
1:B:137:ILE:HG22	1:B:138:PRO:HD3	1.84	0.58
1:B:290:GLN:HE22	1:B:299:GLY:H	1.52	0.58
1:B:352:PRO:HD3	1:B:361:TYR:CE1	2.39	0.58
1:A:469:GLU:HG3	1:A:539:LYS:CE	2.34	0.58
1:B:467:ALA:C	1:B:469:GLU:H	2.08	0.57
1:B:447:VAL:HG23	1:B:496:ILE:HD11	1.85	0.57
1:A:137:ILE:CG2	1:A:138:PRO:HD3	2.34	0.57
1:B:367:SER:HB2	1:B:391:LEU:HD23	1.86	0.57
1:A:367:SER:HB2	1:A:391:LEU:HD23	1.87	0.57
1:B:118:GLN:CG	1:B:130:LEU:HB2	2.34	0.56
1:A:483:HIS:H	1:B:448:GLN:HE21	1.52	0.56
1:B:534:ILE:O	1:B:539:LYS:HE3	2.05	0.56
1:B:137:ILE:CG2	1:B:138:PRO:HD3	2.35	0.56
1:B:469:GLU:HG3	1:B:539:LYS:CE	2.35	0.56
1:B:136:GLN:HA	1:B:139:GLN:NE2	2.21	0.55
1:A:290:GLN:HE22	1:A:299:GLY:H	1.54	0.55
1:A:63:LEU:HD12	1:A:418:ALA:HA	1.89	0.55
1:B:248:VAL:O	1:B:248:VAL:HG12	2.06	0.55
1:B:251:THR:HG21	1:B:260:PHE:HB2	1.89	0.55
1:A:279:ARG:NH1	1:B:106:GLU:OE2	2.38	0.55
1:A:25:THR:O	2:B:611:TPP:HM43	2.07	0.54
1:A:409:ALA:HB2	1:A:438:MET:HB3	1.90	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:136:GLN:HA	1:A:139:GLN:NE2	2.21	0.54
1:A:251:THR:HG21	1:A:260:PHE:HB2	1.89	0.53
1:A:468:MET:O	1:A:534:ILE:HD12	2.08	0.53
1:B:496:ILE:HG23	1:B:520:PRO:HB2	1.90	0.53
1:A:441:GLY:HA3	1:B:437:SER:O	2.09	0.53
1:A:443:PHE:CE2	1:A:491:ALA:HA	2.44	0.53
1:A:345:GLY:HA2	1:A:348:ASP:OD1	2.09	0.53
1:A:545:GLY:HA2	1:B:165:LEU:HD12	1.90	0.53
1:A:308:LEU:HD12	1:A:308:LEU:N	2.25	0.52
1:A:229:PRO:HB2	1:A:248:VAL:HG21	1.91	0.52
1:A:106:GLU:OE2	1:B:279:ARG:NH1	2.42	0.52
1:B:382:THR:N	1:B:383:PRO:CD	2.72	0.52
1:A:534:ILE:O	1:A:539:LYS:HE3	2.09	0.52
1:B:312:ILE:HG12	3:B:612:FAD:C2A	2.40	0.52
1:A:382:THR:N	1:A:383:PRO:CD	2.73	0.51
1:A:437:SER:O	1:B:441:GLY:HA3	2.10	0.51
1:B:443:PHE:CE2	1:B:491:ALA:HA	2.45	0.51
1:A:496:ILE:HG23	1:A:520:PRO:HB2	1.92	0.51
1:B:229:PRO:HB2	1:B:248:VAL:HG21	1.93	0.51
1:B:383:PRO:HD3	2:B:611:TPP:O1B	2.11	0.51
1:A:248:VAL:O	1:A:248:VAL:HG12	2.10	0.50
1:A:446:VAL:HG22	1:A:496:ILE:HD11	1.92	0.50
1:B:409:ALA:HB2	1:B:438:MET:HB3	1.92	0.50
1:A:547:SER:H	1:A:550:MET:CE	2.25	0.50
1:A:118:GLN:CG	1:A:130:LEU:HB2	2.38	0.49
1:A:371:ALA:HB3	1:A:374:ALA:HB2	1.94	0.49
2:A:611:TPP:H7'2	4:B:621:SO4:O3	2.12	0.49
1:B:469:GLU:HG3	1:B:539:LYS:NZ	2.26	0.49
1:B:345:GLY:HA2	1:B:348:ASP:OD1	2.12	0.49
1:A:186:PRO:HG2	1:A:191:LEU:HD21	1.94	0.49
1:B:412:MET:HB3	1:B:413:PRO:HD3	1.95	0.49
1:B:446:VAL:HG22	1:B:496:ILE:HD11	1.94	0.49
1:A:469:GLU:HG3	1:A:539:LYS:NZ	2.27	0.49
1:A:460:ASN:CG	1:A:462:VAL:HG12	2.34	0.48
1:B:241:GLU:O	1:B:241:GLU:HG3	2.12	0.48
1:A:379:ASP:N	1:A:411:ALA:HB2	2.29	0.48
1:A:448:GLN:HE21	1:B:483:HIS:H	1.60	0.48
1:B:307:ALA:C	1:B:308:LEU:HD12	2.34	0.48
1:A:412:MET:HB3	1:A:413:PRO:HD3	1.96	0.48
1:A:279:ARG:HD3	1:B:106:GLU:OE1	2.14	0.48
1:A:227:LYS:HD3	1:A:326:LYS:O	2.13	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:197:LEU:HD22	1:B:289:ILE:HD11	1.96	0.48
1:B:460:ASN:CG	1:B:462:VAL:HG12	2.34	0.48
3:A:612:FAD:H9	3:A:612:FAD:H1'1	1.59	0.47
1:A:293:ILE:HD13	1:A:293:ILE:O	2.15	0.47
1:B:522:LEU:C	1:B:522:LEU:HD23	2.35	0.47
1:B:227:LYS:HD2	1:B:227:LYS:N	2.30	0.47
1:A:467:ALA:HB2	1:A:471:LYS:HA	1.97	0.46
1:A:197:LEU:HD22	1:A:289:ILE:HD11	1.97	0.46
1:B:227:LYS:HD3	1:B:326:LYS:O	2.16	0.46
1:B:8:TYR:CE1	1:B:172:ALA:HB1	2.51	0.46
1:A:467:ALA:HB1	1:A:470:MET:C	2.36	0.46
1:B:467:ALA:HB1	1:B:470:MET:C	2.36	0.46
1:A:522:LEU:C	1:A:522:LEU:HD23	2.35	0.46
1:B:50:GLU:HB2	1:B:80:HIS:HB3	1.98	0.46
1:A:241:GLU:O	1:A:241:GLU:HG3	2.15	0.45
1:B:437:SER:HA	1:B:440:MET:HB2	1.97	0.45
1:B:468:MET:O	1:B:534:ILE:HD12	2.16	0.45
1:A:34:ASP:O	1:A:38:ARG:HG3	2.17	0.45
1:A:50:GLU:HB2	1:A:80:HIS:HB3	1.99	0.45
1:A:165:LEU:HD12	1:B:545:GLY:HA2	1.99	0.45
1:B:74:CYS:HA	1:B:100:ALA:O	2.17	0.45
1:B:186:PRO:HG2	1:B:191:LEU:HD21	1.98	0.45
1:B:464:GLY:HA2	2:B:611:TPP:O2B	2.17	0.45
2:A:611:TPP:HN42	2:A:611:TPP:H2	1.81	0.45
1:B:293:ILE:O	1:B:293:ILE:HD13	2.17	0.45
1:A:367:SER:HB2	1:A:391:LEU:HA	1.98	0.45
1:A:227:LYS:N	1:A:227:LYS:HD2	2.32	0.44
1:B:371:ALA:HB3	1:B:374:ALA:HB2	1.99	0.44
1:A:442:ASP:O	1:A:445:SER:HB2	2.18	0.44
1:A:361:TYR:O	1:A:365:GLN:HG2	2.18	0.44
1:B:379:ASP:N	1:B:411:ALA:HB2	2.32	0.44
1:A:75:GLY:HA3	1:A:76:PRO:HD3	1.83	0.44
1:A:359:PRO:HG2	1:A:530:GLU:HG3	2.00	0.44
1:B:320:LEU:HB2	1:B:321:PRO:HD3	1.99	0.44
1:B:308:LEU:HD12	1:B:308:LEU:N	2.32	0.44
1:A:547:SER:H	1:A:550:MET:HE2	1.83	0.43
1:A:117:PRO:HB2	1:A:158:VAL:CG2	2.49	0.43
1:B:467:ALA:HB2	1:B:471:LYS:HA	1.99	0.43
1:A:74:CYS:HA	1:A:100:ALA:O	2.18	0.43
1:B:367:SER:HB2	1:B:391:LEU:HA	2.01	0.43
4:A:621:SO4:O3	2:B:611:TPP:H7'2	2.18	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:320:LEU:HB2	1:A:321:PRO:HD3	2.01	0.43
1:A:339:TYR:O	1:A:343:ARG:HG3	2.19	0.43
1:A:68:ALA:O	1:A:95:VAL:HA	2.19	0.42
1:A:348:ASP:O	1:A:351:LYS:HE3	2.18	0.42
1:A:437:SER:HA	1:A:440:MET:HB2	2.00	0.42
1:A:464:GLY:HA2	2:A:611:TPP:O2B	2.20	0.42
1:B:179:ALA:HA	1:B:180:PRO:HD2	1.94	0.42
1:B:258:SER:HB3	1:B:339:TYR:HA	2.01	0.42
1:B:359:PRO:HG2	1:B:530:GLU:HG3	2.02	0.42
1:A:513:ARG:HD2	1:A:517:ILE:HD11	2.01	0.42
1:B:253:LEU:HD22	1:B:548:LEU:HB2	2.01	0.42
2:B:611:TPP:C6'	2:B:611:TPP:HM42	2.50	0.42
3:B:612:FAD:H1'1	3:B:612:FAD:H9	1.70	0.42
1:B:242:TYR:HB2	1:B:394:ASN:HA	2.01	0.42
1:A:126:HIS:CE1	1:A:153:GLY:HA3	2.55	0.41
1:A:253:LEU:HD22	1:A:548:LEU:HB2	2.01	0.41
1:A:469:GLU:OE1	1:A:539:LYS:HD3	2.20	0.41
1:A:513:ARG:O	1:A:517:ILE:HG13	2.20	0.41
1:B:290:GLN:NE2	1:B:299:GLY:H	2.16	0.41
1:B:137:ILE:N	1:B:138:PRO:CD	2.83	0.41
1:A:150:LEU:HD23	1:A:150:LEU:HA	1.83	0.41
1:B:352:PRO:HD3	1:B:361:TYR:CZ	2.56	0.41
1:A:251:THR:HG23	1:A:256:PHE:O	2.20	0.41
1:B:50:GLU:HB2	1:B:80:HIS:CB	2.51	0.41
1:B:540:LEU:HD23	1:B:540:LEU:HA	1.75	0.41
1:A:106:GLU:OE1	1:B:279:ARG:HD3	2.21	0.41
1:B:126:HIS:CE1	1:B:153:GLY:HA3	2.56	0.41
1:B:251:THR:HG23	1:B:256:PHE:O	2.19	0.41
1:B:112:PHE:O	1:B:113:GLN:HB2	2.21	0.41
1:A:137:ILE:N	1:A:138:PRO:CD	2.84	0.41
1:B:311:ASP:HA	3:B:612:FAD:N1A	2.36	0.41
1:B:467:ALA:C	1:B:469:GLU:N	2.73	0.41
1:B:86:PHE:O	1:B:90:ARG:HG2	2.20	0.40
1:B:117:PRO:HB2	1:B:158:VAL:HG21	2.03	0.40
1:B:469:GLU:OE1	1:B:539:LYS:HD3	2.21	0.40
1:B:442:ASP:O	1:B:445:SER:HB2	2.20	0.40
1:B:477:THR:C	1:B:479:GLY:N	2.75	0.40
1:A:347:ASP:O	1:A:348:ASP:C	2.59	0.40
1:B:276:PHE:HA	1:B:277:PRO:HD3	1.91	0.40
1:A:242:TYR:HB2	1:A:394:ASN:HA	2.04	0.40
1:A:352:PRO:HD3	1:A:361:TYR:CZ	2.56	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	569/572 (100%)	537 (94%)	30 (5%)	2 (0%)	34	66
1	B	569/572 (100%)	537 (94%)	30 (5%)	2 (0%)	34	66
All	All	1138/1144 (100%)	1074 (94%)	60 (5%)	4 (0%)	34	66

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	468	MET
1	A	469	GLU
1	B	469	GLU
1	A	467	ALA

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	457/458 (100%)	437 (96%)	20 (4%)	28	61
1	B	457/458 (100%)	437 (96%)	20 (4%)	28	61
All	All	914/916 (100%)	874 (96%)	40 (4%)	28	61

All (40) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	25	THR
1	A	36	LEU
1	A	46	SER
1	A	66	GLU
1	A	118	GLN
1	A	139	GLN
1	A	146	ARG
1	A	173	THR
1	A	185	THR
1	A	187	GLU
1	A	210	SER
1	A	231	VAL
1	A	241	GLU
1	A	251	THR
1	A	284	THR
1	A	293	ILE
1	A	347	ASP
1	A	360	GLN
1	A	446	VAL
1	A	508	ASP
1	B	2	LYS
1	B	3	GLN
1	B	25	THR
1	B	36	LEU
1	B	46	SER
1	B	118	GLN
1	B	139	GLN
1	B	146	ARG
1	B	173	THR
1	B	185	THR
1	B	187	GLU
1	B	231	VAL
1	B	241	GLU
1	B	251	THR
1	B	284	THR
1	B	293	ILE
1	B	347	ASP
1	B	360	GLN
1	B	446	VAL
1	B	508	ASP

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (22) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	3	GLN
1	A	92	HIS
1	A	116	HIS
1	A	126	HIS
1	A	139	GLN
1	A	151	ASN
1	A	181	GLN
1	A	290	GLN
1	A	426	GLN
1	A	448	GLN
1	A	542	GLN
1	B	3	GLN
1	B	92	HIS
1	B	116	HIS
1	B	126	HIS
1	B	139	GLN
1	B	151	ASN
1	B	181	GLN
1	B	290	GLN
1	B	426	GLN
1	B	448	GLN
1	B	542	GLN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no monosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 8 ligands modelled in this entry, 2 are monoatomic - leaving 6 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$
4	SO4	B	621	-	4,4,4	0.14	0	6,6,6	0.35	0
4	SO4	A	621	-	4,4,4	0.12	0	6,6,6	0.32	0
2	TPP	A	611	5	22,27,27	1.51	2 (9%)	29,40,40	1.97	9 (31%)
2	TPP	B	611	5	22,27,27	1.36	1 (4%)	29,40,40	2.15	9 (31%)
3	FAD	B	612	-	51,58,58	0.90	2 (3%)	60,89,89	1.64	9 (15%)
3	FAD	A	612	-	51,58,58	1.01	1 (1%)	60,89,89	1.70	10 (16%)

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	FAD	A	612	-	-	7/30/50/50	0/6/6/6
2	TPP	B	611	5	-	2/16/17/17	0/2/2/2
3	FAD	B	612	-	-	10/30/50/50	0/6/6/6
2	TPP	A	611	5	-	2/16/17/17	0/2/2/2

All (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	611	TPP	C4-N3	-5.91	1.34	1.39
2	B	611	TPP	C4-N3	-5.37	1.35	1.39
3	A	612	FAD	C9A-N10	-3.37	1.33	1.38
3	B	612	FAD	O4B-C1B	2.25	1.44	1.41
3	B	612	FAD	C9A-N10	-2.20	1.35	1.38
2	A	611	TPP	C5'-C4'	-2.01	1.39	1.42

All (37) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	612	FAD	C4-N3-C2	7.81	121.74	115.14
3	B	612	FAD	C4-N3-C2	7.19	121.21	115.14
2	B	611	TPP	C6-C5-C4	6.20	132.41	127.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	611	TPP	C6-C5-C4	5.23	131.63	127.43
3	B	612	FAD	N3A-C2A-N1A	-4.90	121.01	128.68
3	A	612	FAD	N3A-C2A-N1A	-4.61	121.48	128.68
2	B	611	TPP	C5'-C7'-N3	-4.28	106.15	113.28
2	A	611	TPP	C5'-C7'-N3	-3.89	106.80	113.28
2	B	611	TPP	CM4-C4-N3	3.20	126.61	122.53
3	A	612	FAD	C4X-C4-N3	-3.19	119.06	123.43
3	B	612	FAD	C4X-C4-N3	-3.12	119.16	123.43
2	A	611	TPP	C6'-N1'-C2'	2.93	120.94	115.96
2	B	611	TPP	C6'-N1'-C2'	2.86	120.84	115.96
2	A	611	TPP	C6'-C5'-C4'	2.81	119.54	115.72
2	B	611	TPP	PA-O3A-PB	-2.76	123.35	132.83
2	A	611	TPP	C5'-C6'-N1'	-2.73	119.28	123.82
3	A	612	FAD	C9A-N10-C10	-2.67	118.41	121.91
3	A	612	FAD	C4-C4X-N5	2.66	121.63	118.60
3	A	612	FAD	C5X-C9A-N10	2.65	119.64	117.72
3	B	612	FAD	C5X-C9A-N10	2.56	119.57	117.72
2	B	611	TPP	C5'-C6'-N1'	-2.55	119.56	123.82
3	A	612	FAD	C5'-C4'-C3'	-2.54	107.29	112.20
2	B	611	TPP	N1'-C2'-N3'	-2.51	121.22	125.54
2	B	611	TPP	C6'-C5'-C4'	2.47	119.08	115.72
2	A	611	TPP	N1'-C2'-N3'	-2.45	121.33	125.54
3	A	612	FAD	C10-C4X-N5	-2.37	119.62	121.26
3	B	612	FAD	C4A-C5A-N7A	-2.29	107.01	109.40
3	B	612	FAD	C4X-N5-C5X	2.23	119.00	116.77
2	A	611	TPP	N4'-C4'-N3'	2.19	120.13	117.03
3	B	612	FAD	C10-C4X-N5	-2.14	119.78	121.26
3	B	612	FAD	C9A-N10-C10	-2.13	119.12	121.91
3	A	612	FAD	C1'-N10-C10	2.11	120.30	118.41
2	B	611	TPP	CM4-C4-C5	-2.10	123.01	127.60
2	A	611	TPP	CM2-C2'-N3'	2.09	120.41	117.15
2	A	611	TPP	CM4-C4-N3	2.05	125.15	122.53
3	B	612	FAD	P-O3P-PA	-2.04	125.83	132.83
3	A	612	FAD	C6-C5X-N5	2.01	121.27	119.05

There are no chirality outliers.

All (21) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	B	611	TPP	PA-O3A-PB-O3B
3	A	612	FAD	O4B-C4B-C5B-O5B
3	A	612	FAD	C3B-C4B-C5B-O5B

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Mol	Chain	Res	Type	Atoms
3	A	612	FAD	C2'-C1'-N10-C9A
3	A	612	FAD	O4'-C4'-C5'-O5'
3	B	612	FAD	C3B-C4B-C5B-O5B
3	B	612	FAD	C2'-C1'-N10-C9A
3	B	612	FAD	C3'-C4'-C5'-O5'
3	B	612	FAD	O4'-C4'-C5'-O5'
3	B	612	FAD	O4B-C4B-C5B-O5B
3	B	612	FAD	O3'-C3'-C4'-C5'
3	B	612	FAD	C2'-C3'-C4'-C5'
3	B	612	FAD	C2'-C3'-C4'-O4'
3	A	612	FAD	C3'-C4'-C5'-O5'
3	B	612	FAD	O3'-C3'-C4'-O4'
3	A	612	FAD	P-O3P-PA-O5B
3	B	612	FAD	P-O3P-PA-O5B
2	A	611	TPP	PA-O3A-PB-O3B
2	A	611	TPP	C4-C5-C6-C7
2	B	611	TPP	PA-O3A-PB-O2B
3	A	612	FAD	N10-C1'-C2'-O2'

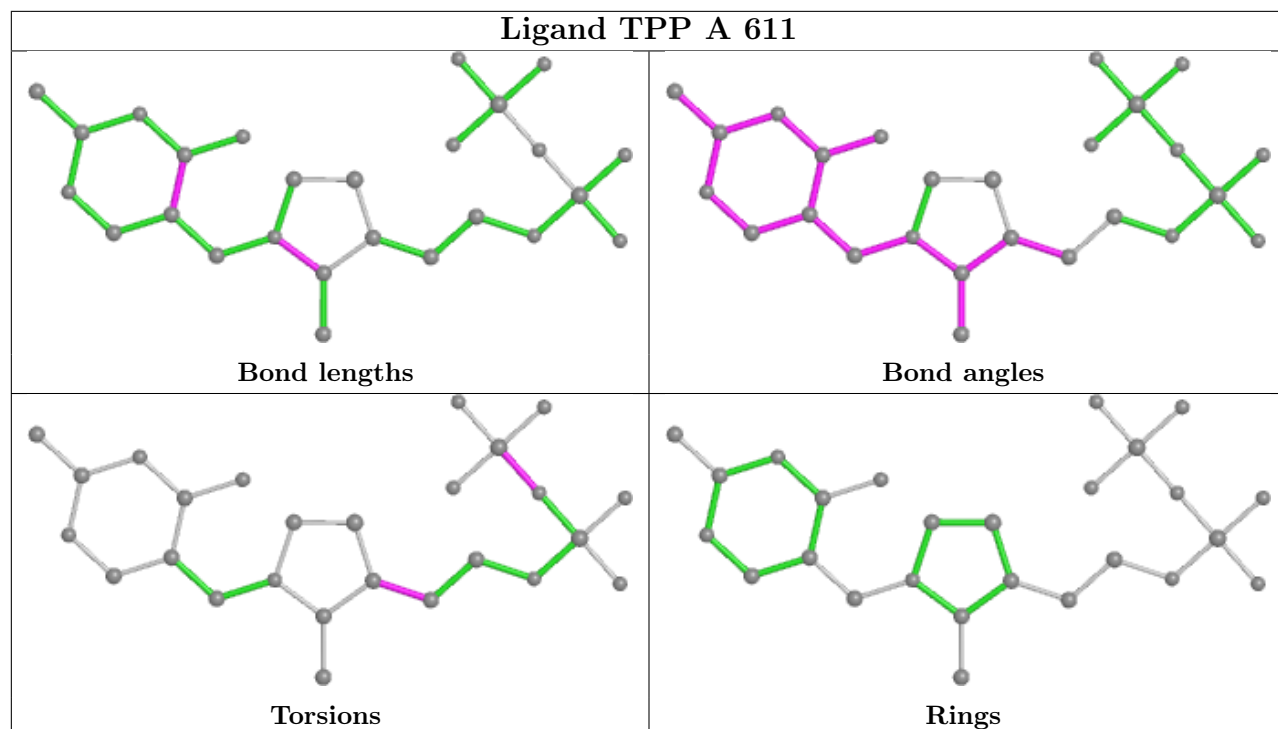
There are no ring outliers.

6 monomers are involved in 16 short contacts:

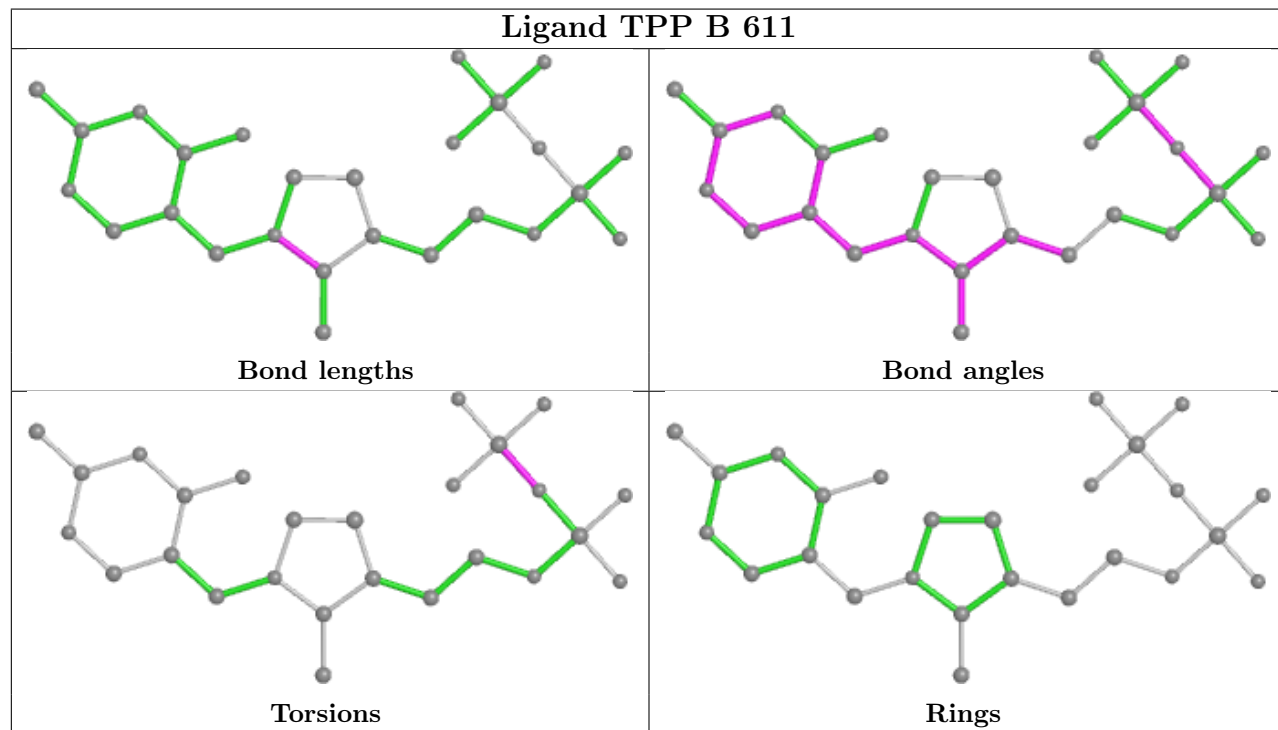
Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	B	621	SO4	1	0
4	A	621	SO4	1	0
2	A	611	TPP	5	0
2	B	611	TPP	6	0
3	B	612	FAD	3	0
3	A	612	FAD	2	0

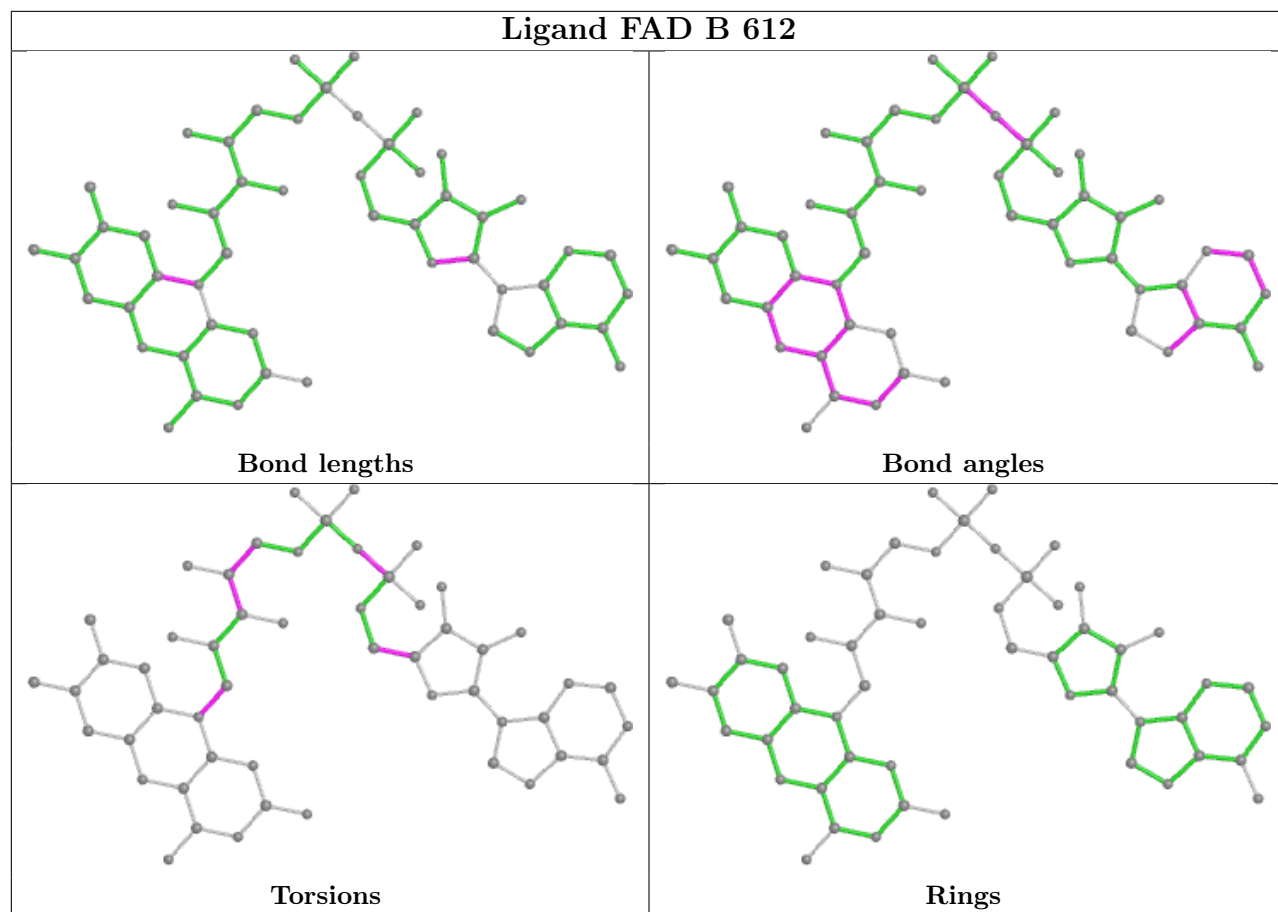
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

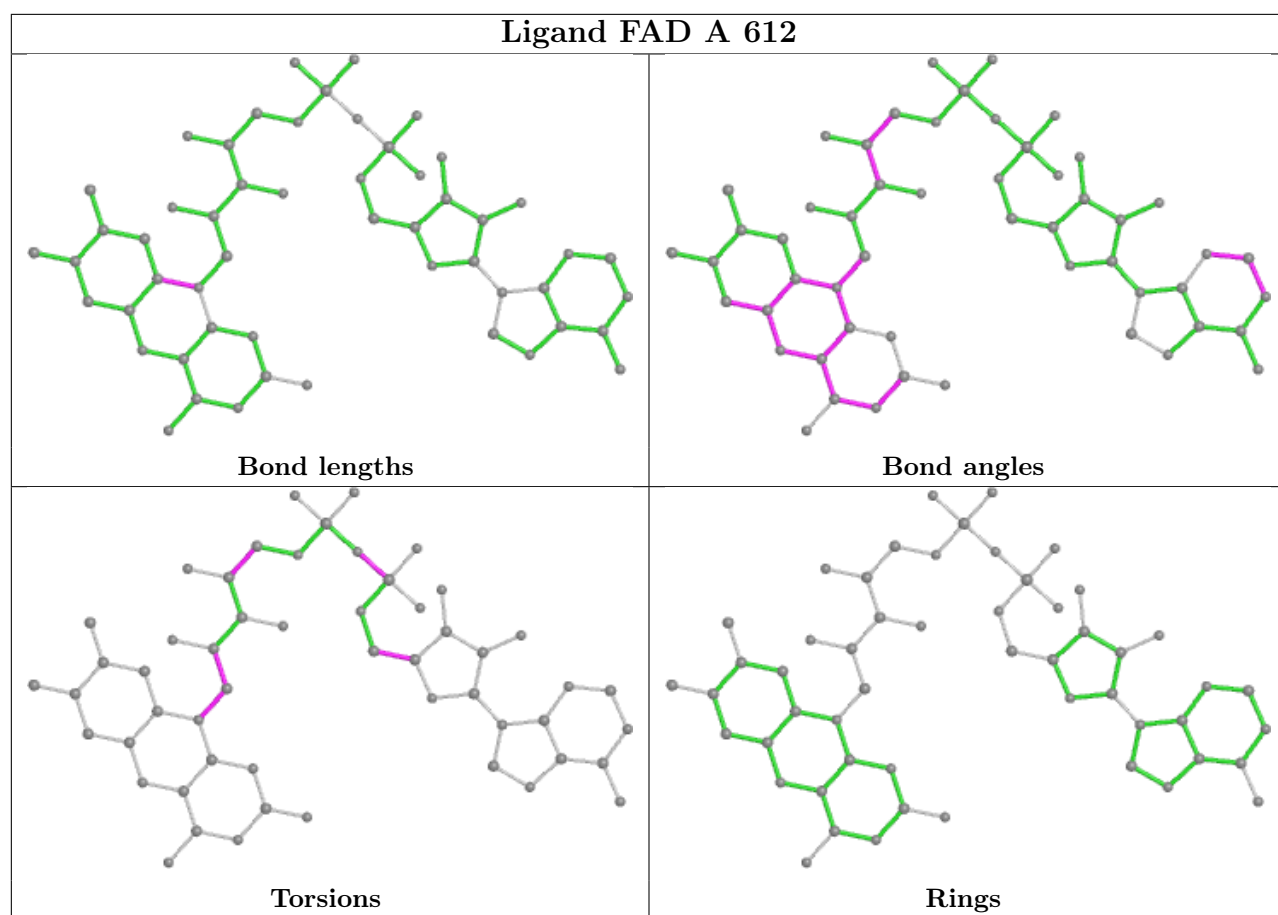
Ligand TPP A 611



Ligand TPP B 611







5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 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	571/572 (99%)	-0.43	15 (2%) 56 52	50, 77, 113, 227	0
1	B	571/572 (99%)	-0.24	14 (2%) 57 55	49, 75, 114, 221	0
All	All	1142/1144 (99%)	-0.34	29 (2%) 57 55	49, 76, 114, 227	0

All (29) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	469	GLU	13.6
1	B	473	GLY	13.1
1	B	468	MET	10.8
1	B	474	GLY	9.8
1	B	475	TYR	9.6
1	A	469	GLU	9.3
1	A	474	GLY	8.4
1	A	468	MET	7.6
1	B	476	LEU	6.4
1	A	475	TYR	6.3
1	A	473	GLY	6.1
1	A	476	LEU	4.5
1	A	472	ALA	4.1
1	A	478	ASP	3.9
1	A	571	LEU	3.5
1	A	572	ARG	3.1
1	B	470	MET	2.9
1	A	470	MET	2.9
1	B	435	GLY	2.9
1	B	567	LYS	2.5
1	B	478	ASP	2.4
1	A	435	GLY	2.3
1	B	432	GLY	2.3
1	B	472	ALA	2.2

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Mol	Chain	Res	Type	RSRZ
1	A	471	LYS	2.1
1	A	477	THR	2.1
1	A	355	LYS	2.1
1	B	355	LYS	2.0
1	B	379	ASP	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 monosaccharides in this entry.

6.4 Ligands [i](#)

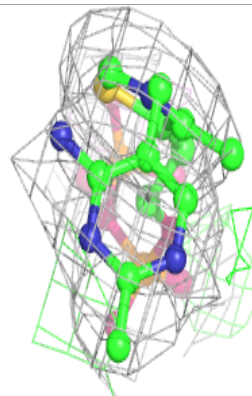
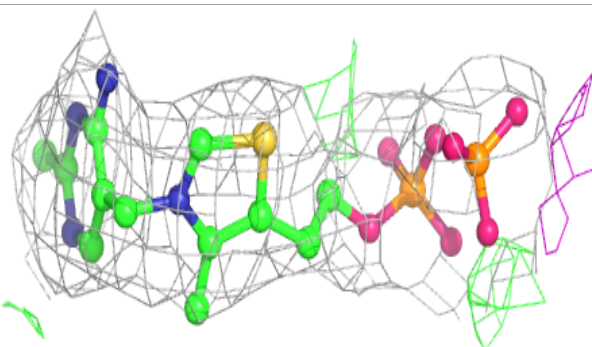
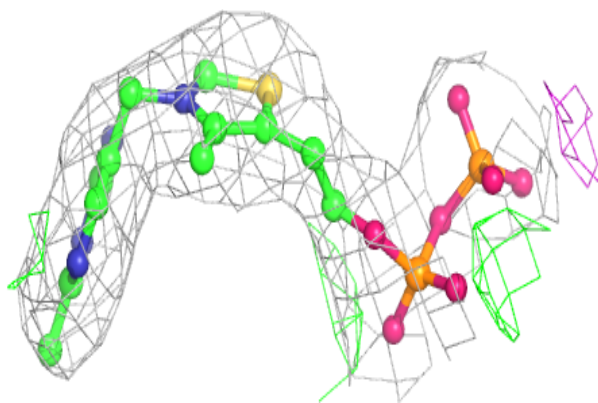
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
5	MG	A	616	1/1	0.92	0.22	57,57,57,57	0
5	MG	B	617	1/1	0.92	0.29	59,59,59,59	0
2	TPP	B	611	26/26	0.97	0.18	34,64,74,122	0
4	SO4	A	621	5/5	0.97	0.15	74,82,95,108	0
3	FAD	B	612	53/53	0.98	0.12	49,66,84,91	0
2	TPP	A	611	26/26	0.98	0.17	46,60,79,82	0
3	FAD	A	612	53/53	0.99	0.12	46,65,79,93	0
4	SO4	B	621	5/5	0.99	0.16	68,71,82,87	0

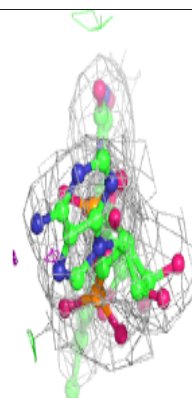
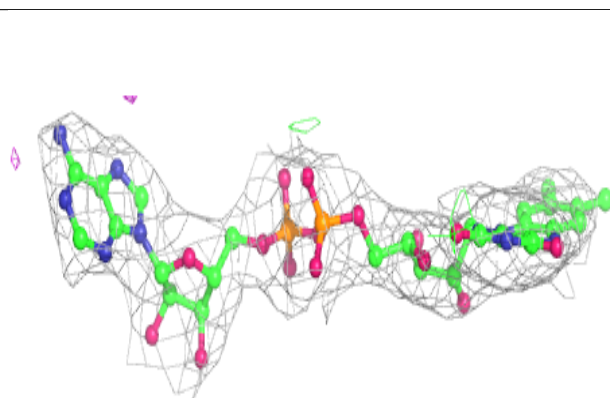
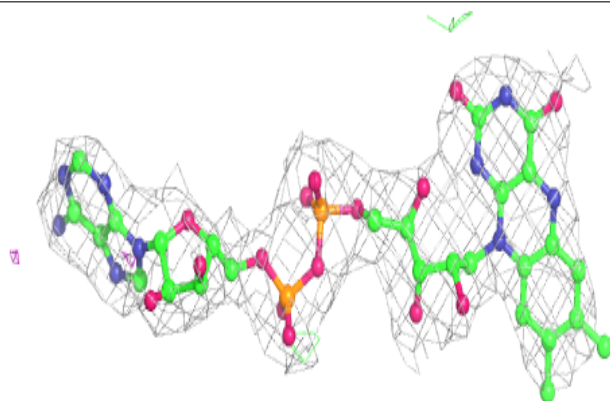
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

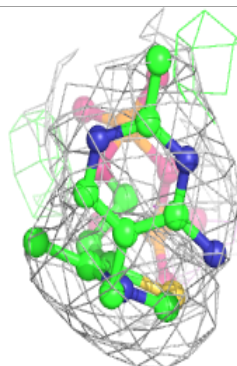
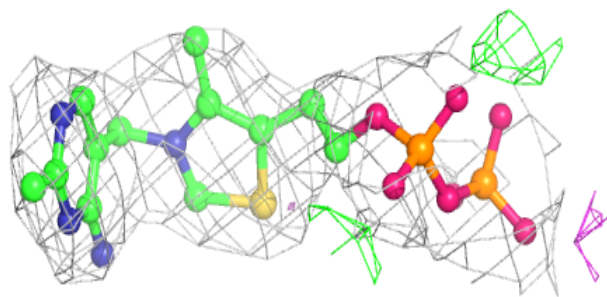
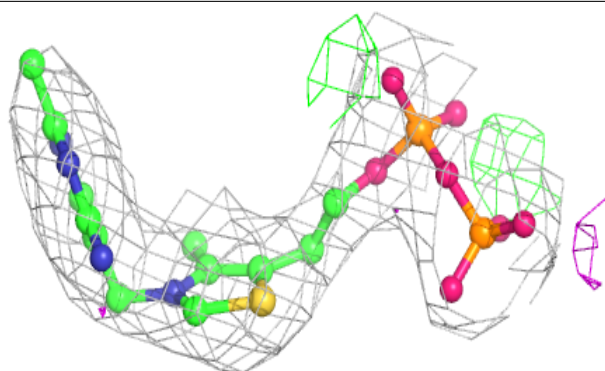
**Electron density around FAD B 612:**

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

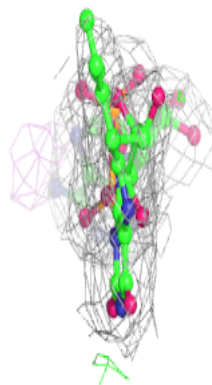
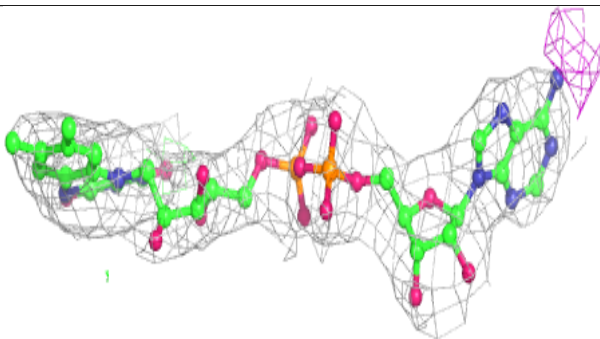
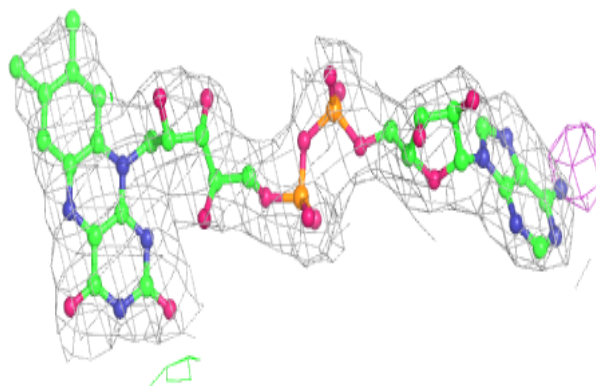


Electron density around TPP A 611:

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

**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)



6.5 Other polymers [i](#)

There are no such residues in this entry.