



wwPDB X-ray Structure Validation Summary Report ⓘ

May 13, 2020 – 04:46 am BST

PDB ID : 5EUJ
Title : PYRUVATE DECARBOXYLASE FROM ZYMOBACTER PALMAE
Authors : Buddrus, L.; Crennell, S.J.; Leak, D.J.; Danson, M.J.; Andrews, E.S.V.; Arcus, V.L.
Deposited on : 2015-11-18
Resolution : 2.15 Å(reported)

This is a wwPDB X-ray Structure Validation Summary 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 : 2.11
buster-report : 1.1.7 (2018)
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac : 5.8.0158
CCP4 : 7.0.044 (Gargrove)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.11

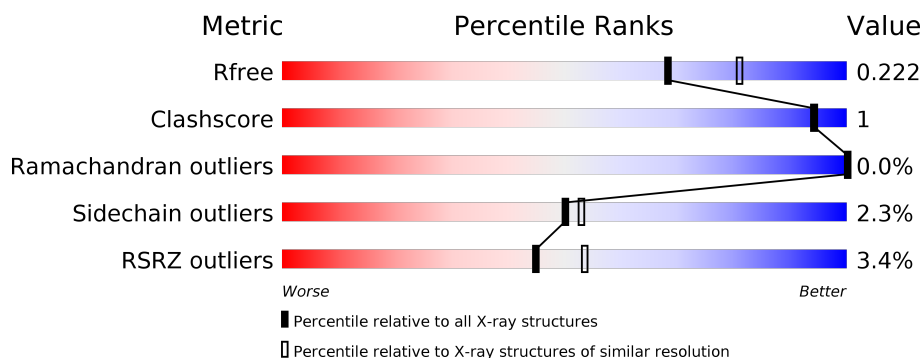
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.15 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.



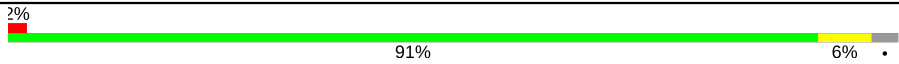
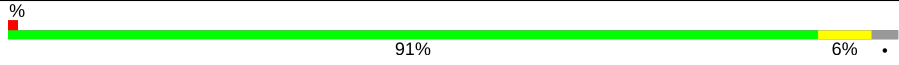
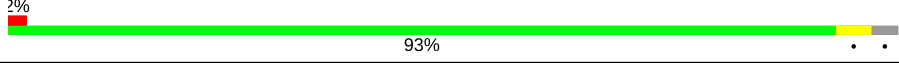
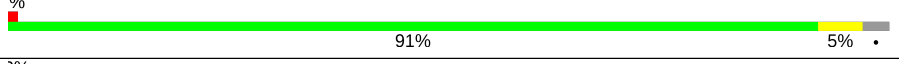
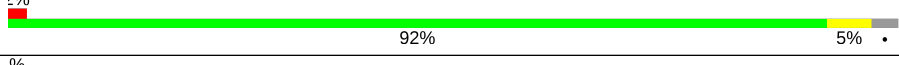
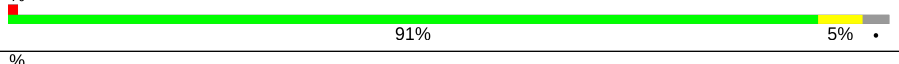
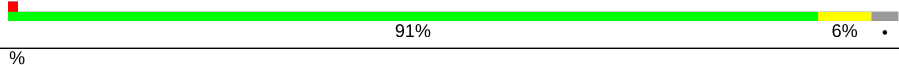
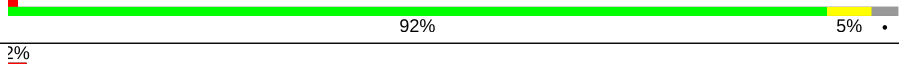
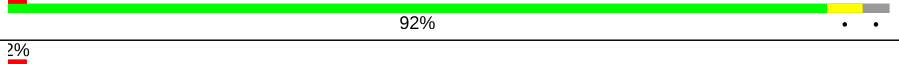
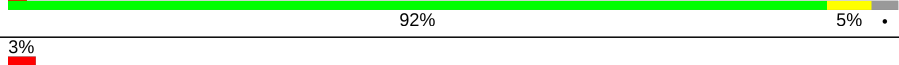
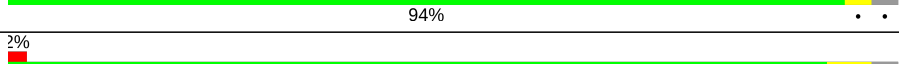
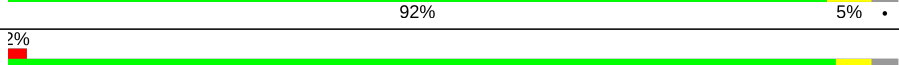
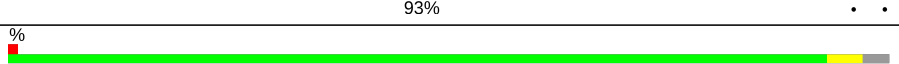
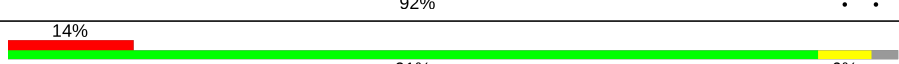
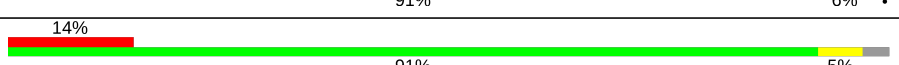
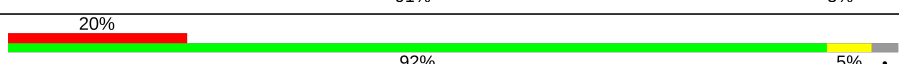
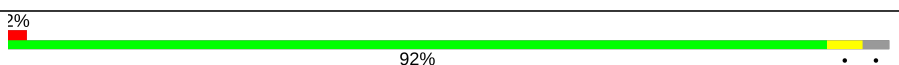

Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	1479 (2.16-2.16)
Clashscore	141614	1585 (2.16-2.16)
Ramachandran outliers	138981	1560 (2.16-2.16)
Sidechain outliers	138945	1559 (2.16-2.16)
RSRZ outliers	127900	1456 (2.16-2.16)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for ≥ 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	573	<div> <div>2%</div> <div> <div></div> <div>91%</div> <div>5%</div> <div>.</div> </div> </div>
1	B	573	<div> <div>2%</div> <div> <div></div> <div>92%</div> <div>5%</div> <div>.</div> </div> </div>
1	C	573	<div> <div>%</div> <div> <div></div> <div>92%</div> <div>5%</div> <div>.</div> </div> </div>
1	D	573	<div> <div>%</div> <div> <div></div> <div>92%</div> <div>.</div> <div>.</div> </div> </div>
1	E	573	<div> <div>%</div> <div> <div></div> <div>92%</div> <div>5%</div> <div>.</div> </div> </div>
1	F	573	<div> <div></div> <div> <div></div> <div>91%</div> <div>5%</div> <div>.</div> </div> </div>

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Mol	Chain	Length	Quality of chain
1	G	573	
1	H	573	
1	I	573	
1	J	573	
1	K	573	
1	L	573	
1	M	573	
1	N	573	
1	O	573	
1	P	573	
1	Q	573	
1	R	573	
1	S	573	
1	T	573	
1	U	573	
1	V	573	
1	W	573	
1	X	573	

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

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
4	EDO	Q	603	-	-	-	X

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 107004 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 decarboxylase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	555	Total	C	N	O	S	0	5	0
			4250	2665	737	823	25			
1	B	555	Total	C	N	O	S	0	4	0
			4237	2658	733	821	25			
1	C	555	Total	C	N	O	S	0	6	0
			4260	2670	742	823	25			
1	D	555	Total	C	N	O	S	0	5	0
			4245	2662	734	824	25			
1	E	556	Total	C	N	O	S	0	4	0
			4244	2662	734	823	25			
1	F	555	Total	C	N	O	S	0	9	0
			4285	2685	745	830	25			
1	G	555	Total	C	N	O	S	0	7	0
			4266	2675	739	827	25			
1	H	555	Total	C	N	O	S	0	6	0
			4252	2666	736	824	26			
1	I	556	Total	C	N	O	S	0	6	0
			4259	2670	737	827	25			
1	J	555	Total	C	N	O	S	0	4	0
			4238	2658	733	822	25			
1	K	555	Total	C	N	O	S	0	7	0
			4266	2673	740	828	25			
1	L	555	Total	C	N	O	S	0	9	0
			4284	2683	745	831	25			
1	M	555	Total	C	N	O	S	0	7	0
			4262	2673	737	827	25			
1	N	555	Total	C	N	O	S	0	7	0
			4265	2672	740	828	25			
1	O	555	Total	C	N	O	S	0	3	0
			4229	2653	732	819	25			
1	P	555	Total	C	N	O	S	0	7	0
			4264	2673	738	828	25			

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	Q	555	Total	C	N	O	S	0	5	0
			4246	2663	734	824	25			
1	R	555	Total	C	N	O	S	0	8	0
			4270	2675	738	832	25			
1	S	555	Total	C	N	O	S	0	2	0
			4221	2649	731	816	25			
1	T	555	Total	C	N	O	S	0	4	0
			4238	2658	733	822	25			
1	U	555	Total	C	N	O	S	0	4	0
			4239	2659	733	822	25			
1	V	555	Total	C	N	O	S	0	4	0
			4238	2658	733	822	25			
1	W	555	Total	C	N	O	S	0	3	0
			4230	2654	732	819	25			
1	X	555	Total	C	N	O	S	0	3	0
			4228	2653	732	818	25			

There are 456 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	134	ALA	ARG	conflict	UNP Q8KTX6
A	245	ALA	GLU	conflict	UNP Q8KTX6
A	557	LEU	-	expression tag	UNP Q8KTX6
A	558	VAL	-	expression tag	UNP Q8KTX6
A	559	PRO	-	expression tag	UNP Q8KTX6
A	560	ARG	-	expression tag	UNP Q8KTX6
A	561	GLY	-	expression tag	UNP Q8KTX6
A	562	SER	-	expression tag	UNP Q8KTX6
A	563	GLY	-	expression tag	UNP Q8KTX6
A	564	GLY	-	expression tag	UNP Q8KTX6
A	565	GLY	-	expression tag	UNP Q8KTX6
A	566	LEU	-	expression tag	UNP Q8KTX6
A	567	GLU	-	expression tag	UNP Q8KTX6
A	568	HIS	-	expression tag	UNP Q8KTX6
A	569	HIS	-	expression tag	UNP Q8KTX6
A	570	HIS	-	expression tag	UNP Q8KTX6
A	571	HIS	-	expression tag	UNP Q8KTX6
A	572	HIS	-	expression tag	UNP Q8KTX6
A	573	HIS	-	expression tag	UNP Q8KTX6
B	134	ALA	ARG	conflict	UNP Q8KTX6
B	245	ALA	GLU	conflict	UNP Q8KTX6
B	557	LEU	-	expression tag	UNP Q8KTX6
B	558	VAL	-	expression tag	UNP Q8KTX6

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Chain	Residue	Modelled	Actual	Comment	Reference
B	559	PRO	-	expression tag	UNP Q8KTX6
B	560	ARG	-	expression tag	UNP Q8KTX6
B	561	GLY	-	expression tag	UNP Q8KTX6
B	562	SER	-	expression tag	UNP Q8KTX6
B	563	GLY	-	expression tag	UNP Q8KTX6
B	564	GLY	-	expression tag	UNP Q8KTX6
B	565	GLY	-	expression tag	UNP Q8KTX6
B	566	LEU	-	expression tag	UNP Q8KTX6
B	567	GLU	-	expression tag	UNP Q8KTX6
B	568	HIS	-	expression tag	UNP Q8KTX6
B	569	HIS	-	expression tag	UNP Q8KTX6
B	570	HIS	-	expression tag	UNP Q8KTX6
B	571	HIS	-	expression tag	UNP Q8KTX6
B	572	HIS	-	expression tag	UNP Q8KTX6
B	573	HIS	-	expression tag	UNP Q8KTX6
C	134	ALA	ARG	conflict	UNP Q8KTX6
C	245	ALA	GLU	conflict	UNP Q8KTX6
C	557	LEU	-	expression tag	UNP Q8KTX6
C	558	VAL	-	expression tag	UNP Q8KTX6
C	559	PRO	-	expression tag	UNP Q8KTX6
C	560	ARG	-	expression tag	UNP Q8KTX6
C	561	GLY	-	expression tag	UNP Q8KTX6
C	562	SER	-	expression tag	UNP Q8KTX6
C	563	GLY	-	expression tag	UNP Q8KTX6
C	564	GLY	-	expression tag	UNP Q8KTX6
C	565	GLY	-	expression tag	UNP Q8KTX6
C	566	LEU	-	expression tag	UNP Q8KTX6
C	567	GLU	-	expression tag	UNP Q8KTX6
C	568	HIS	-	expression tag	UNP Q8KTX6
C	569	HIS	-	expression tag	UNP Q8KTX6
C	570	HIS	-	expression tag	UNP Q8KTX6
C	571	HIS	-	expression tag	UNP Q8KTX6
C	572	HIS	-	expression tag	UNP Q8KTX6
C	573	HIS	-	expression tag	UNP Q8KTX6
D	134	ALA	ARG	conflict	UNP Q8KTX6
D	245	ALA	GLU	conflict	UNP Q8KTX6
D	557	LEU	-	expression tag	UNP Q8KTX6
D	558	VAL	-	expression tag	UNP Q8KTX6
D	559	PRO	-	expression tag	UNP Q8KTX6
D	560	ARG	-	expression tag	UNP Q8KTX6
D	561	GLY	-	expression tag	UNP Q8KTX6
D	562	SER	-	expression tag	UNP Q8KTX6

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Chain	Residue	Modelled	Actual	Comment	Reference
D	563	GLY	-	expression tag	UNP Q8KTX6
D	564	GLY	-	expression tag	UNP Q8KTX6
D	565	GLY	-	expression tag	UNP Q8KTX6
D	566	LEU	-	expression tag	UNP Q8KTX6
D	567	GLU	-	expression tag	UNP Q8KTX6
D	568	HIS	-	expression tag	UNP Q8KTX6
D	569	HIS	-	expression tag	UNP Q8KTX6
D	570	HIS	-	expression tag	UNP Q8KTX6
D	571	HIS	-	expression tag	UNP Q8KTX6
D	572	HIS	-	expression tag	UNP Q8KTX6
D	573	HIS	-	expression tag	UNP Q8KTX6
E	134	ALA	ARG	conflict	UNP Q8KTX6
E	245	ALA	GLU	conflict	UNP Q8KTX6
E	557	LEU	-	expression tag	UNP Q8KTX6
E	558	VAL	-	expression tag	UNP Q8KTX6
E	559	PRO	-	expression tag	UNP Q8KTX6
E	560	ARG	-	expression tag	UNP Q8KTX6
E	561	GLY	-	expression tag	UNP Q8KTX6
E	562	SER	-	expression tag	UNP Q8KTX6
E	563	GLY	-	expression tag	UNP Q8KTX6
E	564	GLY	-	expression tag	UNP Q8KTX6
E	565	GLY	-	expression tag	UNP Q8KTX6
E	566	LEU	-	expression tag	UNP Q8KTX6
E	567	GLU	-	expression tag	UNP Q8KTX6
E	568	HIS	-	expression tag	UNP Q8KTX6
E	569	HIS	-	expression tag	UNP Q8KTX6
E	570	HIS	-	expression tag	UNP Q8KTX6
E	571	HIS	-	expression tag	UNP Q8KTX6
E	572	HIS	-	expression tag	UNP Q8KTX6
E	573	HIS	-	expression tag	UNP Q8KTX6
F	134	ALA	ARG	conflict	UNP Q8KTX6
F	245	ALA	GLU	conflict	UNP Q8KTX6
F	557	LEU	-	expression tag	UNP Q8KTX6
F	558	VAL	-	expression tag	UNP Q8KTX6
F	559	PRO	-	expression tag	UNP Q8KTX6
F	560	ARG	-	expression tag	UNP Q8KTX6
F	561	GLY	-	expression tag	UNP Q8KTX6
F	562	SER	-	expression tag	UNP Q8KTX6
F	563	GLY	-	expression tag	UNP Q8KTX6
F	564	GLY	-	expression tag	UNP Q8KTX6
F	565	GLY	-	expression tag	UNP Q8KTX6
F	566	LEU	-	expression tag	UNP Q8KTX6

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Chain	Residue	Modelled	Actual	Comment	Reference
F	567	GLU	-	expression tag	UNP Q8KTX6
F	568	HIS	-	expression tag	UNP Q8KTX6
F	569	HIS	-	expression tag	UNP Q8KTX6
F	570	HIS	-	expression tag	UNP Q8KTX6
F	571	HIS	-	expression tag	UNP Q8KTX6
F	572	HIS	-	expression tag	UNP Q8KTX6
F	573	HIS	-	expression tag	UNP Q8KTX6
G	134	ALA	ARG	conflict	UNP Q8KTX6
G	245	ALA	GLU	conflict	UNP Q8KTX6
G	557	LEU	-	expression tag	UNP Q8KTX6
G	558	VAL	-	expression tag	UNP Q8KTX6
G	559	PRO	-	expression tag	UNP Q8KTX6
G	560	ARG	-	expression tag	UNP Q8KTX6
G	561	GLY	-	expression tag	UNP Q8KTX6
G	562	SER	-	expression tag	UNP Q8KTX6
G	563	GLY	-	expression tag	UNP Q8KTX6
G	564	GLY	-	expression tag	UNP Q8KTX6
G	565	GLY	-	expression tag	UNP Q8KTX6
G	566	LEU	-	expression tag	UNP Q8KTX6
G	567	GLU	-	expression tag	UNP Q8KTX6
G	568	HIS	-	expression tag	UNP Q8KTX6
G	569	HIS	-	expression tag	UNP Q8KTX6
G	570	HIS	-	expression tag	UNP Q8KTX6
G	571	HIS	-	expression tag	UNP Q8KTX6
G	572	HIS	-	expression tag	UNP Q8KTX6
G	573	HIS	-	expression tag	UNP Q8KTX6
H	134	ALA	ARG	conflict	UNP Q8KTX6
H	245	ALA	GLU	conflict	UNP Q8KTX6
H	557	LEU	-	expression tag	UNP Q8KTX6
H	558	VAL	-	expression tag	UNP Q8KTX6
H	559	PRO	-	expression tag	UNP Q8KTX6
H	560	ARG	-	expression tag	UNP Q8KTX6
H	561	GLY	-	expression tag	UNP Q8KTX6
H	562	SER	-	expression tag	UNP Q8KTX6
H	563	GLY	-	expression tag	UNP Q8KTX6
H	564	GLY	-	expression tag	UNP Q8KTX6
H	565	GLY	-	expression tag	UNP Q8KTX6
H	566	LEU	-	expression tag	UNP Q8KTX6
H	567	GLU	-	expression tag	UNP Q8KTX6
H	568	HIS	-	expression tag	UNP Q8KTX6
H	569	HIS	-	expression tag	UNP Q8KTX6
H	570	HIS	-	expression tag	UNP Q8KTX6

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Chain	Residue	Modelled	Actual	Comment	Reference
H	571	HIS	-	expression tag	UNP Q8KTX6
H	572	HIS	-	expression tag	UNP Q8KTX6
H	573	HIS	-	expression tag	UNP Q8KTX6
I	134	ALA	ARG	conflict	UNP Q8KTX6
I	245	ALA	GLU	conflict	UNP Q8KTX6
I	557	LEU	-	expression tag	UNP Q8KTX6
I	558	VAL	-	expression tag	UNP Q8KTX6
I	559	PRO	-	expression tag	UNP Q8KTX6
I	560	ARG	-	expression tag	UNP Q8KTX6
I	561	GLY	-	expression tag	UNP Q8KTX6
I	562	SER	-	expression tag	UNP Q8KTX6
I	563	GLY	-	expression tag	UNP Q8KTX6
I	564	GLY	-	expression tag	UNP Q8KTX6
I	565	GLY	-	expression tag	UNP Q8KTX6
I	566	LEU	-	expression tag	UNP Q8KTX6
I	567	GLU	-	expression tag	UNP Q8KTX6
I	568	HIS	-	expression tag	UNP Q8KTX6
I	569	HIS	-	expression tag	UNP Q8KTX6
I	570	HIS	-	expression tag	UNP Q8KTX6
I	571	HIS	-	expression tag	UNP Q8KTX6
I	572	HIS	-	expression tag	UNP Q8KTX6
I	573	HIS	-	expression tag	UNP Q8KTX6
J	134	ALA	ARG	conflict	UNP Q8KTX6
J	245	ALA	GLU	conflict	UNP Q8KTX6
J	557	LEU	-	expression tag	UNP Q8KTX6
J	558	VAL	-	expression tag	UNP Q8KTX6
J	559	PRO	-	expression tag	UNP Q8KTX6
J	560	ARG	-	expression tag	UNP Q8KTX6
J	561	GLY	-	expression tag	UNP Q8KTX6
J	562	SER	-	expression tag	UNP Q8KTX6
J	563	GLY	-	expression tag	UNP Q8KTX6
J	564	GLY	-	expression tag	UNP Q8KTX6
J	565	GLY	-	expression tag	UNP Q8KTX6
J	566	LEU	-	expression tag	UNP Q8KTX6
J	567	GLU	-	expression tag	UNP Q8KTX6
J	568	HIS	-	expression tag	UNP Q8KTX6
J	569	HIS	-	expression tag	UNP Q8KTX6
J	570	HIS	-	expression tag	UNP Q8KTX6
J	571	HIS	-	expression tag	UNP Q8KTX6
J	572	HIS	-	expression tag	UNP Q8KTX6
J	573	HIS	-	expression tag	UNP Q8KTX6
K	134	ALA	ARG	conflict	UNP Q8KTX6

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Chain	Residue	Modelled	Actual	Comment	Reference
K	245	ALA	GLU	conflict	UNP Q8KTX6
K	557	LEU	-	expression tag	UNP Q8KTX6
K	558	VAL	-	expression tag	UNP Q8KTX6
K	559	PRO	-	expression tag	UNP Q8KTX6
K	560	ARG	-	expression tag	UNP Q8KTX6
K	561	GLY	-	expression tag	UNP Q8KTX6
K	562	SER	-	expression tag	UNP Q8KTX6
K	563	GLY	-	expression tag	UNP Q8KTX6
K	564	GLY	-	expression tag	UNP Q8KTX6
K	565	GLY	-	expression tag	UNP Q8KTX6
K	566	LEU	-	expression tag	UNP Q8KTX6
K	567	GLU	-	expression tag	UNP Q8KTX6
K	568	HIS	-	expression tag	UNP Q8KTX6
K	569	HIS	-	expression tag	UNP Q8KTX6
K	570	HIS	-	expression tag	UNP Q8KTX6
K	571	HIS	-	expression tag	UNP Q8KTX6
K	572	HIS	-	expression tag	UNP Q8KTX6
K	573	HIS	-	expression tag	UNP Q8KTX6
L	134	ALA	ARG	conflict	UNP Q8KTX6
L	245	ALA	GLU	conflict	UNP Q8KTX6
L	557	LEU	-	expression tag	UNP Q8KTX6
L	558	VAL	-	expression tag	UNP Q8KTX6
L	559	PRO	-	expression tag	UNP Q8KTX6
L	560	ARG	-	expression tag	UNP Q8KTX6
L	561	GLY	-	expression tag	UNP Q8KTX6
L	562	SER	-	expression tag	UNP Q8KTX6
L	563	GLY	-	expression tag	UNP Q8KTX6
L	564	GLY	-	expression tag	UNP Q8KTX6
L	565	GLY	-	expression tag	UNP Q8KTX6
L	566	LEU	-	expression tag	UNP Q8KTX6
L	567	GLU	-	expression tag	UNP Q8KTX6
L	568	HIS	-	expression tag	UNP Q8KTX6
L	569	HIS	-	expression tag	UNP Q8KTX6
L	570	HIS	-	expression tag	UNP Q8KTX6
L	571	HIS	-	expression tag	UNP Q8KTX6
L	572	HIS	-	expression tag	UNP Q8KTX6
L	573	HIS	-	expression tag	UNP Q8KTX6
M	134	ALA	ARG	conflict	UNP Q8KTX6
M	245	ALA	GLU	conflict	UNP Q8KTX6
M	557	LEU	-	expression tag	UNP Q8KTX6
M	558	VAL	-	expression tag	UNP Q8KTX6
M	559	PRO	-	expression tag	UNP Q8KTX6

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Chain	Residue	Modelled	Actual	Comment	Reference
M	560	ARG	-	expression tag	UNP Q8KTX6
M	561	GLY	-	expression tag	UNP Q8KTX6
M	562	SER	-	expression tag	UNP Q8KTX6
M	563	GLY	-	expression tag	UNP Q8KTX6
M	564	GLY	-	expression tag	UNP Q8KTX6
M	565	GLY	-	expression tag	UNP Q8KTX6
M	566	LEU	-	expression tag	UNP Q8KTX6
M	567	GLU	-	expression tag	UNP Q8KTX6
M	568	HIS	-	expression tag	UNP Q8KTX6
M	569	HIS	-	expression tag	UNP Q8KTX6
M	570	HIS	-	expression tag	UNP Q8KTX6
M	571	HIS	-	expression tag	UNP Q8KTX6
M	572	HIS	-	expression tag	UNP Q8KTX6
M	573	HIS	-	expression tag	UNP Q8KTX6
N	134	ALA	ARG	conflict	UNP Q8KTX6
N	245	ALA	GLU	conflict	UNP Q8KTX6
N	557	LEU	-	expression tag	UNP Q8KTX6
N	558	VAL	-	expression tag	UNP Q8KTX6
N	559	PRO	-	expression tag	UNP Q8KTX6
N	560	ARG	-	expression tag	UNP Q8KTX6
N	561	GLY	-	expression tag	UNP Q8KTX6
N	562	SER	-	expression tag	UNP Q8KTX6
N	563	GLY	-	expression tag	UNP Q8KTX6
N	564	GLY	-	expression tag	UNP Q8KTX6
N	565	GLY	-	expression tag	UNP Q8KTX6
N	566	LEU	-	expression tag	UNP Q8KTX6
N	567	GLU	-	expression tag	UNP Q8KTX6
N	568	HIS	-	expression tag	UNP Q8KTX6
N	569	HIS	-	expression tag	UNP Q8KTX6
N	570	HIS	-	expression tag	UNP Q8KTX6
N	571	HIS	-	expression tag	UNP Q8KTX6
N	572	HIS	-	expression tag	UNP Q8KTX6
N	573	HIS	-	expression tag	UNP Q8KTX6
O	134	ALA	ARG	conflict	UNP Q8KTX6
O	245	ALA	GLU	conflict	UNP Q8KTX6
O	557	LEU	-	expression tag	UNP Q8KTX6
O	558	VAL	-	expression tag	UNP Q8KTX6
O	559	PRO	-	expression tag	UNP Q8KTX6
O	560	ARG	-	expression tag	UNP Q8KTX6
O	561	GLY	-	expression tag	UNP Q8KTX6
O	562	SER	-	expression tag	UNP Q8KTX6
O	563	GLY	-	expression tag	UNP Q8KTX6

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Chain	Residue	Modelled	Actual	Comment	Reference
O	564	GLY	-	expression tag	UNP Q8KTX6
O	565	GLY	-	expression tag	UNP Q8KTX6
O	566	LEU	-	expression tag	UNP Q8KTX6
O	567	GLU	-	expression tag	UNP Q8KTX6
O	568	HIS	-	expression tag	UNP Q8KTX6
O	569	HIS	-	expression tag	UNP Q8KTX6
O	570	HIS	-	expression tag	UNP Q8KTX6
O	571	HIS	-	expression tag	UNP Q8KTX6
O	572	HIS	-	expression tag	UNP Q8KTX6
O	573	HIS	-	expression tag	UNP Q8KTX6
P	134	ALA	ARG	conflict	UNP Q8KTX6
P	245	ALA	GLU	conflict	UNP Q8KTX6
P	557	LEU	-	expression tag	UNP Q8KTX6
P	558	VAL	-	expression tag	UNP Q8KTX6
P	559	PRO	-	expression tag	UNP Q8KTX6
P	560	ARG	-	expression tag	UNP Q8KTX6
P	561	GLY	-	expression tag	UNP Q8KTX6
P	562	SER	-	expression tag	UNP Q8KTX6
P	563	GLY	-	expression tag	UNP Q8KTX6
P	564	GLY	-	expression tag	UNP Q8KTX6
P	565	GLY	-	expression tag	UNP Q8KTX6
P	566	LEU	-	expression tag	UNP Q8KTX6
P	567	GLU	-	expression tag	UNP Q8KTX6
P	568	HIS	-	expression tag	UNP Q8KTX6
P	569	HIS	-	expression tag	UNP Q8KTX6
P	570	HIS	-	expression tag	UNP Q8KTX6
P	571	HIS	-	expression tag	UNP Q8KTX6
P	572	HIS	-	expression tag	UNP Q8KTX6
P	573	HIS	-	expression tag	UNP Q8KTX6
Q	134	ALA	ARG	conflict	UNP Q8KTX6
Q	245	ALA	GLU	conflict	UNP Q8KTX6
Q	557	LEU	-	expression tag	UNP Q8KTX6
Q	558	VAL	-	expression tag	UNP Q8KTX6
Q	559	PRO	-	expression tag	UNP Q8KTX6
Q	560	ARG	-	expression tag	UNP Q8KTX6
Q	561	GLY	-	expression tag	UNP Q8KTX6
Q	562	SER	-	expression tag	UNP Q8KTX6
Q	563	GLY	-	expression tag	UNP Q8KTX6
Q	564	GLY	-	expression tag	UNP Q8KTX6
Q	565	GLY	-	expression tag	UNP Q8KTX6
Q	566	LEU	-	expression tag	UNP Q8KTX6
Q	567	GLU	-	expression tag	UNP Q8KTX6

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Chain	Residue	Modelled	Actual	Comment	Reference
Q	568	HIS	-	expression tag	UNP Q8KTX6
Q	569	HIS	-	expression tag	UNP Q8KTX6
Q	570	HIS	-	expression tag	UNP Q8KTX6
Q	571	HIS	-	expression tag	UNP Q8KTX6
Q	572	HIS	-	expression tag	UNP Q8KTX6
Q	573	HIS	-	expression tag	UNP Q8KTX6
R	134	ALA	ARG	conflict	UNP Q8KTX6
R	245	ALA	GLU	conflict	UNP Q8KTX6
R	557	LEU	-	expression tag	UNP Q8KTX6
R	558	VAL	-	expression tag	UNP Q8KTX6
R	559	PRO	-	expression tag	UNP Q8KTX6
R	560	ARG	-	expression tag	UNP Q8KTX6
R	561	GLY	-	expression tag	UNP Q8KTX6
R	562	SER	-	expression tag	UNP Q8KTX6
R	563	GLY	-	expression tag	UNP Q8KTX6
R	564	GLY	-	expression tag	UNP Q8KTX6
R	565	GLY	-	expression tag	UNP Q8KTX6
R	566	LEU	-	expression tag	UNP Q8KTX6
R	567	GLU	-	expression tag	UNP Q8KTX6
R	568	HIS	-	expression tag	UNP Q8KTX6
R	569	HIS	-	expression tag	UNP Q8KTX6
R	570	HIS	-	expression tag	UNP Q8KTX6
R	571	HIS	-	expression tag	UNP Q8KTX6
R	572	HIS	-	expression tag	UNP Q8KTX6
R	573	HIS	-	expression tag	UNP Q8KTX6
S	134	ALA	ARG	conflict	UNP Q8KTX6
S	245	ALA	GLU	conflict	UNP Q8KTX6
S	557	LEU	-	expression tag	UNP Q8KTX6
S	558	VAL	-	expression tag	UNP Q8KTX6
S	559	PRO	-	expression tag	UNP Q8KTX6
S	560	ARG	-	expression tag	UNP Q8KTX6
S	561	GLY	-	expression tag	UNP Q8KTX6
S	562	SER	-	expression tag	UNP Q8KTX6
S	563	GLY	-	expression tag	UNP Q8KTX6
S	564	GLY	-	expression tag	UNP Q8KTX6
S	565	GLY	-	expression tag	UNP Q8KTX6
S	566	LEU	-	expression tag	UNP Q8KTX6
S	567	GLU	-	expression tag	UNP Q8KTX6
S	568	HIS	-	expression tag	UNP Q8KTX6
S	569	HIS	-	expression tag	UNP Q8KTX6
S	570	HIS	-	expression tag	UNP Q8KTX6
S	571	HIS	-	expression tag	UNP Q8KTX6

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Chain	Residue	Modelled	Actual	Comment	Reference
S	572	HIS	-	expression tag	UNP Q8KTX6
S	573	HIS	-	expression tag	UNP Q8KTX6
T	134	ALA	ARG	conflict	UNP Q8KTX6
T	245	ALA	GLU	conflict	UNP Q8KTX6
T	557	LEU	-	expression tag	UNP Q8KTX6
T	558	VAL	-	expression tag	UNP Q8KTX6
T	559	PRO	-	expression tag	UNP Q8KTX6
T	560	ARG	-	expression tag	UNP Q8KTX6
T	561	GLY	-	expression tag	UNP Q8KTX6
T	562	SER	-	expression tag	UNP Q8KTX6
T	563	GLY	-	expression tag	UNP Q8KTX6
T	564	GLY	-	expression tag	UNP Q8KTX6
T	565	GLY	-	expression tag	UNP Q8KTX6
T	566	LEU	-	expression tag	UNP Q8KTX6
T	567	GLU	-	expression tag	UNP Q8KTX6
T	568	HIS	-	expression tag	UNP Q8KTX6
T	569	HIS	-	expression tag	UNP Q8KTX6
T	570	HIS	-	expression tag	UNP Q8KTX6
T	571	HIS	-	expression tag	UNP Q8KTX6
T	572	HIS	-	expression tag	UNP Q8KTX6
T	573	HIS	-	expression tag	UNP Q8KTX6
U	134	ALA	ARG	conflict	UNP Q8KTX6
U	245	ALA	GLU	conflict	UNP Q8KTX6
U	557	LEU	-	expression tag	UNP Q8KTX6
U	558	VAL	-	expression tag	UNP Q8KTX6
U	559	PRO	-	expression tag	UNP Q8KTX6
U	560	ARG	-	expression tag	UNP Q8KTX6
U	561	GLY	-	expression tag	UNP Q8KTX6
U	562	SER	-	expression tag	UNP Q8KTX6
U	563	GLY	-	expression tag	UNP Q8KTX6
U	564	GLY	-	expression tag	UNP Q8KTX6
U	565	GLY	-	expression tag	UNP Q8KTX6
U	566	LEU	-	expression tag	UNP Q8KTX6
U	567	GLU	-	expression tag	UNP Q8KTX6
U	568	HIS	-	expression tag	UNP Q8KTX6
U	569	HIS	-	expression tag	UNP Q8KTX6
U	570	HIS	-	expression tag	UNP Q8KTX6
U	571	HIS	-	expression tag	UNP Q8KTX6
U	572	HIS	-	expression tag	UNP Q8KTX6
U	573	HIS	-	expression tag	UNP Q8KTX6
V	134	ALA	ARG	conflict	UNP Q8KTX6
V	245	ALA	GLU	conflict	UNP Q8KTX6

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Chain	Residue	Modelled	Actual	Comment	Reference
V	557	LEU	-	expression tag	UNP Q8KTX6
V	558	VAL	-	expression tag	UNP Q8KTX6
V	559	PRO	-	expression tag	UNP Q8KTX6
V	560	ARG	-	expression tag	UNP Q8KTX6
V	561	GLY	-	expression tag	UNP Q8KTX6
V	562	SER	-	expression tag	UNP Q8KTX6
V	563	GLY	-	expression tag	UNP Q8KTX6
V	564	GLY	-	expression tag	UNP Q8KTX6
V	565	GLY	-	expression tag	UNP Q8KTX6
V	566	LEU	-	expression tag	UNP Q8KTX6
V	567	GLU	-	expression tag	UNP Q8KTX6
V	568	HIS	-	expression tag	UNP Q8KTX6
V	569	HIS	-	expression tag	UNP Q8KTX6
V	570	HIS	-	expression tag	UNP Q8KTX6
V	571	HIS	-	expression tag	UNP Q8KTX6
V	572	HIS	-	expression tag	UNP Q8KTX6
V	573	HIS	-	expression tag	UNP Q8KTX6
W	134	ALA	ARG	conflict	UNP Q8KTX6
W	245	ALA	GLU	conflict	UNP Q8KTX6
W	557	LEU	-	expression tag	UNP Q8KTX6
W	558	VAL	-	expression tag	UNP Q8KTX6
W	559	PRO	-	expression tag	UNP Q8KTX6
W	560	ARG	-	expression tag	UNP Q8KTX6
W	561	GLY	-	expression tag	UNP Q8KTX6
W	562	SER	-	expression tag	UNP Q8KTX6
W	563	GLY	-	expression tag	UNP Q8KTX6
W	564	GLY	-	expression tag	UNP Q8KTX6
W	565	GLY	-	expression tag	UNP Q8KTX6
W	566	LEU	-	expression tag	UNP Q8KTX6
W	567	GLU	-	expression tag	UNP Q8KTX6
W	568	HIS	-	expression tag	UNP Q8KTX6
W	569	HIS	-	expression tag	UNP Q8KTX6
W	570	HIS	-	expression tag	UNP Q8KTX6
W	571	HIS	-	expression tag	UNP Q8KTX6
W	572	HIS	-	expression tag	UNP Q8KTX6
W	573	HIS	-	expression tag	UNP Q8KTX6
X	134	ALA	ARG	conflict	UNP Q8KTX6
X	245	ALA	GLU	conflict	UNP Q8KTX6
X	557	LEU	-	expression tag	UNP Q8KTX6
X	558	VAL	-	expression tag	UNP Q8KTX6
X	559	PRO	-	expression tag	UNP Q8KTX6
X	560	ARG	-	expression tag	UNP Q8KTX6

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Chain	Residue	Modelled	Actual	Comment	Reference
X	561	GLY	-	expression tag	UNP Q8KTX6
X	562	SER	-	expression tag	UNP Q8KTX6
X	563	GLY	-	expression tag	UNP Q8KTX6
X	564	GLY	-	expression tag	UNP Q8KTX6
X	565	GLY	-	expression tag	UNP Q8KTX6
X	566	LEU	-	expression tag	UNP Q8KTX6
X	567	GLU	-	expression tag	UNP Q8KTX6
X	568	HIS	-	expression tag	UNP Q8KTX6
X	569	HIS	-	expression tag	UNP Q8KTX6
X	570	HIS	-	expression tag	UNP Q8KTX6
X	571	HIS	-	expression tag	UNP Q8KTX6
X	572	HIS	-	expression tag	UNP Q8KTX6
X	573	HIS	-	expression tag	UNP Q8KTX6

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

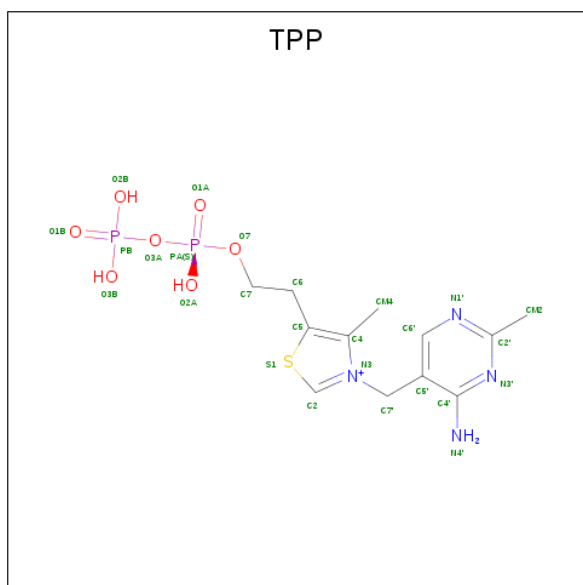
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	P	1	Total Mg 1 1	0	0
2	K	1	Total Mg 1 1	0	0
2	B	1	Total Mg 1 1	0	0
2	W	1	Total Mg 1 1	0	0
2	N	1	Total Mg 1 1	0	0
2	X	1	Total Mg 1 1	0	0
2	S	1	Total Mg 1 1	0	0
2	J	1	Total Mg 1 1	0	0
2	E	1	Total Mg 1 1	0	0
2	V	1	Total Mg 1 1	0	0
2	A	1	Total Mg 1 1	0	0
2	R	1	Total Mg 1 1	0	0
2	M	1	Total Mg 1 1	0	0

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	D	1	Total	Mg	0	0
			1	1		
2	I	1	Total	Mg	0	0
			1	1		
2	U	1	Total	Mg	0	0
			1	1		
2	L	1	Total	Mg	0	0
			1	1		
2	G	1	Total	Mg	0	0
			1	1		
2	Q	1	Total	Mg	0	0
			1	1		
2	H	1	Total	Mg	0	0
			1	1		
2	C	1	Total	Mg	0	0
			1	1		
2	T	1	Total	Mg	0	0
			1	1		
2	O	1	Total	Mg	0	0
			1	1		
2	F	1	Total	Mg	0	0
			1	1		

- Molecule 3 is THIAMINE DIPHOSPHATE (three-letter code: TPP) (formula: $C_{12}H_{19}N_4O_7P_2S$).



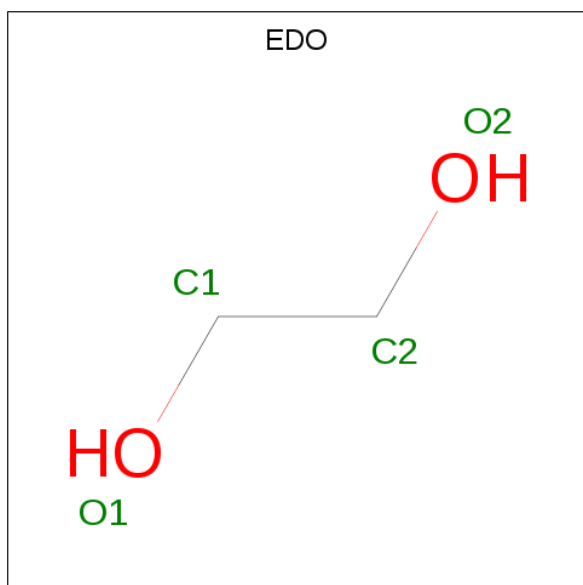
Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
3	A	1	Total 26	C 12	N 4	O 7	P 2	S 1	0	0
3	B	1	Total 26	C 12	N 4	O 7	P 2	S 1	0	0
3	C	1	Total 26	C 12	N 4	O 7	P 2	S 1	0	0
3	D	1	Total 26	C 12	N 4	O 7	P 2	S 1	0	0
3	E	1	Total 26	C 12	N 4	O 7	P 2	S 1	0	0
3	F	1	Total 26	C 12	N 4	O 7	P 2	S 1	0	0
3	G	1	Total 26	C 12	N 4	O 7	P 2	S 1	0	0
3	H	1	Total 26	C 12	N 4	O 7	P 2	S 1	0	0
3	I	1	Total 26	C 12	N 4	O 7	P 2	S 1	0	0
3	J	1	Total 26	C 12	N 4	O 7	P 2	S 1	0	0
3	K	1	Total 26	C 12	N 4	O 7	P 2	S 1	0	0
3	L	1	Total 26	C 12	N 4	O 7	P 2	S 1	0	0
3	M	1	Total 26	C 12	N 4	O 7	P 2	S 1	0	0
3	N	1	Total 26	C 12	N 4	O 7	P 2	S 1	0	0
3	O	1	Total 26	C 12	N 4	O 7	P 2	S 1	0	0
3	P	1	Total 26	C 12	N 4	O 7	P 2	S 1	0	0
3	Q	1	Total 26	C 12	N 4	O 7	P 2	S 1	0	0
3	R	1	Total 26	C 12	N 4	O 7	P 2	S 1	0	0
3	S	1	Total 26	C 12	N 4	O 7	P 2	S 1	0	0
3	T	1	Total 26	C 12	N 4	O 7	P 2	S 1	0	0
3	U	1	Total 26	C 12	N 4	O 7	P 2	S 1	0	0
3	V	1	Total 26	C 12	N 4	O 7	P 2	S 1	0	0

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

- Molecule 4 is 1,2-ETHANEDIOL (three-letter code: EDO) (formula: C₂H₆O₂).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total	C	O	0	0
			4	2	2		
4	F	1	Total	C	O	0	0
			4	2	2		
4	I	1	Total	C	O	0	0
			4	2	2		
4	N	1	Total	C	O	0	0
			4	2	2		
4	Q	1	Total	C	O	0	0
			4	2	2		
4	R	1	Total	C	O	0	0
			4	2	2		

- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	139	Total	O	0	0
			139	139		

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	B	157	Total 157	O 157	0	0
5	C	246	Total 246	O 246	0	0
5	D	199	Total 199	O 199	0	0
5	E	221	Total 221	O 221	0	0
5	F	275	Total 275	O 275	0	0
5	G	192	Total 192	O 192	0	0
5	H	150	Total 150	O 150	0	0
5	I	176	Total 176	O 176	0	0
5	J	217	Total 217	O 217	0	0
5	K	206	Total 206	O 206	0	0
5	L	200	Total 200	O 200	0	0
5	M	288	Total 288	O 288	0	0
5	N	269	Total 269	O 269	0	0
5	O	185	Total 185	O 185	0	0
5	P	212	Total 212	O 212	0	0
5	Q	149	Total 149	O 149	0	0
5	R	151	Total 151	O 151	0	0
5	S	184	Total 184	O 184	0	0
5	T	184	Total 184	O 184	0	0
5	U	81	Total 81	O 81	0	0
5	V	66	Total 66	O 66	0	0

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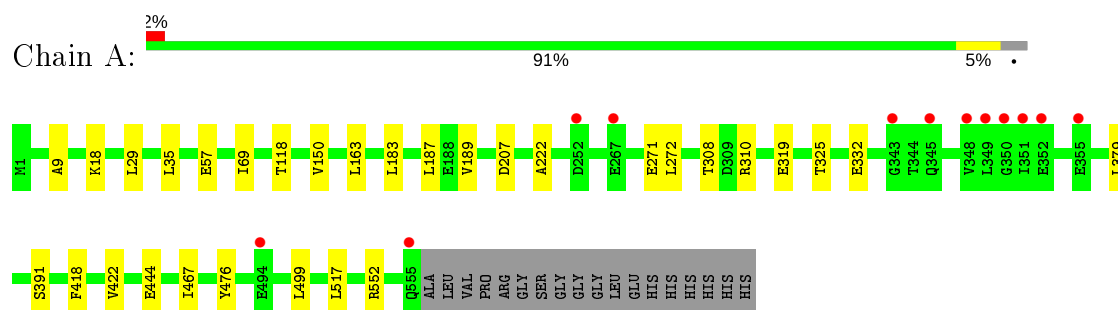
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	W	55	Total 55	O 55	0	0
5	X	114	Total 114	O 114	0	0

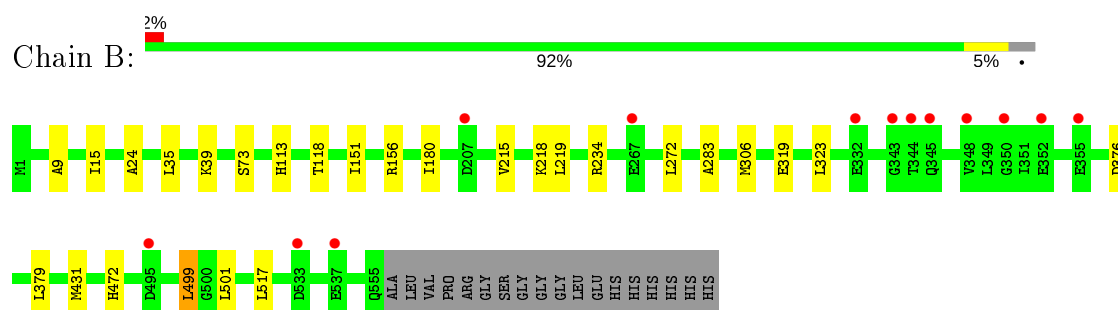
3 Residue-property plots [i](#)

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

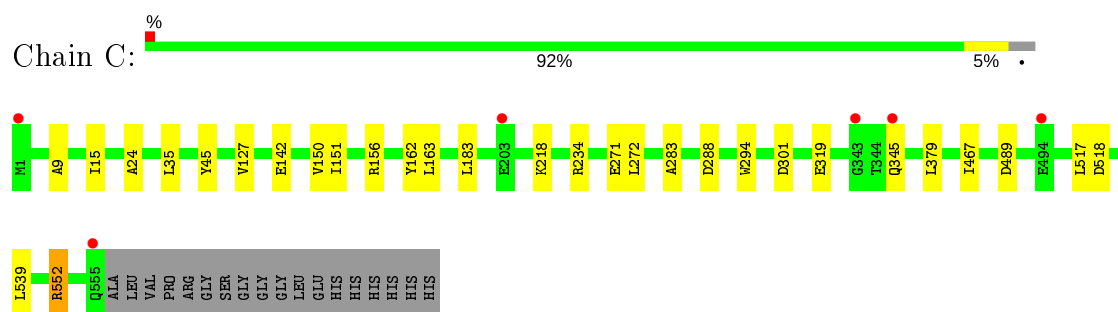
• Molecule 1: Pyruvate decarboxylase



• Molecule 1: Pyruvate decarboxylase

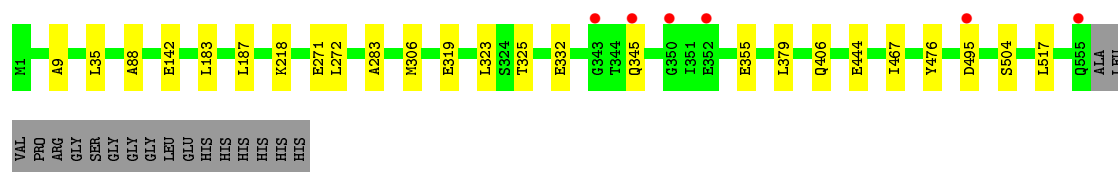


• Molecule 1: Pyruvate decarboxylase

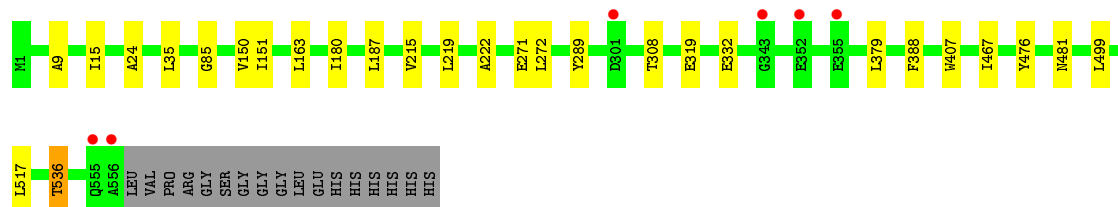
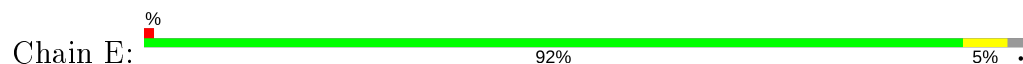


• Molecule 1: Pyruvate decarboxylase

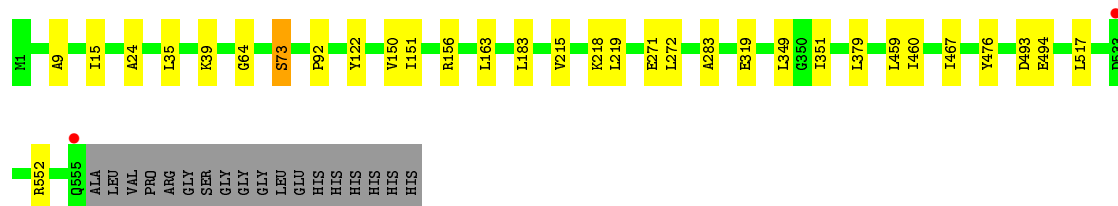




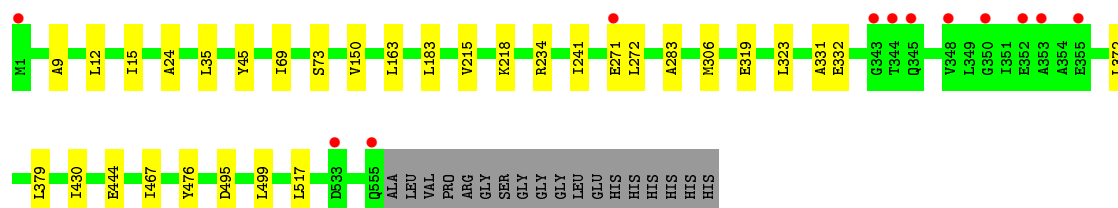
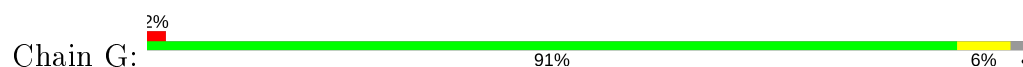
- Molecule 1: Pyruvate decarboxylase



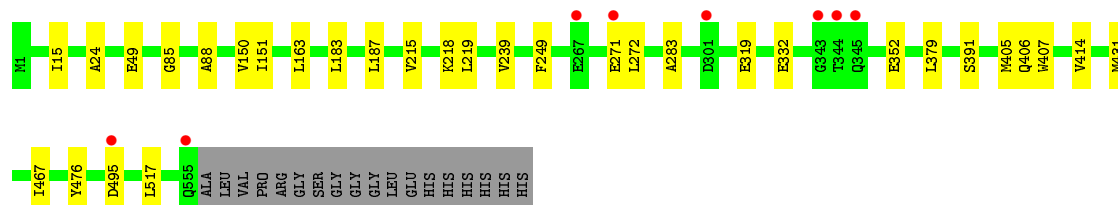
- Molecule 1: Pyruvate decarboxylase



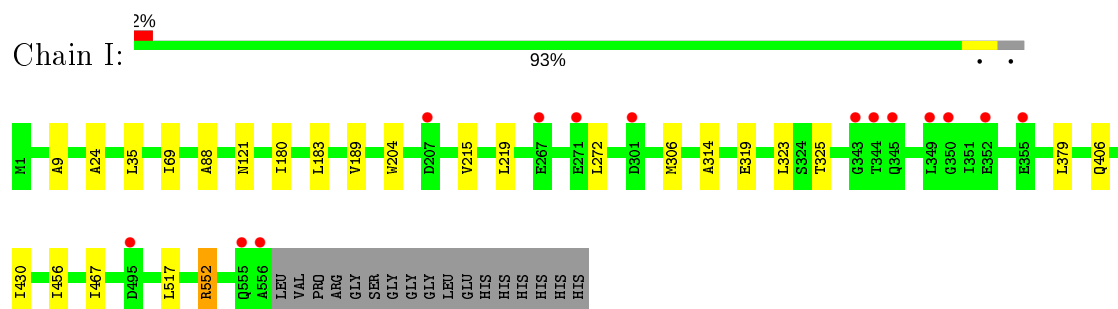
- Molecule 1: Pyruvate decarboxylase



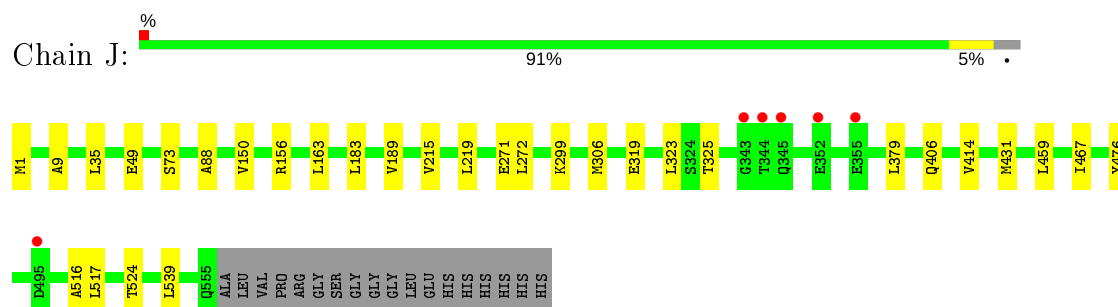
- Molecule 1: Pyruvate decarboxylase



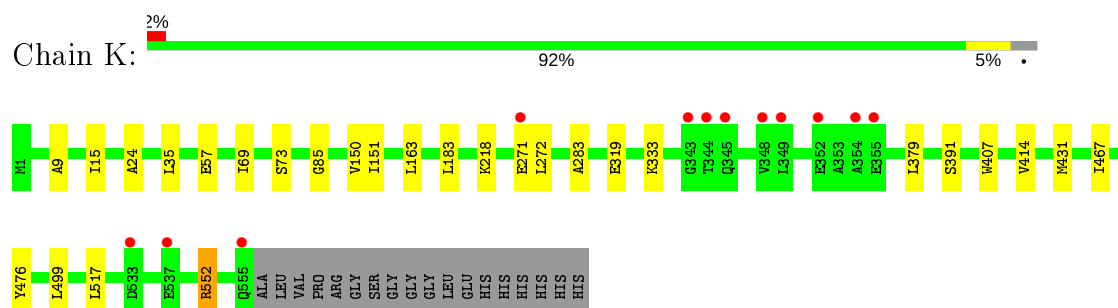
● Molecule 1: Pyruvate decarboxylase



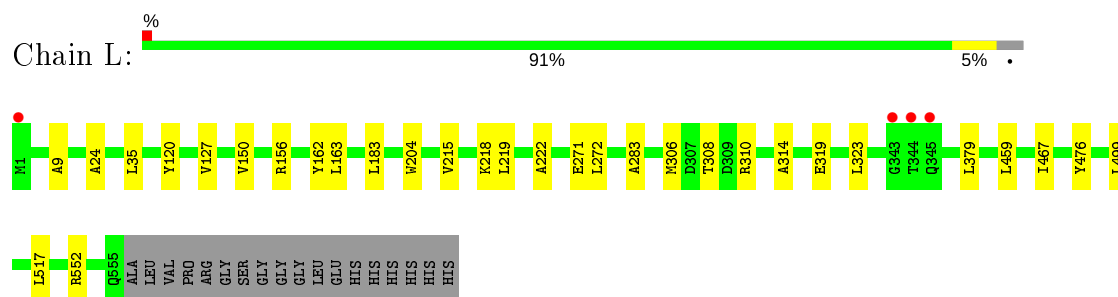
● Molecule 1: Pyruvate decarboxylase



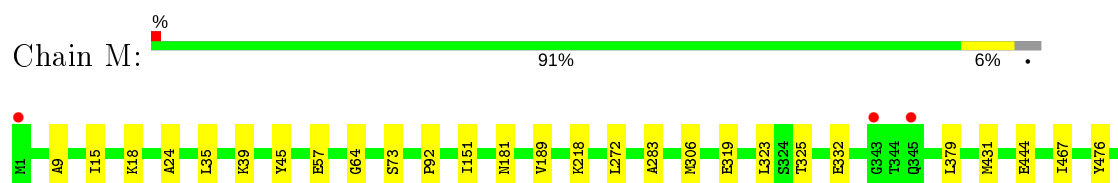
● Molecule 1: Pyruvate decarboxylase

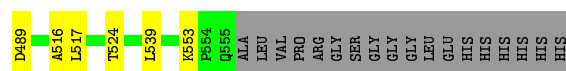


● Molecule 1: Pyruvate decarboxylase

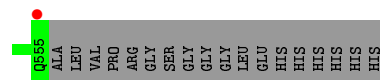
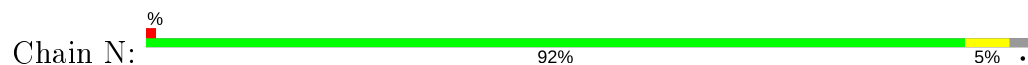


● Molecule 1: Pyruvate decarboxylase

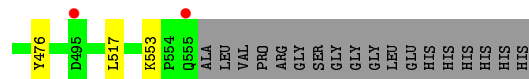




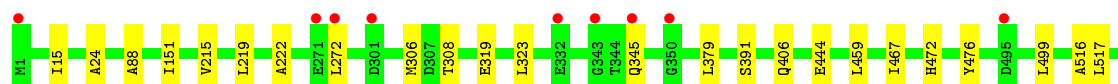
- Molecule 1: Pyruvate decarboxylase



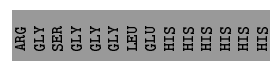
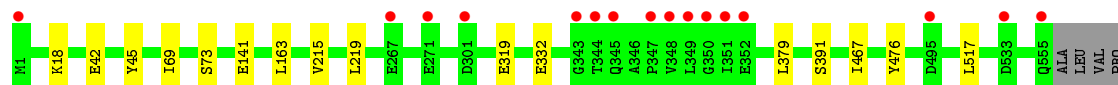
- Molecule 1: Pyruvate decarboxylase



- Molecule 1: Pyruvate decarboxylase

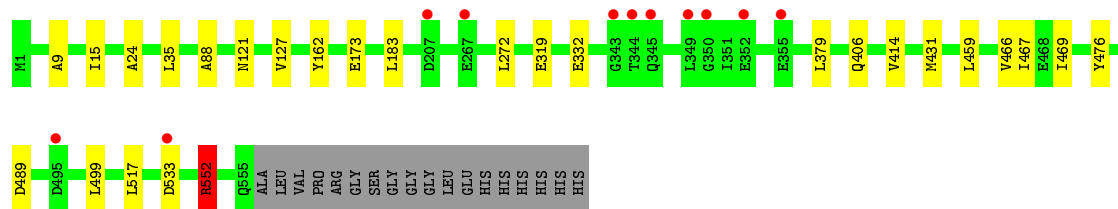


- Molecule 1: Pyruvate decarboxylase

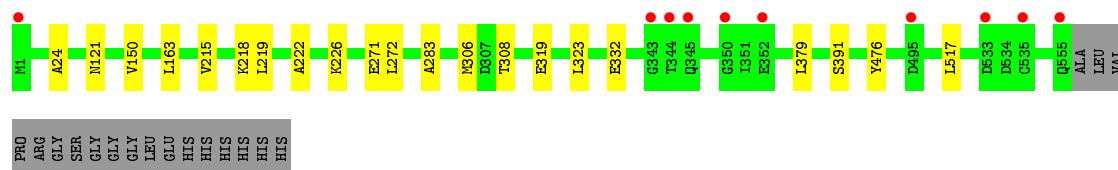
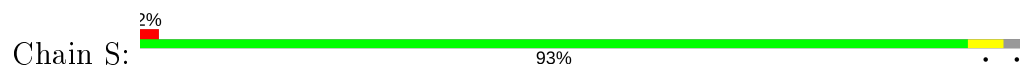


- Molecule 1: Pyruvate decarboxylase

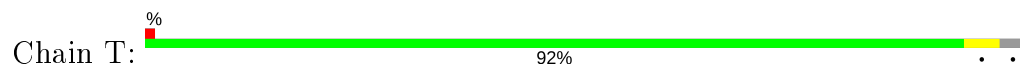




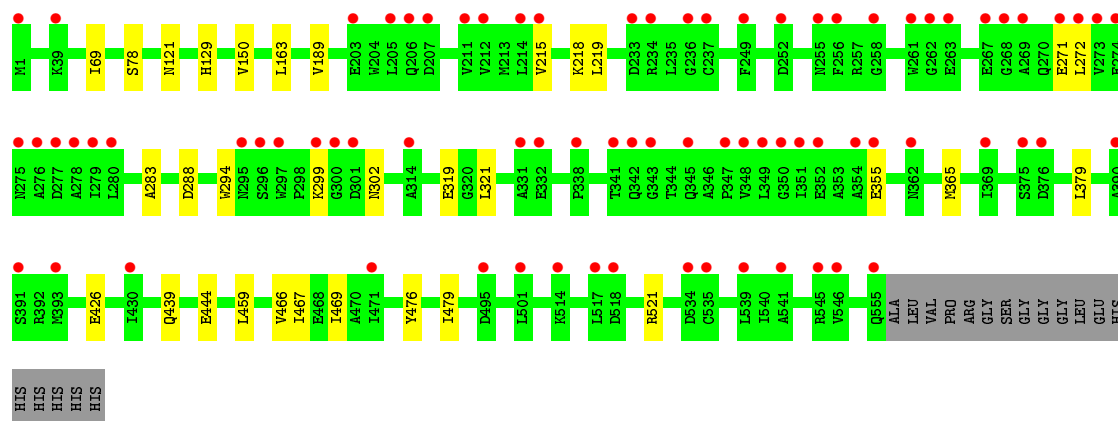
• Molecule 1: Pyruvate decarboxylase



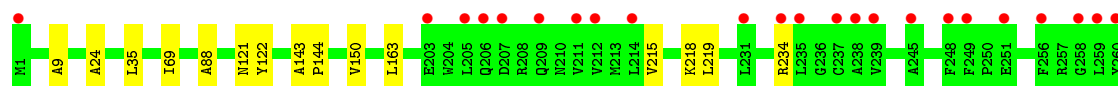
• Molecule 1: Pyruvate decarboxylase

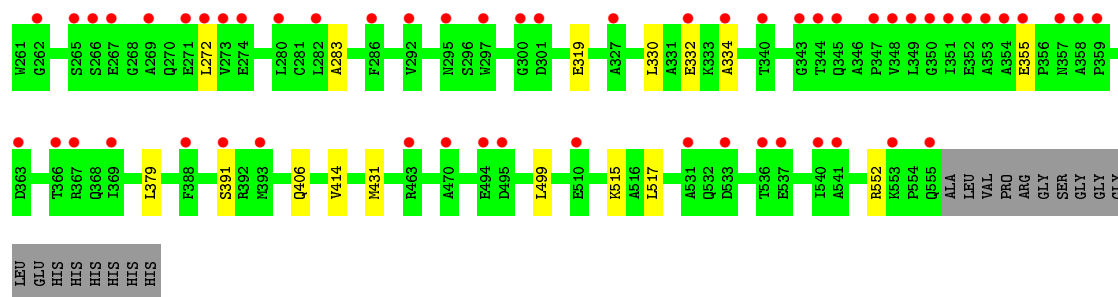


• Molecule 1: Pyruvate decarboxylase

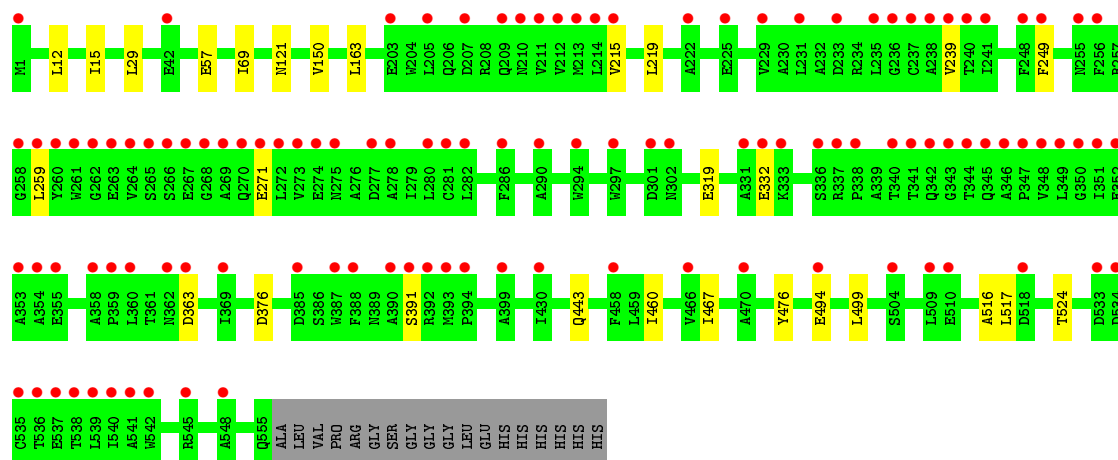


• Molecule 1: Pyruvate decarboxylase

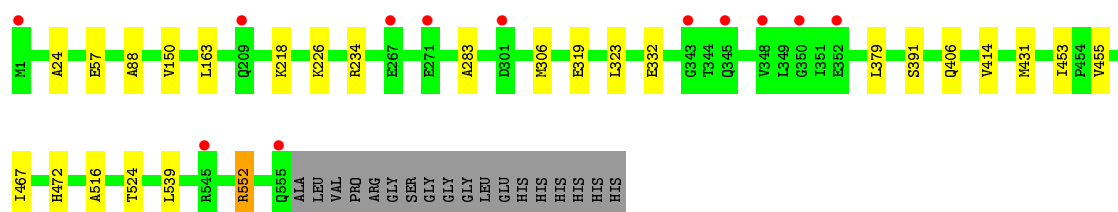
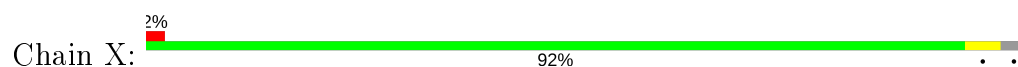




• Molecule 1: Pyruvate decarboxylase



• Molecule 1: Pyruvate decarboxylase



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	204.56Å 177.39Å 244.55Å 90.00° 112.94° 90.00°	Depositor
Resolution (Å)	75.40 – 2.15 75.47 – 2.15	Depositor EDS
% Data completeness (in resolution range)	98.8 (75.40-2.15) 98.8 (75.47-2.15)	Depositor EDS
R_{merge}	0.16	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.13 (at 2.14Å)	Xtriage
Refinement program	REFMAC 5.8.0103	Depositor
R, R_{free}	0.186 , 0.220 0.191 , 0.222	Depositor DCC
R_{free} test set	42940 reflections (5.01%)	wwPDB-VP
Wilson B-factor (Å ²)	22.8	Xtriage
Anisotropy	0.163	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 32.1	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	0.014 for h,-k,-h-l	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	107004	wwPDB-VP
Average B, all atoms (Å ²)	26.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 10.54% 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 [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: MG, EDO, 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	0.43	0/4334	0.65	2/5898 (0.0%)
1	B	0.43	0/4321	0.64	1/5882 (0.0%)
1	C	0.43	0/4344	0.67	3/5911 (0.1%)
1	D	0.44	0/4329	0.66	0/5893
1	E	0.45	0/4327	0.67	0/5888
1	F	0.45	0/4369	0.68	1/5945 (0.0%)
1	G	0.43	0/4350	0.65	0/5921
1	H	0.44	0/4336	0.64	0/5901
1	I	0.42	0/4342	0.67	2/5908 (0.0%)
1	J	0.43	0/4322	0.67	1/5883 (0.0%)
1	K	0.44	0/4350	0.64	0/5920
1	L	0.44	0/4368	0.65	2/5945 (0.0%)
1	M	0.44	0/4346	0.68	0/5916
1	N	0.45	0/4349	0.68	1/5919 (0.0%)
1	O	0.43	0/4313	0.65	0/5870
1	P	0.44	0/4348	0.67	0/5917
1	Q	0.43	0/4330	0.65	0/5894
1	R	0.42	0/4354	0.66	1/5927 (0.0%)
1	S	0.42	0/4305	0.65	0/5860
1	T	0.43	0/4322	0.65	1/5883 (0.0%)
1	U	0.42	0/4323	0.62	0/5884
1	V	0.41	0/4322	0.61	0/5883
1	W	0.43	0/4314	0.61	0/5872
1	X	0.41	0/4312	0.63	0/5870
All	All	0.43	0/104030	0.65	15/141590 (0.0%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	T	0	1

There are no bond length outliers.

The worst 5 of 15 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	I	552	ARG	NE-CZ-NH1	-7.24	116.68	120.30
1	I	552	ARG	NE-CZ-NH2	7.12	123.86	120.30
1	C	552	ARG	NE-CZ-NH2	6.50	123.55	120.30
1	C	552	ARG	NE-CZ-NH1	-5.64	117.48	120.30
1	A	310	ARG	NE-CZ-NH1	5.59	123.10	120.30

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	T	494	GLU	Peptide

5.2 Too-close contacts [i](#)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	4250	0	4149	11	0
1	B	4237	0	4138	11	0
1	C	4260	0	4161	16	0
1	D	4245	0	4141	12	0
1	E	4244	0	4141	17	0
1	F	4285	0	4179	14	0
1	G	4266	0	4163	14	0
1	H	4252	0	4148	18	0
1	I	4259	0	4151	11	0
1	J	4238	0	4135	13	0
1	K	4266	0	4157	13	0
1	L	4284	0	4176	12	0
1	M	4262	0	4158	15	0
1	N	4265	0	4155	13	0
1	O	4229	0	4129	11	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	P	4264	0	4157	11	0
1	Q	4246	0	4143	8	0
1	R	4270	0	4154	12	0
1	S	4221	0	4127	7	0
1	T	4238	0	4135	10	0
1	U	4239	0	4137	13	0
1	V	4238	0	4135	15	0
1	W	4230	0	4132	10	0
1	X	4228	0	4133	13	0
2	A	1	0	0	0	0
2	B	1	0	0	0	0
2	C	1	0	0	0	0
2	D	1	0	0	0	0
2	E	1	0	0	0	0
2	F	1	0	0	0	0
2	G	1	0	0	0	0
2	H	1	0	0	0	0
2	I	1	0	0	0	0
2	J	1	0	0	0	0
2	K	1	0	0	0	0
2	L	1	0	0	0	0
2	M	1	0	0	0	0
2	N	1	0	0	0	0
2	O	1	0	0	0	0
2	P	1	0	0	0	0
2	Q	1	0	0	0	0
2	R	1	0	0	0	0
2	S	1	0	0	0	0
2	T	1	0	0	0	0
2	U	1	0	0	0	0
2	V	1	0	0	0	0
2	W	1	0	0	0	0
2	X	1	0	0	0	0
3	A	26	0	16	1	0
3	B	26	0	16	0	0
3	C	26	0	16	2	0
3	D	26	0	16	2	0
3	E	26	0	16	4	0
3	F	26	0	16	1	0
3	G	26	0	16	3	0
3	H	26	0	16	2	0
3	I	26	0	16	2	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	J	26	0	16	2	0
3	K	26	0	16	2	0
3	L	26	0	16	2	0
3	M	26	0	16	2	0
3	N	26	0	16	2	0
3	O	26	0	16	2	0
3	P	26	0	16	2	0
3	Q	26	0	16	2	0
3	R	26	0	16	2	0
3	S	26	0	16	0	0
3	T	26	0	16	1	0
3	U	26	0	16	1	0
3	V	26	0	16	0	0
3	W	26	0	16	1	0
3	X	26	0	16	2	0
4	A	4	0	6	0	0
4	F	4	0	6	2	0
4	I	4	0	6	0	0
4	N	4	0	6	0	0
4	Q	4	0	6	0	0
4	R	4	0	6	0	0
5	A	139	0	0	0	0
5	B	157	0	0	0	0
5	C	246	0	0	2	0
5	D	199	0	0	1	0
5	E	221	0	0	0	0
5	F	275	0	0	0	0
5	G	192	0	0	0	0
5	H	150	0	0	1	0
5	I	176	0	0	0	0
5	J	217	0	0	0	0
5	K	206	0	0	1	0
5	L	200	0	0	0	0
5	M	288	0	0	0	0
5	N	269	0	0	0	0
5	O	185	0	0	0	0
5	P	212	0	0	0	0
5	Q	149	0	0	0	0
5	R	151	0	0	1	0
5	S	184	0	0	0	0
5	T	184	0	0	0	0
5	U	81	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
5	V	66	0	0	1	0
5	W	55	0	0	0	0
5	X	114	0	0	1	0
All	All	107004	0	99954	269	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 1.

The worst 5 of 269 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:9:ALA:HB2	1:A:35:LEU:HD23	1.70	0.73
1:C:9:ALA:HB2	1:C:35:LEU:HD23	1.72	0.70
1:F:9:ALA:HB2	1:F:35:LEU:HD23	1.77	0.67
1:X:414:VAL:HG22	1:X:431:MET:HE1	1.77	0.66
1:W:215:VAL:HG13	1:W:219:LEU:HD22	1.80	0.64

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	558/573 (97%)	551 (99%)	7 (1%)	0	100	100
1	B	557/573 (97%)	547 (98%)	10 (2%)	0	100	100
1	C	559/573 (98%)	549 (98%)	10 (2%)	0	100	100
1	D	558/573 (97%)	548 (98%)	10 (2%)	0	100	100
1	E	557/573 (97%)	550 (99%)	7 (1%)	0	100	100
1	F	562/573 (98%)	552 (98%)	10 (2%)	0	100	100
1	G	560/573 (98%)	552 (99%)	7 (1%)	1 (0%)	47	46

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	H	559/573 (98%)	549 (98%)	10 (2%)	0	100	100
1	I	559/573 (98%)	549 (98%)	10 (2%)	0	100	100
1	J	557/573 (97%)	546 (98%)	10 (2%)	1 (0%)	47	46
1	K	560/573 (98%)	554 (99%)	5 (1%)	1 (0%)	47	46
1	L	562/573 (98%)	550 (98%)	12 (2%)	0	100	100
1	M	560/573 (98%)	548 (98%)	11 (2%)	1 (0%)	47	46
1	N	560/573 (98%)	554 (99%)	6 (1%)	0	100	100
1	O	556/573 (97%)	546 (98%)	9 (2%)	1 (0%)	47	46
1	P	560/573 (98%)	549 (98%)	11 (2%)	0	100	100
1	Q	558/573 (97%)	547 (98%)	11 (2%)	0	100	100
1	R	561/573 (98%)	553 (99%)	8 (1%)	0	100	100
1	S	555/573 (97%)	545 (98%)	10 (2%)	0	100	100
1	T	557/573 (97%)	548 (98%)	9 (2%)	0	100	100
1	U	557/573 (97%)	536 (96%)	21 (4%)	0	100	100
1	V	557/573 (97%)	536 (96%)	21 (4%)	0	100	100
1	W	556/573 (97%)	537 (97%)	19 (3%)	0	100	100
1	X	556/573 (97%)	545 (98%)	11 (2%)	0	100	100
All	All	13401/13752 (97%)	13141 (98%)	255 (2%)	5 (0%)	100	100

All (5) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	J	73	SER
1	K	73	SER
1	O	73	SER
1	M	73	SER
1	G	73	SER

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	440/448 (98%)	424 (96%)	16 (4%)	35	33
1	B	439/448 (98%)	430 (98%)	9 (2%)	53	57
1	C	441/448 (98%)	432 (98%)	9 (2%)	55	59
1	D	440/448 (98%)	429 (98%)	11 (2%)	47	49
1	E	439/448 (98%)	431 (98%)	8 (2%)	59	63
1	F	444/448 (99%)	432 (97%)	12 (3%)	44	46
1	G	442/448 (99%)	432 (98%)	10 (2%)	50	53
1	H	441/448 (98%)	429 (97%)	12 (3%)	44	46
1	I	441/448 (98%)	433 (98%)	8 (2%)	59	63
1	J	439/448 (98%)	430 (98%)	9 (2%)	53	57
1	K	442/448 (99%)	429 (97%)	13 (3%)	42	42
1	L	444/448 (99%)	433 (98%)	11 (2%)	47	49
1	M	442/448 (99%)	430 (97%)	12 (3%)	44	46
1	N	442/448 (99%)	433 (98%)	9 (2%)	55	59
1	O	438/448 (98%)	428 (98%)	10 (2%)	50	53
1	P	442/448 (99%)	431 (98%)	11 (2%)	47	49
1	Q	440/448 (98%)	429 (98%)	11 (2%)	47	49
1	R	443/448 (99%)	430 (97%)	13 (3%)	42	42
1	S	437/448 (98%)	427 (98%)	10 (2%)	50	53
1	T	439/448 (98%)	429 (98%)	10 (2%)	50	53
1	U	439/448 (98%)	425 (97%)	14 (3%)	39	38
1	V	439/448 (98%)	428 (98%)	11 (2%)	47	49
1	W	438/448 (98%)	424 (97%)	14 (3%)	39	38
1	X	438/448 (98%)	429 (98%)	9 (2%)	53	57
All	All	10569/10752 (98%)	10307 (98%)	262 (2%)	50	49

5 of 262 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	L	183	LEU
1	N	379	LEU
1	W	271	GLU
1	L	379	LEU
1	M	332	GLU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (2) such sidechains are listed below:

Mol	Chain	Res	Type
1	C	34	GLN
1	M	181	ASN

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 carbohydrates in this entry.

5.6 Ligand geometry ⓘ

Of 54 ligands modelled in this entry, 24 are monoatomic - leaving 30 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	W	602	2	22,27,27	1.36	2 (9%)	29,40,40	1.81	8 (27%)
3	TPP	D	602	2	22,27,27	1.60	2 (9%)	29,40,40	1.57	7 (24%)
3	TPP	N	602	2	22,27,27	1.89	4 (18%)	29,40,40	1.55	6 (20%)
3	TPP	R	602	2	22,27,27	1.72	2 (9%)	29,40,40	1.60	4 (13%)
3	TPP	E	602	2	22,27,27	1.78	2 (9%)	29,40,40	1.48	6 (20%)
3	TPP	T	602	2	22,27,27	1.62	2 (9%)	29,40,40	1.75	5 (17%)
3	TPP	I	602	2	22,27,27	1.61	2 (9%)	29,40,40	1.72	6 (20%)
3	TPP	C	602	2	22,27,27	1.53	2 (9%)	29,40,40	1.56	5 (17%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
3	TPP	M	602	2	22,27,27	1.77	2 (9%)	29,40,40	1.58	5 (17%)
3	TPP	J	602	2	22,27,27	1.66	2 (9%)	29,40,40	1.72	8 (27%)
4	EDO	N	603	-	3,3,3	0.48	0	2,2,2	0.37	0
3	TPP	S	602	2	22,27,27	1.53	2 (9%)	29,40,40	1.82	6 (20%)
3	TPP	A	602	2	22,27,27	1.32	2 (9%)	29,40,40	1.79	7 (24%)
3	TPP	G	602	2	22,27,27	1.54	2 (9%)	29,40,40	1.61	4 (13%)
4	EDO	I	603	-	3,3,3	0.53	0	2,2,2	0.21	0
3	TPP	B	602	2	22,27,27	1.39	2 (9%)	29,40,40	1.66	3 (10%)
3	TPP	Q	602	2	22,27,27	1.50	2 (9%)	29,40,40	1.71	5 (17%)
3	TPP	K	602	2	22,27,27	1.46	2 (9%)	29,40,40	1.66	5 (17%)
3	TPP	H	602	2	22,27,27	1.60	2 (9%)	29,40,40	1.40	5 (17%)
3	TPP	V	602	2	22,27,27	1.43	2 (9%)	29,40,40	1.84	5 (17%)
4	EDO	Q	603	-	3,3,3	0.48	0	2,2,2	0.07	0
3	TPP	X	602	2	22,27,27	1.48	2 (9%)	29,40,40	1.80	8 (27%)
4	EDO	R	603	-	3,3,3	0.57	0	2,2,2	0.01	0
4	EDO	A	603	-	3,3,3	0.60	0	2,2,2	0.28	0
3	TPP	U	602	2	22,27,27	1.34	2 (9%)	29,40,40	1.96	8 (27%)
4	EDO	F	601	-	3,3,3	0.48	0	2,2,2	0.20	0
3	TPP	F	603	2	22,27,27	1.67	2 (9%)	29,40,40	1.58	7 (24%)
3	TPP	L	602	2	22,27,27	1.64	3 (13%)	29,40,40	1.72	4 (13%)
3	TPP	P	602	2	22,27,27	1.51	2 (9%)	29,40,40	1.55	5 (17%)
3	TPP	O	602	2	22,27,27	1.46	2 (9%)	29,40,40	1.58	5 (17%)

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	W	602	2	-	0/16/17/17	0/2/2/2
3	TPP	D	602	2	-	3/16/17/17	0/2/2/2
3	TPP	N	602	2	-	0/16/17/17	0/2/2/2
3	TPP	R	602	2	-	0/16/17/17	0/2/2/2
3	TPP	E	602	2	-	1/16/17/17	0/2/2/2
3	TPP	T	602	2	-	0/16/17/17	0/2/2/2
3	TPP	I	602	2	-	1/16/17/17	0/2/2/2
3	TPP	C	602	2	-	0/16/17/17	0/2/2/2
3	TPP	M	602	2	-	0/16/17/17	0/2/2/2
3	TPP	J	602	2	-	0/16/17/17	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	EDO	N	603	-	-	1/1/1/1	-
3	TPP	S	602	2	-	0/16/17/17	0/2/2/2
3	TPP	A	602	2	-	3/16/17/17	0/2/2/2
3	TPP	G	602	2	-	0/16/17/17	0/2/2/2
4	EDO	I	603	-	-	0/1/1/1	-
3	TPP	B	602	2	-	0/16/17/17	0/2/2/2
3	TPP	Q	602	2	-	2/16/17/17	0/2/2/2
3	TPP	K	602	2	-	0/16/17/17	0/2/2/2
3	TPP	H	602	2	-	2/16/17/17	0/2/2/2
3	TPP	V	602	2	-	1/16/17/17	0/2/2/2
4	EDO	Q	603	-	-	1/1/1/1	-
3	TPP	X	602	2	-	0/16/17/17	0/2/2/2
4	EDO	R	603	-	-	1/1/1/1	-
4	EDO	A	603	-	-	1/1/1/1	-
3	TPP	U	602	2	-	3/16/17/17	0/2/2/2
4	EDO	F	601	-	-	1/1/1/1	-
3	TPP	F	603	2	-	0/16/17/17	0/2/2/2
3	TPP	L	602	2	-	3/16/17/17	0/2/2/2
3	TPP	P	602	2	-	2/16/17/17	0/2/2/2
3	TPP	O	602	2	-	0/16/17/17	0/2/2/2

The worst 5 of 51 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	E	602	TPP	C4-N3	-6.95	1.33	1.39
3	N	602	TPP	C4-N3	-6.70	1.33	1.39
3	M	602	TPP	C4-N3	-6.31	1.34	1.39
3	R	602	TPP	C4-N3	-6.11	1.34	1.39
3	H	602	TPP	C4-N3	-6.01	1.34	1.39

The worst 5 of 137 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	U	602	TPP	C6-C5-C4	6.81	132.90	127.43
3	V	602	TPP	C6-C5-C4	5.86	132.14	127.43
3	Q	602	TPP	C6-C5-C4	5.67	131.98	127.43
3	T	602	TPP	C6-C5-C4	5.60	131.93	127.43
3	L	602	TPP	C6-C5-C4	5.46	131.81	127.43

There are no chirality outliers.

5 of 26 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	I	602	TPP	C4-C5-C6-C7
3	A	602	TPP	PA-O3A-PB-O3B
3	L	602	TPP	PA-O3A-PB-O2B
3	L	602	TPP	PA-O3A-PB-O3B
3	P	602	TPP	PA-O3A-PB-O2B

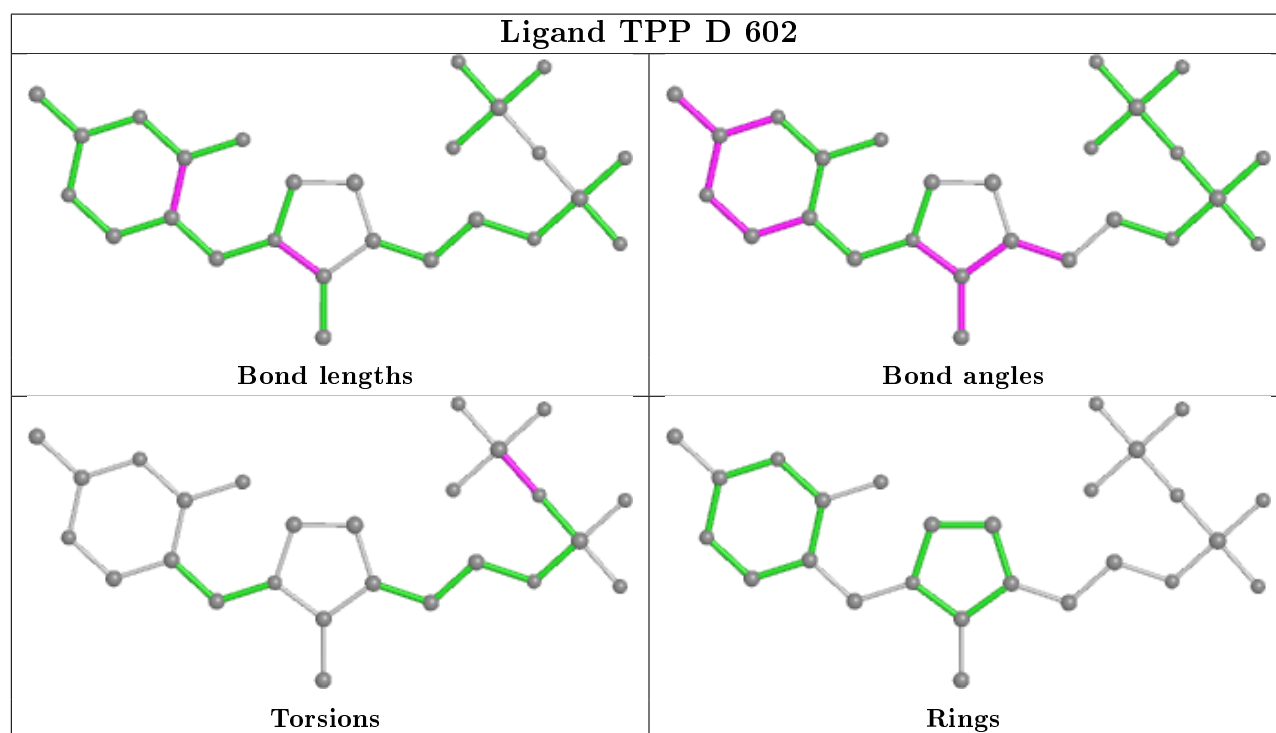
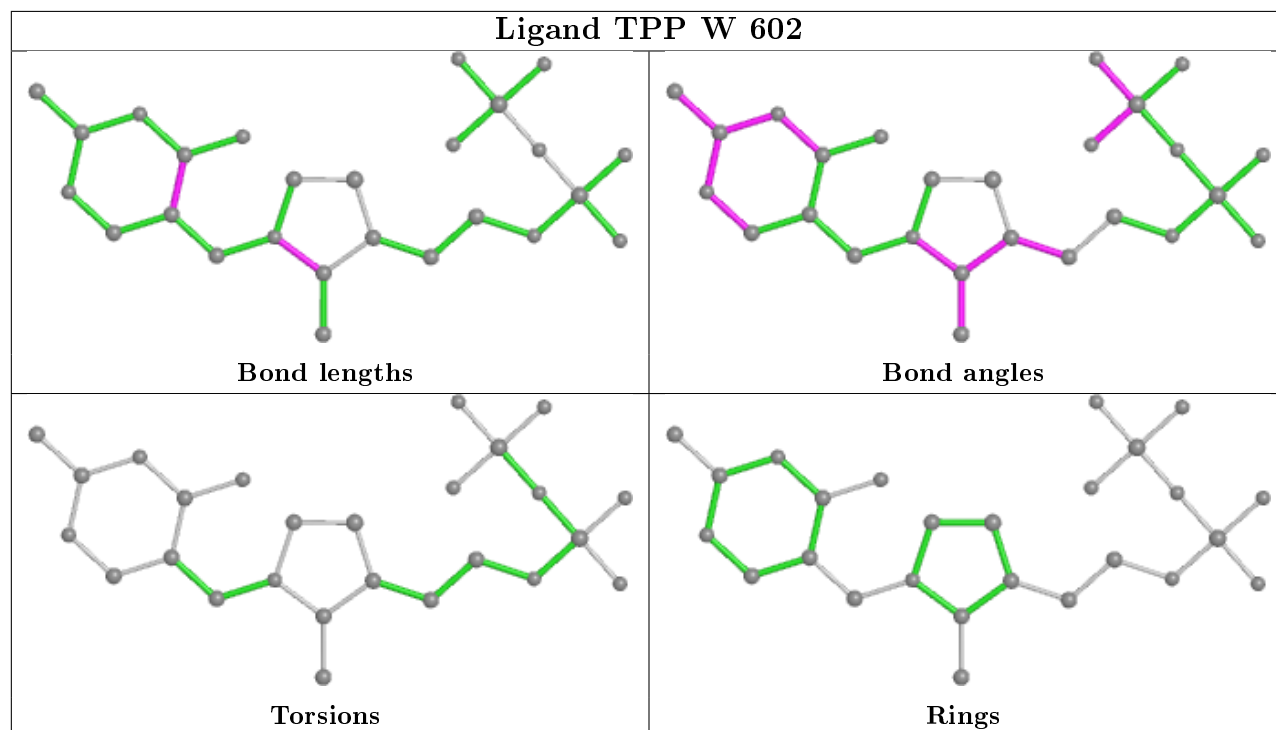
There are no ring outliers.

22 monomers are involved in 41 short contacts:

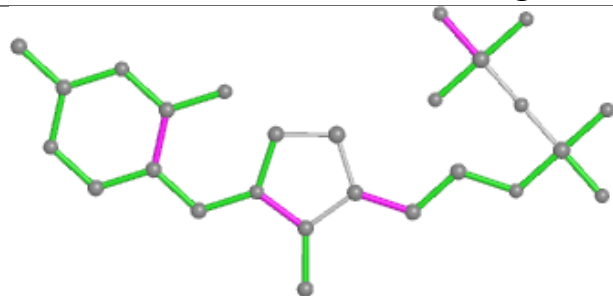
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	W	602	TPP	1	0
3	D	602	TPP	2	0
3	N	602	TPP	2	0
3	R	602	TPP	2	0
3	E	602	TPP	4	0
3	T	602	TPP	1	0
3	I	602	TPP	2	0
3	C	602	TPP	2	0
3	M	602	TPP	2	0
3	J	602	TPP	2	0
3	A	602	TPP	1	0
3	G	602	TPP	3	0
3	Q	602	TPP	2	0
3	K	602	TPP	2	0
3	H	602	TPP	2	0
3	X	602	TPP	2	0
3	U	602	TPP	1	0
4	F	601	EDO	2	0
3	F	603	TPP	1	0
3	L	602	TPP	2	0
3	P	602	TPP	2	0
3	O	602	TPP	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

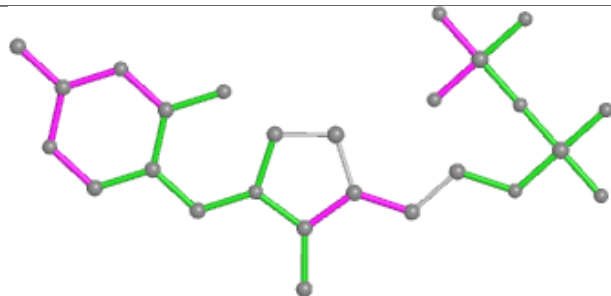
any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.



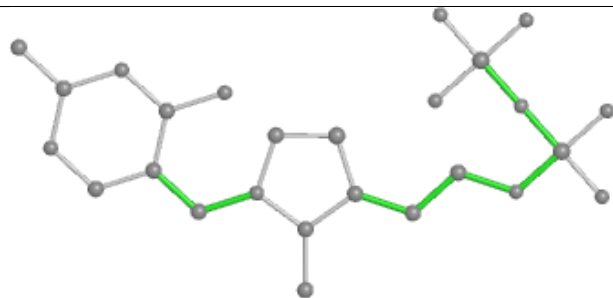
Ligand TPP N 602



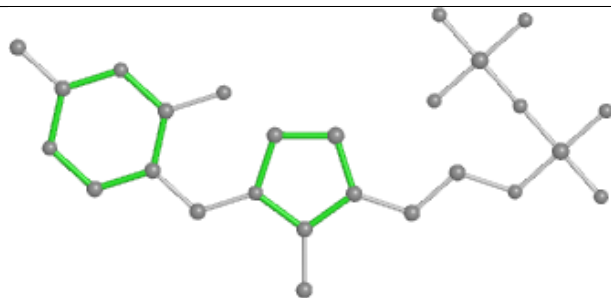
Bond lengths



Bond angles

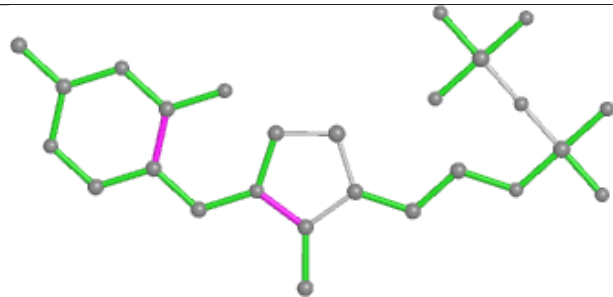


Torsions

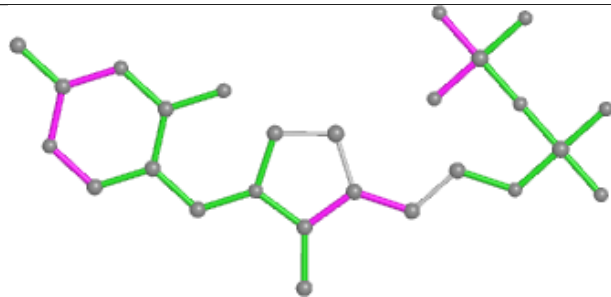


Rings

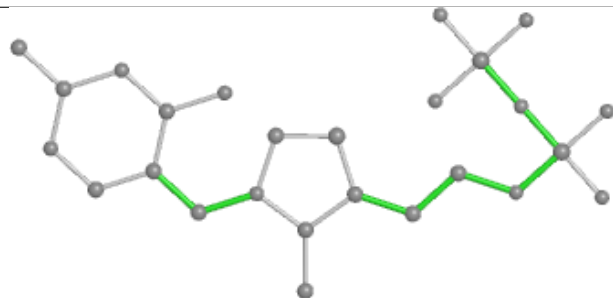
Ligand TPP R 602



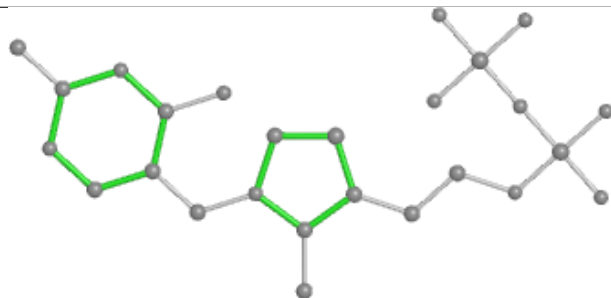
Bond lengths



Bond angles

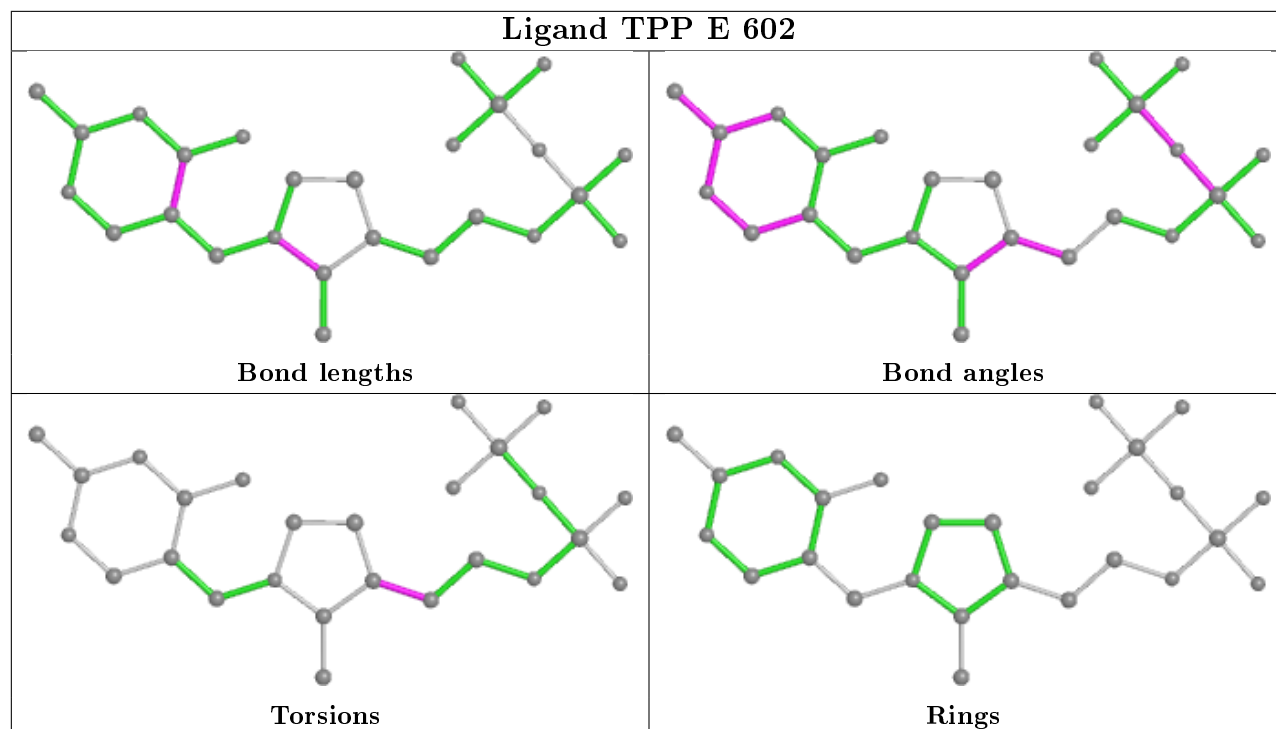


Torsions

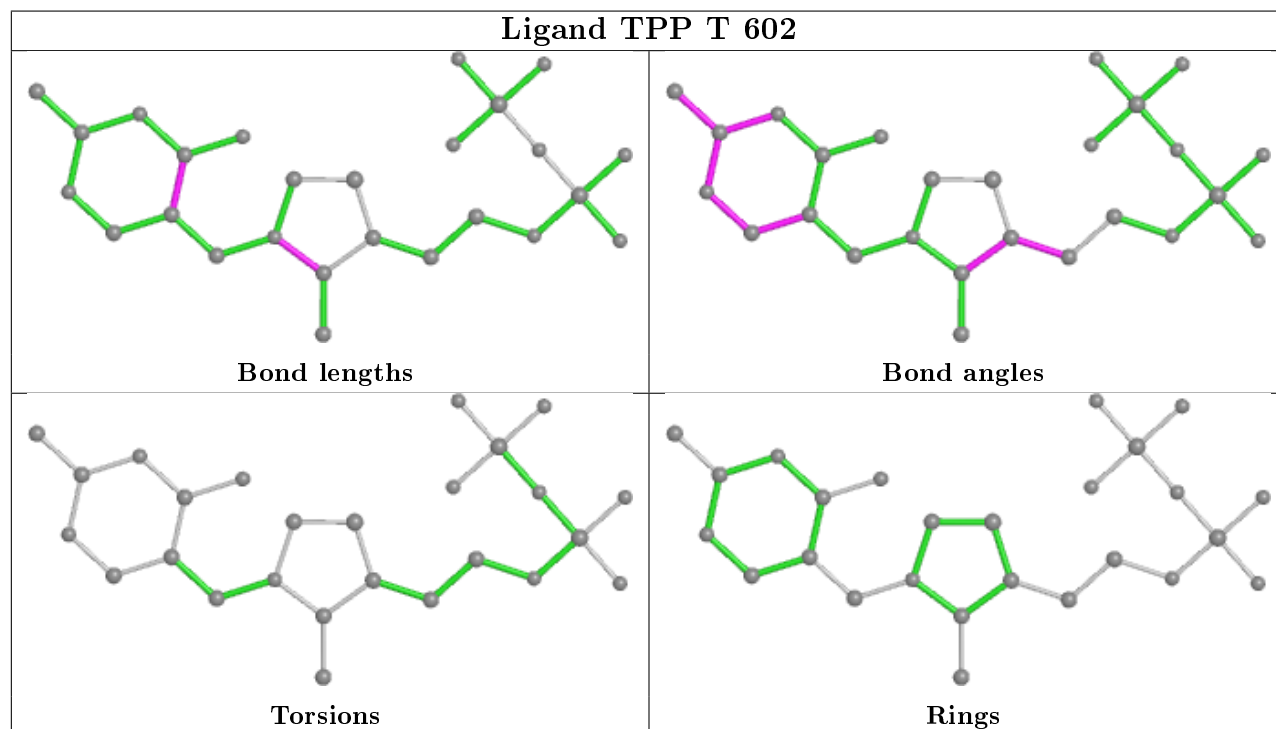


Rings

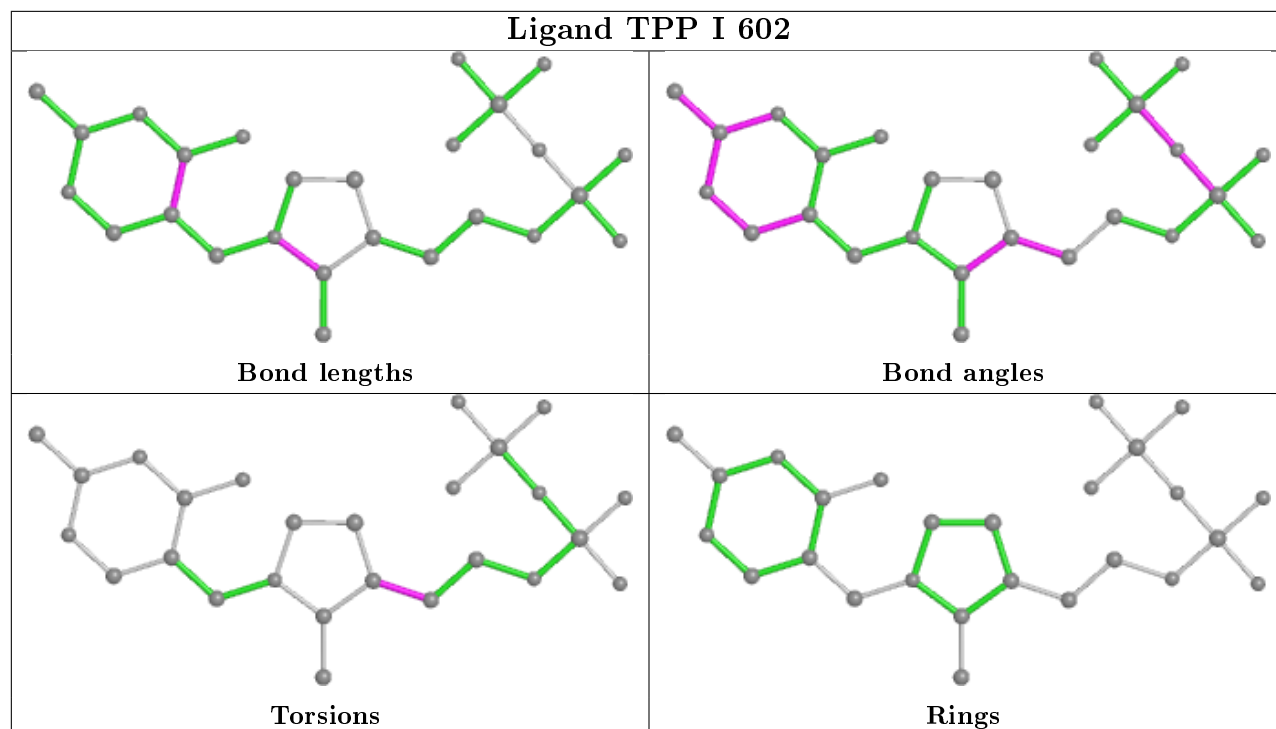
Ligand TPP E 602



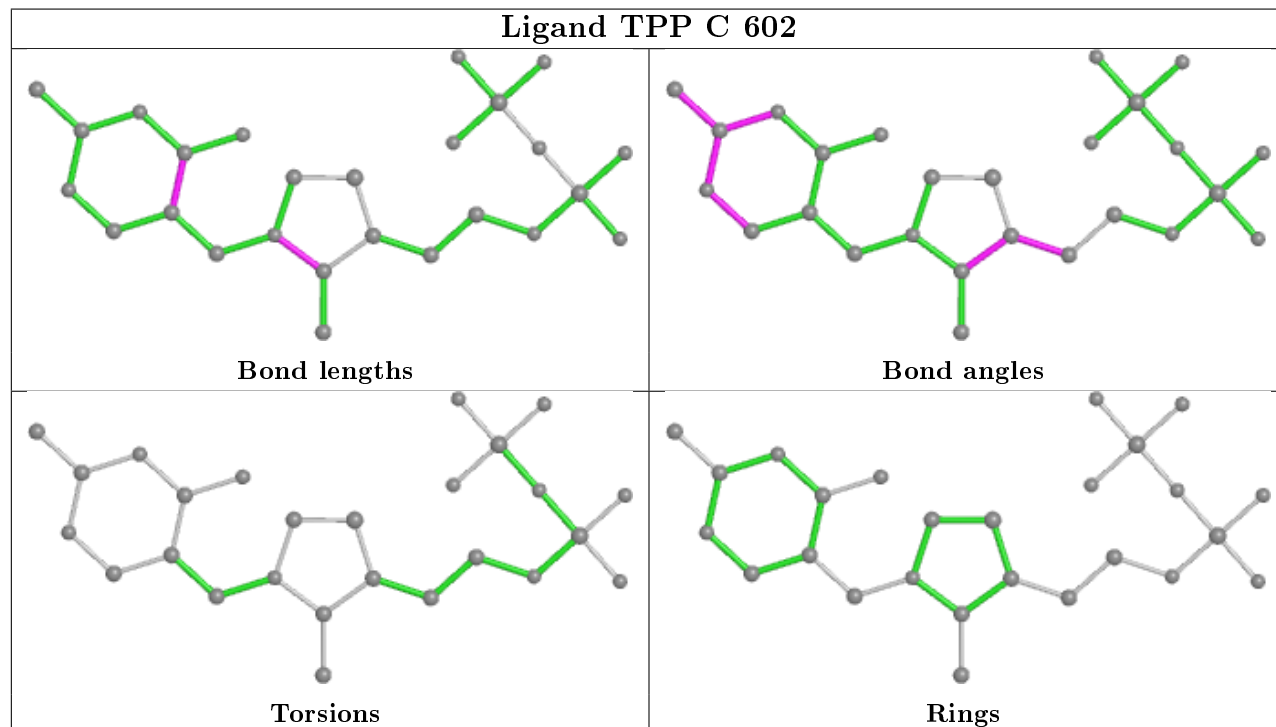
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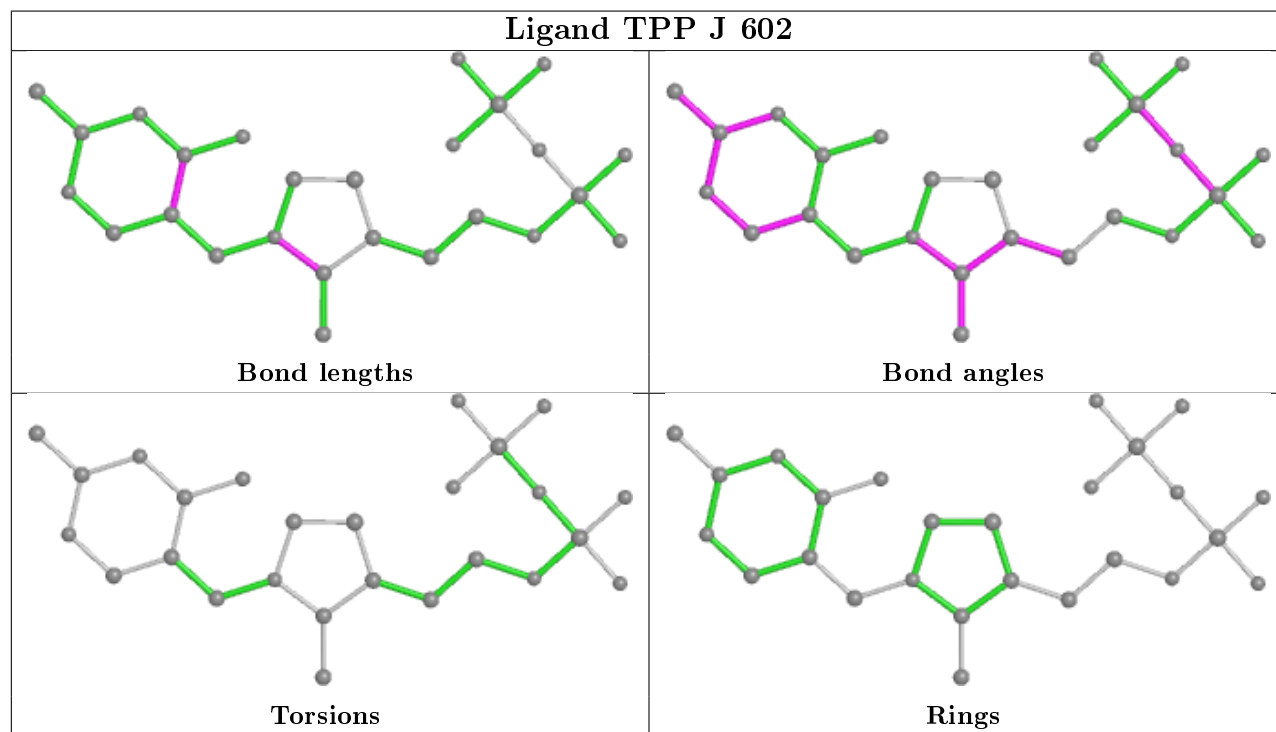
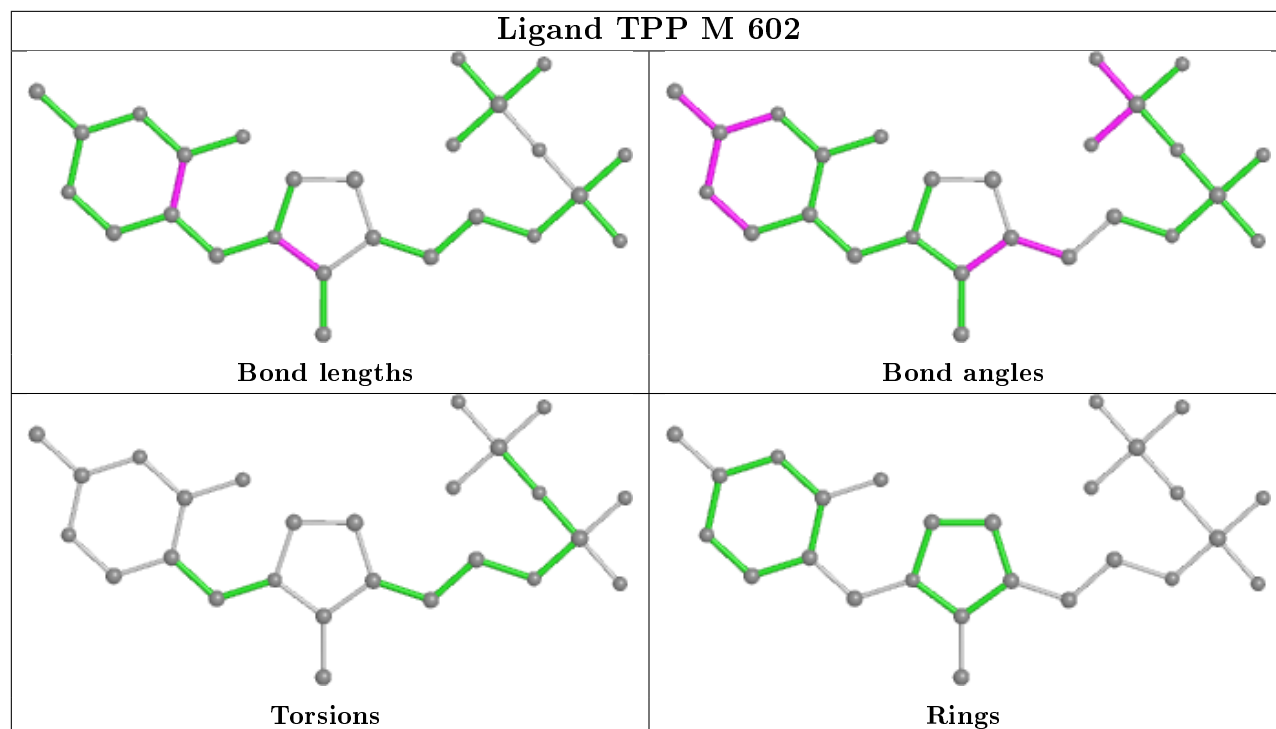


Ligand TPP I 602

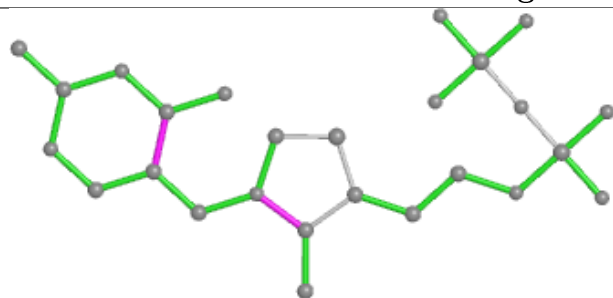


Ligand TPP C 602

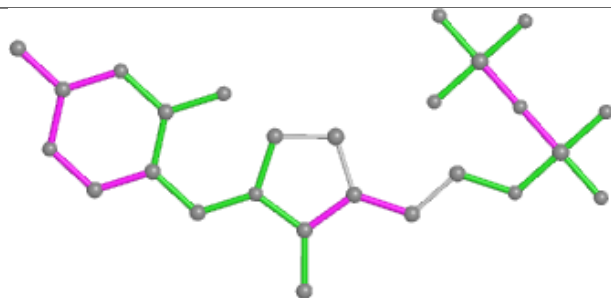




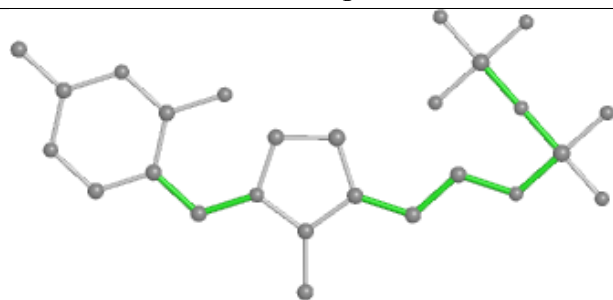
Ligand TPP S 602



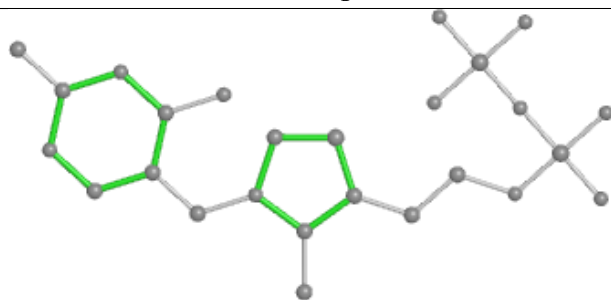
Bond lengths



Bond angles

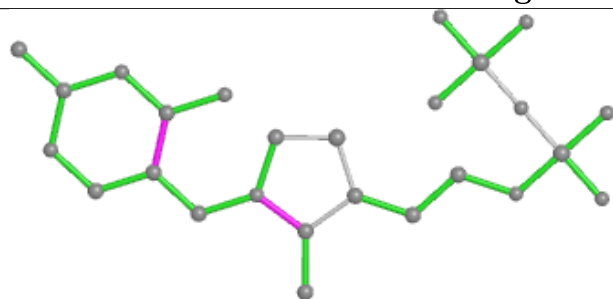


Torsions

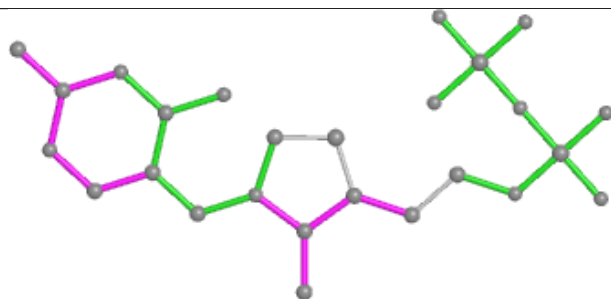


Rings

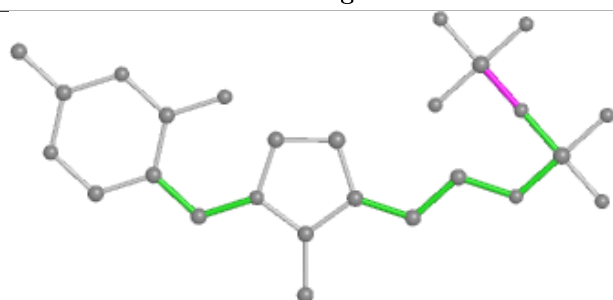
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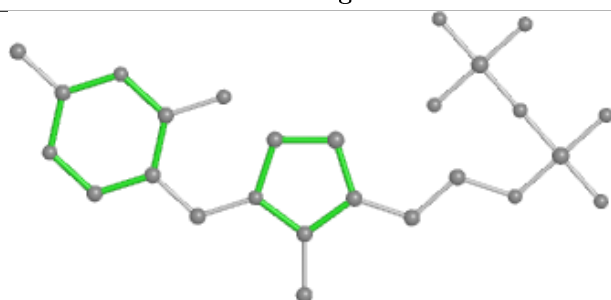
Bond lengths



Bond angles

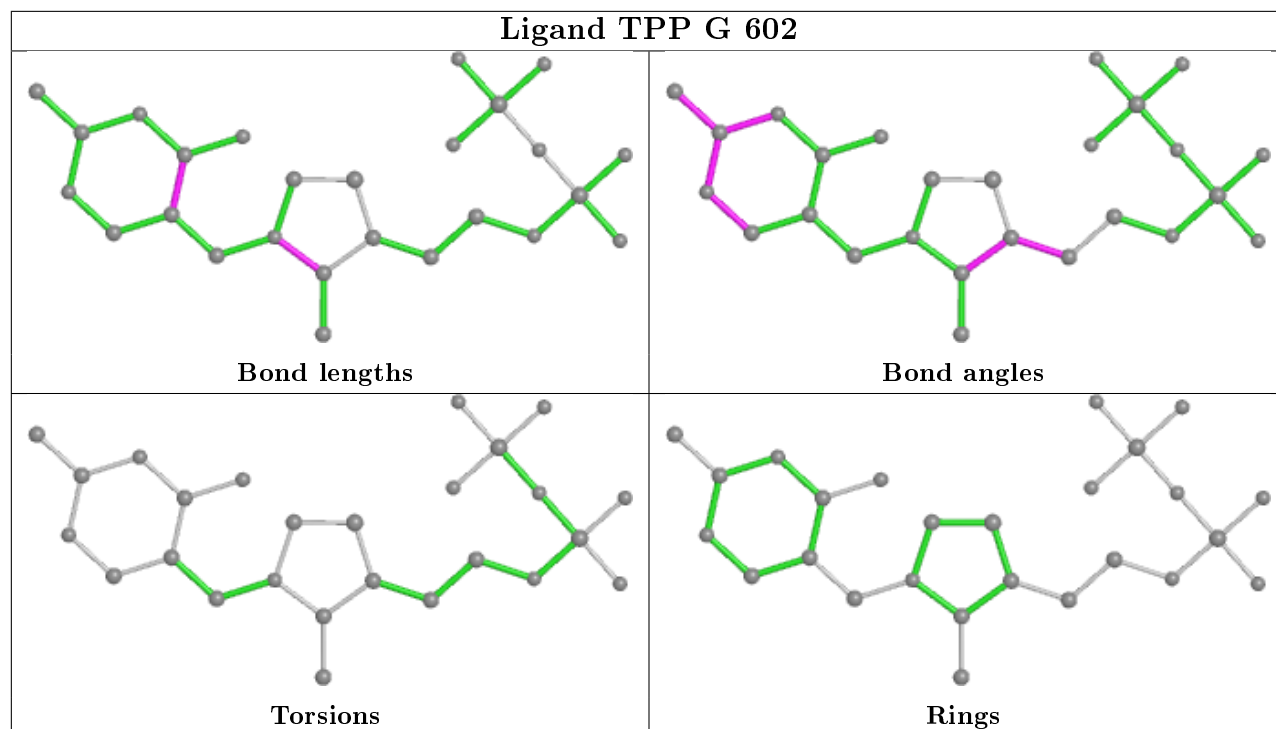


Torsions

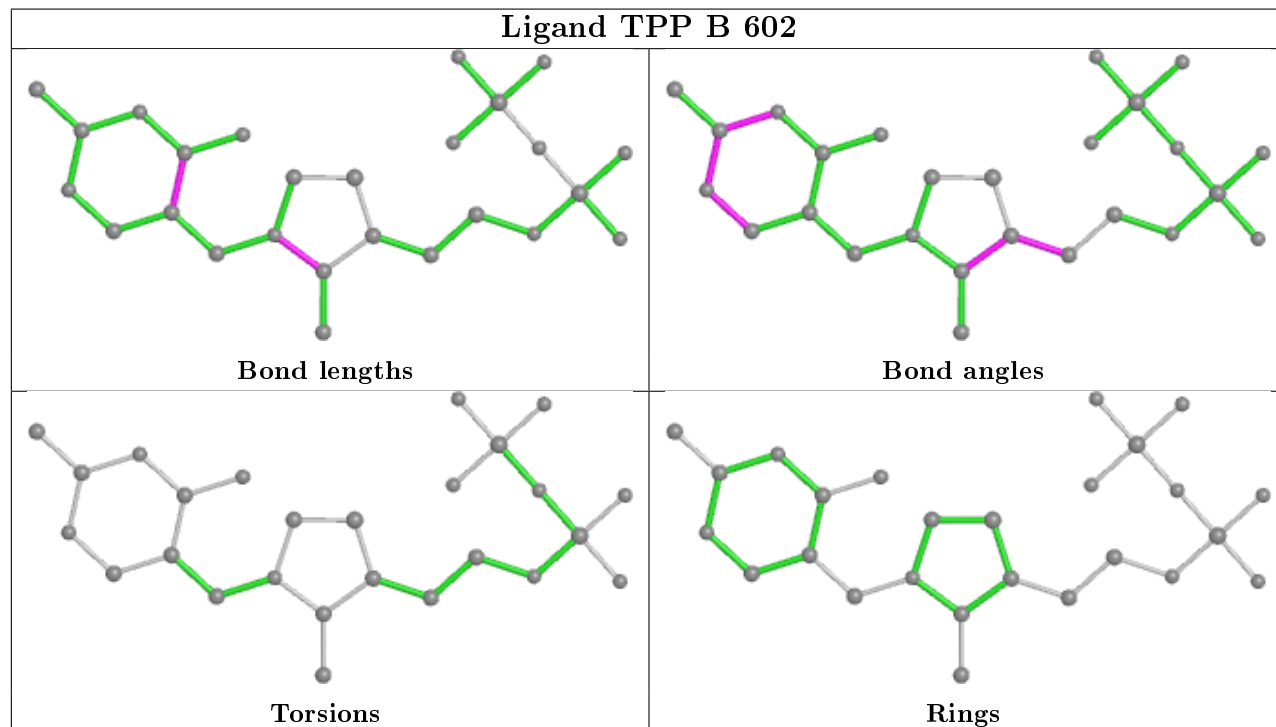


Rings

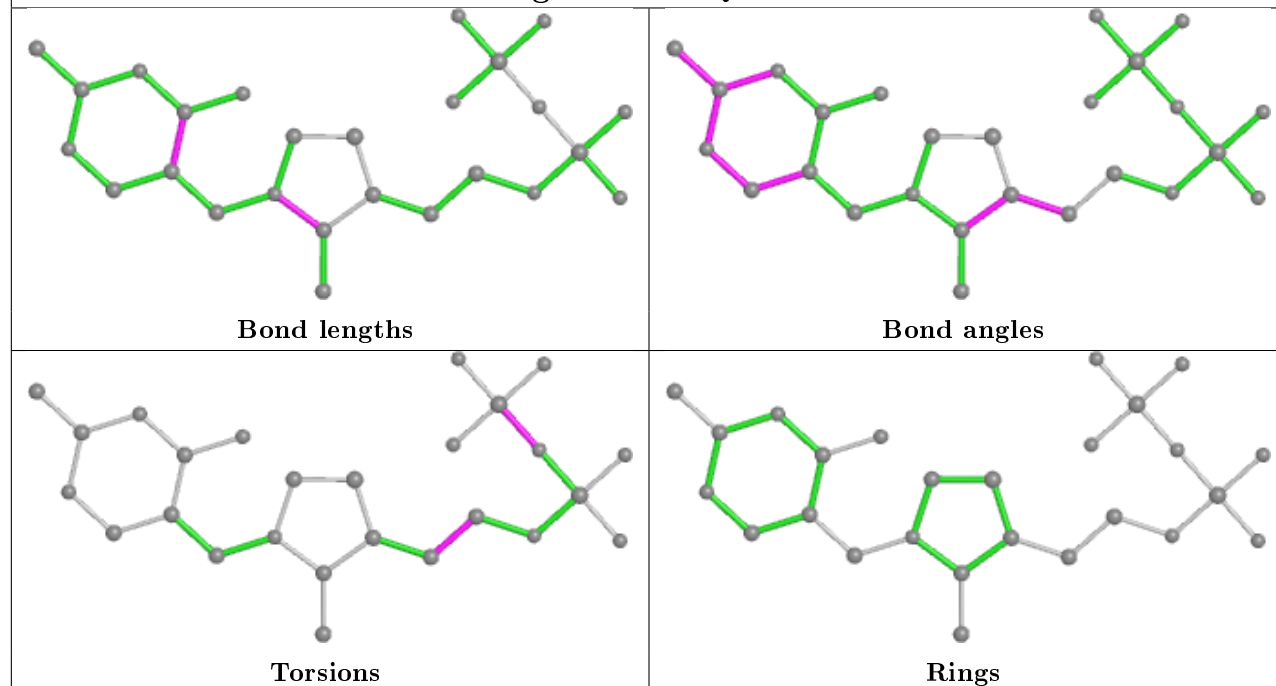
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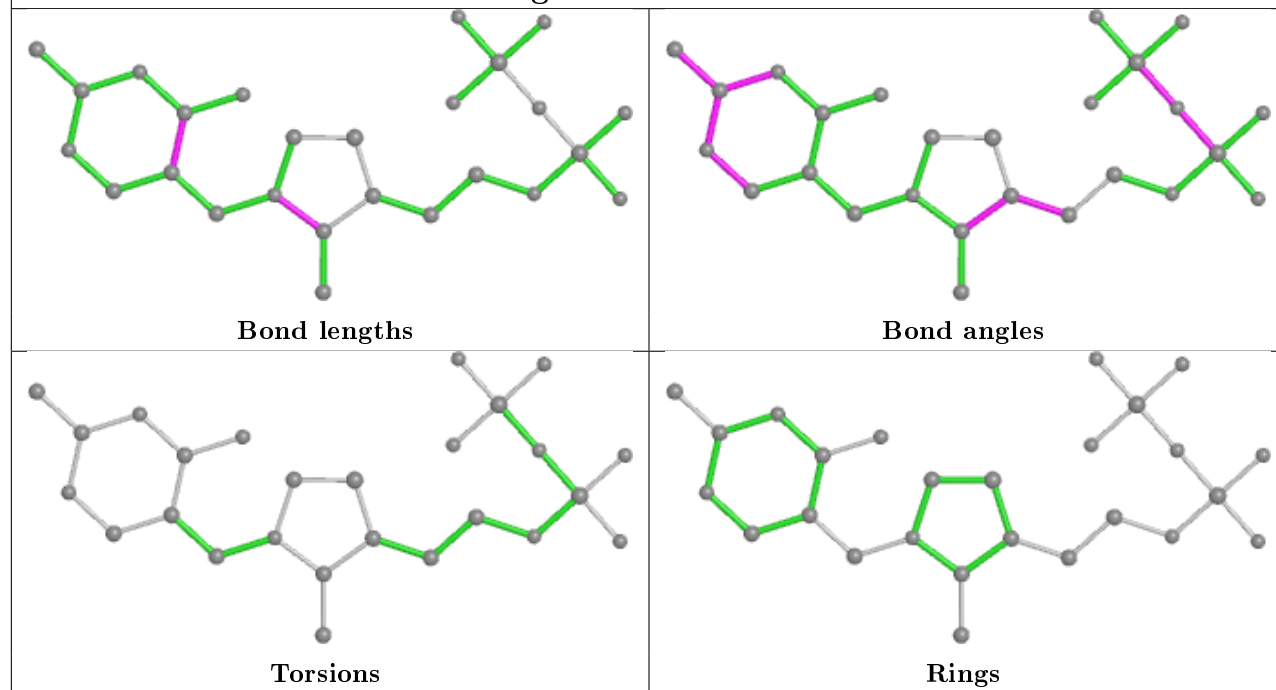
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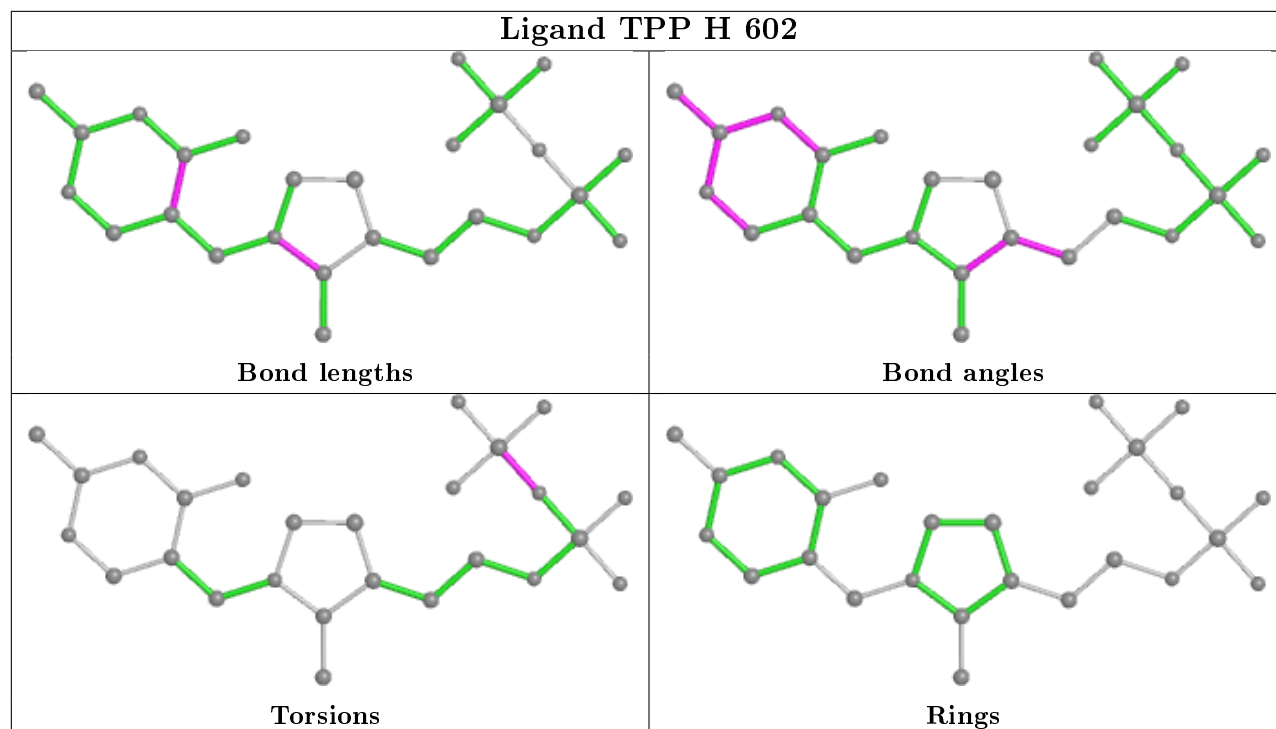
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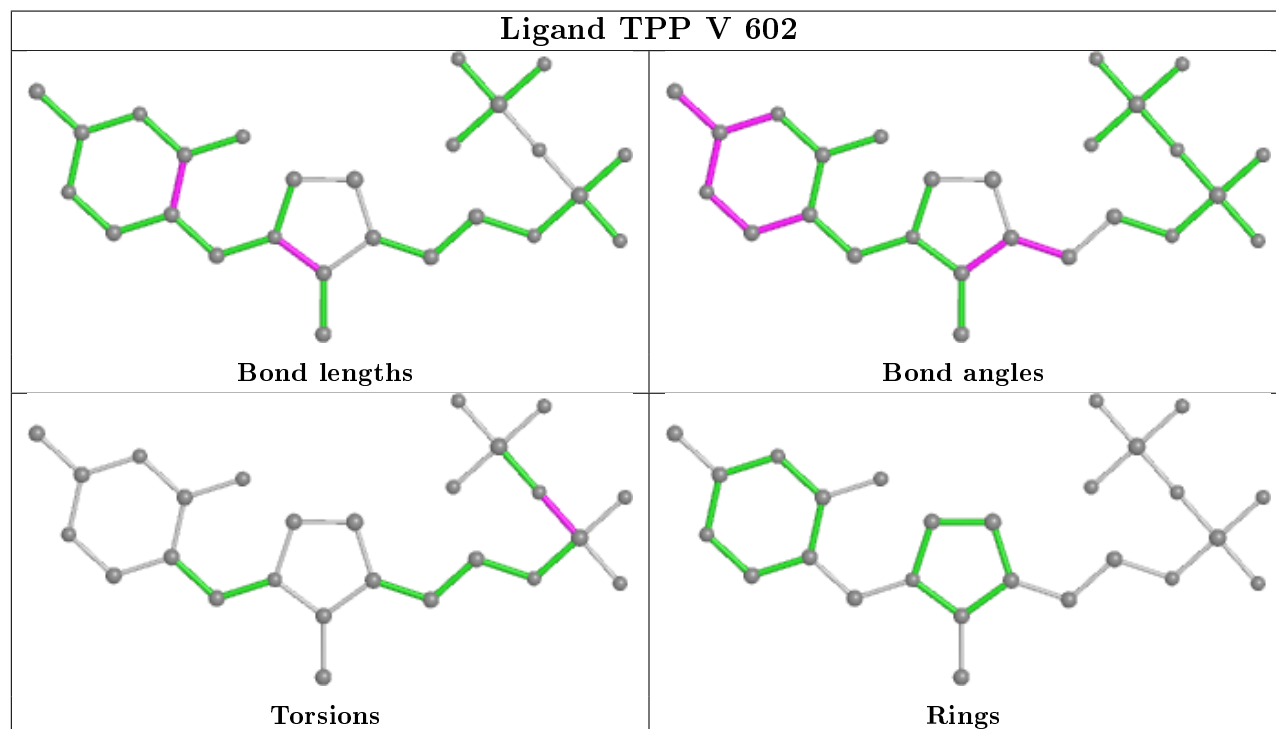
Ligand TPP K 602



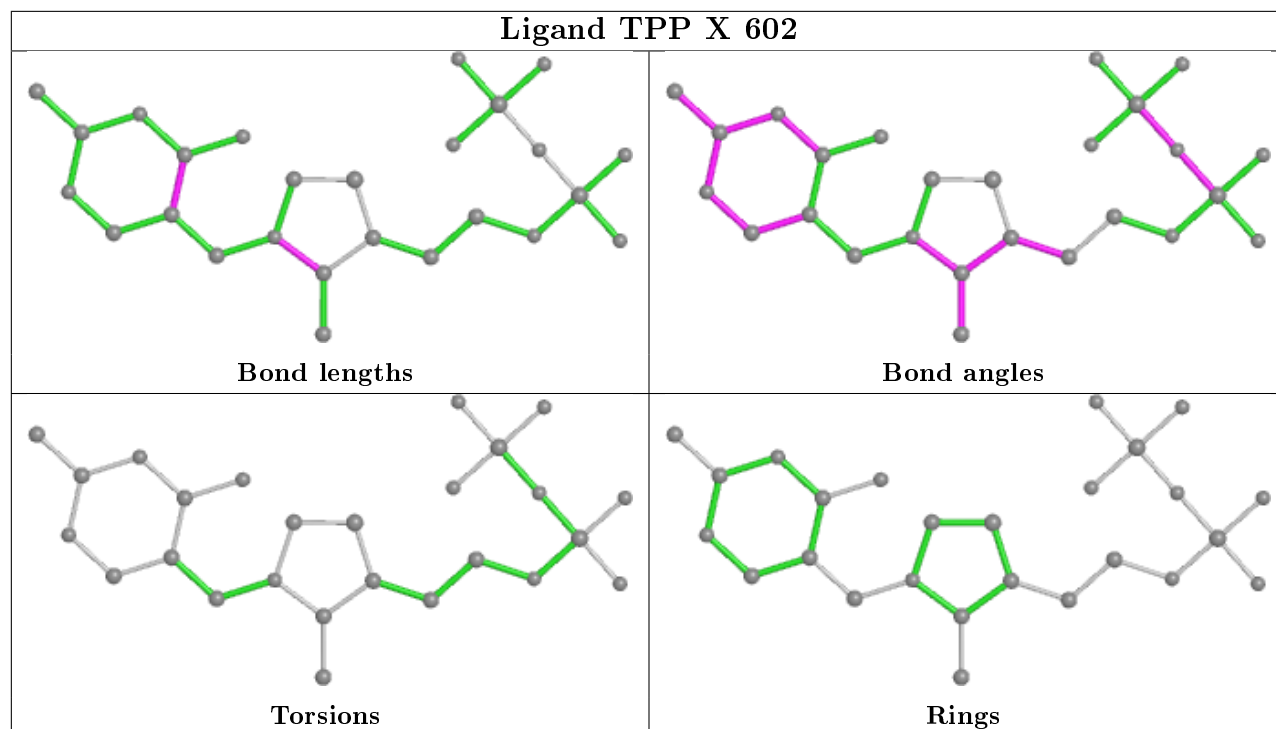
Ligand TPP H 602



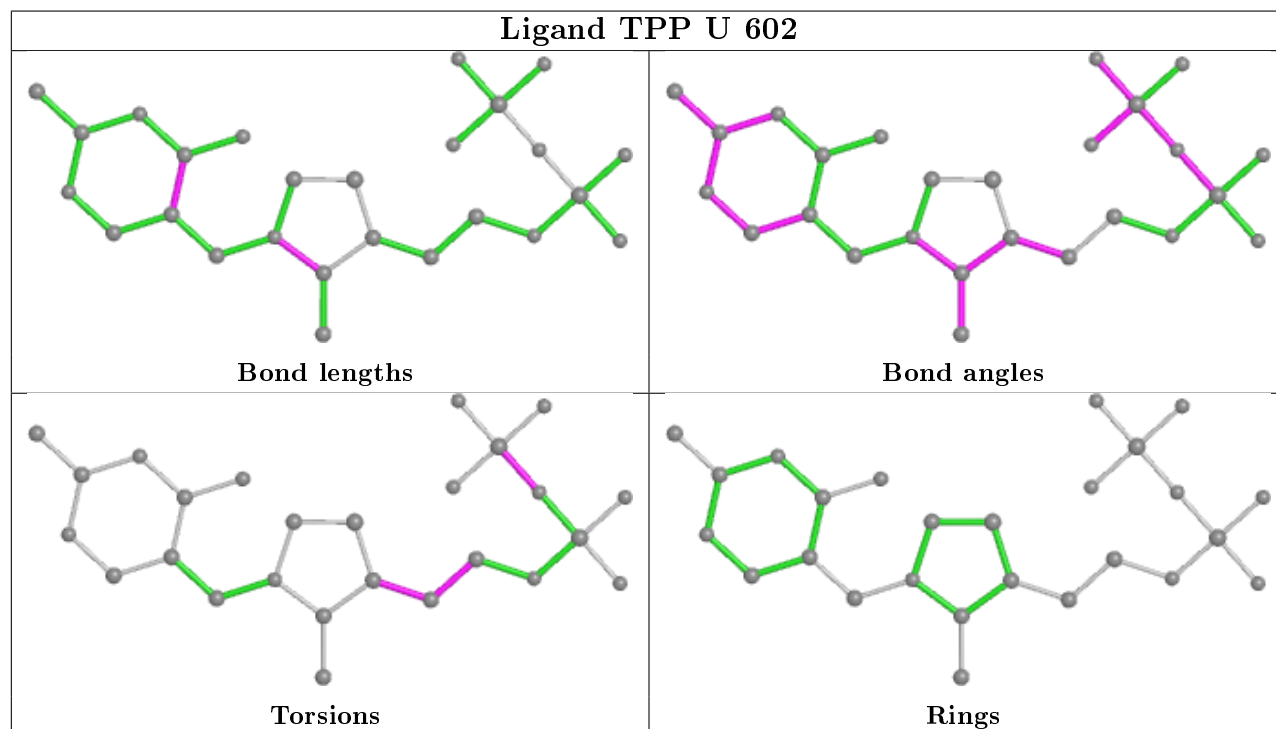
Ligand TPP V 602



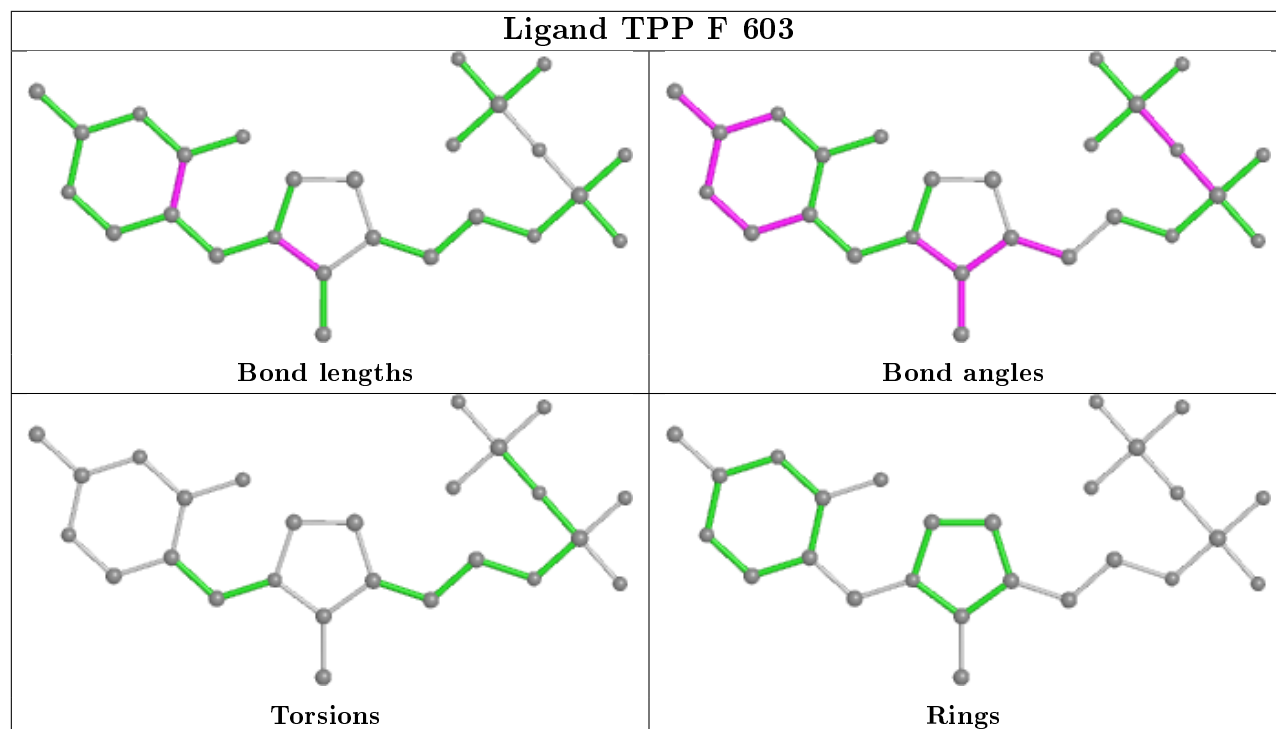
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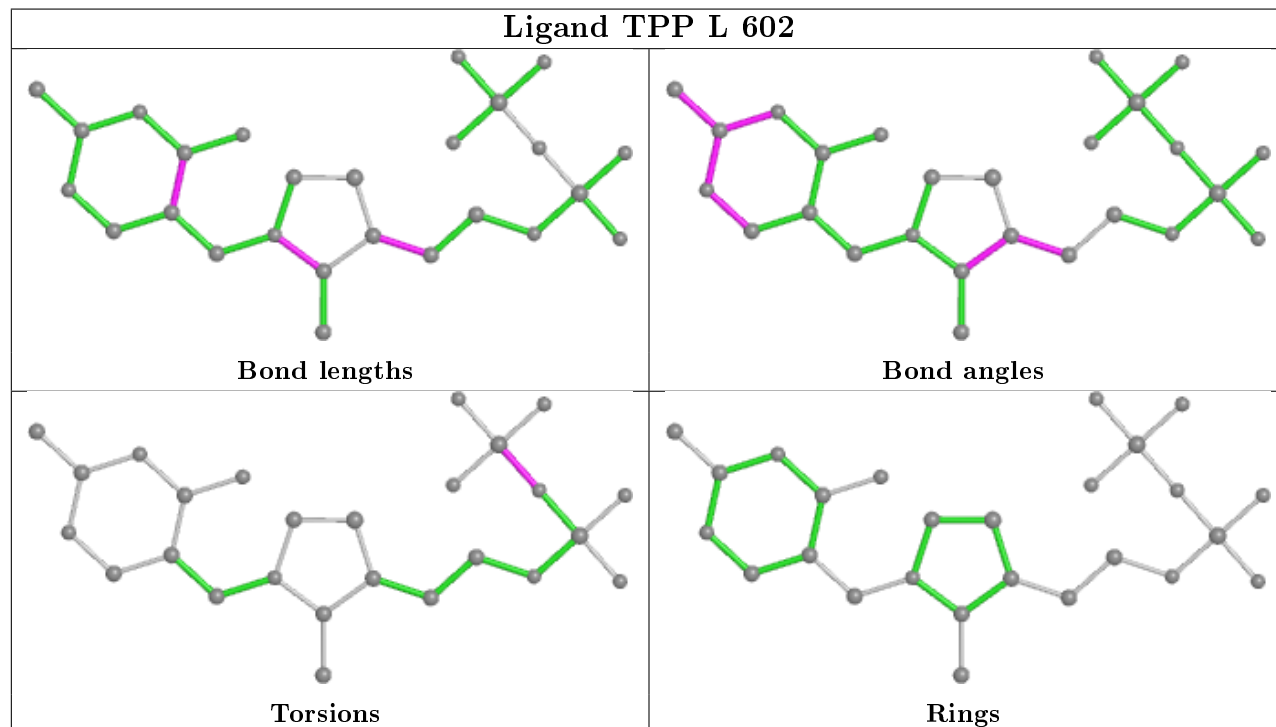
Ligand TPP U 602

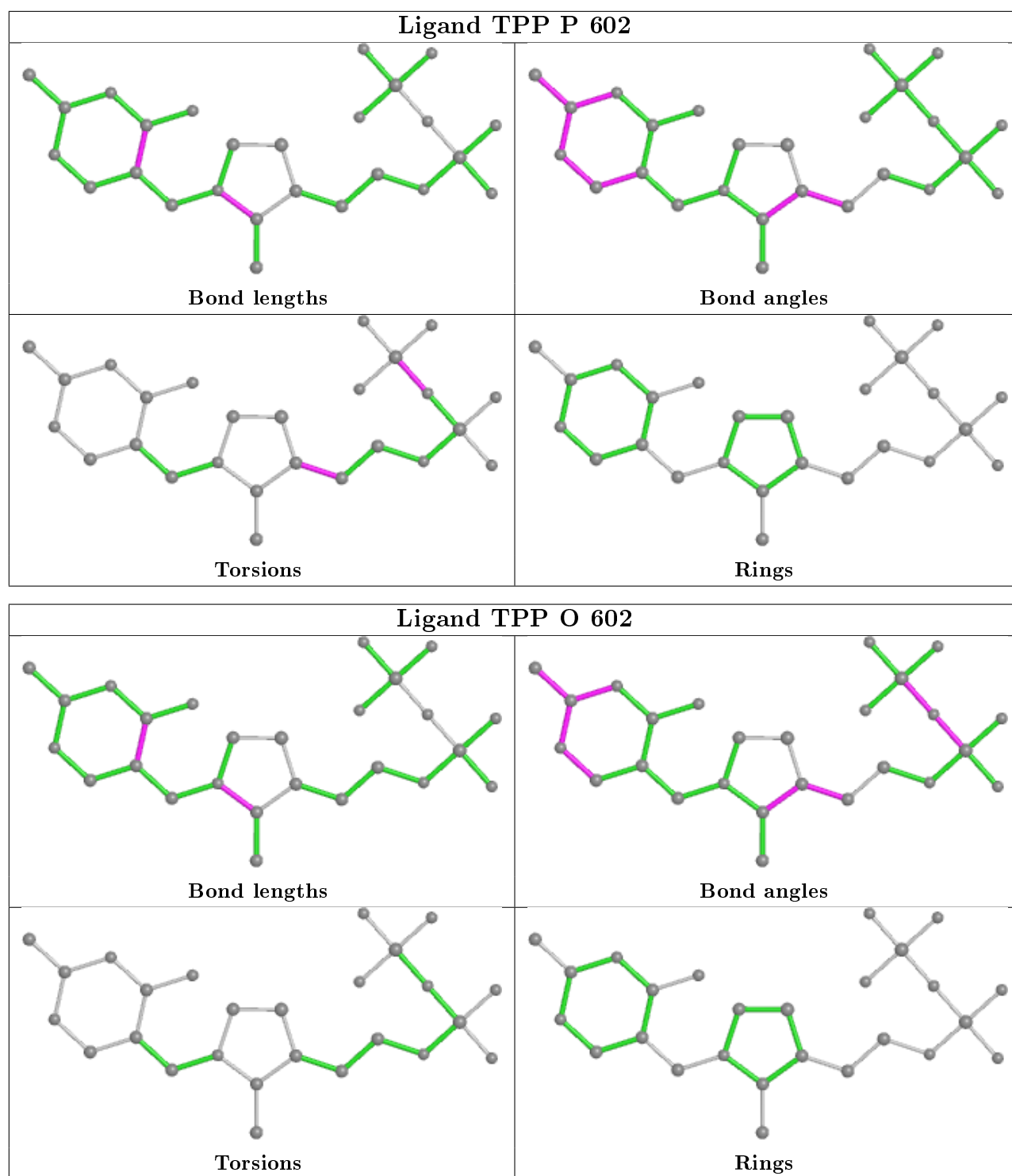


Ligand TPP F 603



Ligand TPP L 602





5.7 Other polymers [\(i\)](#)

There are no such residues in this entry.

5.8 Polymer linkage issues

The following chains have linkage breaks:

Mol	Chain	Number of breaks
1	I	1
1	E	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	I	555:GLN	C	556:ALA	N	5.35
1	E	555:GLN	C	556:ALA	N	3.78

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	555/573 (96%)	0.16	12 (2%) 62 69	15, 27, 44, 68	0
1	B	555/573 (96%)	0.10	13 (2%) 60 68	12, 25, 44, 66	0
1	C	555/573 (96%)	-0.08	6 (1%) 80 85	10, 19, 36, 57	0
1	D	555/573 (96%)	-0.04	6 (1%) 80 85	12, 21, 37, 58	0
1	E	556/573 (97%)	-0.16	6 (1%) 80 85	11, 20, 35, 76	0
1	F	555/573 (96%)	-0.18	2 (0%) 92 94	9, 17, 31, 55	0
1	G	555/573 (96%)	0.04	12 (2%) 62 69	13, 24, 41, 62	0
1	H	555/573 (96%)	0.11	8 (1%) 75 80	14, 26, 43, 66	0
1	I	556/573 (97%)	0.10	14 (2%) 57 65	12, 23, 44, 88	0
1	J	555/573 (96%)	-0.04	6 (1%) 80 85	12, 21, 38, 66	0
1	K	555/573 (96%)	0.00	12 (2%) 62 69	12, 22, 40, 58	0
1	L	555/573 (96%)	-0.13	4 (0%) 87 91	13, 21, 37, 58	0
1	M	555/573 (96%)	-0.16	3 (0%) 91 93	9, 16, 32, 50	0
1	N	555/573 (96%)	-0.10	3 (0%) 91 93	8, 17, 31, 51	0
1	O	555/573 (96%)	0.06	12 (2%) 62 69	12, 23, 41, 62	0
1	P	555/573 (96%)	-0.06	10 (1%) 68 75	10, 22, 42, 63	0
1	Q	555/573 (96%)	0.11	16 (2%) 51 61	13, 26, 43, 63	0
1	R	555/573 (96%)	0.06	11 (1%) 65 72	13, 25, 44, 74	0
1	S	555/573 (96%)	0.00	10 (1%) 68 75	13, 23, 42, 64	0
1	T	555/573 (96%)	-0.04	5 (0%) 84 88	13, 24, 40, 59	0
1	U	555/573 (96%)	0.85	78 (14%) 2 3	19, 43, 73, 94	0
1	V	555/573 (96%)	0.74	79 (14%) 2 3	21, 41, 68, 98	0
1	W	555/573 (96%)	1.03	115 (20%) 1 1	21, 47, 73, 97	0
1	X	555/573 (96%)	0.14	12 (2%) 62 69	16, 31, 50, 77	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
All	All	13322/13752 (96%)	0.10	455 (3%) 45 53	8, 24, 52, 98	0

The worst 5 of 455 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	I	556	ALA	12.3
1	E	556	ALA	6.5
1	U	343	GLY	6.3
1	V	349	LEU	5.5
1	W	348	VAL	5.4

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

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

6.3 Carbohydrates ⓘ

There are no carbohydrates in this entry.

6.4 Ligands ⓘ

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
4	EDO	N	603	4/4	0.67	0.26	48,51,52,54	0
4	EDO	Q	603	4/4	0.73	0.42	57,59,60,60	0
4	EDO	R	603	4/4	0.73	0.33	53,55,55,57	0
4	EDO	I	603	4/4	0.75	0.30	56,58,58,58	0
4	EDO	A	603	4/4	0.78	0.36	42,42,43,44	0
2	MG	K	601	1/1	0.87	0.05	23,23,23,23	0
2	MG	W	601	1/1	0.88	0.05	37,37,37,37	0
4	EDO	F	601	4/4	0.88	0.26	50,50,51,51	0
3	TPP	W	602	26/26	0.90	0.17	34,39,50,53	0
2	MG	P	601	1/1	0.91	0.07	21,21,21,21	0
2	MG	R	601	1/1	0.92	0.08	25,25,25,25	0
3	TPP	U	602	26/26	0.92	0.14	27,36,42,46	0
2	MG	B	601	1/1	0.92	0.04	25,25,25,25	0

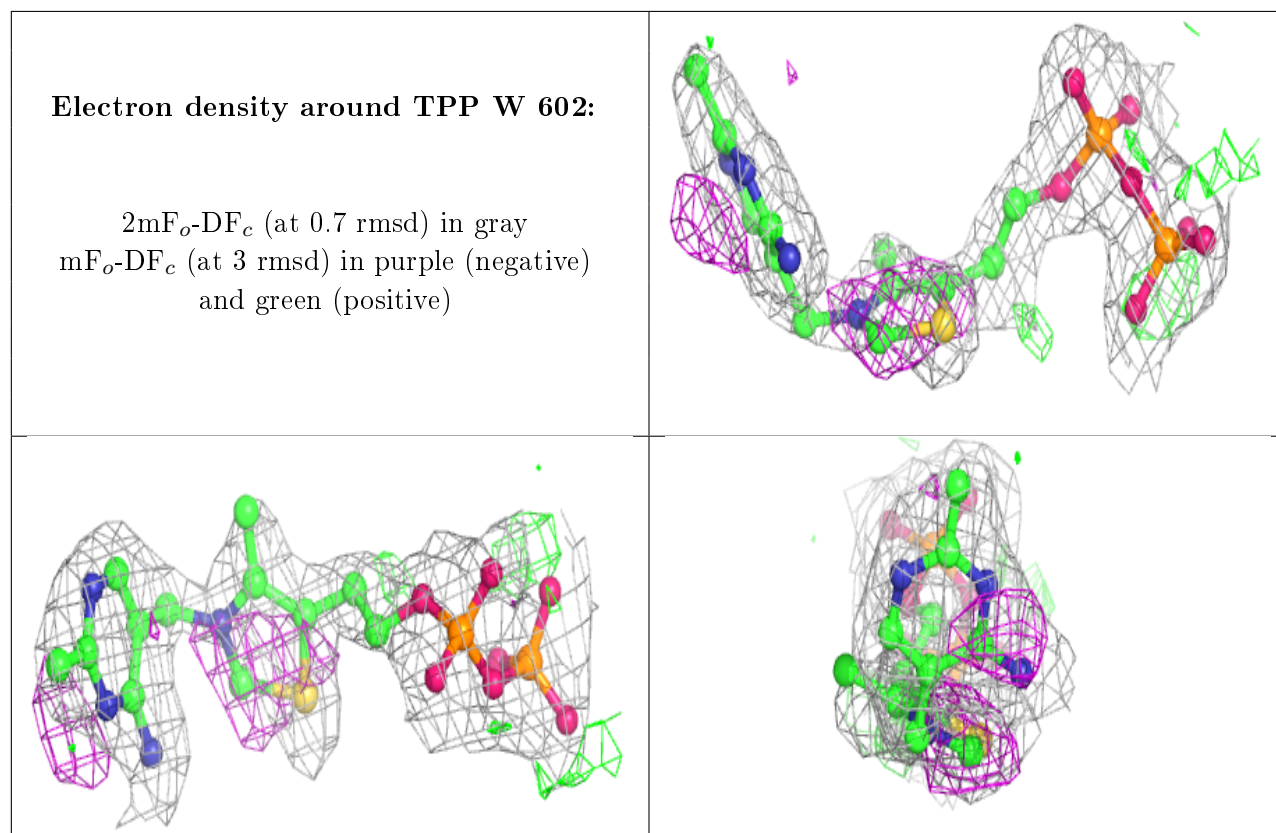
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
3	TPP	V	602	26/26	0.93	0.12	27,38,41,45	0
2	MG	S	601	1/1	0.93	0.06	23,23,23,23	0
2	MG	A	601	1/1	0.93	0.06	25,25,25,25	0
3	TPP	K	602	26/26	0.93	0.13	19,21,29,34	0
3	TPP	Q	602	26/26	0.94	0.13	17,22,27,30	0
3	TPP	A	602	26/26	0.94	0.14	19,23,31,36	0
3	TPP	D	602	26/26	0.94	0.14	15,17,22,25	0
2	MG	H	601	1/1	0.94	0.09	19,19,19,19	0
3	TPP	L	602	26/26	0.94	0.13	17,20,24,27	0
2	MG	V	601	1/1	0.94	0.05	34,34,34,34	0
3	TPP	B	602	26/26	0.94	0.14	21,27,32,36	0
3	TPP	X	602	26/26	0.94	0.12	23,27,32,35	0
2	MG	U	601	1/1	0.94	0.06	31,31,31,31	0
3	TPP	T	602	26/26	0.95	0.13	19,23,28,34	0
3	TPP	S	602	26/26	0.95	0.12	18,20,26,30	0
3	TPP	I	602	26/26	0.95	0.12	16,19,25,29	0
3	TPP	G	602	26/26	0.95	0.12	18,23,27,29	0
3	TPP	F	603	26/26	0.95	0.13	13,16,20,24	0
2	MG	D	601	1/1	0.95	0.04	22,22,22,22	0
2	MG	I	601	1/1	0.95	0.08	19,19,19,19	0
3	TPP	P	602	26/26	0.95	0.13	16,22,26,29	0
3	TPP	H	602	26/26	0.95	0.14	19,23,27,30	0
3	TPP	R	602	26/26	0.95	0.12	17,22,27,32	0
3	TPP	O	602	26/26	0.95	0.13	18,19,25,27	0
3	TPP	N	602	26/26	0.95	0.12	12,14,19,24	0
2	MG	G	601	1/1	0.96	0.08	21,21,21,21	0
3	TPP	C	602	26/26	0.96	0.14	14,16,20,23	0
3	TPP	E	602	26/26	0.96	0.12	13,15,21,23	0
3	TPP	J	602	26/26	0.96	0.12	16,18,22,25	0
3	TPP	M	602	26/26	0.96	0.13	13,15,19,22	0
2	MG	X	601	1/1	0.96	0.06	32,32,32,32	0
2	MG	T	601	1/1	0.97	0.05	19,19,19,19	0
2	MG	J	601	1/1	0.97	0.03	15,15,15,15	0
2	MG	L	601	1/1	0.97	0.07	24,24,24,24	0
2	MG	C	601	1/1	0.97	0.12	13,13,13,13	0
2	MG	M	601	1/1	0.97	0.08	13,13,13,13	0
2	MG	Q	601	1/1	0.98	0.04	22,22,22,22	0
2	MG	E	601	1/1	0.98	0.06	14,14,14,14	0
2	MG	N	601	1/1	0.99	0.05	11,11,11,11	0
2	MG	F	602	1/1	0.99	0.05	15,15,15,15	0
2	MG	O	601	1/1	0.99	0.02	17,17,17,17	0

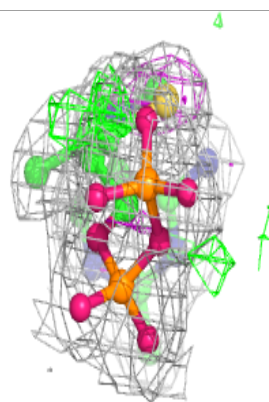
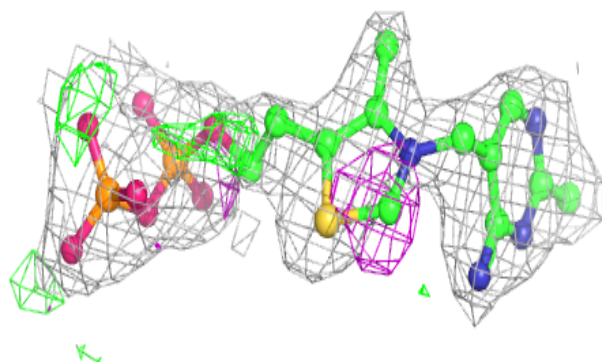
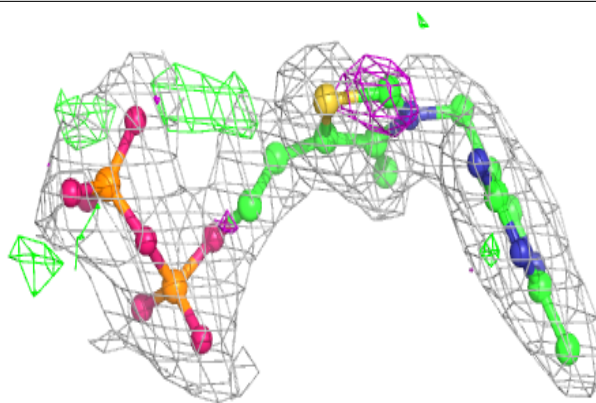
The following is a graphical depiction of the model fit to experimental electron density of all

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.

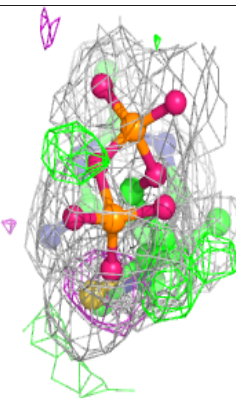
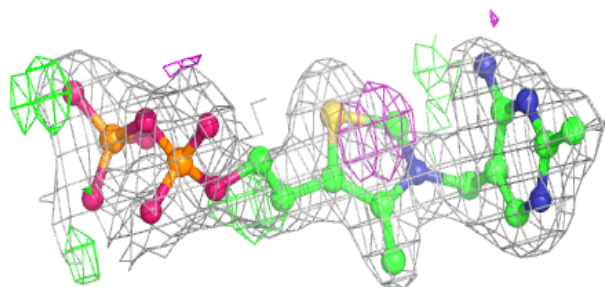
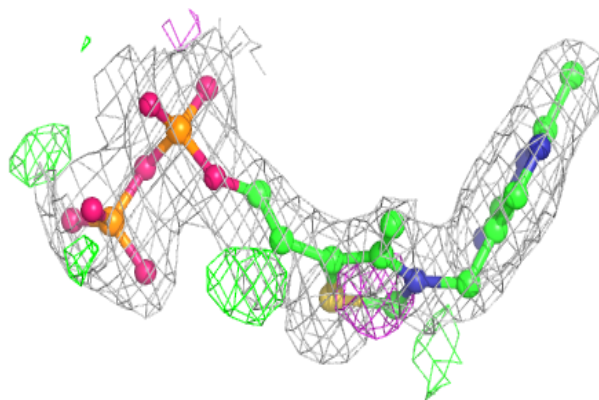


Electron density around TPP U 602:

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

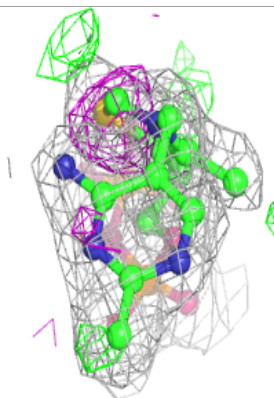
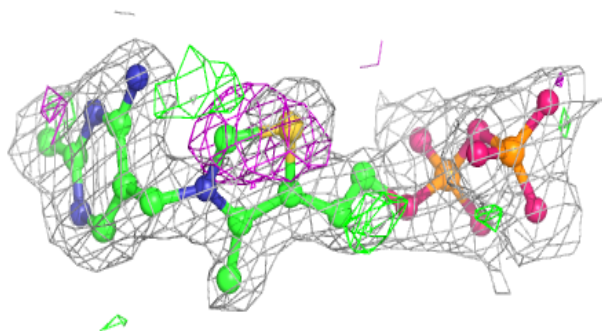
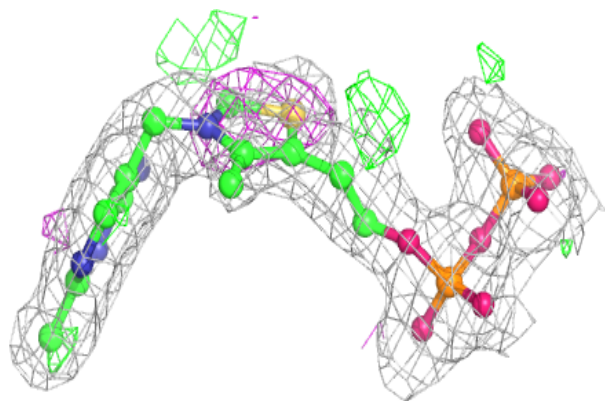
**Electron density around TPP V 602:**

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

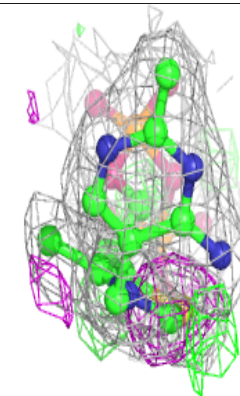
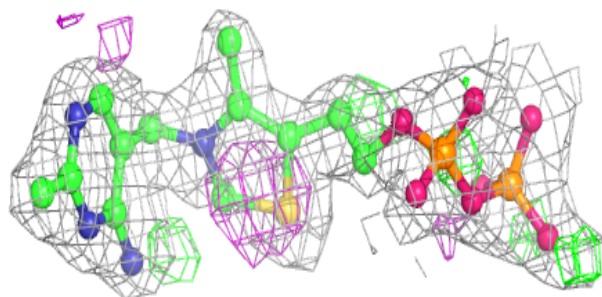
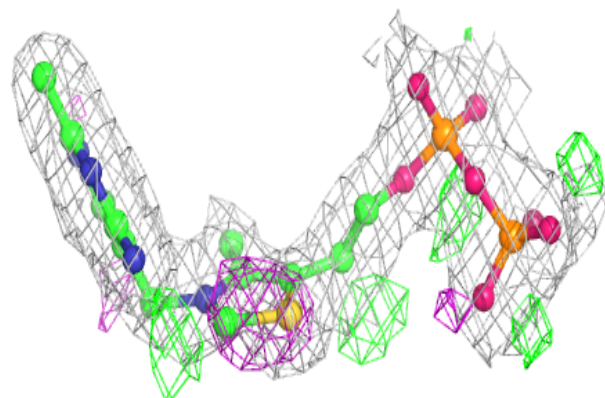


Electron density around TPP K 602:

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

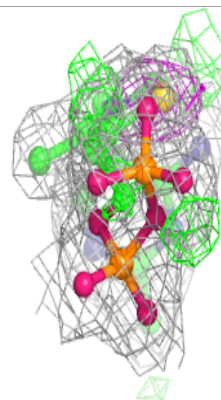
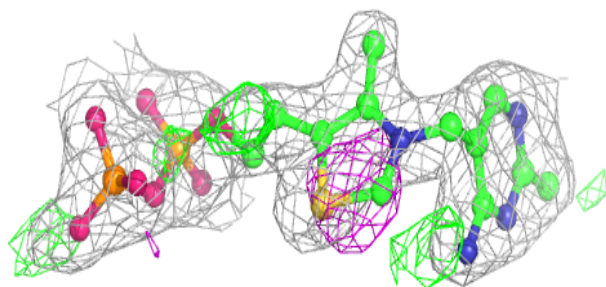
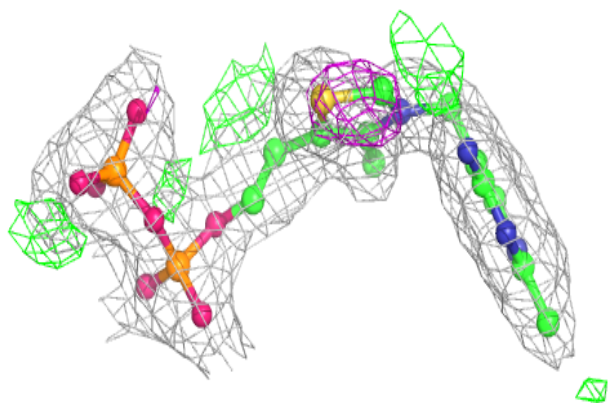
**Electron density around TPP Q 602:**

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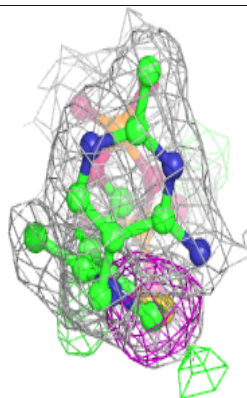
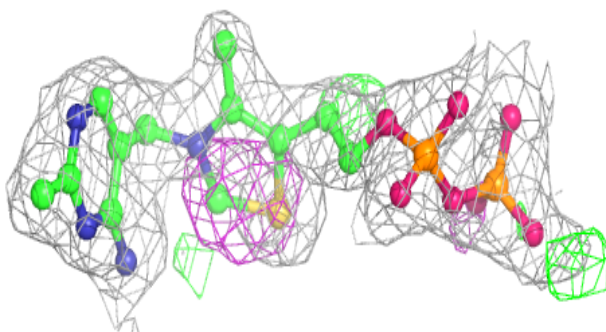
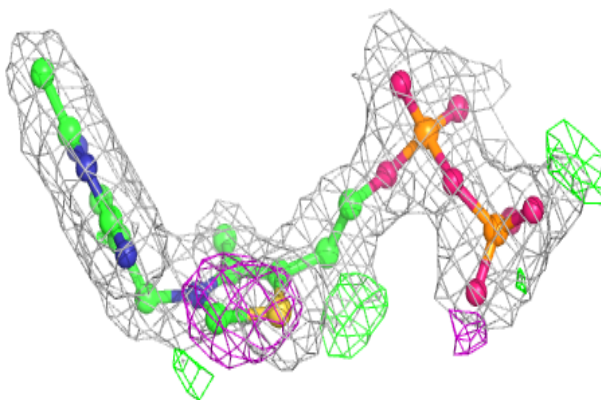


Electron density around TPP A 602:

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

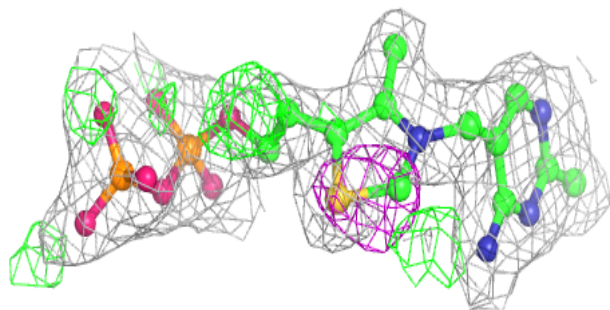
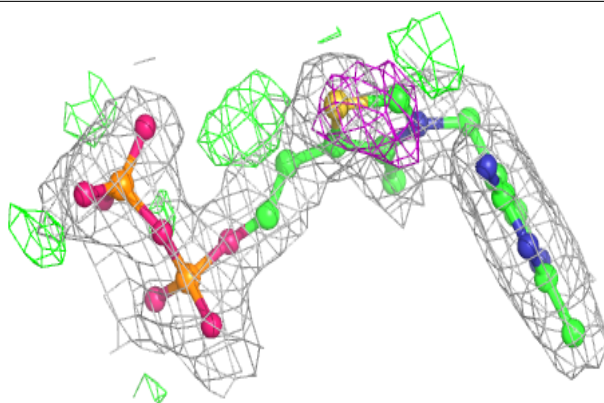
**Electron density around TPP D 602:**

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

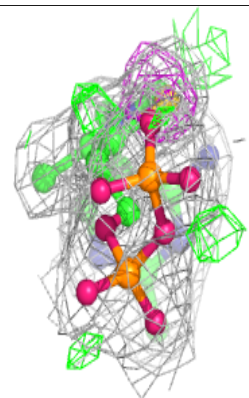
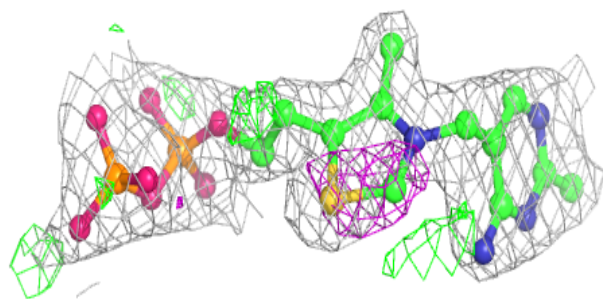
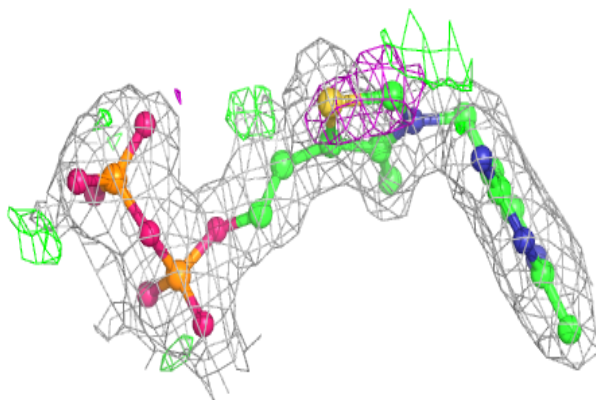


Electron density around TPP L 602:

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

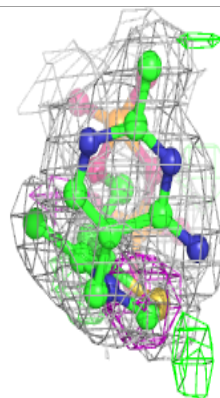
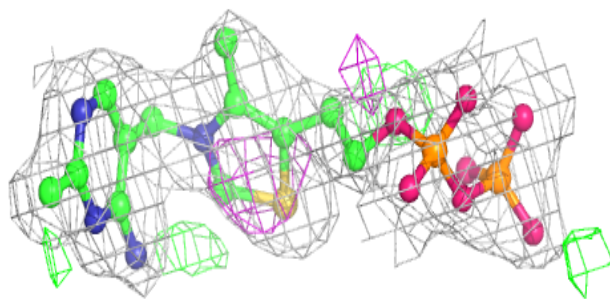
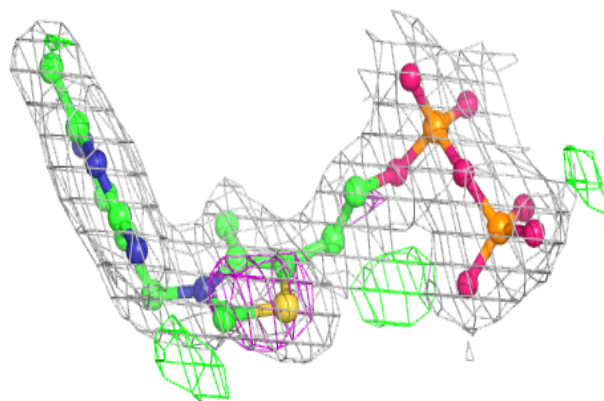
**Electron density around TPP B 602:**

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and green (positive)

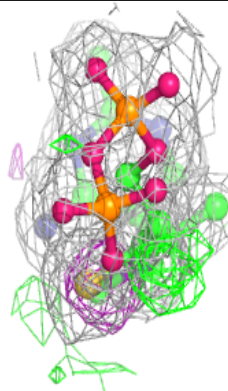
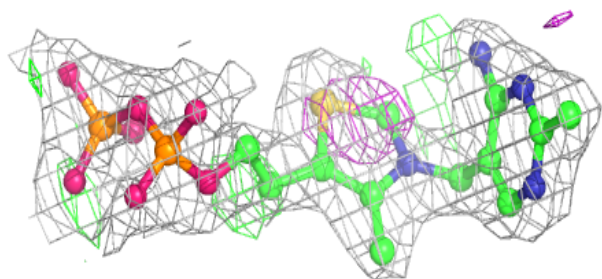
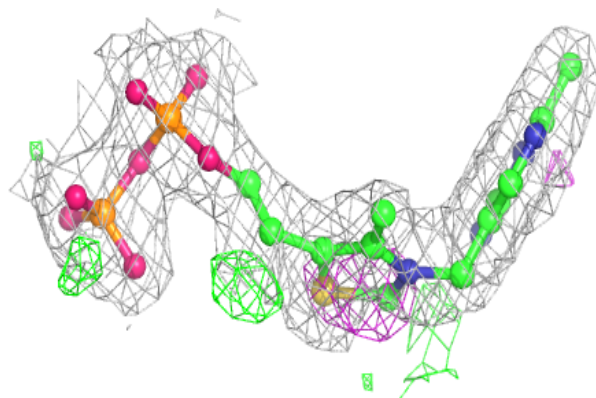


Electron density around TPP X 602:

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

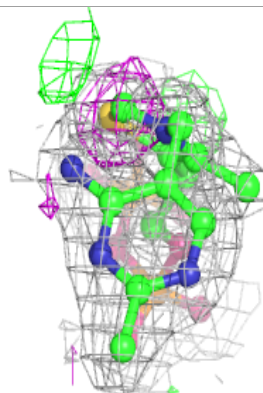
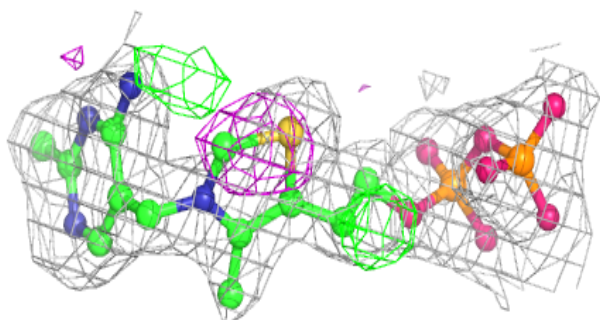
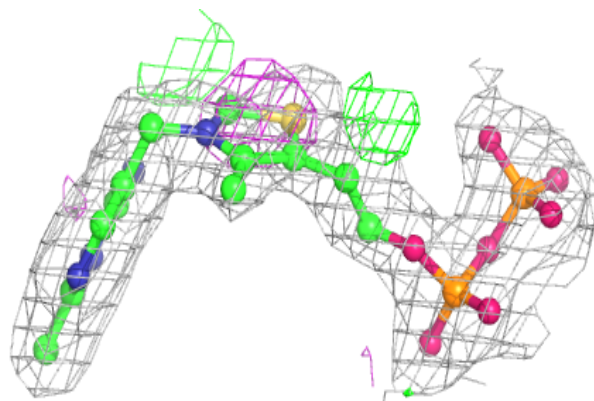
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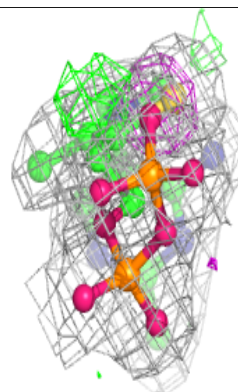
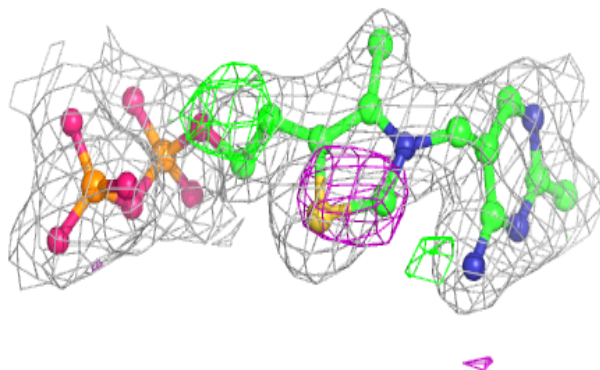
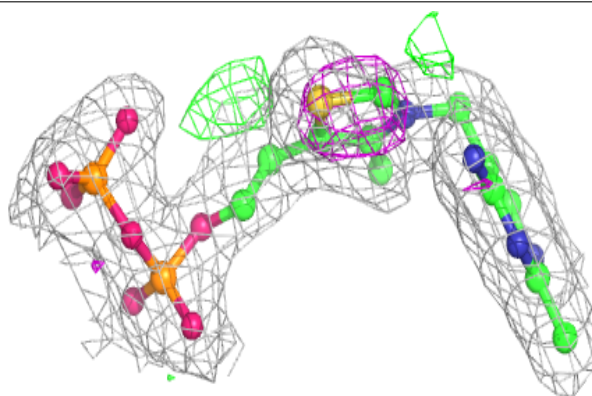


Electron density around TPP S 602:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
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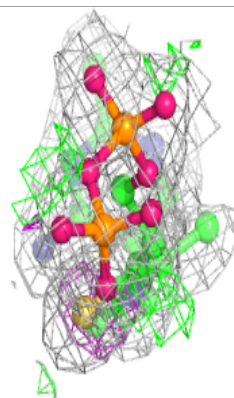
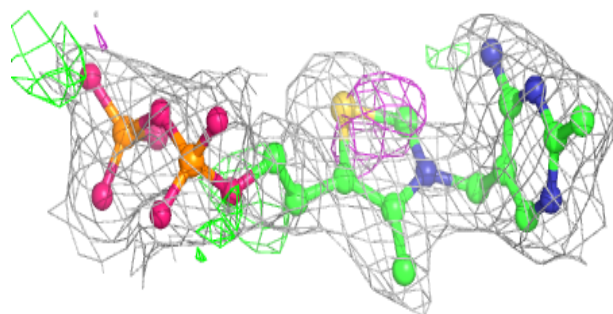
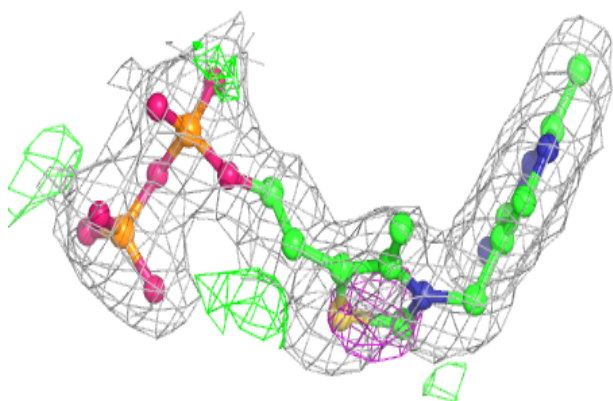
**Electron density around TPP I 602:**

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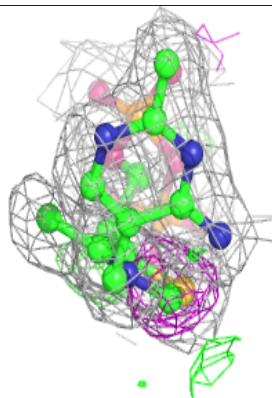
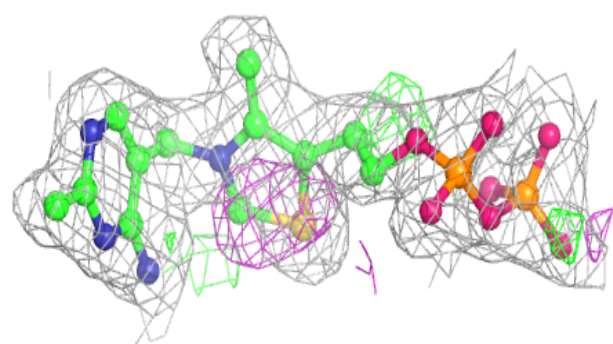
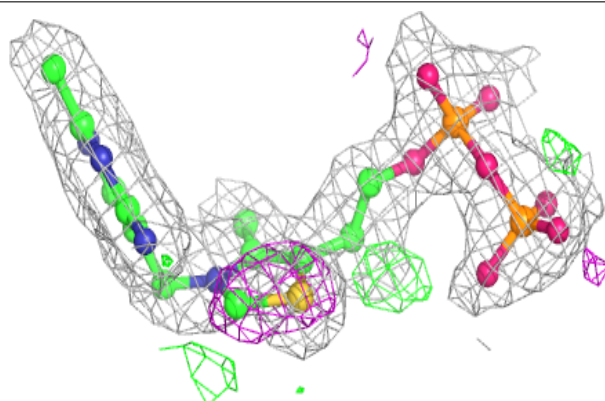


Electron density around TPP G 602:

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and green (positive)

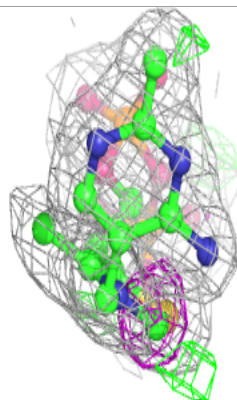
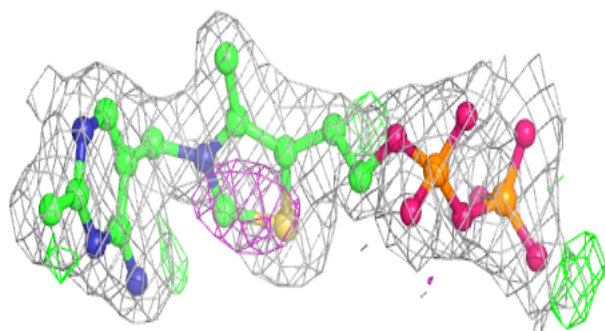
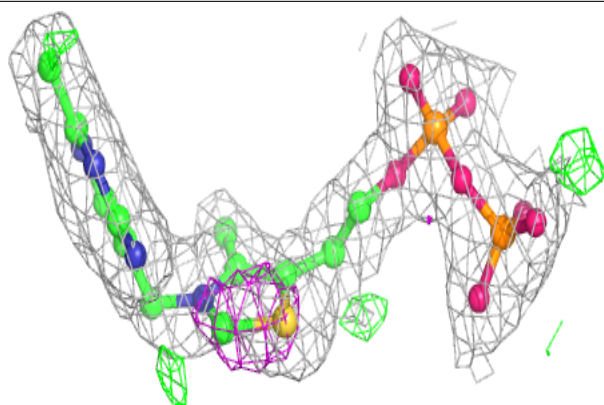
**Electron density around TPP F 603:**

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and green (positive)

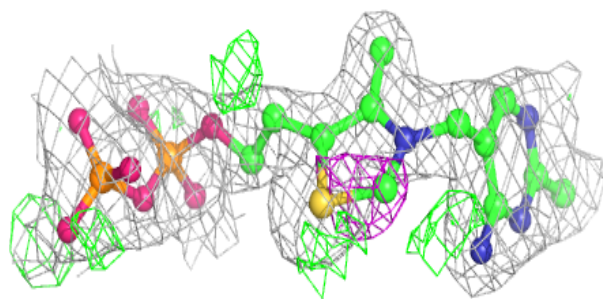
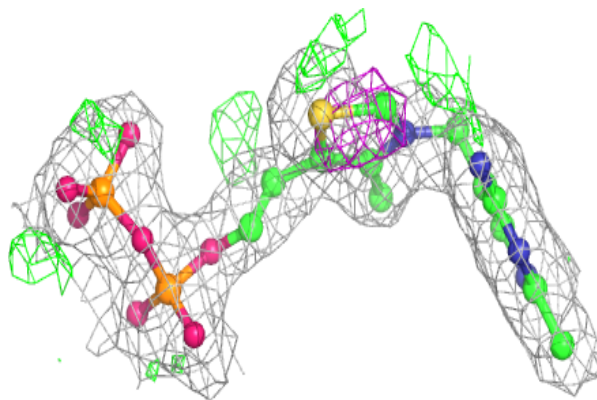


Electron density around TPP P 602:

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

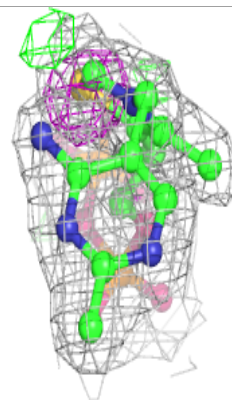
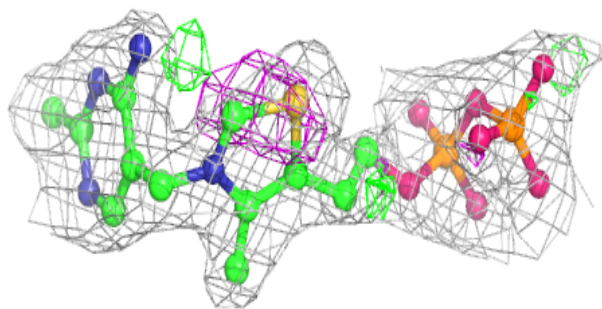
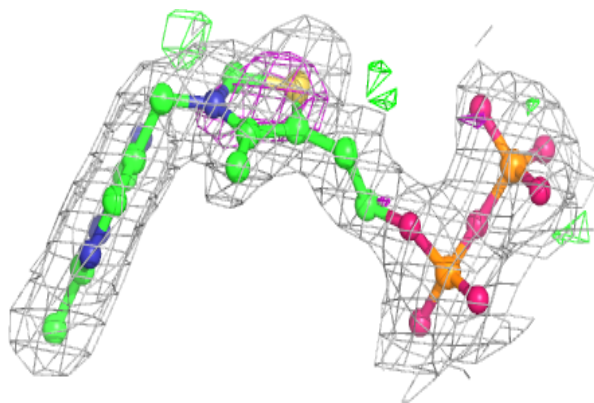
**Electron density around TPP H 602:**

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and green (positive)

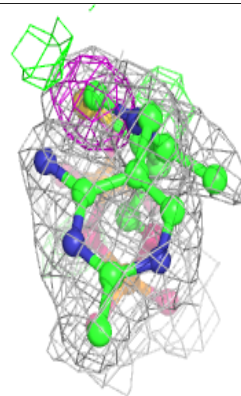
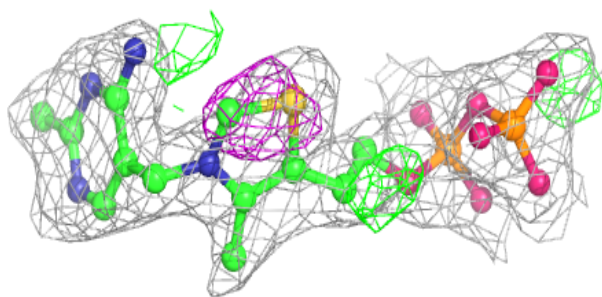
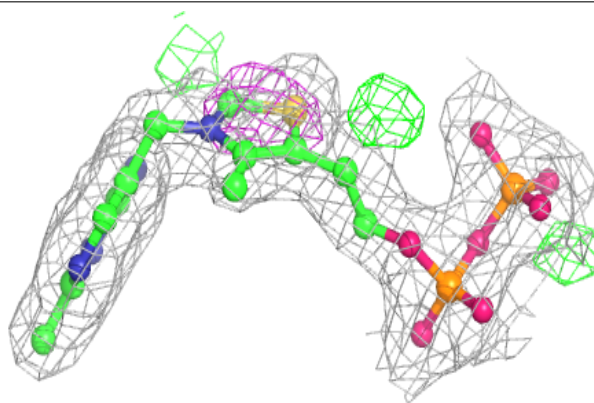


Electron density around TPP R 602:

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and green (positive)

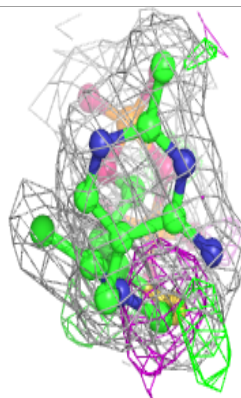
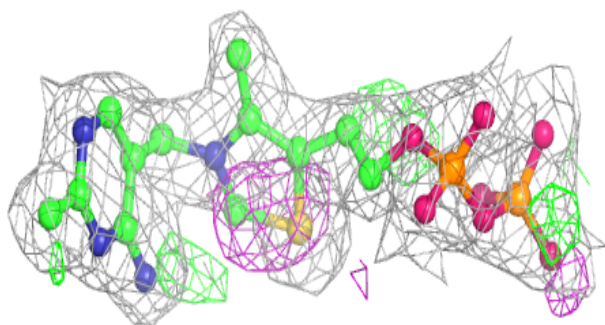
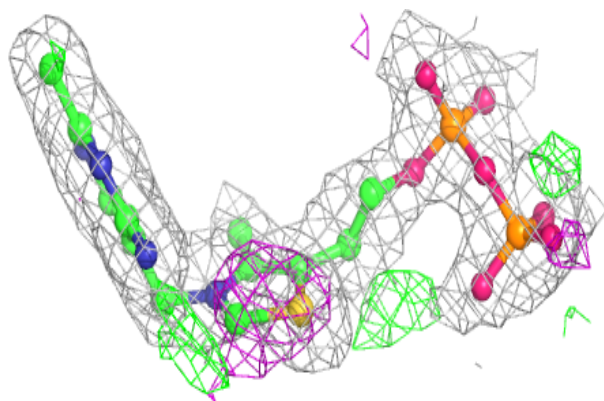
**Electron density around TPP O 602:**

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

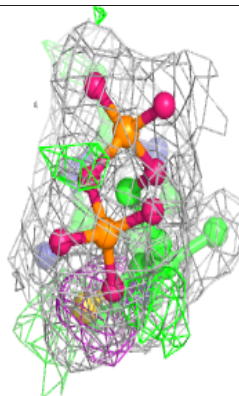
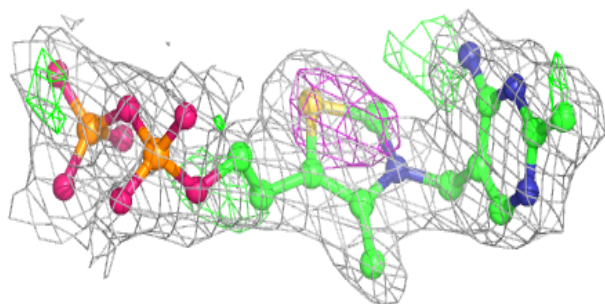
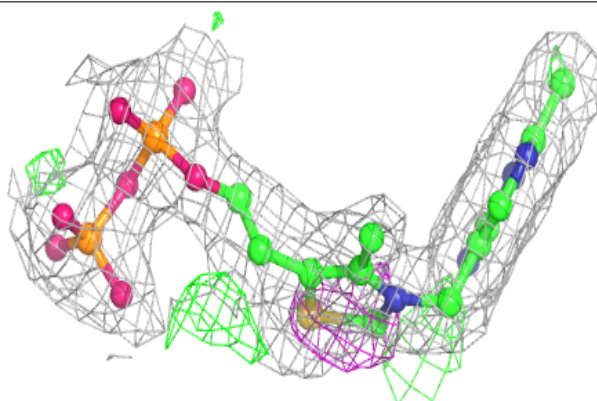


Electron density around TPP N 602:

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

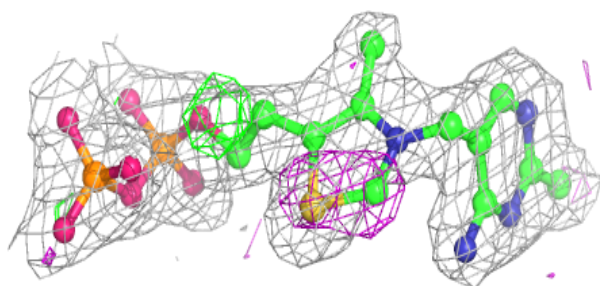
**Electron density around TPP C 602:**

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

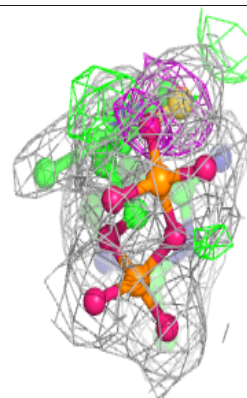
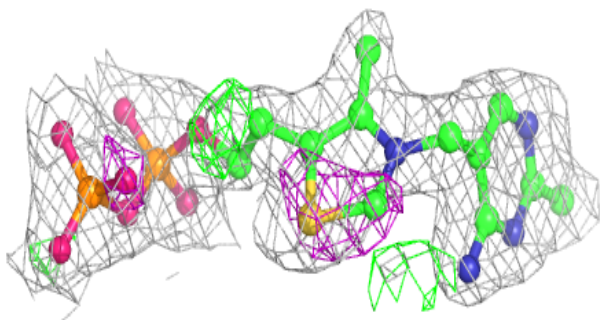
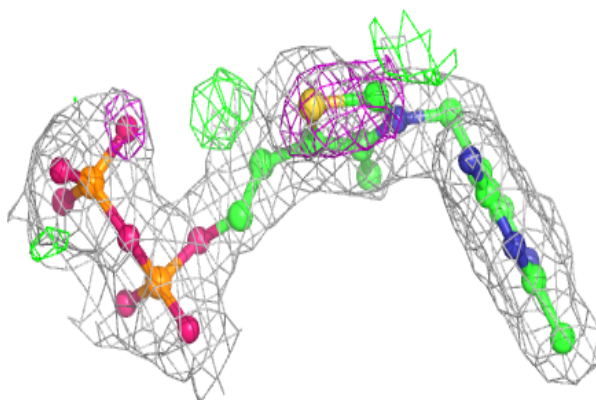


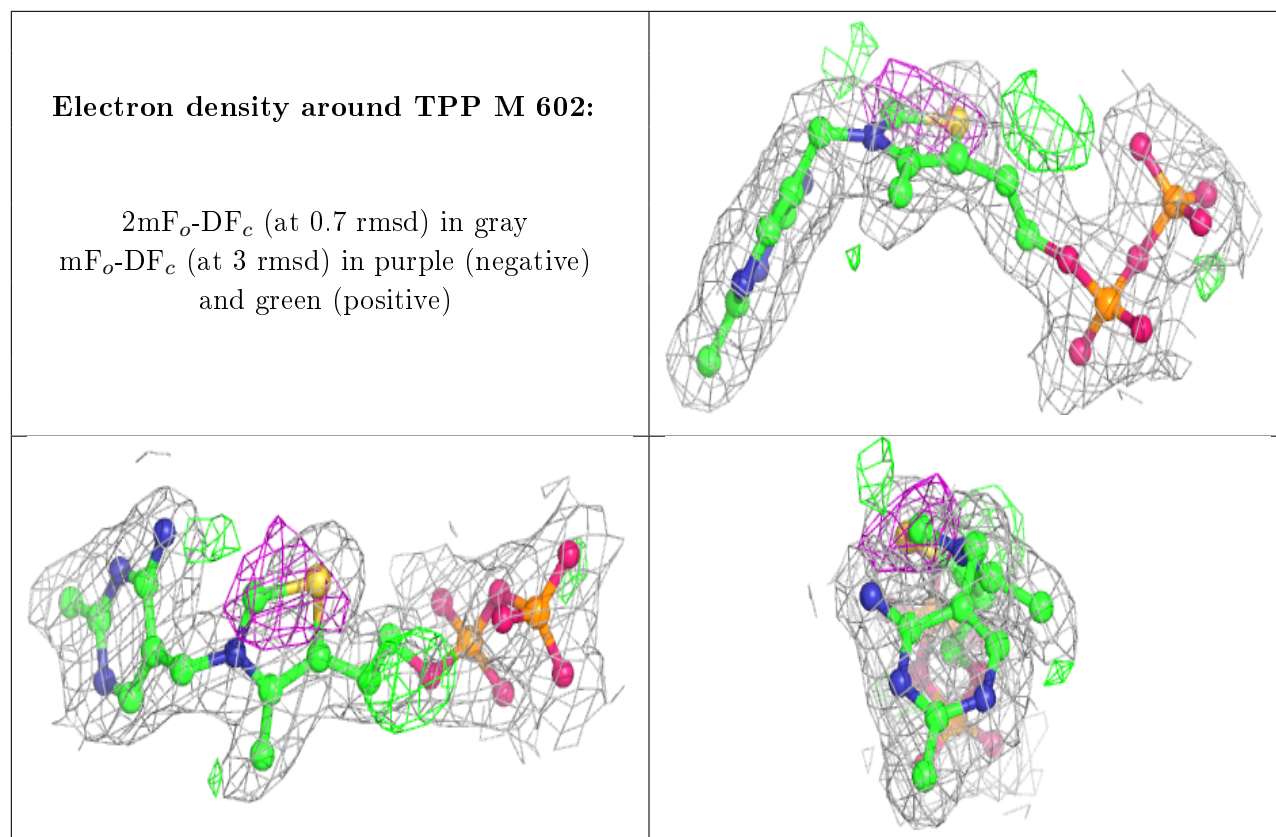
Electron density around TPP E 602:

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

**Electron density around TPP J 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 [i](#)

There are no such residues in this entry.