



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 20, 2026 – 09:46 AM UTC

PDB ID : 9EV5 / pdb_00009ev5
Title : Corynebacterium glutamicum CS176 pyruvate:quinone oxidoreductase (PQO)
in complex with FAD and thiamine diphosphate-magnesium ion
Authors : Da Silva Lameira, C.; Muenssinger, S.; Yang, L.; Eikmanns, B.J.; Bellinzoni,
M.
Deposited on : 2024-03-28
Resolution : 1.86 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

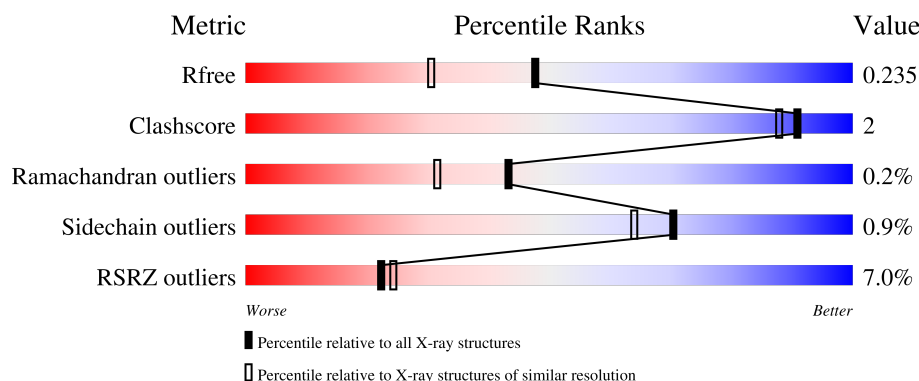
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.86 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}	180053	3428 (1.86-1.86)
Clashscore	190562	3579 (1.86-1.86)
Ramachandran outliers	187476	3553 (1.86-1.86)
Sidechain outliers	187428	3553 (1.86-1.86)
RSRZ outliers	180081	3429 (1.86-1.86)

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	581	3% 94% 5%
1	B	581	3% 95% 2%
1	C	581	7% 92% 7%
1	D	581	14% 94% 5%

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 18843 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 Thiamine pyrophosphate-requiring enzymes [acetolactate synthase, pyruvate dehydrogenase (Cytochrome), glyoxylate carboligase, phosphonopyruvate decarboxylase].

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	575	Total	C	N	O	S	0	0	0
			4282	2692	744	826	20			
1	B	576	Total	C	N	O	S	0	0	0
			4291	2698	745	828	20			
1	C	576	Total	C	N	O	S	0	0	0
			4287	2697	745	825	20			
1	D	576	Total	C	N	O	S	0	0	0
			4238	2665	738	815	20			

There are 32 discrepancies between the modelled and reference sequences:

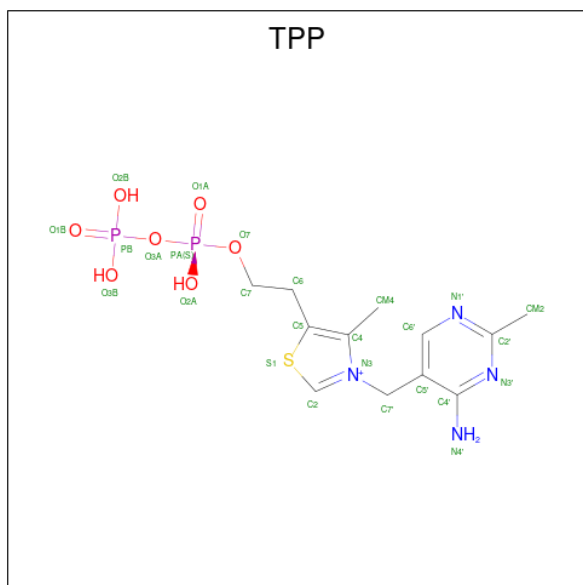
Chain	Residue	Modelled	Actual	Comment	Reference
A	-1	GLY	-	expression tag	UNP Q8NMG5
A	0	HIS	-	expression tag	UNP Q8NMG5
A	3	ARG	HIS	variant	UNP Q8NMG5
A	40	GLY	ASP	variant	UNP Q8NMG5
A	453	LYS	GLN	variant	UNP Q8NMG5
A	492	ASP	GLU	variant	UNP Q8NMG5
A	508	THR	LYS	variant	UNP Q8NMG5
A	516	ASP	GLU	variant	UNP Q8NMG5
B	-1	GLY	-	expression tag	UNP Q8NMG5
B	0	HIS	-	expression tag	UNP Q8NMG5
B	3	ARG	HIS	variant	UNP Q8NMG5
B	40	GLY	ASP	variant	UNP Q8NMG5
B	453	LYS	GLN	variant	UNP Q8NMG5
B	492	ASP	GLU	variant	UNP Q8NMG5
B	508	THR	LYS	variant	UNP Q8NMG5
B	516	ASP	GLU	variant	UNP Q8NMG5
C	-1	GLY	-	expression tag	UNP Q8NMG5
C	0	HIS	-	expression tag	UNP Q8NMG5
C	3	ARG	HIS	variant	UNP Q8NMG5

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Chain	Residue	Modelled	Actual	Comment	Reference
C	40	GLY	ASP	variant	UNP Q8NMG5
C	453	LYS	GLN	variant	UNP Q8NMG5
C	492	ASP	GLU	variant	UNP Q8NMG5
C	508	THR	LYS	variant	UNP Q8NMG5
C	516	ASP	GLU	variant	UNP Q8NMG5
D	-1	GLY	-	expression tag	UNP Q8NMG5
D	0	HIS	-	expression tag	UNP Q8NMG5
D	3	ARG	HIS	variant	UNP Q8NMG5
D	40	GLY	ASP	variant	UNP Q8NMG5
D	453	LYS	GLN	variant	UNP Q8NMG5
D	492	ASP	GLU	variant	UNP Q8NMG5
D	508	THR	LYS	variant	UNP Q8NMG5
D	516	ASP	GLU	variant	UNP Q8NMG5

- Molecule 2 is THIAMINE DIPHOSPHATE (CCD ID: TPP) (formula: $C_{12}H_{19}N_4O_7P_2S$) (labeled as "Ligand of Interest" by depositor).

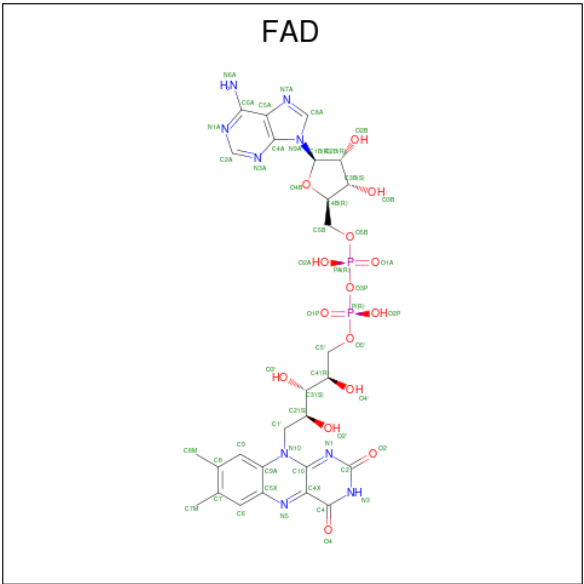


Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
2	A	1	Total	C	N	O	P	S	0	0
			26	12	4	7	2	1		
2	B	1	Total	C	N	O	P	S	0	0
			26	12	4	7	2	1		
2	C	1	Total	C	N	O	P	S	0	0
			26	12	4	7	2	1		
2	D	1	Total	C	N	O	P	S	0	0
			26	12	4	7	2	1		

- Molecule 3 is MAGNESIUM ION (CCD ID: MG) (formula: Mg) (labeled as "Ligand of Interest" by depositor).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	1	Total	Mg	0	0
			1	1		
3	B	1	Total	Mg	0	0
			1	1		
3	C	1	Total	Mg	0	0
			1	1		
3	D	1	Total	Mg	0	0
			1	1		

- Molecule 4 is FLAVIN-ADENINE DINUCLEOTIDE (CCD ID: FAD) (formula: C₂₇H₃₃N₉O₁₅P₂) (labeled as "Ligand of Interest" by depositor).



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

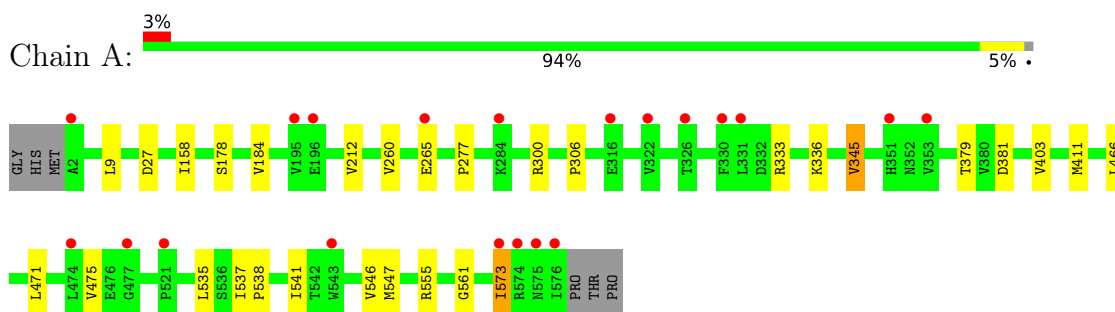
- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	408	Total 408	O 408	0	0
5	B	393	Total 393	O 393	0	0
5	C	338	Total 338	O 338	0	0
5	D	286	Total 286	O 286	0	0

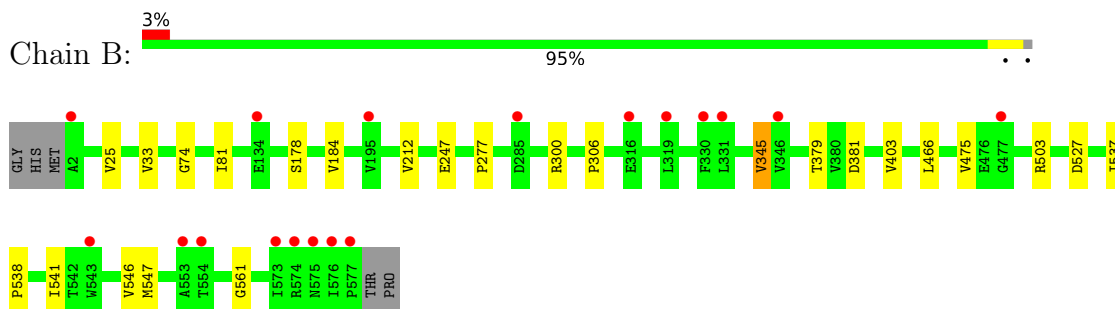
3 Residue-property plots

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ($RSRZ > 2$). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

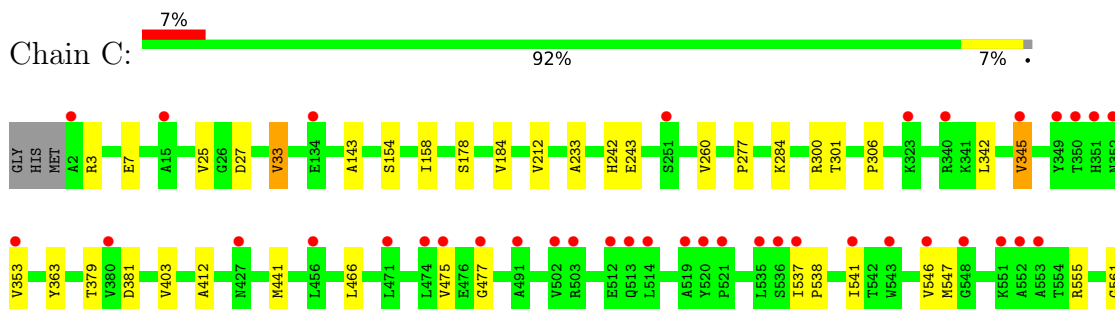
- Molecule 1: Thiamine pyrophosphate-requiring enzymes [acetolactate synthase, pyruvate dehydrogenase (Cytochrome), glyoxylate carboligase, phosphonopyruvate decarboxylase]

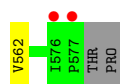


- Molecule 1: Thiamine pyrophosphate-requiring enzymes [acetolactate synthase, pyruvate dehydrogenase (Cytochrome), glyoxylate carboligase, phosphonopyruvate decarboxylase]



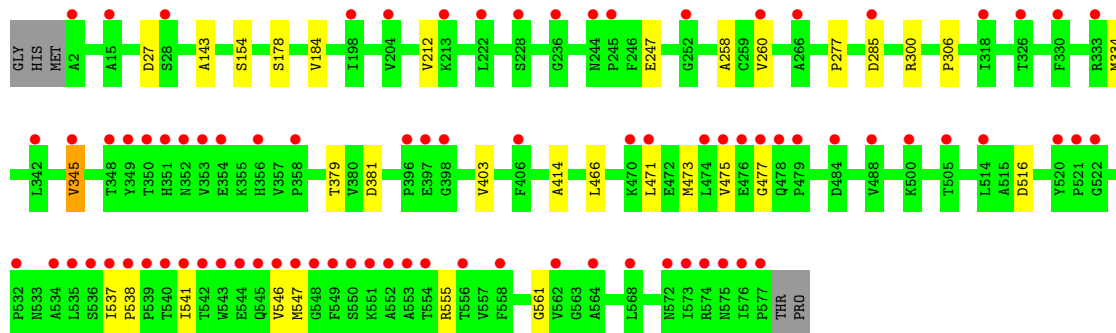
- Molecule 1: Thiamine pyrophosphate-requiring enzymes [acetolactate synthase, pyruvate dehydrogenase (Cytochrome), glyoxylate carboligase, phosphonopyruvate decarboxylase]





- Molecule 1: Thiamine pyrophosphate-requiring enzymes [acetolactate synthase, pyruvate dehydrogenase (Cytochrome), glyoxylate carboligase, phosphonopyruvate decarboxylase]

Chain D: 14% 94% 5%



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	104.19Å 77.94Å 158.04Å 90.00° 100.63° 90.00°	Depositor
Resolution (Å)	155.33 – 1.86 155.33 – 1.86	Depositor EDS
% Data completeness (in resolution range)	64.9 (155.33-1.86) 64.9 (155.33-1.86)	Depositor EDS
R_{merge}	0.20	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.50 (at 1.86Å)	Xtriage
Refinement program	BUSTER 2.10.4	Depositor
R, R_{free}	0.207 , 0.239 0.200 , 0.235	Depositor DCC
R_{free} test set	6723 reflections (4.98%)	wwPDB-VP
Wilson B-factor (Å ²)	20.4	Xtriage
Anisotropy	0.589	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.37 , 62.4	EDS
L-test for twinning ²	$\langle L \rangle = 0.47$, $\langle L^2 \rangle = 0.30$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	18843	wwPDB-VP
Average B, all atoms (Å ²)	32.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 22.74 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 5.3594e-03. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

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: 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	0.80	0/4364	1.05	3/5935 (0.1%)
1	B	0.77	0/4374	1.05	5/5951 (0.1%)
1	C	0.73	0/4370	1.04	6/5946 (0.1%)
1	D	0.71	0/4318	1.05	7/5877 (0.1%)
All	All	0.75	0/17426	1.05	21/23709 (0.1%)

There are no bond length outliers.

All (21) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	158	ILE	N-CA-C	7.96	116.12	107.60
1	C	158	ILE	N-CA-C	7.58	115.65	108.15
1	B	466	LEU	N-CA-C	-6.89	99.28	109.62
1	D	477	GLY	CA-C-N	6.10	128.85	120.67
1	D	477	GLY	C-N-CA	6.10	128.85	120.67
1	A	466	LEU	N-CA-C	-6.00	98.13	108.56
1	C	466	LEU	N-CA-C	-5.90	98.30	108.56
1	D	466	LEU	N-CA-C	-5.66	98.71	108.56
1	B	81	ILE	N-CA-C	5.63	116.27	110.36
1	B	466	LEU	CA-C-N	5.58	126.30	119.99
1	B	466	LEU	C-N-CA	5.58	126.30	119.99
1	B	184	VAL	N-CA-C	5.54	114.59	106.55
1	D	285	ASP	N-CA-C	5.50	116.96	111.07
1	D	184	VAL	N-CA-C	5.44	114.44	106.55
1	C	184	VAL	N-CA-C	5.43	114.42	106.55
1	A	184	VAL	N-CA-C	5.28	114.20	106.55
1	C	477	GLY	CA-C-N	5.23	127.68	120.67
1	C	477	GLY	C-N-CA	5.23	127.68	120.67
1	D	516	ASP	CA-CB-CG	5.18	117.78	112.60
1	D	414	ALA	N-CA-C	5.13	116.56	111.07

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	233	ALA	N-CA-C	-5.10	103.95	110.53

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	4282	0	4215	16	0
1	B	4291	0	4224	11	0
1	C	4287	0	4219	19	0
1	D	4238	0	4145	15	0
2	A	26	0	16	1	0
2	B	26	0	16	1	0
2	C	26	0	16	0	0
2	D	26	0	16	0	0
3	A	1	0	0	0	0
3	B	1	0	0	0	0
3	C	1	0	0	0	0
3	D	1	0	0	0	0
4	A	53	0	31	1	0
4	B	53	0	31	0	0
4	C	53	0	31	0	0
4	D	53	0	31	0	0
5	A	408	0	0	0	0
5	B	393	0	0	0	0
5	C	338	0	0	0	0
5	D	286	0	0	0	0
All	All	18843	0	16991	57	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 (57) 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:C:25:VAL:HG22	1:C:33:VAL:HG11	1.72	0.71
1:B:306:PRO:HB2	1:D:178:SER:HB2	1.78	0.66
1:A:306:PRO:HB2	1:C:178:SER:HB2	1.77	0.65
1:D:258:ALA:HB1	1:D:334:MET:CE	2.27	0.65
1:B:178:SER:HB2	1:D:306:PRO:HB2	1.79	0.64
1:D:345:VAL:HG13	1:D:561:GLY:HA2	1.83	0.60
1:A:336:LYS:HA	1:A:573:ILE:HD11	1.84	0.59
1:B:25:VAL:HG21	1:B:33:VAL:HG21	1.85	0.59
1:C:277:PRO:HA	1:C:300:ARG:HD2	1.85	0.58
1:C:345:VAL:HG13	1:C:561:GLY:HA2	1.84	0.58
1:B:345:VAL:HG13	1:B:561:GLY:HA2	1.86	0.57
1:D:475:VAL:HG22	1:D:537:ILE:HG21	1.86	0.57
1:A:345:VAL:HG13	1:A:561:GLY:HA2	1.85	0.57
1:A:178:SER:HB2	1:C:306:PRO:HB2	1.86	0.56
1:B:277:PRO:HA	1:B:300:ARG:HD2	1.87	0.56
1:A:260:VAL:HG12	1:A:555:ARG:HG2	1.86	0.56
1:C:475:VAL:HG22	1:C:537:ILE:HG21	1.88	0.55
1:A:277:PRO:HA	1:A:300:ARG:HD2	1.88	0.55
1:D:277:PRO:HA	1:D:300:ARG:HD2	1.88	0.55
1:D:546:VAL:HG12	1:D:547:MET:HE2	1.89	0.54
1:B:538:PRO:HD2	1:B:541:ILE:HD12	1.90	0.52
1:C:3:ARG:HG2	1:C:7:GLU:OE2	2.08	0.52
1:A:411:MET:HG2	2:A:601:TPP:C2'	2.40	0.52
1:C:538:PRO:HD2	1:C:541:ILE:HD12	1.91	0.52
1:A:546:VAL:HG12	1:A:547:MET:HE2	1.92	0.51
1:B:546:VAL:HG12	1:B:547:MET:HE2	1.92	0.51
1:A:265:GLU:OE1	1:A:333:ARG:NH2	2.35	0.50
1:C:546:VAL:HG13	1:C:547:MET:HE2	1.95	0.48
1:A:475:VAL:HG22	1:A:537:ILE:HG21	1.96	0.47
1:D:260:VAL:HG11	1:D:555:ARG:HA	1.96	0.47
1:B:25:VAL:CG2	1:B:33:VAL:HG21	2.46	0.46
1:C:284:LYS:HD3	1:C:301:THR:OG1	2.16	0.46
1:A:260:VAL:HG11	1:A:555:ARG:HA	1.98	0.45
1:C:260:VAL:HG11	1:C:555:ARG:HA	1.97	0.45
1:A:538:PRO:HD2	1:A:541:ILE:HD12	1.99	0.44
1:A:471:LEU:HD12	1:A:535:LEU:HD22	2.00	0.44
1:B:475:VAL:HG22	1:B:537:ILE:HG21	1.99	0.44
1:B:379:THR:HA	1:B:403:VAL:O	2.18	0.44
1:B:503:ARG:NH1	1:B:527:ASP:OD2	2.50	0.44
1:D:143:ALA:HB1	1:D:154:SER:HB3	1.99	0.43
1:C:143:ALA:HB1	1:C:154:SER:HB3	2.00	0.43
4:A:603:FAD:H9	4:A:603:FAD:H1'1	1.89	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:412:ALA:HB2	1:C:441:MET:HB3	2.01	0.42
1:A:260:VAL:CG1	1:A:555:ARG:HG2	2.49	0.42
2:B:601:TPP:HN42	2:B:601:TPP:H2	1.84	0.42
1:D:475:VAL:CG2	1:D:537:ILE:HG21	2.49	0.42
1:C:242:HIS:HD2	1:C:243:GLU:OE1	2.02	0.42
1:D:538:PRO:HD2	1:D:541:ILE:HD12	2.00	0.42
1:C:25:VAL:HG11	1:D:473:MET:HE1	2.02	0.42
1:D:379:THR:HA	1:D:403:VAL:O	2.20	0.42
1:C:342:LEU:HD22	1:C:562:VAL:HG21	2.01	0.41
1:A:379:THR:HA	1:A:403:VAL:O	2.21	0.41
1:C:379:THR:HA	1:C:403:VAL:O	2.21	0.41
1:C:353:VAL:HG22	1:C:363:TYR:HB2	2.02	0.41
1:A:475:VAL:CG2	1:A:537:ILE:HG21	2.51	0.40
1:C:25:VAL:HG11	1:D:473:MET:CE	2.51	0.40
1:D:471:LEU:HD23	1:D:471:LEU:C	2.46	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	573/581 (99%)	563 (98%)	9 (2%)	1 (0%)	43	31
1	B	574/581 (99%)	566 (99%)	7 (1%)	1 (0%)	43	31
1	C	574/581 (99%)	563 (98%)	10 (2%)	1 (0%)	43	31
1	D	574/581 (99%)	564 (98%)	9 (2%)	1 (0%)	43	31
All	All	2295/2324 (99%)	2256 (98%)	35 (2%)	4 (0%)	43	31

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	27	ASP
1	D	27	ASP
1	C	27	ASP
1	B	74	GLY

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	450/464 (97%)	445 (99%)	5 (1%)	65	57
1	B	452/464 (97%)	448 (99%)	4 (1%)	70	64
1	C	450/464 (97%)	446 (99%)	4 (1%)	70	64
1	D	438/464 (94%)	434 (99%)	4 (1%)	70	64
All	All	1790/1856 (96%)	1773 (99%)	17 (1%)	70	64

All (17) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	9	LEU
1	A	212	VAL
1	A	345	VAL
1	A	381	ASP
1	A	573	ILE
1	B	212	VAL
1	B	247	GLU
1	B	345	VAL
1	B	381	ASP
1	C	33	VAL
1	C	212	VAL
1	C	345	VAL
1	C	381	ASP
1	D	212	VAL
1	D	247	GLU
1	D	345	VAL
1	D	381	ASP

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

Mol	Chain	Res	Type
1	A	238	GLN
1	A	321	HIS
1	A	422	GLN
1	B	200	ASN
1	B	238	GLN
1	C	30	ASN
1	C	242	HIS
1	C	533	ASN
1	D	112	GLN
1	D	238	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

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

5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry ⓘ

Of 12 ligands modelled in this entry, 4 are monoatomic - leaving 8 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
2	TPP	C	601	3	26,27,27	0.45	0	38,40,40	0.51	0
2	TPP	B	601	3	26,27,27	0.42	0	38,40,40	0.57	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
4	FAD	C	603	-	58,58,58	0.35	0	85,89,89	0.46	0
4	FAD	A	603	-	58,58,58	0.48	0	85,89,89	0.43	0
2	TPP	D	601	3	26,27,27	0.42	0	38,40,40	0.58	0
4	FAD	B	603	-	58,58,58	0.43	0	85,89,89	0.48	0
4	FAD	D	603	-	58,58,58	0.44	0	85,89,89	0.51	0
2	TPP	A	601	3	26,27,27	0.51	0	38,40,40	0.66	0

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
2	TPP	C	601	3	-	2/17/17/17	0/2/2/2
2	TPP	B	601	3	-	2/17/17/17	0/2/2/2
4	FAD	C	603	-	-	4/34/50/50	0/6/6/6
4	FAD	A	603	-	-	5/34/50/50	0/6/6/6
2	TPP	D	601	3	-	2/17/17/17	0/2/2/2
4	FAD	B	603	-	-	4/34/50/50	0/6/6/6
4	FAD	D	603	-	-	5/34/50/50	0/6/6/6
2	TPP	A	601	3	-	2/17/17/17	0/2/2/2

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (26) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	601	TPP	PA-O3A-PB-O2B
2	B	601	TPP	PA-O3A-PB-O2B
2	C	601	TPP	PA-O3A-PB-O2B
2	D	601	TPP	PA-O3A-PB-O2B
4	A	603	FAD	PA-O3P-P-O1P
4	C	603	FAD	PA-O3P-P-O1P
4	D	603	FAD	PA-O3P-P-O1P
4	A	603	FAD	P-O3P-PA-O5B
4	C	603	FAD	P-O3P-PA-O5B
4	D	603	FAD	P-O3P-PA-O5B
2	A	601	TPP	PA-O3A-PB-O1B

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Mol	Chain	Res	Type	Atoms
4	A	603	FAD	C2'-C1'-N10-C10
4	B	603	FAD	C2'-C1'-N10-C10
4	C	603	FAD	C2'-C1'-N10-C10
4	D	603	FAD	C2'-C1'-N10-C10
2	D	601	TPP	PA-O3A-PB-O1B
4	A	603	FAD	PA-O3P-P-O2P
4	B	603	FAD	PA-O3P-P-O1P
4	C	603	FAD	PA-O3P-P-O2P
4	D	603	FAD	PA-O3P-P-O2P
2	B	601	TPP	PA-O3A-PB-O1B
2	C	601	TPP	PA-O3A-PB-O1B
4	B	603	FAD	C3'-C4'-C5'-O5'
4	D	603	FAD	O4B-C4B-C5B-O5B
4	B	603	FAD	PA-O3P-P-O2P
4	A	603	FAD	O4B-C4B-C5B-O5B

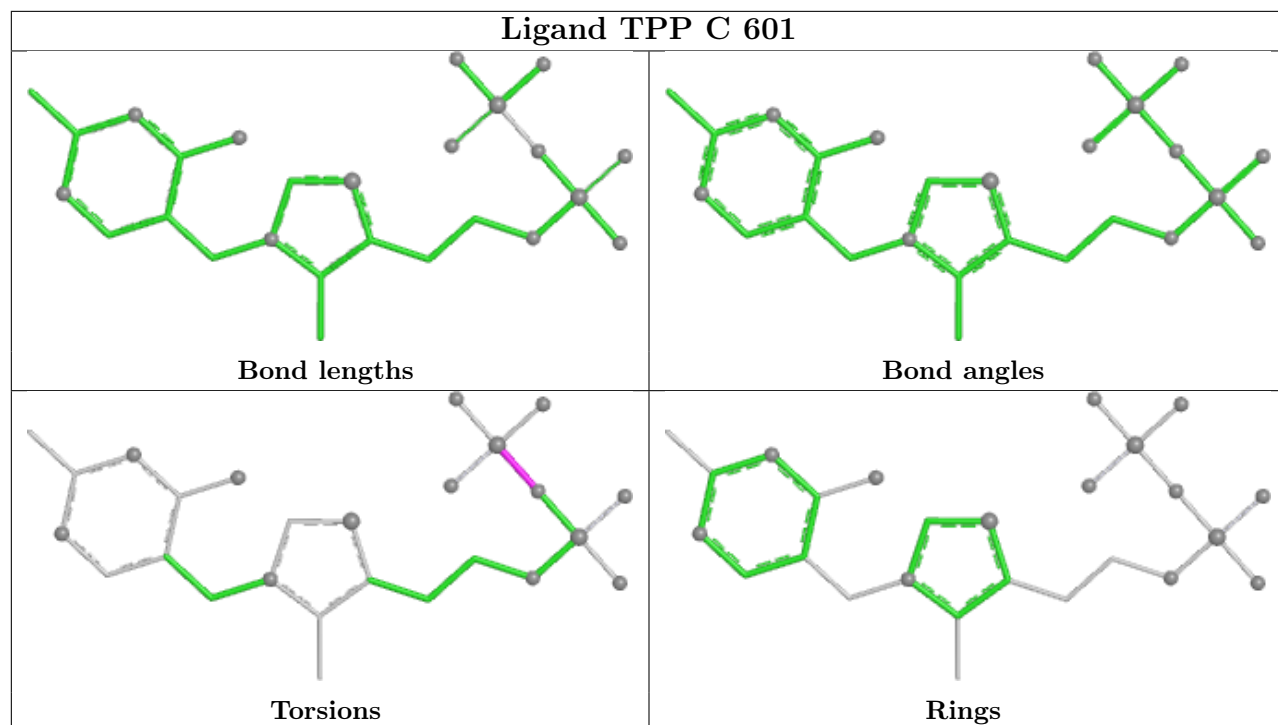
There are no ring outliers.

3 monomers are involved in 3 short contacts:

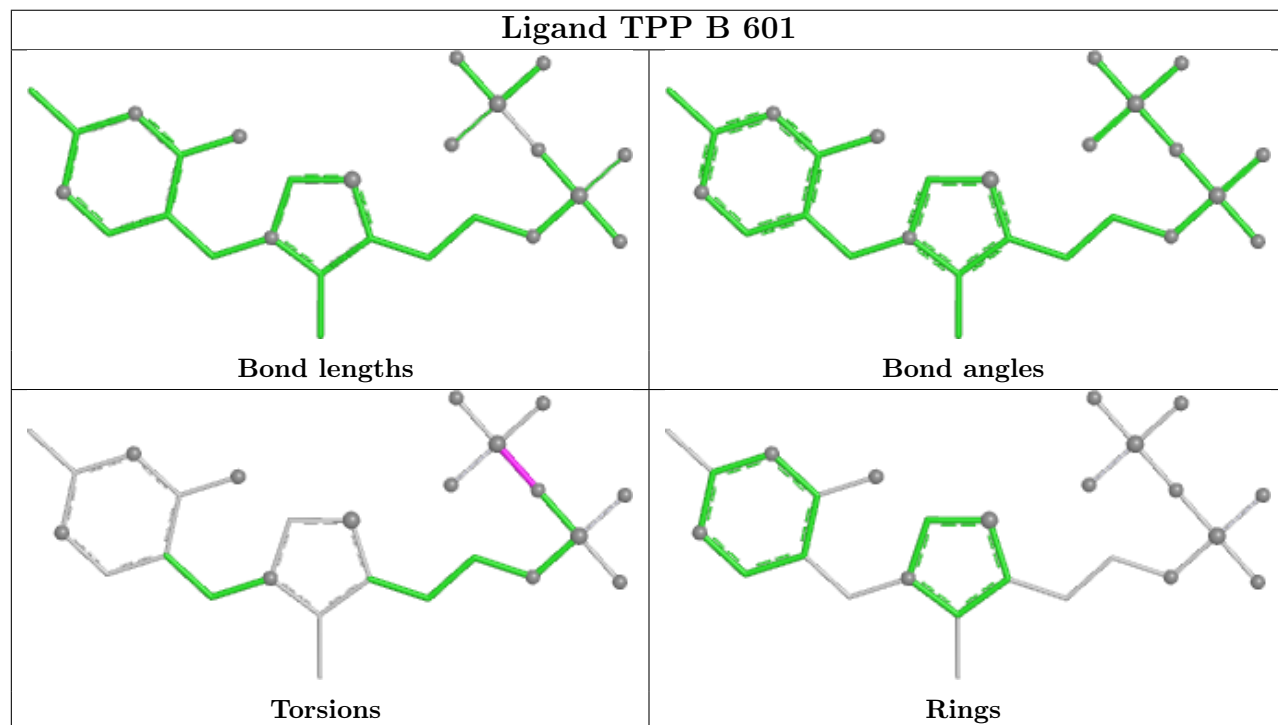
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	601	TPP	1	0
4	A	603	FAD	1	0
2	A	601	TPP	1	0

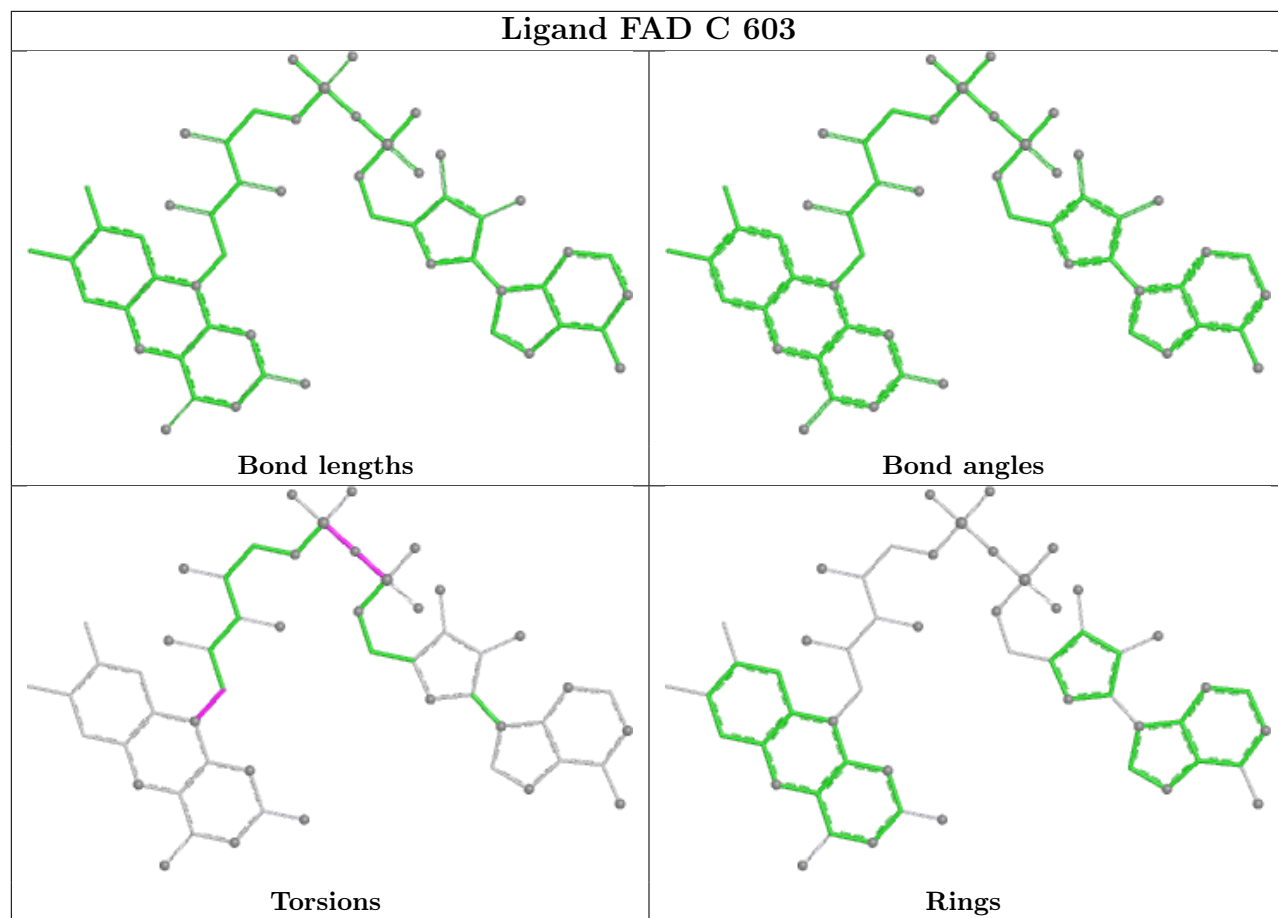
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

Ligand TPP C 601

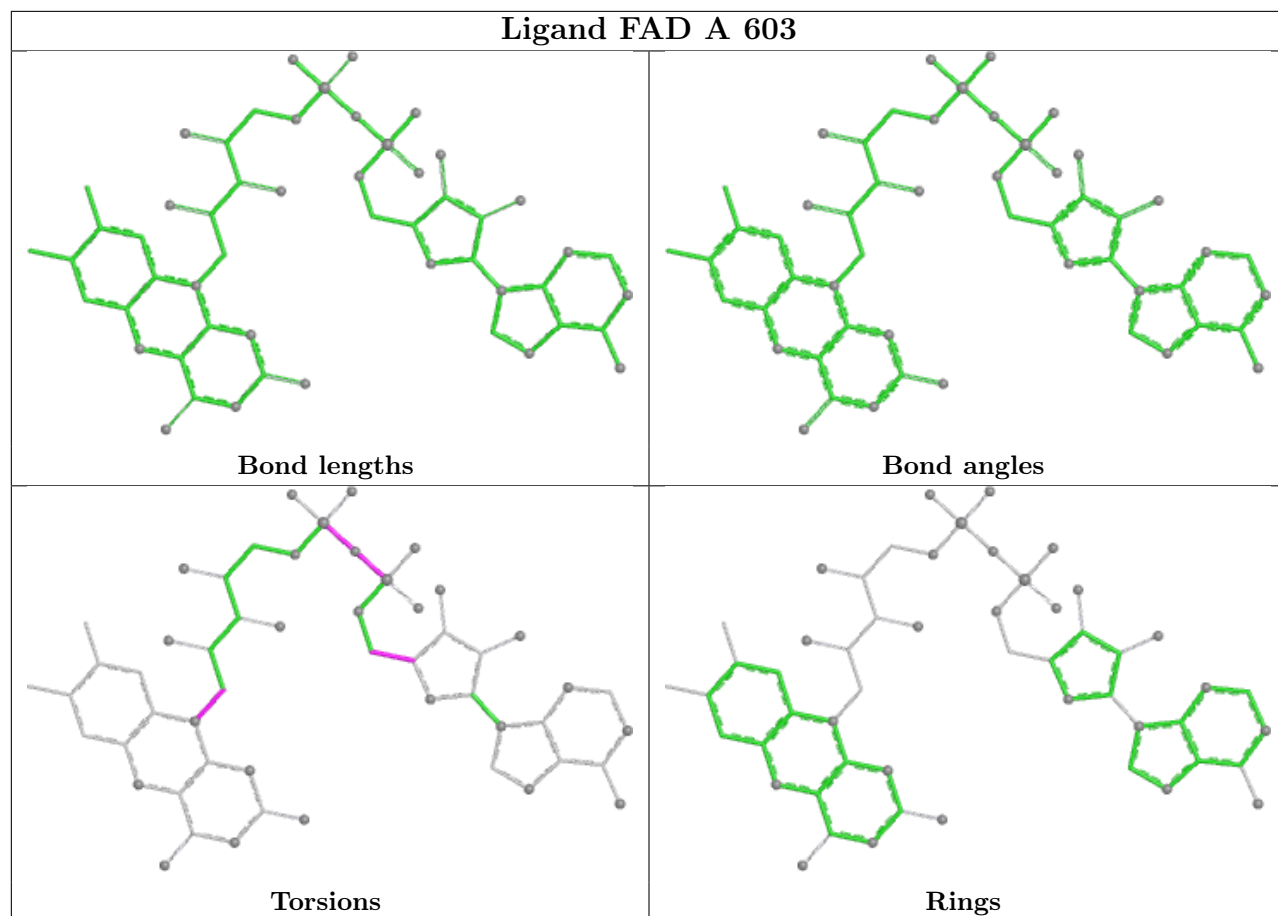


Ligand TPP B 601

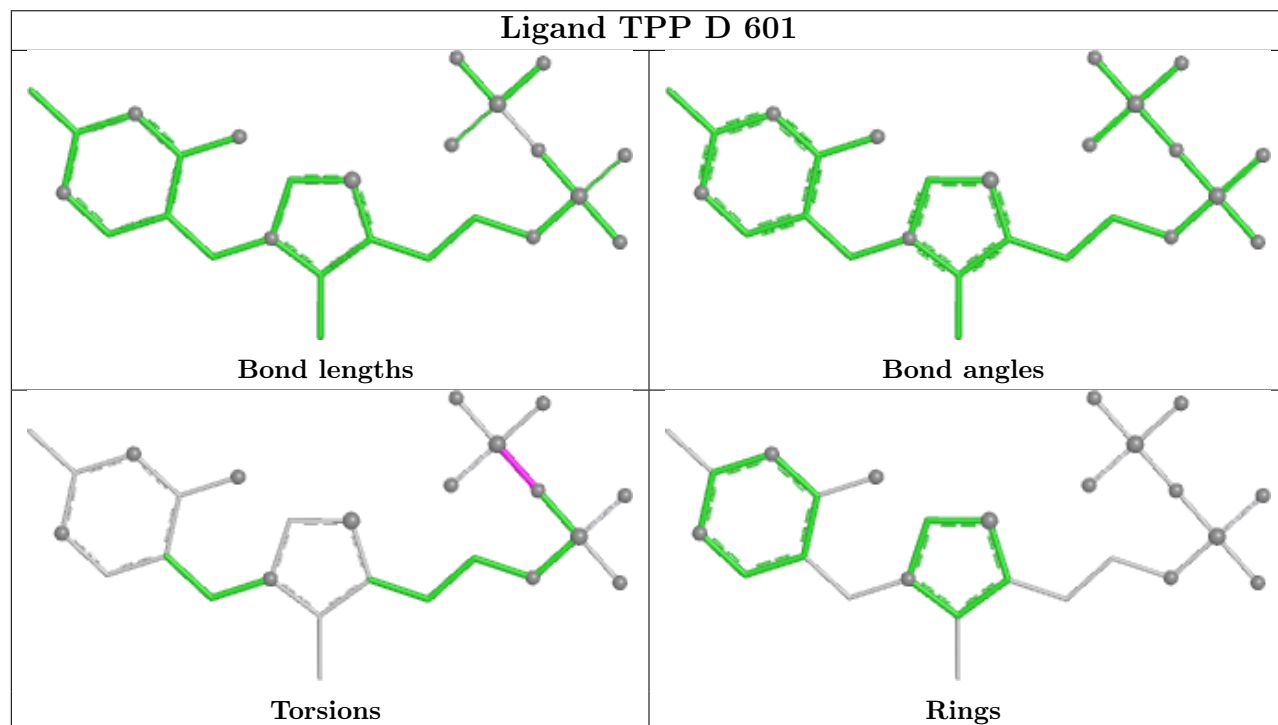


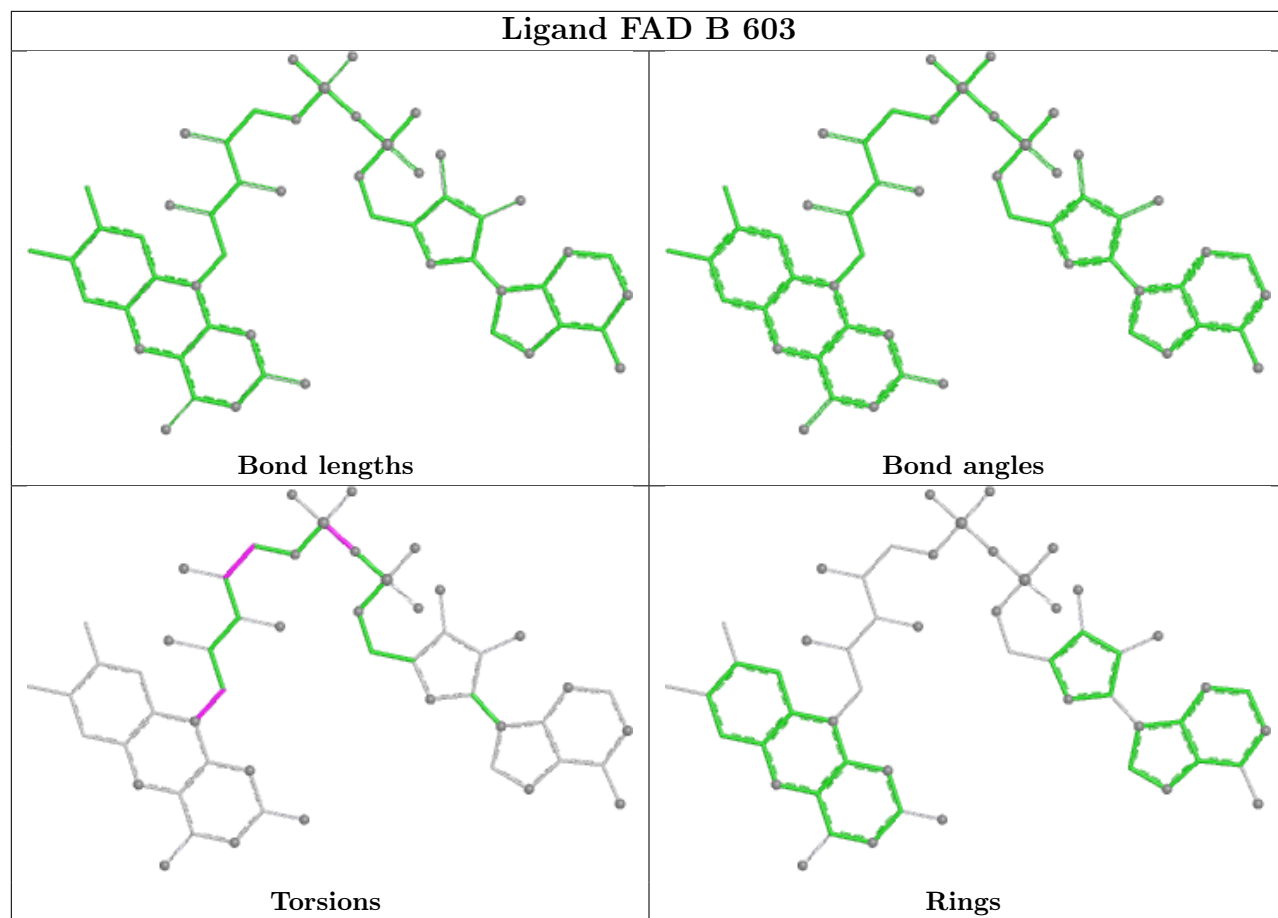


Ligand FAD A 603

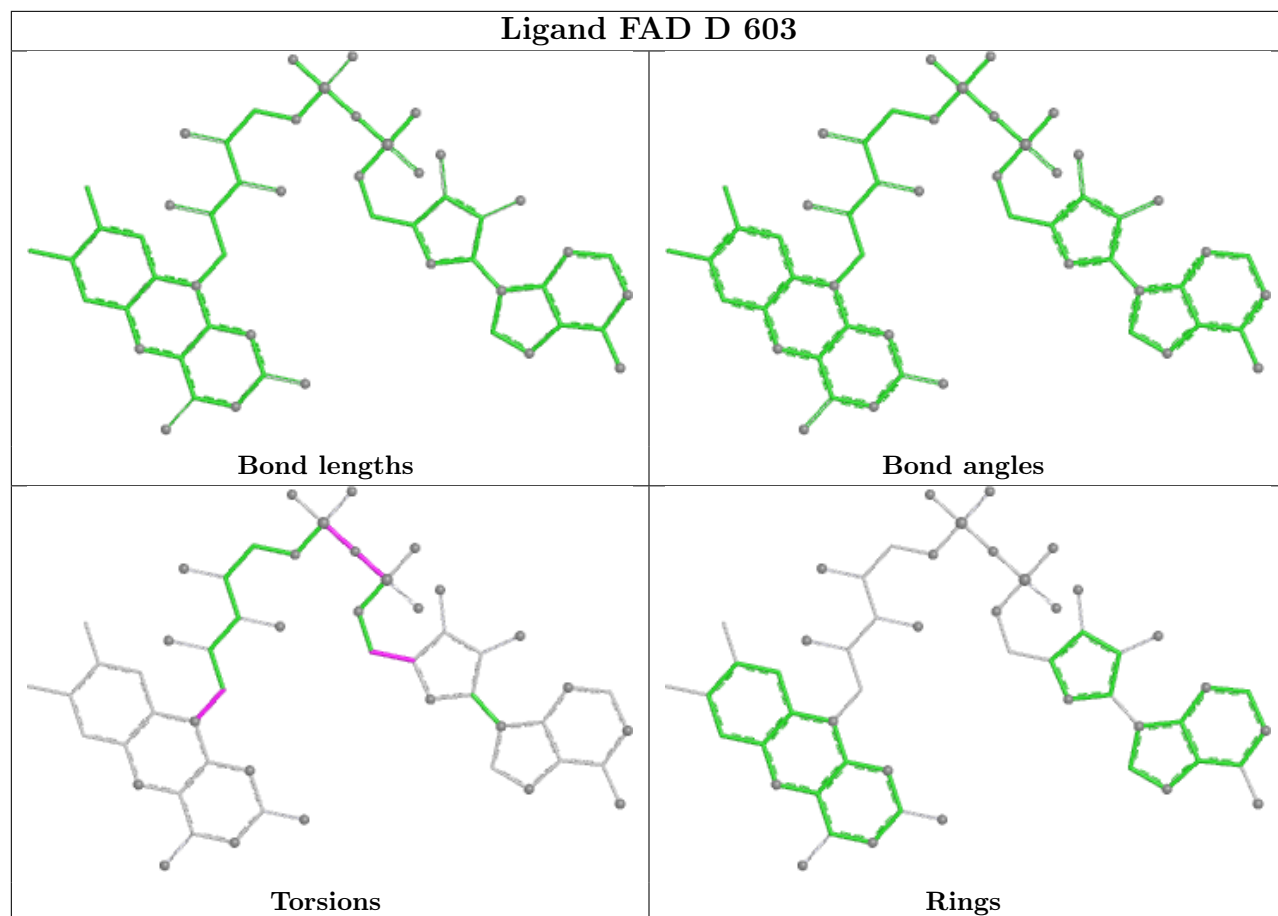


Ligand TPP D 601

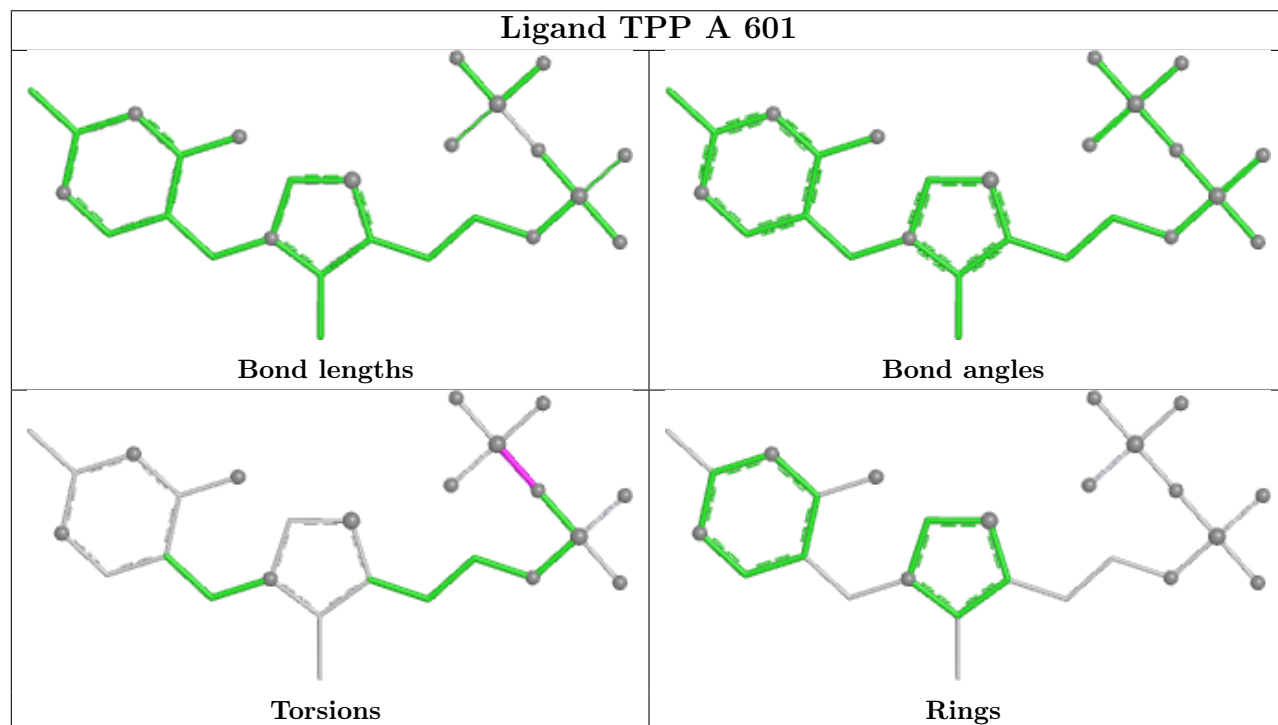




Ligand FAD D 603



Ligand TPP A 601



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	575/581 (98%)	0.04	20 (3%)	47	51	12, 23, 44, 62	0
1	B	576/581 (99%)	0.05	18 (3%)	51	55	13, 25, 45, 69	0
1	C	576/581 (99%)	0.64	40 (6%)	23	25	18, 33, 55, 70	0
1	D	576/581 (99%)	0.84	83 (14%)	6	6	16, 41, 69, 84	0
All	All	2303/2324 (99%)	0.39	161 (6%)	22	24	12, 30, 58, 84	0

All (161) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	2	ALA	7.0
1	D	535	LEU	6.6
1	D	2	ALA	6.5
1	C	2	ALA	6.3
1	D	477	GLY	5.7
1	D	541	ILE	5.2
1	A	2	ALA	4.8
1	D	537	ILE	4.8
1	D	474	LEU	4.5
1	C	353	VAL	4.4
1	D	577	PRO	4.3
1	D	543	TRP	4.3
1	C	502	VAL	4.2
1	D	475	VAL	4.2
1	D	553	ALA	4.1
1	D	576	ILE	4.0
1	C	552	ALA	4.0
1	D	353	VAL	4.0
1	D	552	ALA	4.0
1	D	471	LEU	4.0
1	C	541	ILE	4.0

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Mol	Chain	Res	Type	RSRZ
1	D	521	PRO	4.0
1	D	350	THR	3.9
1	D	549	PHE	3.8
1	D	568	LEU	3.7
1	C	543	TRP	3.7
1	D	222	LEU	3.6
1	D	352	ASN	3.6
1	A	576	ILE	3.6
1	C	521	PRO	3.6
1	B	330	PHE	3.5
1	D	558	PHE	3.5
1	D	544	GLU	3.5
1	C	474	LEU	3.5
1	C	514	LEU	3.4
1	D	534	ALA	3.4
1	B	346	VAL	3.3
1	A	543	TRP	3.3
1	D	476	GLU	3.2
1	A	573	ILE	3.2
1	D	536	SER	3.2
1	C	475	VAL	3.2
1	B	573	ILE	3.2
1	C	576	ILE	3.2
1	D	542	THR	3.2
1	A	574	ARG	3.2
1	C	537	ILE	3.1
1	C	551	LYS	3.1
1	D	349	TYR	3.1
1	C	503	ARG	3.1
1	D	358	PRO	3.1
1	A	477	GLY	3.1
1	D	345	VAL	3.1
1	A	330	PHE	3.0
1	B	331	LEU	3.0
1	B	543	TRP	3.0
1	D	574	ARG	3.0
1	C	513	GLN	3.0
1	D	342	LEU	2.9
1	D	351	HIS	2.9
1	A	353	VAL	2.9
1	D	546	VAL	2.9
1	A	326	THR	2.9

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Mol	Chain	Res	Type	RSRZ
1	D	547	MET	2.9
1	C	519	ALA	2.9
1	C	553	ALA	2.9
1	C	351	HIS	2.9
1	D	348	THR	2.9
1	A	575	ASN	2.9
1	C	352	ASN	2.9
1	B	576	ILE	2.9
1	C	477	GLY	2.9
1	D	548	GLY	2.9
1	D	572	ASN	2.8
1	A	474	LEU	2.8
1	D	575	ASN	2.8
1	B	316	GLU	2.7
1	D	545	GLN	2.6
1	B	577	PRO	2.6
1	D	398	GLY	2.6
1	D	213	LYS	2.6
1	C	548	GLY	2.6
1	D	470	LYS	2.6
1	C	535	LEU	2.6
1	C	512	GLU	2.6
1	D	551	LYS	2.6
1	D	540	THR	2.6
1	D	554	THR	2.6
1	A	521	PRO	2.5
1	C	340	ARG	2.5
1	D	245	PRO	2.5
1	C	349	TYR	2.5
1	D	520	TYR	2.5
1	C	15	ALA	2.5
1	D	236	GLY	2.5
1	D	406	PHE	2.5
1	D	573	ILE	2.5
1	D	484	ASP	2.5
1	D	539	PRO	2.5
1	C	471	LEU	2.4
1	C	350	THR	2.4
1	A	351	HIS	2.4
1	C	536	SER	2.4
1	D	514	LEU	2.4
1	D	330	PHE	2.4

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Mol	Chain	Res	Type	RSRZ
1	D	326	THR	2.4
1	B	553	ALA	2.4
1	B	134	GLU	2.4
1	D	228	SER	2.4
1	D	500	LYS	2.4
1	D	354	GLU	2.3
1	C	577	PRO	2.3
1	C	380	VAL	2.3
1	D	28	SER	2.3
1	D	260	VAL	2.3
1	D	198	ILE	2.3
1	D	505	THR	2.3
1	D	266	ALA	2.3
1	D	333	ARG	2.3
1	D	562	VAL	2.3
1	B	574	ARG	2.2
1	D	479	PRO	2.2
1	D	538	PRO	2.2
1	C	456	LEU	2.2
1	D	15	ALA	2.2
1	B	575	ASN	2.2
1	A	195	VAL	2.2
1	A	316	GLU	2.2
1	A	284	LYS	2.2
1	A	265	GLU	2.2
1	A	331	LEU	2.2
1	D	252	GLY	2.2
1	C	491	ALA	2.2
1	C	323	LYS	2.2
1	C	134	GLU	2.1
1	C	520	TYR	2.1
1	D	532	PRO	2.1
1	B	285	ASP	2.1
1	D	285	ASP	2.1
1	A	322	VAL	2.1
1	B	195	VAL	2.1
1	C	546	VAL	2.1
1	D	204	VAL	2.1
1	A	196	GLU	2.1
1	C	427	ASN	2.1
1	D	318	ILE	2.1
1	B	554	THR	2.1

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Mol	Chain	Res	Type	RSRZ
1	D	488	VAL	2.1
1	B	319	LEU	2.1
1	D	397	GLU	2.0
1	D	550	SER	2.0
1	D	556	THR	2.0
1	B	477	GLY	2.0
1	D	356	HIS	2.0
1	D	522	GLY	2.0
1	D	564	ALA	2.0
1	C	251	SER	2.0
1	D	478	GLN	2.0
1	D	244	ASN	2.0
1	D	396	PRO	2.0
1	C	345	VAL	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 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
3	MG	D	602	1/1	0.81	0.11	50,50,50,50	0
2	TPP	D	601	26/26	0.90	0.11	25,33,37,37	0
3	MG	A	602	1/1	0.92	0.07	24,24,24,24	0
2	TPP	C	601	26/26	0.93	0.10	22,31,33,34	0
4	FAD	D	603	53/53	0.93	0.09	23,25,28,29	0
4	FAD	C	603	53/53	0.95	0.07	19,22,25,26	0
4	FAD	B	603	53/53	0.96	0.06	14,18,20,20	0
3	MG	C	602	1/1	0.96	0.06	29,29,29,29	0
4	FAD	A	603	53/53	0.96	0.06	13,16,19,19	0

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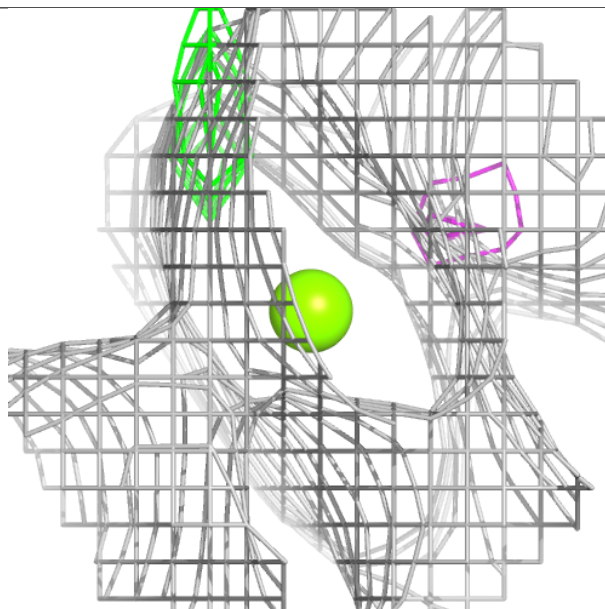
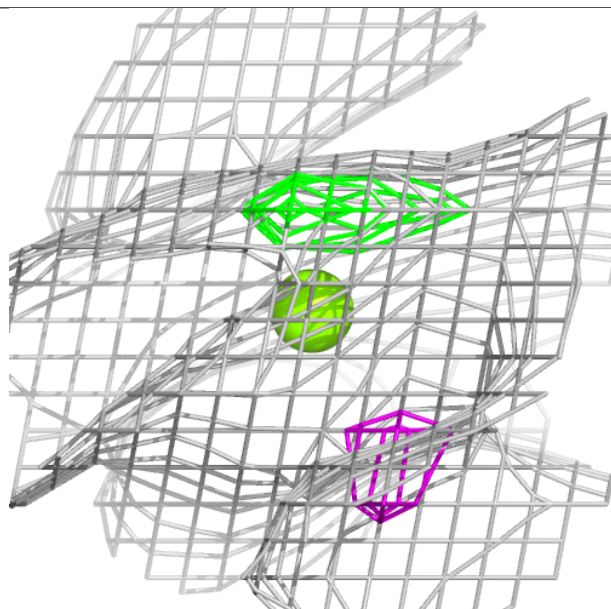
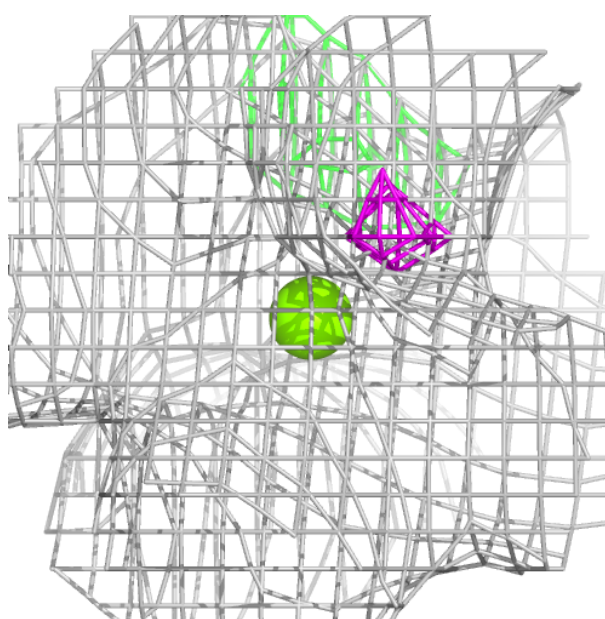
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
2	TPP	B	601	26/26	0.97	0.06	11,17,19,20	0
2	TPP	A	601	26/26	0.97	0.06	12,17,18,20	0
3	MG	B	602	1/1	0.99	0.04	18,18,18,18	0

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

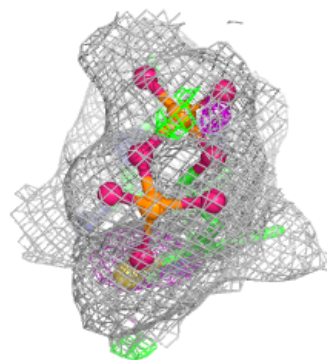
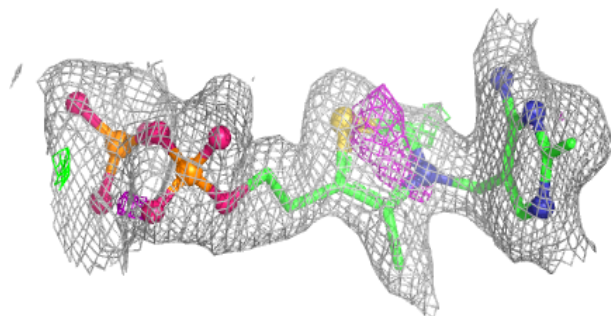
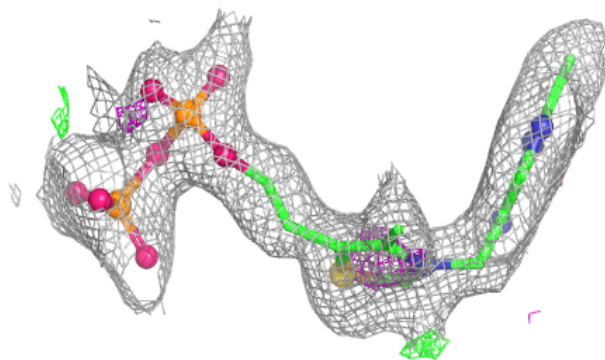
Electron density around MG D 602:

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



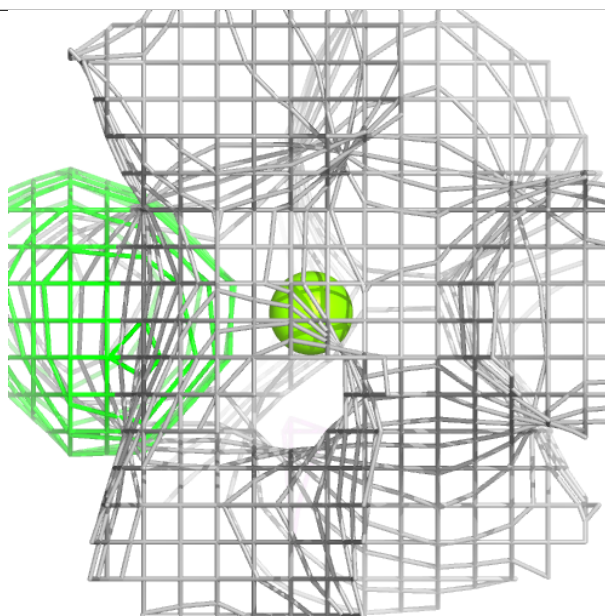
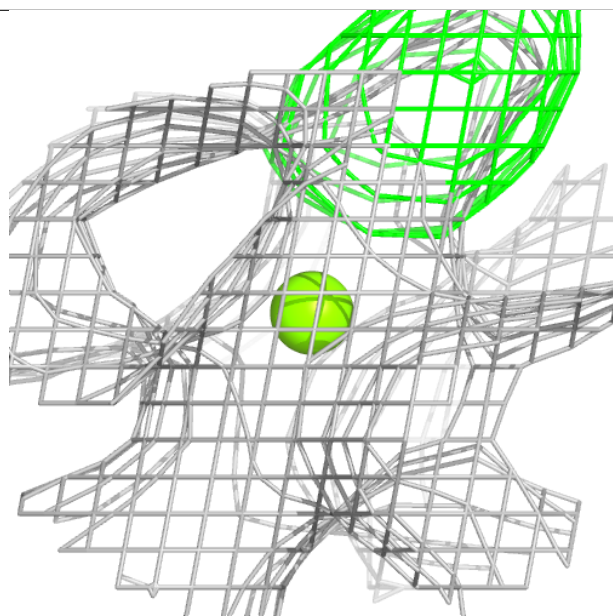
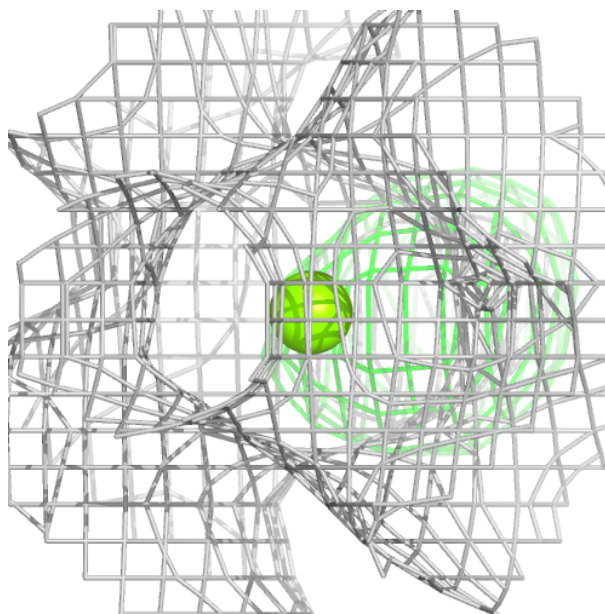
Electron density around TPP D 601:

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



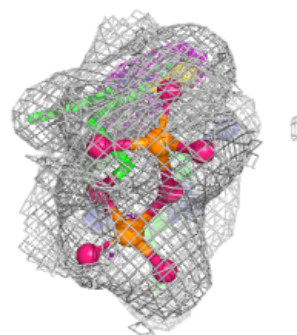
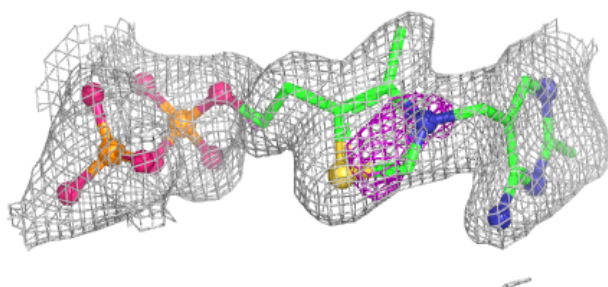
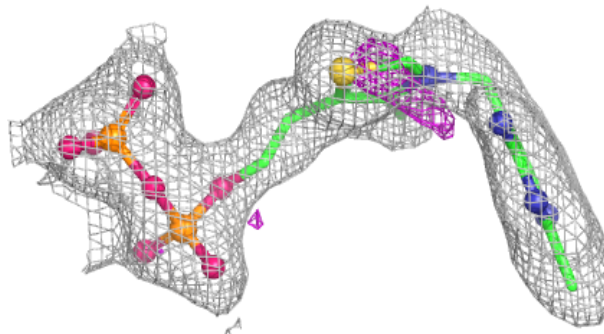
Electron density around MG A 602:

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

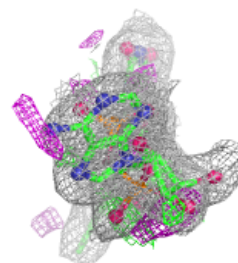
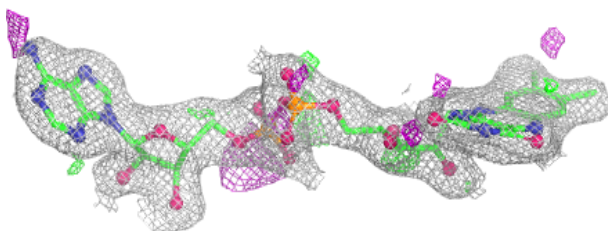
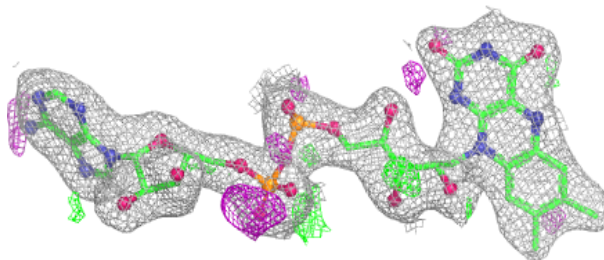


Electron density around TPP C 601:

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

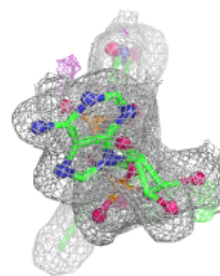
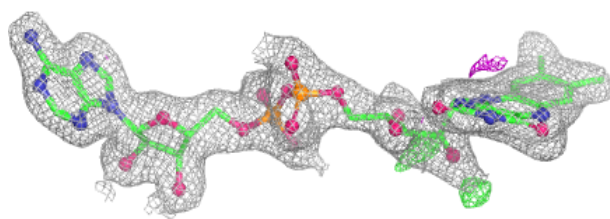
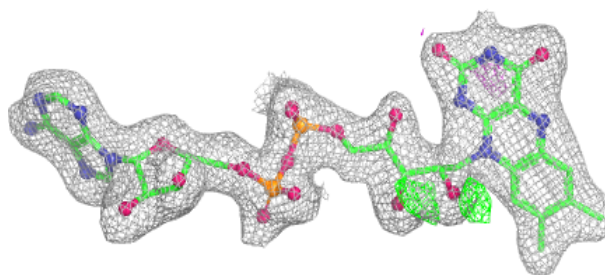
**Electron density around FAD D 603:**

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

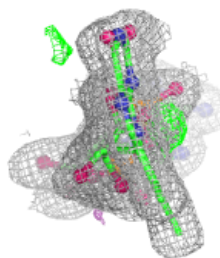
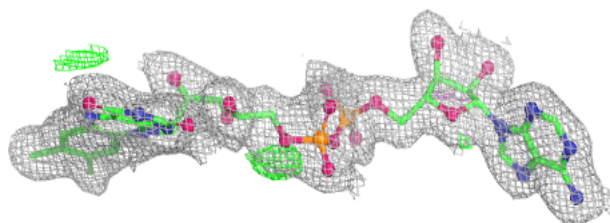
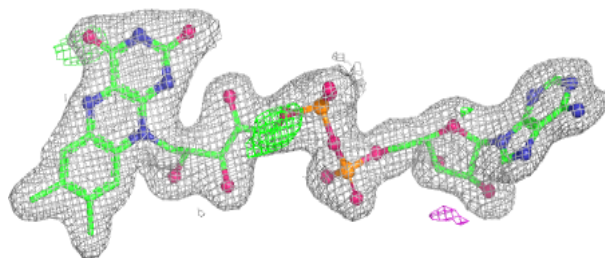


Electron density around FAD C 603:

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

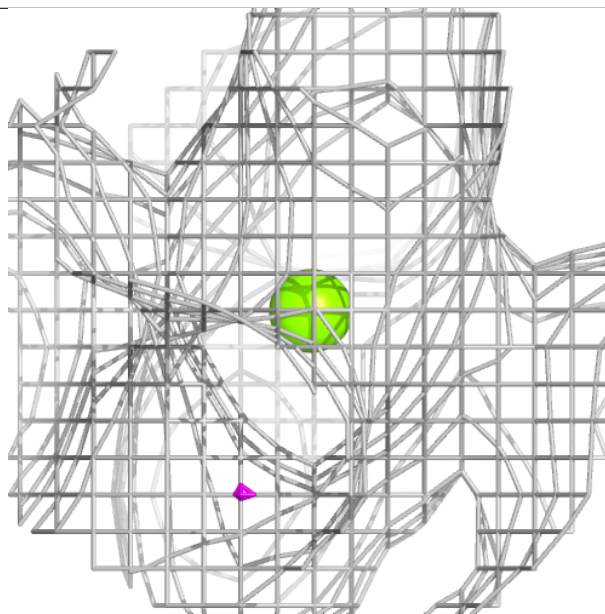
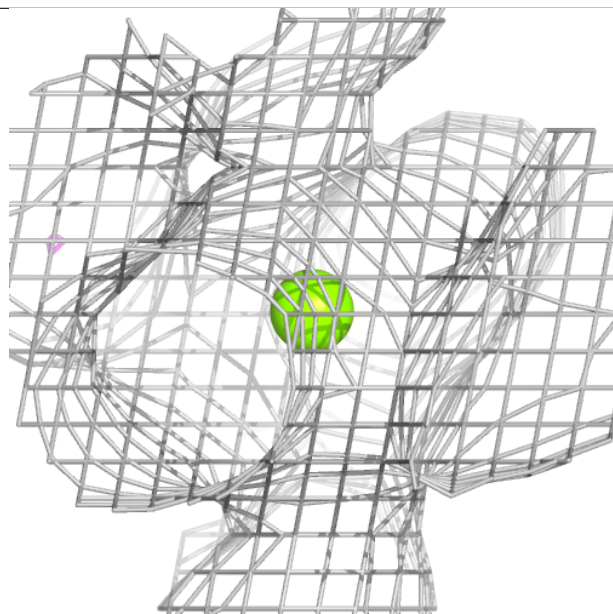
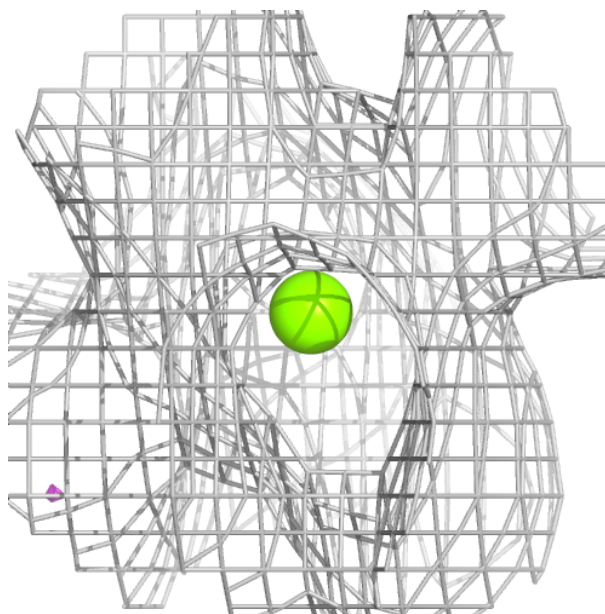
**Electron density around FAD B 603:**

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



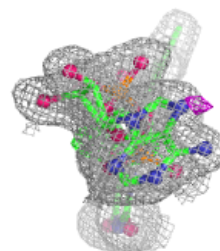
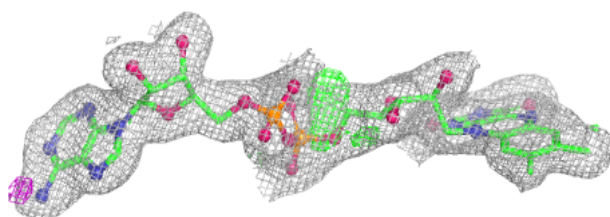
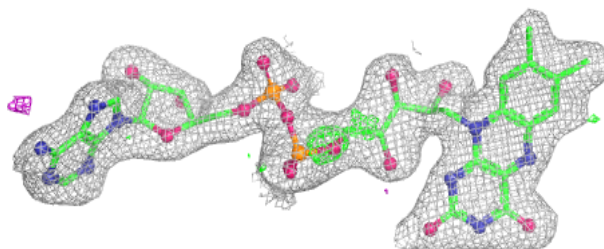
Electron density around MG C 602:

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

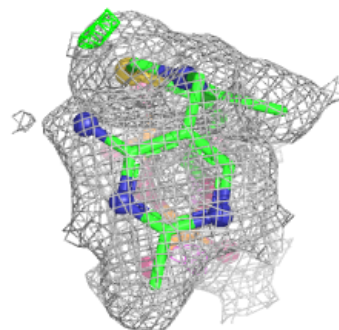
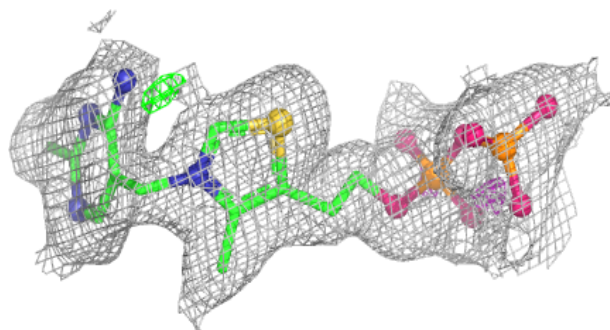
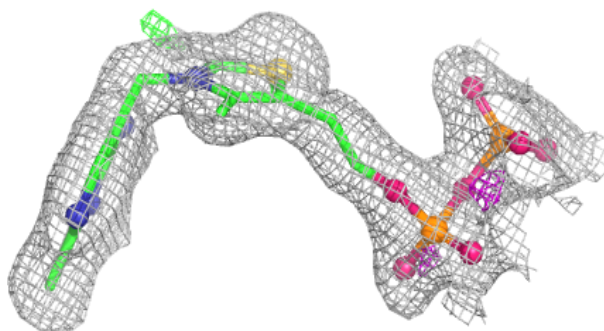


Electron density around FAD A 603:

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

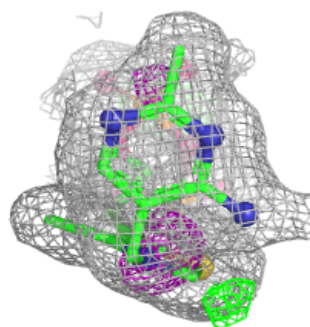
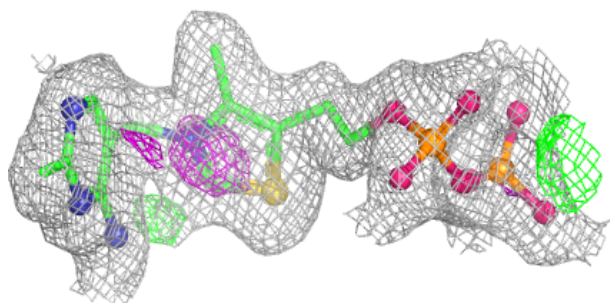
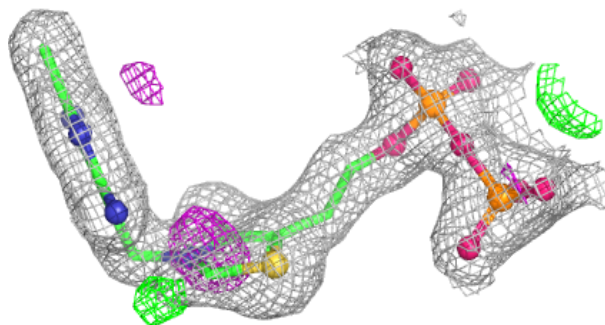
**Electron density around TPP B 601:**

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



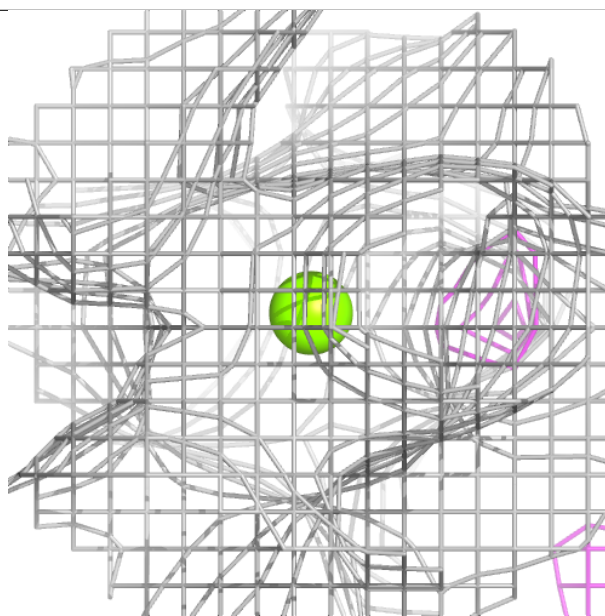
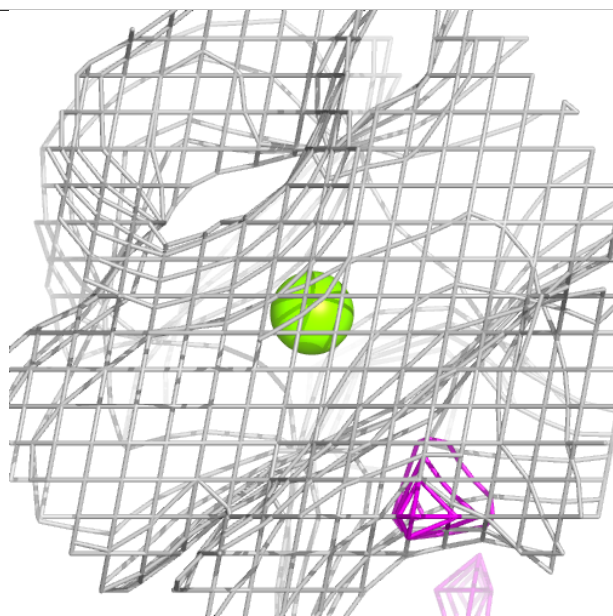
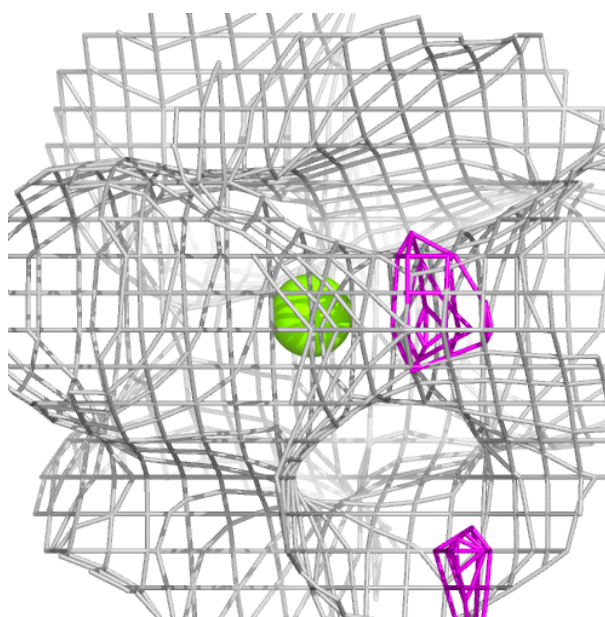
Electron density around TPP A 601:

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



Electron density around MG B 602:

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



6.5 Other polymers ⓘ

There are no such residues in this entry.