



Full wwPDB X-ray Structure Validation Report ⓘ

May 21, 2020 – 11:27 pm BST

PDB ID : 6EFH
Title : Pyruvate decarboxylase from Kluyveromyces lactis soaked with pyruvamide
Authors : Kutter, S.; Konig, S.
Deposited on : 2018-08-16
Resolution : 2.99 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

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

MolProbity : 4.02b-467
Mogul : 1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix) : 1.13
EDS : 2.11
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

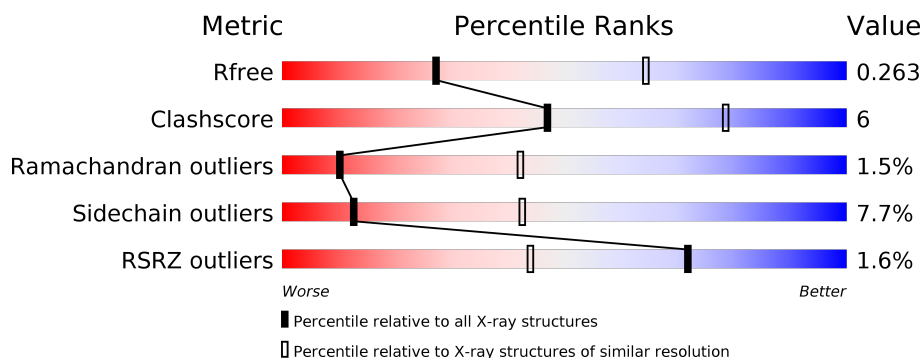
1 Overall quality at a glance ⓘ

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.99 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	2092 (3.00-3.00)
Clashscore	141614	2416 (3.00-3.00)
Ramachandran outliers	138981	2333 (3.00-3.00)
Sidechain outliers	138945	2336 (3.00-3.00)
RSRZ outliers	127900	1990 (3.00-3.00)

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	563	<div> <div>2%</div> <div> <div></div> <div>82%</div> <div>15%</div> <div>..</div> </div> </div>
1	B	563	<div> <div>%</div> <div> <div></div> <div>77%</div> <div>19%</div> <div>..</div> </div> </div>

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
2	PY0	A	601	-	-	X	-
2	PY0	B	600	-	-	X	-

2 Entry composition [i](#)

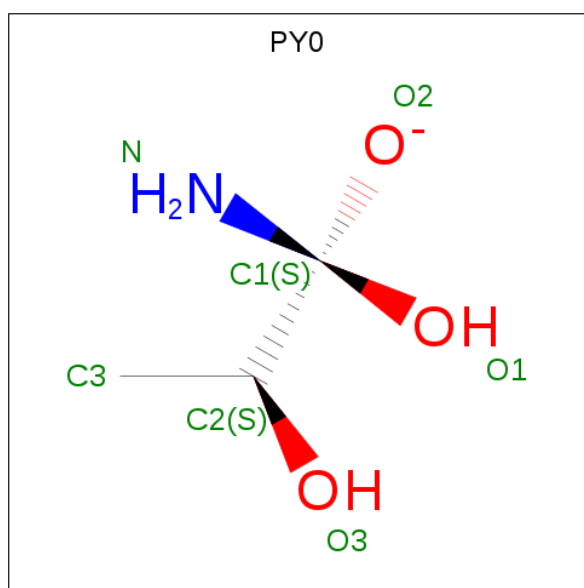
There are 6 unique types of molecules in this entry. The entry contains 8712 atoms, of which 0 are hydrogens and 0 are deuteriums.

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.

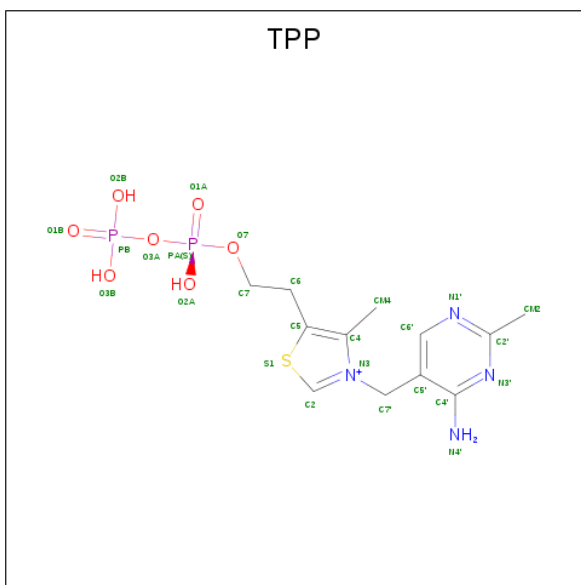
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	557	Total	C	N	O	S	0	0	0
			4299	2739	717	829	14			
1	B	556	Total	C	N	O	S	0	0	0
			4288	2729	716	829	14			

- Molecule 2 is (1S,2S)-1-amino-1,2-dihydroxypropan-1-olate (three-letter code: PY0) (formula: $C_3H_8NO_3$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	1	Total	C	N	O	0	0
			7	3	1	3		
2	B	1	Total	C	N	O	0	0
			7	3	1	3		

- 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

- Molecule 4 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

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

- Molecule 5 is PENTAETHYLENE GLYCOL (three-letter code: 1PE) (formula: $\text{C}_{10}\text{H}_{22}\text{O}_6$).



Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	1	Total	C O	0	0
			16	10 6		

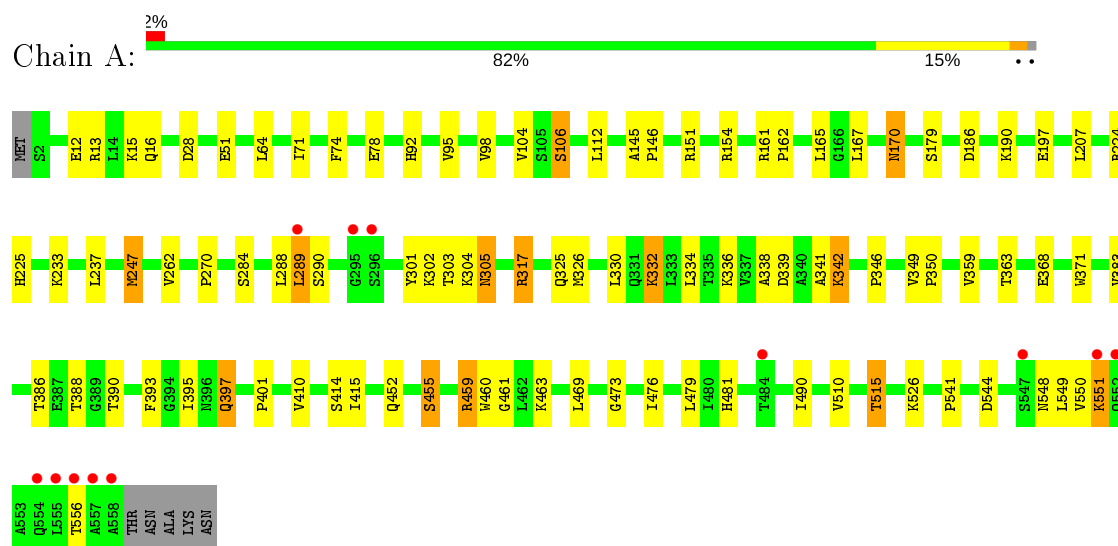
- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	30	Total	O	0	0
			30	30		
6	B	11	Total	O	0	0
			11	11		

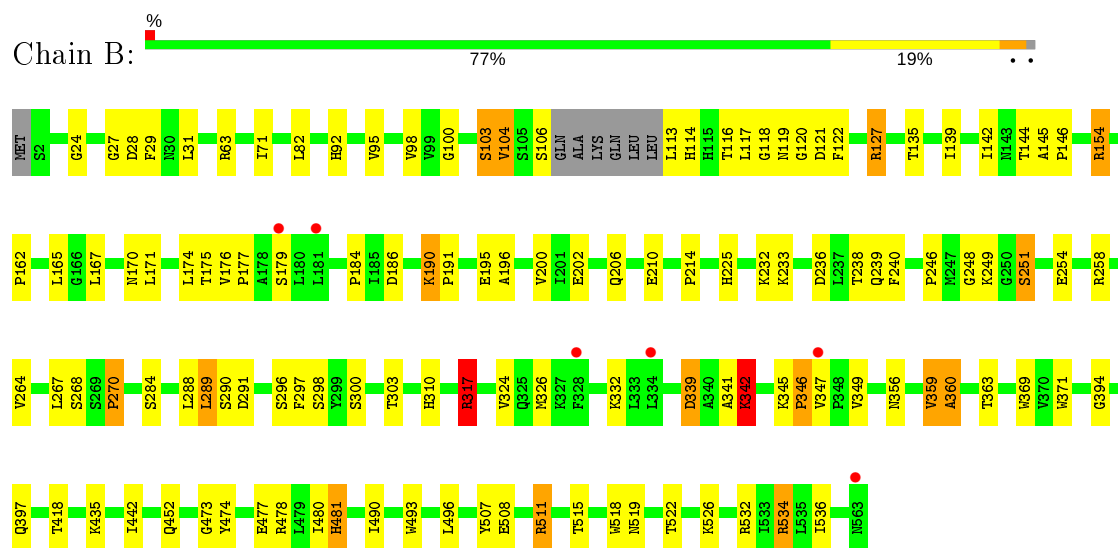
3 Residue-property plots [i](#)

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



4 Data and refinement statistics

Property	Value	Source
Space group	I 4 2 2	Depositor
Cell constants a, b, c, α , β , γ	172.76 Å 172.76 Å 210.08 Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	55.60 – 2.99 55.54 – 2.99	Depositor EDS
% Data completeness (in resolution range)	100.0 (55.60-2.99) 100.0 (55.54-2.99)	Depositor EDS
R_{merge}	0.33	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.88 (at 3.01 Å)	Xtriage
Refinement program	REFMAC 5.8.0230	Depositor
R, R_{free}	0.178 , 0.265 0.185 , 0.263	Depositor DCC
R_{free} test set	1055 reflections (3.27%)	wwPDB-VP
Wilson B-factor (Å ²)	45.0	Xtriage
Anisotropy	0.073	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 40.0	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	8712	wwPDB-VP
Average B, all atoms (Å ²)	43.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.45% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: PY0, MG, 1PE, 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	0.58	1/4391 (0.0%)	0.73	1/5978 (0.0%)
1	B	0.53	0/4379	0.75	1/5961 (0.0%)
All	All	0.56	1/8770 (0.0%)	0.74	2/11939 (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	A	0	4
1	B	0	7
All	All	0	11

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	78	GLU	CD-OE1	5.16	1.31	1.25

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	151	ARG	NE-CZ-NH2	-5.51	117.54	120.30
1	B	28	ASP	CB-CA-C	5.02	120.44	110.40

There are no chirality outliers.

All (11) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	13	ARG	Sidechain
1	A	161	ARG	Sidechain
1	A	317	ARG	Sidechain
1	A	459	ARG	Sidechain
1	B	120	GLY	Peptide
1	B	127	ARG	Sidechain
1	B	154	ARG	Sidechain
1	B	342	LYS	Peptide
1	B	511	ARG	Sidechain
1	B	534	ARG	Sidechain
1	B	63	ARG	Sidechain

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	4299	0	4273	47	0
1	B	4288	0	4253	61	0
2	A	7	0	7	4	0
2	B	7	0	7	5	0
3	A	26	0	16	2	0
3	B	26	0	16	2	0
4	A	1	0	0	0	0
4	B	1	0	0	0	0
5	A	16	0	22	0	0
6	A	30	0	0	0	0
6	B	11	0	0	0	0
All	All	8712	0	8594	107	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 6.

All (107) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:248:GLY:O	1:B:251:SER:OG	2.06	0.74
1:A:288:LEU:HD12	2:A:601:PY0:H33C	1.72	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:92:HIS:O	1:A:224:ARG:CD	2.43	0.67
1:A:154:ARG:HD2	1:A:186:ASP:O	1.95	0.66
1:B:480:ILE:O	1:B:481:HIS:HB2	1.96	0.65
1:A:92:HIS:O	1:A:224:ARG:HD3	1.98	0.64
1:B:104:VAL:HG23	1:B:170:ASN:HD21	1.62	0.64
1:B:258:ARG:NH1	1:B:349:VAL:HG13	2.14	0.63
1:A:330:LEU:O	1:A:334:LEU:HG	1.99	0.62
1:B:225:HIS:HE1	2:B:600:PY0:H31C	1.66	0.61
1:B:225:HIS:CE1	2:B:600:PY0:H31C	2.36	0.60
1:B:356:ASN:ND2	1:B:369:TRP:CD1	2.70	0.60
1:B:480:ILE:O	1:B:481:HIS:CB	2.49	0.59
1:A:390:THR:HG23	3:A:602:TPP:O2B	2.03	0.59
1:A:247:MET:HE1	1:A:288:LEU:HD23	1.85	0.58
1:A:71:ILE:HA	1:A:98:VAL:O	2.03	0.58
1:B:515:THR:O	1:B:519:ASN:ND2	2.36	0.58
1:A:145:ALA:HB3	1:A:146:PRO:HD3	1.87	0.57
1:B:154:ARG:NH2	1:B:186:ASP:O	2.37	0.56
1:A:455:SER:HB2	1:B:493:TRP:HE1	1.70	0.56
1:B:369:TRP:CZ2	1:B:515:THR:OG1	2.59	0.55
1:B:534:ARG:HG3	1:B:534:ARG:HH11	1.73	0.54
1:A:339:ASP:O	1:A:342:LYS:HB2	2.08	0.53
1:B:142:ILE:HD13	1:B:174:LEU:HB3	1.92	0.51
1:A:92:HIS:O	1:A:224:ARG:HD2	2.11	0.50
1:A:51:GLU:OE2	3:B:601:TPP:N1'	2.44	0.50
1:A:288:LEU:HD12	2:A:601:PY0:C3	2.42	0.50
1:A:541:PRO:HB2	1:A:544:ASP:HB2	1.94	0.50
1:B:200:VAL:HG21	1:B:324:VAL:HG21	1.94	0.50
1:A:469:LEU:N	1:A:469:LEU:HD23	2.27	0.49
1:A:95:VAL:O	1:A:162:PRO:HA	2.12	0.49
1:A:359:VAL:HG23	1:A:515:THR:HG21	1.95	0.48
1:B:106:SER:HB3	1:B:113:LEU:HD22	1.95	0.48
1:A:104:VAL:HG23	1:A:104:VAL:O	2.13	0.48
1:B:92:HIS:HB3	2:B:600:PY0:H33C	1.95	0.48
1:A:288:LEU:O	1:A:289:LEU:HG	2.14	0.47
1:B:536:ILE:HD12	1:B:536:ILE:N	2.29	0.47
1:B:317:ARG:HH11	1:B:317:ARG:HB3	1.79	0.47
1:B:165:LEU:HG	1:B:167:LEU:HD13	1.97	0.47
1:B:27:GLY:O	1:B:31:LEU:HG	2.15	0.47
1:A:473:GLY:HA2	1:A:490:ILE:HG12	1.97	0.46
1:B:214:PRO:HG2	1:B:240:PHE:CD1	2.51	0.46
1:A:225:HIS:HB2	1:A:326:MET:CE	2.45	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:190:LYS:O	1:A:325:GLN:NE2	2.49	0.46
1:B:473:GLY:HA2	1:B:490:ILE:HG12	1.98	0.46
1:A:12:GLU:O	1:A:16:GLN:HG3	2.16	0.45
1:B:258:ARG:HH12	1:B:349:VAL:HG13	1.80	0.45
1:B:29:PHE:O	1:B:100:GLY:HA3	2.16	0.45
1:B:176:VAL:HB	1:B:177:PRO:CD	2.46	0.45
1:B:24:GLY:HA3	1:B:71:ILE:O	2.17	0.45
1:A:397:GLN:HB3	1:A:397:GLN:HE21	1.65	0.45
1:B:121:ASP:OD2	1:B:127:ARG:NH1	2.50	0.45
1:A:165:LEU:HD11	1:A:167:LEU:HD21	1.99	0.44
1:A:386:THR:HG21	1:A:395:ILE:HB	1.99	0.44
1:B:196:ALA:O	1:B:200:VAL:HG23	2.17	0.44
1:A:349:VAL:HB	1:A:350:PRO:CD	2.48	0.44
2:A:601:PY0:H32C	2:A:601:PY0:HN1	1.51	0.44
1:B:238:THR:HB	1:B:240:PHE:CE2	2.52	0.44
1:B:359:VAL:O	1:B:360:ALA:O	2.35	0.44
1:B:518:TRP:O	1:B:522:THR:HG23	2.18	0.44
1:B:474:TYR:CD1	3:B:601:TPP:H61	2.52	0.44
1:B:342:LYS:HE2	1:B:342:LYS:HA	2.00	0.43
1:B:206:GLN:NE2	1:B:210:GLU:OE1	2.46	0.43
1:B:508:GLU:HG3	1:B:532:ARG:HD2	2.00	0.43
1:B:339:ASP:O	1:B:341:ALA:N	2.52	0.43
1:A:170:ASN:ND2	1:A:170:ASN:C	2.72	0.43
1:A:64:LEU:HD11	1:A:383:VAL:HG21	2.00	0.43
1:B:249:LYS:NZ	1:B:254:GLU:OE2	2.47	0.43
1:B:190:LYS:O	1:B:191:PRO:C	2.55	0.43
1:A:455:SER:HB2	1:B:493:TRP:NE1	2.33	0.43
1:A:170:ASN:HD22	1:A:170:ASN:C	2.22	0.43
1:B:236:ASP:O	1:B:239:GLN:HG2	2.19	0.43
1:B:95:VAL:O	1:B:162:PRO:HA	2.19	0.43
1:B:310:HIS:O	1:B:326:MET:HB2	2.18	0.42
1:B:371:TRP:CE2	1:B:394:GLY:HA3	2.54	0.42
1:A:207:LEU:HA	1:A:207:LEU:HD23	1.84	0.42
1:A:197:GLU:OE2	1:A:332:LYS:HD2	2.19	0.42
1:A:371:TRP:CE3	1:A:371:TRP:HA	2.54	0.42
1:B:418:THR:OG1	1:B:442:ILE:HD12	2.20	0.42
1:B:92:HIS:CG	2:B:600:PY0:H33C	2.54	0.42
1:A:341:ALA:O	1:A:342:LYS:C	2.58	0.42
1:A:247:MET:CE	1:A:288:LEU:HD23	2.49	0.42
1:B:267:LEU:HD12	1:B:297:PHE:HB3	2.01	0.42
1:B:103:SER:O	1:B:104:VAL:C	2.58	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:103:SER:HB3	1:B:170:ASN:H	1.83	0.42
1:B:496:LEU:CD1	1:B:511:ARG:NH1	2.83	0.41
1:A:548:ASN:HA	1:A:551:LYS:HB2	2.01	0.41
1:B:310:HIS:ND1	2:B:600:PYO:N	2.64	0.41
1:A:92:HIS:CE1	2:A:601:PYO:H31C	2.55	0.41
1:B:246:PRO:HG3	1:B:264:VAL:HG22	2.02	0.41
1:B:258:ARG:NH1	1:B:347:VAL:O	2.52	0.41
1:A:237:LEU:HD22	1:A:338:ALA:HB2	2.03	0.41
1:A:303:THR:OG1	1:A:305:ASN:HB2	2.21	0.41
1:B:288:LEU:O	1:B:289:LEU:HD13	2.20	0.41
1:B:474:TYR:O	1:B:478:ARG:HG3	2.21	0.41
1:A:225:HIS:HB2	1:A:326:MET:HE1	2.03	0.41
1:B:71:ILE:HA	1:B:98:VAL:O	2.21	0.41
1:A:393:PHE:HE2	1:A:476:ILE:HD11	1.85	0.41
1:B:145:ALA:HB3	1:B:146:PRO:HD3	2.02	0.40
1:A:363:THR:HB	1:A:515:THR:HB	2.02	0.40
1:B:290:SER:O	1:B:291:ASP:HB2	2.20	0.40
1:A:415:ILE:HG12	3:A:602:TPP:C4'	2.51	0.40
1:A:481:HIS:C	1:A:481:HIS:CD2	2.94	0.40
1:B:190:LYS:O	1:B:191:PRO:O	2.40	0.40
1:A:460:TRP:O	1:A:461:GLY:C	2.60	0.40
1:B:139:ILE:HG22	1:B:171:LEU:HD12	2.03	0.40
1:B:238:THR:HB	1:B:240:PHE:CZ	2.56	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	A	555/563 (99%)	519 (94%)	30 (5%)	6 (1%)	14 50
1	B	552/563 (98%)	506 (92%)	35 (6%)	11 (2%)	7 34

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
All	All	1107/1126 (98%)	1025 (93%)	65 (6%)	17 (2%)	10	42

All (17) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	106	SER
1	A	289	LEU
1	A	342	LYS
1	B	117	LEU
1	B	360	ALA
1	B	481	HIS
1	B	184	PRO
1	B	317	ARG
1	A	346	PRO
1	B	300	SER
1	B	346	PRO
1	A	74	PHE
1	B	339	ASP
1	B	104	VAL
1	B	270	PRO
1	A	401	PRO
1	B	118	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	469/474 (99%)	433 (92%)	36 (8%)	13	42
1	B	468/474 (99%)	432 (92%)	36 (8%)	13	42
All	All	937/948 (99%)	865 (92%)	72 (8%)	13	42

All (72) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	15	LYS

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Mol	Chain	Res	Type
1	A	28	ASP
1	A	106	SER
1	A	112	LEU
1	A	170	ASN
1	A	179	SER
1	A	233	LYS
1	A	247	MET
1	A	262	VAL
1	A	270	PRO
1	A	284	SER
1	A	290	SER
1	A	301	TYR
1	A	302	LYS
1	A	304	LYS
1	A	305	ASN
1	A	317	ARG
1	A	332	LYS
1	A	336	LYS
1	A	368	GLU
1	A	388	THR
1	A	397	GLN
1	A	410	VAL
1	A	414	SER
1	A	452	GLN
1	A	455	SER
1	A	459	ARG
1	A	463	LYS
1	A	479	LEU
1	A	510	VAL
1	A	515	THR
1	A	526	LYS
1	A	549	LEU
1	A	550	VAL
1	A	551	LYS
1	A	556	THR
1	B	82	LEU
1	B	103	SER
1	B	114	HIS
1	B	116	THR
1	B	119	ASN
1	B	122	PHE
1	B	135	THR

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Mol	Chain	Res	Type
1	B	144	THR
1	B	175	THR
1	B	179	SER
1	B	190	LYS
1	B	195	GLU
1	B	202	GLU
1	B	232	LYS
1	B	233	LYS
1	B	251	SER
1	B	268	SER
1	B	270	PRO
1	B	284	SER
1	B	289	LEU
1	B	296	SER
1	B	298	SER
1	B	303	THR
1	B	317	ARG
1	B	332	LYS
1	B	342	LYS
1	B	345	LYS
1	B	346	PRO
1	B	359	VAL
1	B	363	THR
1	B	397	GLN
1	B	435	LYS
1	B	452	GLN
1	B	477	GLU
1	B	507	TYR
1	B	526	LYS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (1) such sidechains are listed below:

Mol	Chain	Res	Type
1	B	225	HIS

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 7 ligands modelled in this entry, 2 are monoatomic - leaving 5 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	A	602	4	22,27,27	1.42	3 (13%)	29,40,40	2.48	10 (34%)
2	PY0	A	601	1	4,6,6	3.71	2 (50%)	1,9,9	1.31	0
5	1PE	A	604	-	15,15,15	0.74	0	14,14,14	0.68	0
3	TPP	B	601	4	22,27,27	1.40	3 (13%)	29,40,40	1.99	7 (24%)
2	PY0	B	600	1	4,6,6	4.32	2 (50%)	1,9,9	0.76	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
3	TPP	A	602	4	-	1/16/17/17	0/2/2/2
2	PY0	A	601	1	-	0/0/6/6	-
5	1PE	A	604	-	-	6/13/13/13	-
3	TPP	B	601	4	-	1/16/17/17	0/2/2/2
2	PY0	B	600	1	-	0/0/6/6	-

All (10) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	600	PY0	O1-C1	6.25	1.46	1.38
2	B	600	PY0	O2-C1	5.80	1.46	1.38
2	A	601	PY0	O2-C1	5.41	1.45	1.38
2	A	601	PY0	O1-C1	4.86	1.44	1.38
3	A	602	TPP	C5'-C4'	4.18	1.50	1.42
3	B	601	TPP	C4-N3	-3.70	1.36	1.39
3	B	601	TPP	C6-C5	3.14	1.52	1.50
3	B	601	TPP	C5'-C4'	2.63	1.47	1.42
3	A	602	TPP	C7'-C5'	2.29	1.56	1.51
3	A	602	TPP	C2'-N1'	2.01	1.37	1.34

All (17) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	602	TPP	C6-C5-C4	6.78	132.88	127.43
3	A	602	TPP	CM2-C2'-N1'	6.22	123.98	117.14
3	B	601	TPP	CM4-C4-N3	4.69	128.51	122.53
3	B	601	TPP	C6-C5-C4	4.40	130.96	127.43
3	A	602	TPP	CM4-C4-N3	4.15	127.82	122.53
3	A	602	TPP	C6'-N1'-C2'	3.80	122.42	115.96
3	B	601	TPP	CM4-C4-C5	-3.47	120.02	127.60
3	B	601	TPP	O2B-PB-O3A	-3.42	93.18	104.64
3	A	602	TPP	N1'-C2'-N3'	-3.19	120.05	125.54
3	A	602	TPP	CM4-C4-C5	-2.85	121.38	127.60
3	A	602	TPP	O2B-PB-O3A	-2.69	95.61	104.64
3	B	601	TPP	C6'-N1'-C2'	2.66	120.49	115.96
3	B	601	TPP	C7'-N3-C2	-2.62	120.63	125.35
3	A	602	TPP	O3B-PB-O3A	2.60	113.36	104.64
3	B	601	TPP	O2A-PA-O1A	2.55	124.86	112.24
3	A	602	TPP	O2B-PB-O1B	2.19	119.26	110.68
3	A	602	TPP	C2'-N3'-C4'	2.14	121.42	118.08

There are no chirality outliers.

All (8) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	A	604	1PE	OH4-C13-C23-OH3
5	A	604	1PE	OH6-C15-C25-OH5
3	A	602	TPP	C5-C6-C7-O7
3	B	601	TPP	C4-C5-C6-C7
5	A	604	1PE	C23-C13-OH4-C24
5	A	604	1PE	C16-C26-OH6-C15

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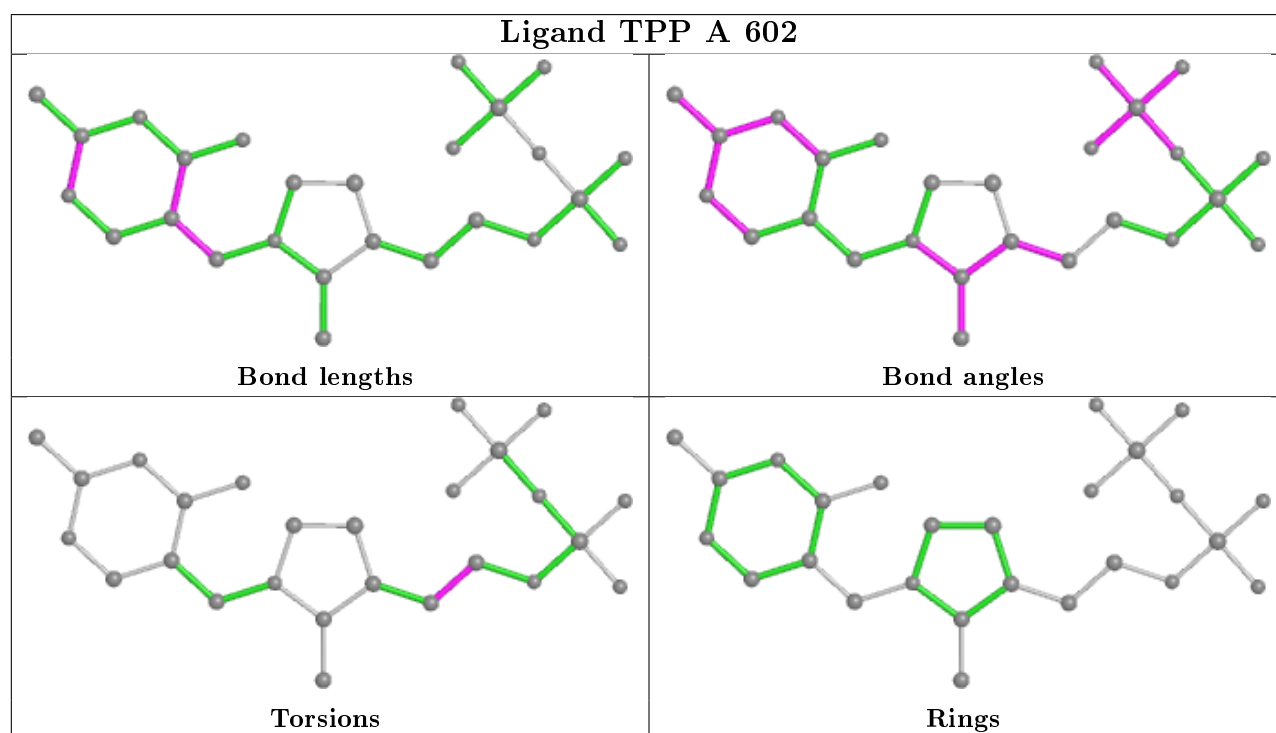
Mol	Chain	Res	Type	Atoms
5	A	604	1PE	C13-C23-OH3-C22
5	A	604	1PE	OH7-C16-C26-OH6

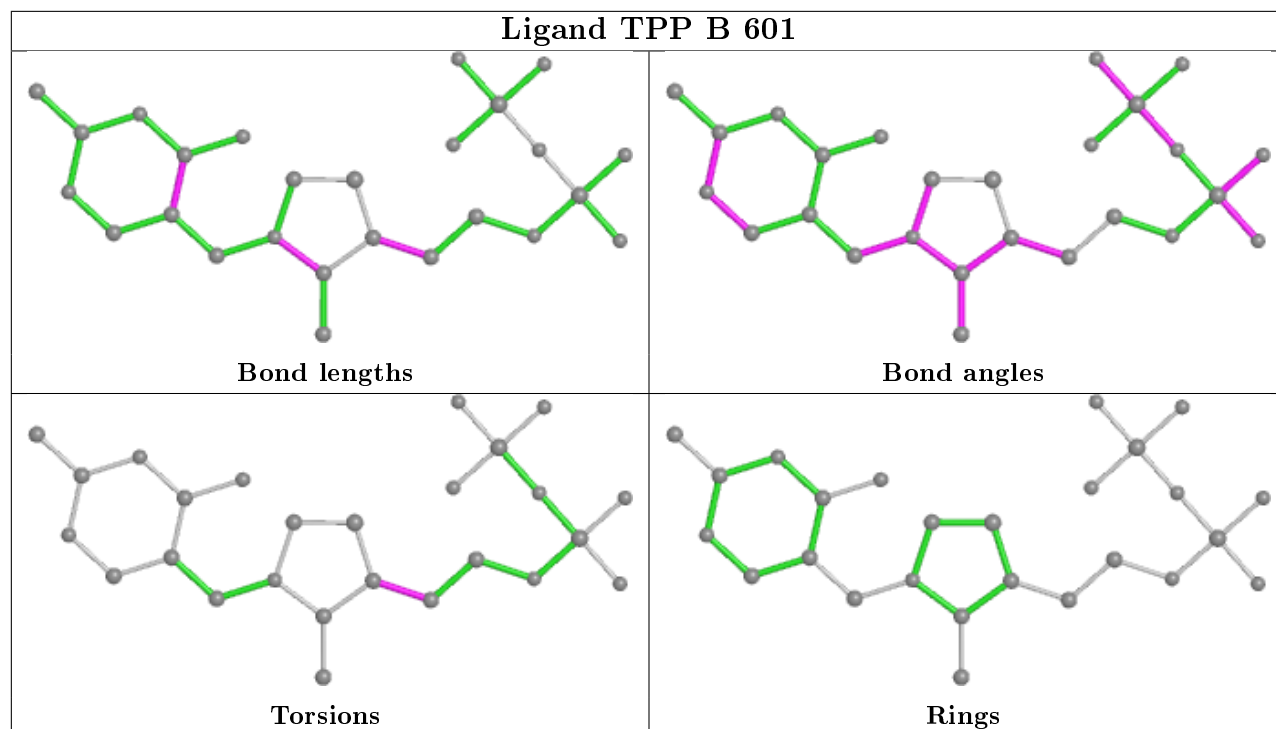
There are no ring outliers.

4 monomers are involved in 13 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	602	TPP	2	0
2	A	601	PY0	4	0
3	B	601	TPP	2	0
2	B	600	PY0	5	0

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





5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data [i](#)

6.1 Protein, DNA and RNA chains [i](#)

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 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	557/563 (98%)	-0.17	12 (2%) 62 33	16, 34, 88, 135	0
1	B	556/563 (98%)	-0.17	6 (1%) 80 56	18, 43, 84, 105	0
All	All	1113/1126 (98%)	-0.17	18 (1%) 72 44	16, 38, 85, 135	0

All (18) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	556	THR	5.2
1	A	555	LEU	4.7
1	A	295	GLY	4.1
1	A	558	ALA	3.7
1	A	554	GLN	3.6
1	B	563	ASN	3.2
1	A	547	SER	2.9
1	A	551	LYS	2.8
1	A	552	GLN	2.8
1	A	557	ALA	2.7
1	A	484	THR	2.6
1	A	296	SER	2.4
1	B	328	PHE	2.4
1	B	179	SER	2.2
1	A	289	LEU	2.2
1	B	181	LEU	2.1
1	B	334	LEU	2.0
1	B	347	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

There are no carbohydrates in this entry.

6.4 Ligands

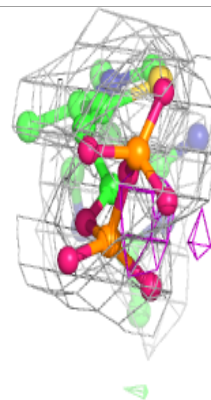
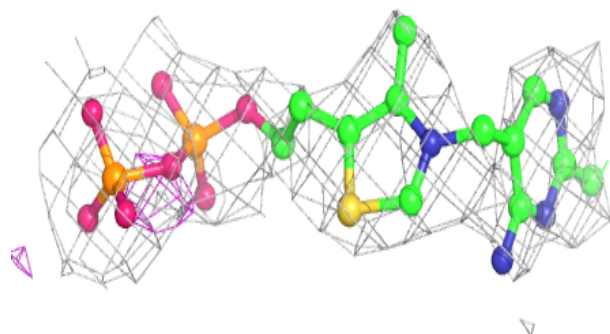
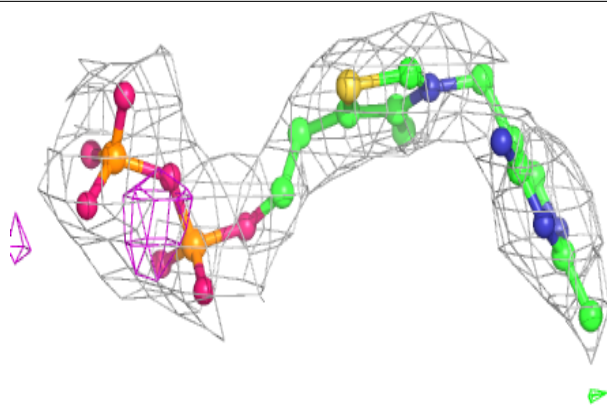
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
4	MG	A	603	1/1	0.89	0.11	40,40,40,40	0
5	1PE	A	604	16/16	0.93	0.36	34,52,62,62	0
2	PY0	B	600	7/7	0.93	0.24	37,45,54,58	0
2	PY0	A	601	7/7	0.94	0.31	54,62,64,67	0
3	TPP	A	602	26/26	0.95	0.16	51,62,76,78	0
4	MG	B	602	1/1	0.98	0.11	17,17,17,17	0
3	TPP	B	601	26/26	0.99	0.12	24,26,29,31	0

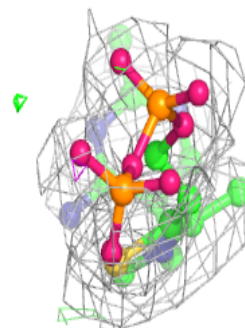
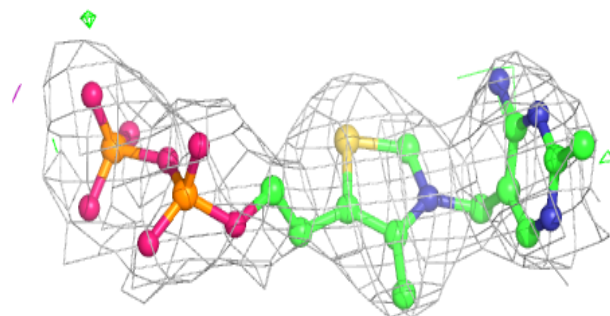
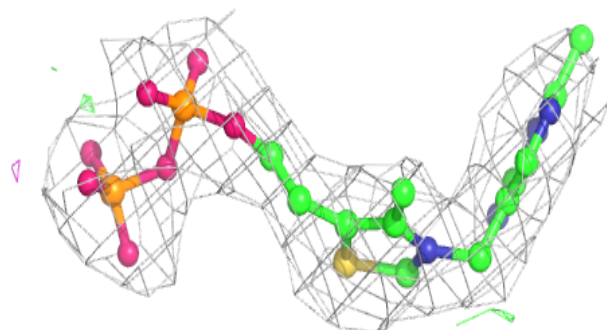
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around TPP 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 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)



6.5 Other polymers [i](#)

There are no such residues in this entry.