



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 6, 2026 – 06:34 AM UTC

PDB ID : 6EFH / pdb_00006efh
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 types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

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

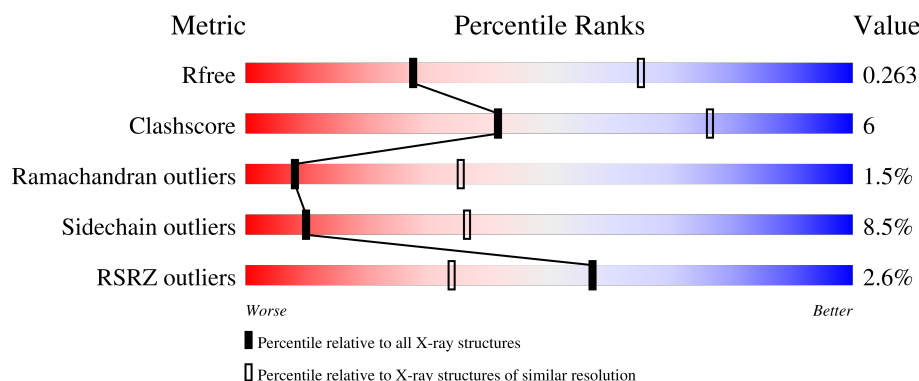
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.99 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}	180053	2672 (3.00-3.00)
Clashscore	190562	2977 (3.00-3.00)
Ramachandran outliers	187476	2877 (3.00-3.00)
Sidechain outliers	187428	2880 (3.00-3.00)
RSRZ outliers	180081	2671 (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 of the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	563	3% 81% 15% ..
1	B	563	2% 75% 20% ..

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](#)

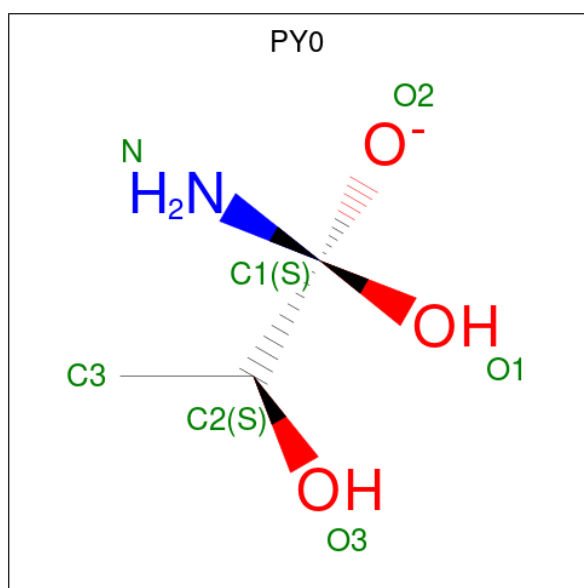
There are 6 unique types of molecules in this entry. The entry contains 8712 atoms, of which 0 are hydrogens and 0 are deuteriums.

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.

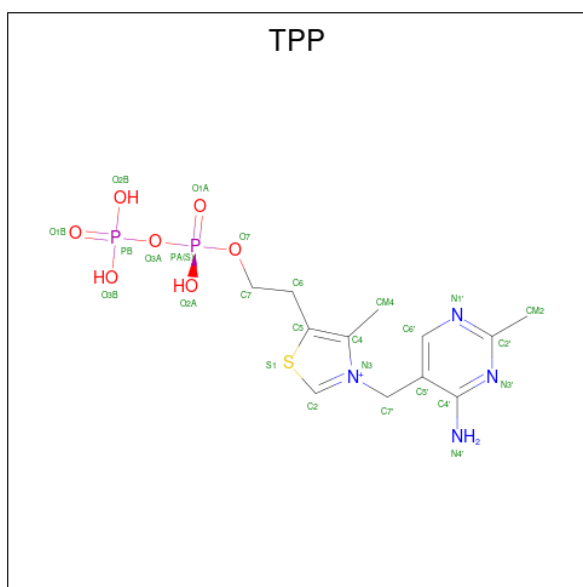
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	557	Total	C	N	O	S	0	0	0
			4299	2739	717	829	14			
1	B	556	Total	C	N	O	S	0	0	0
			4288	2729	716	829	14			

- Molecule 2 is (1S,2S)-1-amino-1,2-dihydroxypropan-1-olate (CCD ID: 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 (CCD ID: TPP) (formula: $C_{12}H_{19}N_4O_7P_2S$).

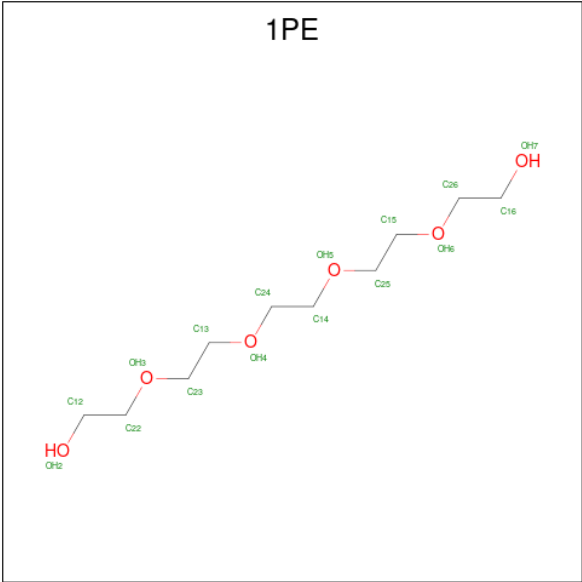


Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
3	A	1	Total 26	C 12	N 4	O 7	P 2	S 1	0	0
3	B	1	Total 26	C 12	N 4	O 7	P 2	S 1	0	0

- Molecule 4 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

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

- Molecule 5 is PENTAETHYLENE GLYCOL (CCD ID: 1PE) (formula: $C_{10}H_{22}O_6$).



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

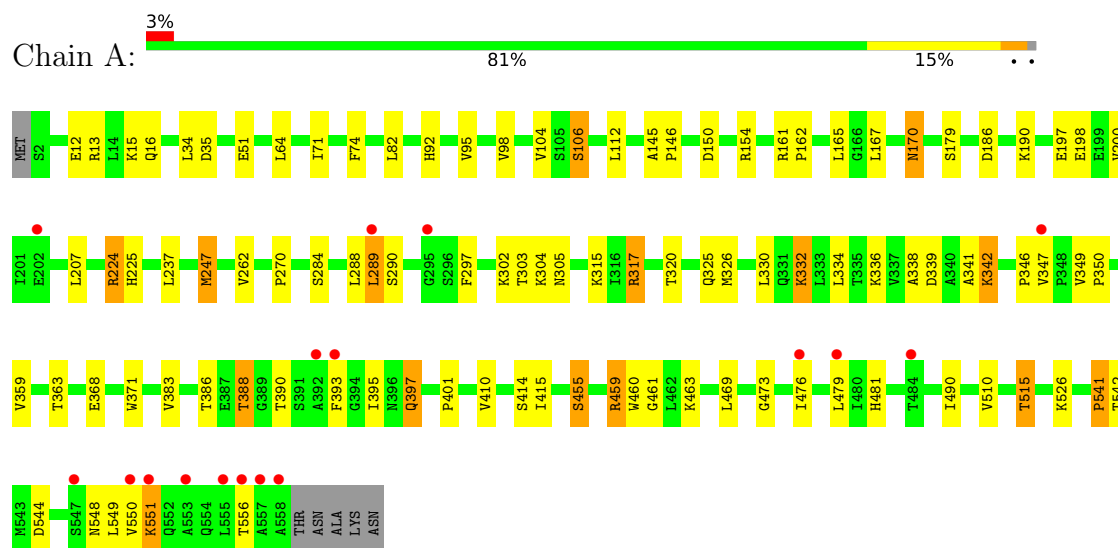
- Molecule 6 is water.

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

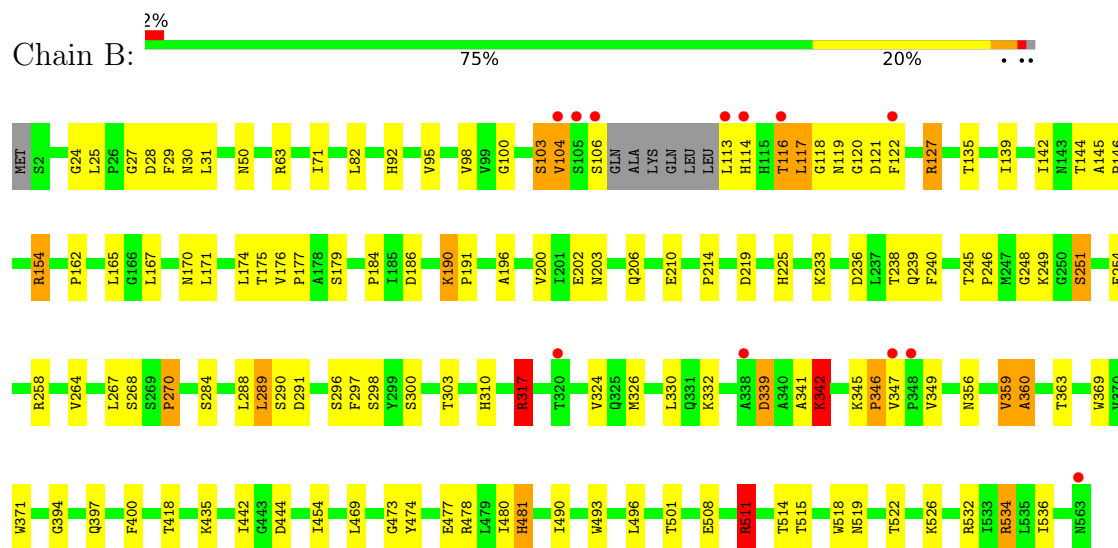
3 Residue-property plots [i](#)

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

• Molecule 1: Pyruvate 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	172.76Å 172.76Å 210.08Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	55.60 – 2.99 55.60 – 2.99	Depositor EDS
% Data completeness (in resolution range)	100.0 (55.60-2.99) 100.0 (55.60-2.99)	Depositor EDS
R_{merge}	0.33	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.88 (at 3.01Å)	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)	0.34 , 46.4	EDS
L-test for twinning ²	$\langle L \rangle = 0.47$, $\langle L^2 \rangle = 0.30$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	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: 1PE, PY0, MG, 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	0.89	0/4391	1.12	3/5978 (0.1%)
1	B	0.83	1/4379 (0.0%)	1.16	4/5961 (0.1%)
All	All	0.86	1/8770 (0.0%)	1.14	7/11939 (0.1%)

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	B	117	LEU	N-CA	6.70	1.54	1.46

All (7) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	116	THR	CB-CA-C	7.18	122.25	110.90
1	B	28	ASP	CB-CA-C	6.02	120.44	110.81
1	B	444	ASP	CA-CB-CG	5.79	118.39	112.60
1	A	297	PHE	CA-CB-CG	5.53	119.33	113.80
1	A	388	THR	CB-CA-C	5.41	117.95	109.84
1	B	400	PHE	CA-CB-CG	5.40	119.20	113.80
1	A	150	ASP	CA-CB-CG	5.27	117.87	112.60

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	46	0
1	B	4288	0	4253	65	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	110	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 (110) 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:247:MET:HE1	1:A:288:LEU:HD23	1.68	0.73
1:B:356:ASN:HD22	1:B:369:TRP:NE1	1.88	0.72
1:A:288:LEU:HD12	2:A:601:PY0:H33C	1.72	0.71
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: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:HH11	1:B:534:ARG:HG3	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:B:190:LYS:O	1:B:191:PRO:C	2.55	0.48
1:A:170:ASN:HD22	1:A:170:ASN:C	2.22	0.47
1:A:288:LEU:O	1:A:289:LEU:HG	2.14	0.47
1:B:536:ILE:N	1:B:536:ILE:HD12	2.29	0.47
1:A:170:ASN:C	1:A:170:ASN:ND2	2.72	0.47
1:B:165:LEU:HG	1:B:167:LEU:HD13	1.97	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:317:ARG:HH11	1:B:317:ARG:HB3	1.79	0.47
1:A:341:ALA:O	1:A:342:LYS:C	2.58	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:103:SER:O	1:B:104:VAL:C	2.58	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
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:A:481:HIS:C	1:A:481:HIS:CD2	2.94	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:A:460:TRP:O	1:A:461:GLY:C	2.60	0.45
1:B:24:GLY:HA3	1:B:71:ILE:O	2.17	0.45
1:A:397:GLN:HE21	1:A:397:GLN:HB3	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:HN1	2:A:601:PY0:H32C	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:HA	1:B:342:LYS:HE2	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:30:ASN:C	1:B:30:ASN:OD1	2.61	0.43
1:B:339:ASP:O	1:B:341:ALA:N	2.52	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:219:ASP:CG	1:B:245:THR:HG21	2.44	0.43
1:A:455:SER:HB2	1:B:493:TRP:NE1	2.33	0.43
1:B:50:ASN:OD1	1:B:50:ASN:C	2.62	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:207:LEU:HD23	1:A:207:LEU:HA	1.84	0.42
1:A:197:GLU:OE2	1:A:332:LYS:HD2	2.19	0.42
1:A:371:TRP:HA	1:A:371:TRP:CE3	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:B:267:LEU:HD12	1:B:297:PHE:HB3	2.01	0.42
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:PY0:N	2.64	0.41
1:A:92:HIS:CE1	2:A:601:PY0: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: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:34:LEU:O	1:A:35:ASP:C	2.64	0.40
1:B:190:LYS:O	1:B:191:PRO:O	2.40	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 ⓘ

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	555/563 (99%)	519 (94%)	30 (5%)	6 (1%)	11	43
1	B	552/563 (98%)	506 (92%)	35 (6%)	11 (2%)	6	28
All	All	1107/1126 (98%)	1025 (93%)	65 (6%)	17 (2%)	8	35

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%)	429 (92%)	40 (8%)	10	36
1	B	468/474 (99%)	428 (92%)	40 (8%)	10	36
All	All	937/948 (99%)	857 (92%)	80 (8%)	10	36

All (80) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	15	LYS
1	A	82	LEU
1	A	106	SER
1	A	112	LEU
1	A	170	ASN
1	A	179	SER
1	A	198	GLU
1	A	200	VAL
1	A	224	ARG
1	A	247	MET
1	A	262	VAL
1	A	270	PRO
1	A	284	SER
1	A	290	SER
1	A	302	LYS
1	A	304	LYS
1	A	315	LYS
1	A	317	ARG
1	A	320	THR
1	A	332	LYS
1	A	336	LYS
1	A	347	VAL
1	A	368	GLU
1	A	388	THR
1	A	397	GLN
1	A	410	VAL
1	A	414	SER
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	541	PRO
1	A	542	THR
1	A	549	LEU
1	A	550	VAL
1	A	551	LYS
1	A	556	THR
1	B	25	LEU
1	B	82	LEU
1	B	103	SER

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Mol	Chain	Res	Type
1	B	114	HIS
1	B	116	THR
1	B	119	ASN
1	B	122	PHE
1	B	135	THR
1	B	144	THR
1	B	175	THR
1	B	179	SER
1	B	190	LYS
1	B	202	GLU
1	B	203	ASN
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	330	LEU
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	454	ILE
1	B	469	LEU
1	B	477	GLU
1	B	501	THR
1	B	511	ARG
1	B	514	THR
1	B	526	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (13) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	20	GLN

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Mol	Chain	Res	Type
1	A	53	ASN
1	A	114	HIS
1	A	239	GLN
1	A	293	ASN
1	A	356	ASN
1	A	373	GLN
1	A	397	GLN
1	A	486	GLN
1	B	83	ASN
1	B	114	HIS
1	B	213	ASN
1	B	492	ASN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 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
2	PY0	A	601	1	4,6,6	3.72	2 (50%)	1,9,9	1.29	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
3	TPP	B	601	4	26,27,27	1.68	3 (11%)	38,40,40	1.87	7 (18%)
5	1PE	A	604	-	15,15,15	0.75	0	14,14,14	0.68	0
2	PY0	B	600	1	4,6,6	4.33	2 (50%)	1,9,9	0.72	0
3	TPP	A	602	4	26,27,27	2.18	5 (19%)	38,40,40	2.36	14 (36%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	PY0	A	601	1	-	0/0/6/6	-
3	TPP	B	601	4	-	0/17/17/17	0/2/2/2
5	1PE	A	604	-	-	6/13/13/13	-
2	PY0	B	600	1	-	0/0/6/6	-
3	TPP	A	602	4	-	1/17/17/17	0/2/2/2

All (12) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	602	TPP	C5-C4	6.77	1.49	1.35
2	B	600	PY0	O1-C1	6.25	1.46	1.38
2	B	600	PY0	O2-C1	5.80	1.46	1.38
3	B	601	TPP	C5-C4	5.46	1.46	1.35
2	A	601	PY0	O2-C1	5.41	1.45	1.38
3	A	602	TPP	PA-O3A	5.37	1.65	1.59
2	A	601	PY0	O1-C1	4.86	1.44	1.38
3	A	602	TPP	C5'-C4'	4.37	1.50	1.42
3	B	601	TPP	PA-O3A	4.12	1.63	1.59
3	B	601	TPP	C5'-C4'	2.75	1.47	1.42
3	A	602	TPP	C7'-C5'	2.65	1.56	1.51
3	A	602	TPP	C2'-N1'	2.13	1.37	1.34

All (21) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	602	TPP	CM2-C2'-N1'	6.37	123.98	117.20
3	A	602	TPP	C2-S1-C5	-6.14	87.15	91.22
3	B	601	TPP	C2-S1-C5	-5.38	87.65	91.22
3	A	602	TPP	S1-C2-N3	4.68	118.23	112.30
3	B	601	TPP	S1-C2-N3	3.95	117.30	112.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	602	TPP	C6'-N1'-C2'	3.87	122.42	116.07
3	B	601	TPP	CM4-C4-N3	3.44	128.51	120.57
3	B	601	TPP	O2B-PB-O3A	-3.42	93.18	104.64
3	A	602	TPP	N1'-C2'-N3'	-3.29	120.05	125.53
3	A	602	TPP	CM4-C4-N3	3.14	127.82	120.57
3	B	601	TPP	CM4-C4-C5	-3.01	120.02	127.75
3	A	602	TPP	C6-C5-S1	-2.80	114.34	120.90
3	A	602	TPP	O2B-PB-O3A	-2.69	95.61	104.64
3	B	601	TPP	C6'-N1'-C2'	2.69	120.49	116.07
3	B	601	TPP	O2A-PA-O1A	2.67	124.86	112.44
3	A	602	TPP	O3B-PB-O3A	2.60	113.36	104.64
3	A	602	TPP	CM4-C4-C5	-2.49	121.38	127.75
3	A	602	TPP	O3A-PA-O1A	-2.48	103.23	110.70
3	A	602	TPP	C2-N3-C4	-2.25	111.02	114.06
3	A	602	TPP	C2'-N3'-C4'	2.16	121.42	118.10
3	A	602	TPP	O2B-PB-O1B	2.16	119.26	110.83

There are no chirality outliers.

All (7) 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
5	A	604	1PE	C23-C13-OH4-C24
5	A	604	1PE	C16-C26-OH6-C15
5	A	604	1PE	C13-C23-OH3-C22
5	A	604	1PE	OH7-C16-C26-OH6

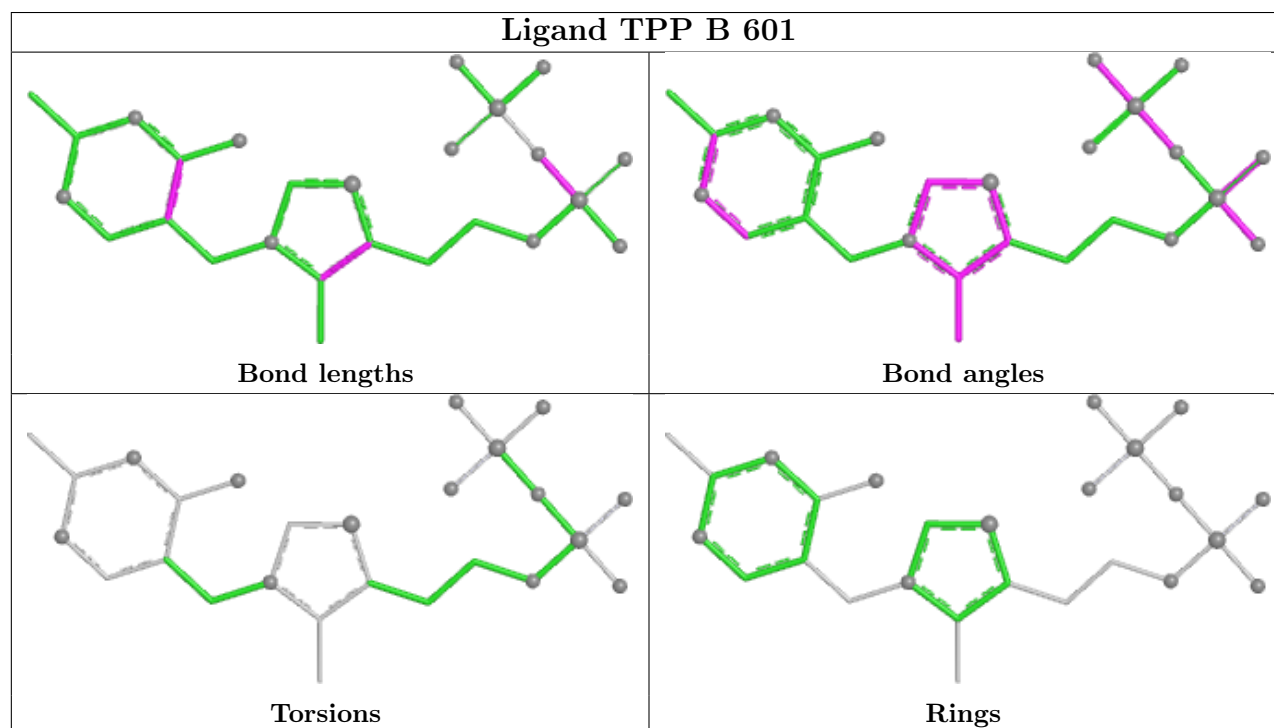
There are no ring outliers.

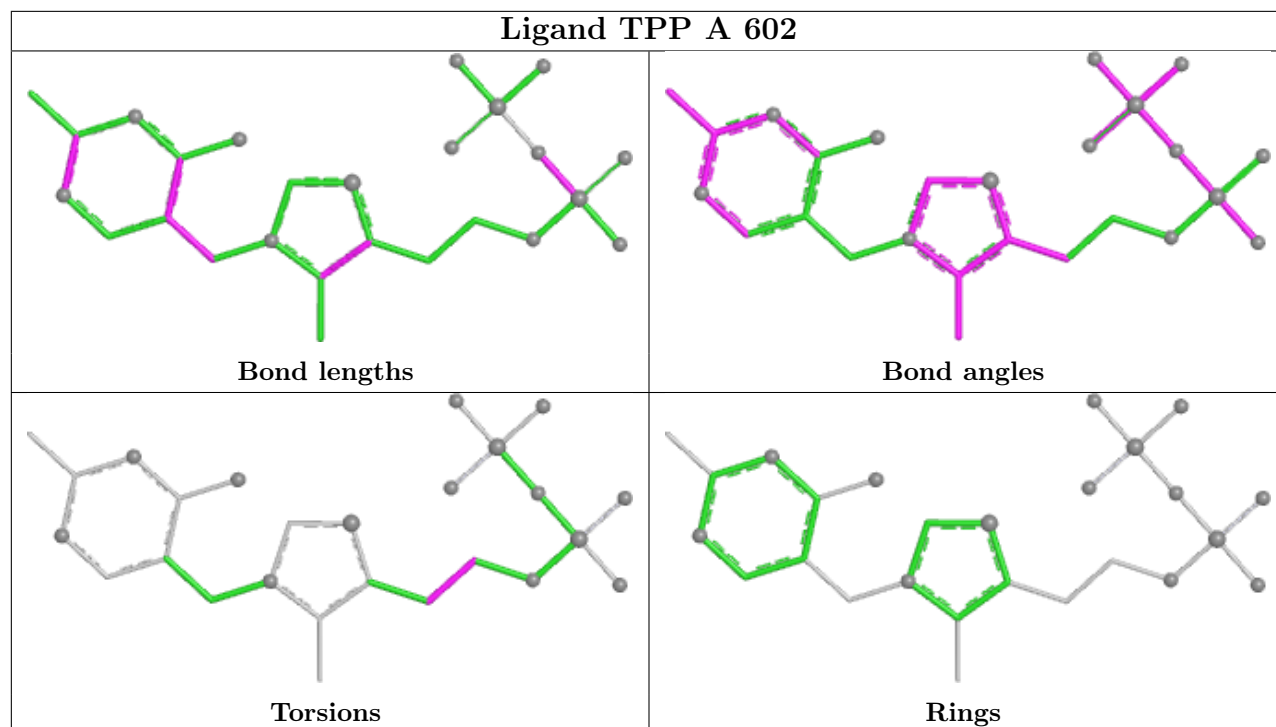
4 monomers are involved in 13 short contacts:

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





5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2		OWAB(Å ²)	Q<0.9
1	A	557/563 (98%)	-0.24	17 (3%)	51 30	16, 34, 88, 135	0
1	B	556/563 (98%)	-0.13	12 (2%)	62 39	18, 43, 84, 105	0
All	All	1113/1126 (98%)	-0.19	29 (2%)	57 34	16, 38, 85, 135	0

All (29) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	347	VAL	4.5
1	B	116	THR	4.0
1	A	558	ALA	4.0
1	B	104	VAL	4.0
1	A	555	LEU	4.0
1	B	113	LEU	3.9
1	B	563	ASN	3.8
1	A	289	LEU	3.6
1	A	556	THR	3.5
1	B	114	HIS	3.3
1	A	551	LYS	3.2
1	B	105	SER	3.1
1	B	106	SER	3.1
1	A	553	ALA	3.1
1	B	122	PHE	2.9
1	A	347	VAL	2.9
1	A	479	LEU	2.8
1	A	393	PHE	2.7
1	A	550	VAL	2.6
1	A	392	ALA	2.5
1	A	295	GLY	2.4
1	B	348	PRO	2.4
1	A	557	ALA	2.3
1	A	547	SER	2.3

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Mol	Chain	Res	Type	RSRZ
1	B	338	ALA	2.2
1	A	202	GLU	2.1
1	A	484	THR	2.1
1	A	476	ILE	2.1
1	B	320	THR	2.0

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

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

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

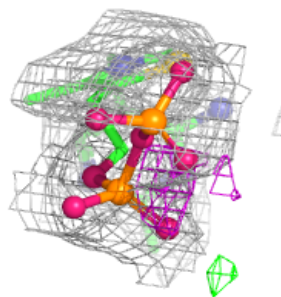
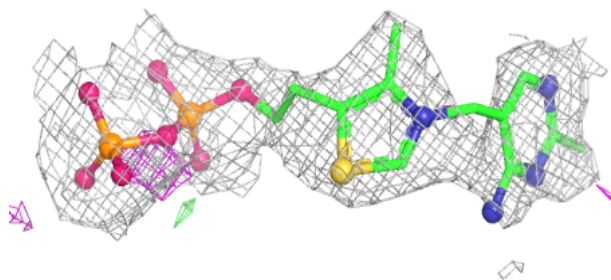
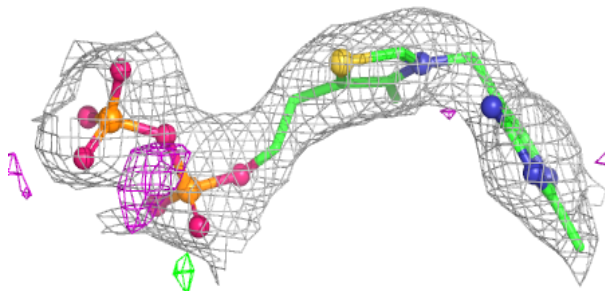
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
2	PY0	B	600	7/7	0.80	0.18	37,45,54,58	0
2	PY0	A	601	7/7	0.93	0.15	54,62,64,67	0
3	TPP	A	602	26/26	0.94	0.11	51,62,76,78	0
5	1PE	A	604	16/16	0.94	0.13	34,52,62,62	0
4	MG	A	603	1/1	0.99	0.05	40,40,40,40	0
4	MG	B	602	1/1	0.99	0.03	17,17,17,17	0
3	TPP	B	601	26/26	0.99	0.05	24,26,29,31	0

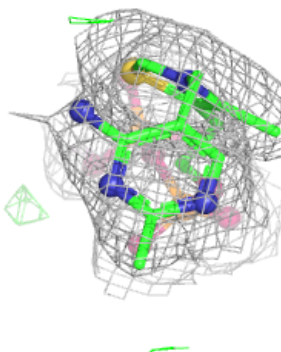
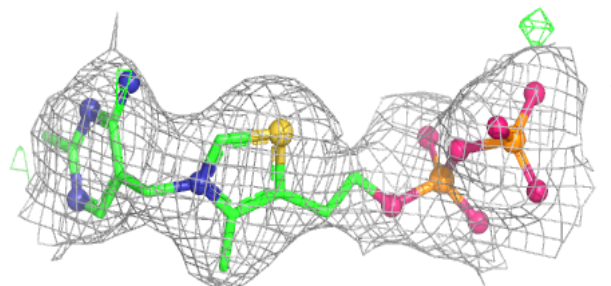
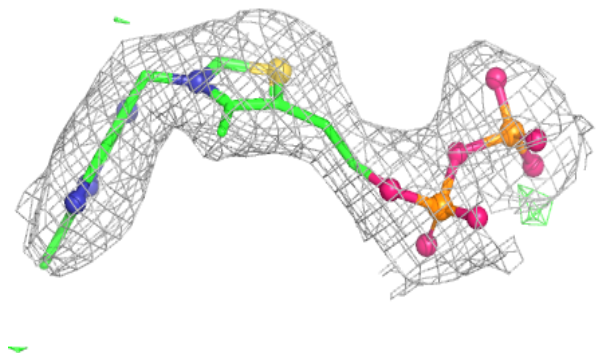
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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