



wwPDB X-ray Structure Validation Summary Report ⓘ

Mar 5, 2026 – 07:11 PM UTC

PDB ID : 1QPB / pdb_00001qpb
Title : PYRUVATE DECARBOXYLASE FROM YEAST (FORM B) COMPLEXED
WITH PYRUVAMIDE
Authors : Lu, G.; Dobritsch, D.; Schneider, G.
Deposited on : 1999-11-26
Resolution : 2.40 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 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

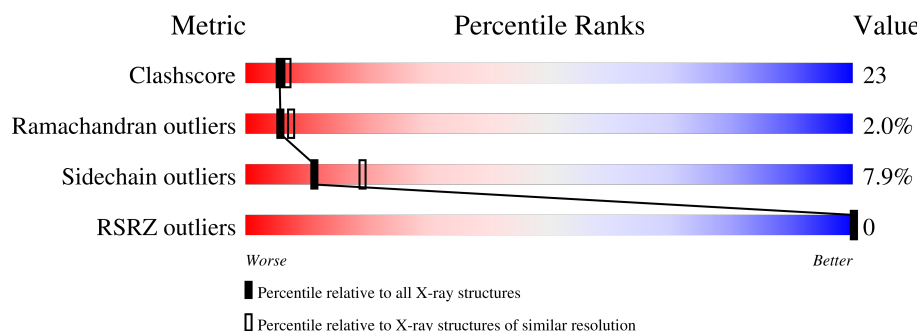
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.40 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))
Clashscore	190562	5391 (2.40-2.40)
Ramachandran outliers	187476	5320 (2.40-2.40)
Sidechain outliers	187428	5321 (2.40-2.40)
RSRZ outliers	180081	4916 (2.40-2.40)

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	
1	B	563	

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	PYM	A	602	-	X	-	-
4	PYM	B	602	-	X	-	-

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 8757 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.

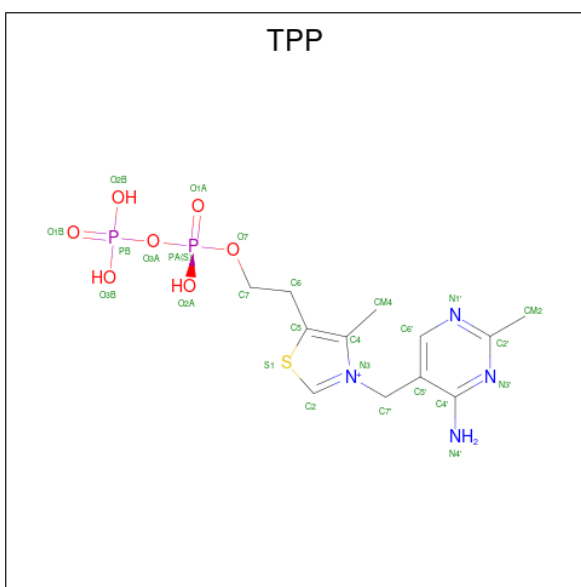
- Molecule 1 is a protein called PYRUVATE DECARBOXYLASE (FORM B).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	555	Total	C	N	O	S	75	0	0
			4275	2734	714	811	16			
1	B	555	Total	C	N	O	S	126	0	0
			4275	2734	714	811	16			

There are 8 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	206	VAL	ALA	variant	UNP P06169
A	208	ILE	VAL	variant	UNP P06169
A	336	ALA	THR	variant	UNP P06169
A	538	VAL	ILE	variant	UNP P06169
B	206	VAL	ALA	variant	UNP P06169
B	208	ILE	VAL	variant	UNP P06169
B	336	ALA	THR	variant	UNP P06169
B	538	VAL	ILE	variant	UNP P06169

- Molecule 2 is THIAMINE DIPHOSPHATE (CCD ID: TPP) (formula: C₁₂H₁₉N₄O₇P₂S).

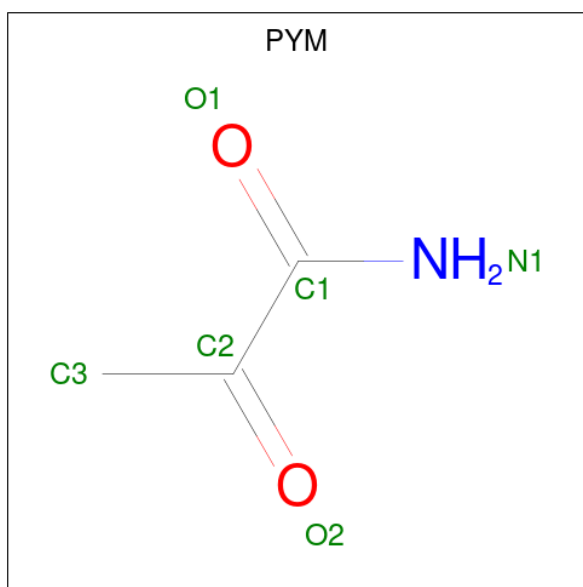


Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
2	A	1	Total 26	C 12	N 4	O 7	P 2	S 1	0	0
2	B	1	Total 26	C 12	N 4	O 7	P 2	S 1	0	0

- Molecule 3 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

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

- Molecule 4 is PYRUVAMIDE (CCD ID: PYM) (formula: $\text{C}_3\text{H}_5\text{NO}_2$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	A	1	Total	C	N	O	0	0
			6	3	1	2		
4	B	1	Total	C	N	O	0	0
			6	3	1	2		

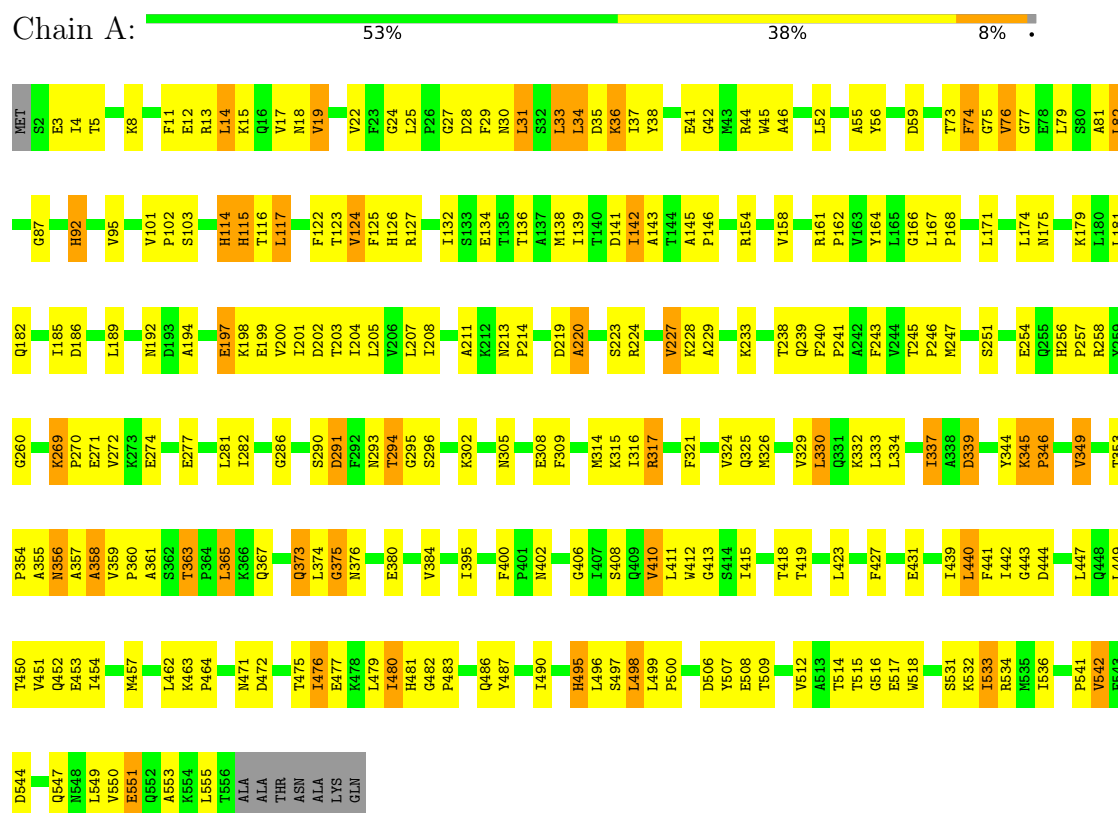
- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	85	Total	O	0	0
			85	85		
5	B	56	Total	O	0	0
			56	56		

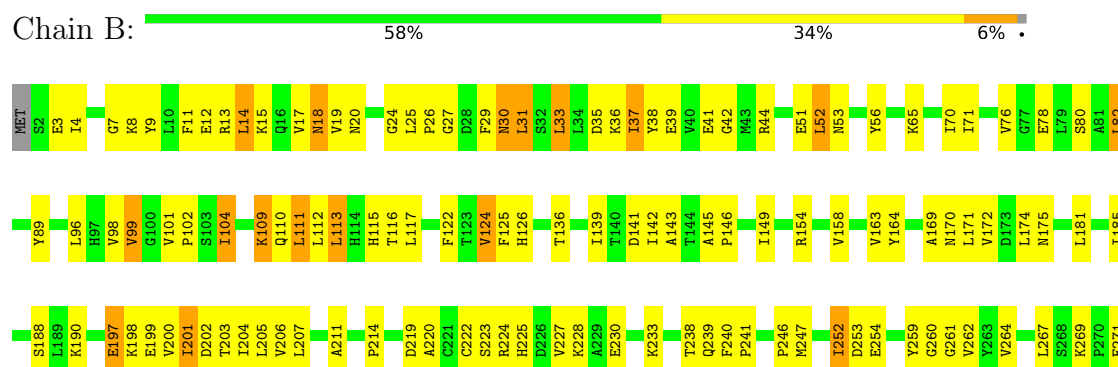
3 Residue-property plots

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

• Molecule 1: PYRUVATE DECARBOXYLASE (FORM B)



• Molecule 1: PYRUVATE DECARBOXYLASE (FORM B)



V272	K273	E274	E277	D280	L281	L282	L288	L289	S296	Y299	S300	Y301	I306	V307	E308	F309	H310	S311	D312	H313	M314	K315	I316	R317	F321	V324	Q325	M326	K327	F328	V329	L330	Q331	K332	L333	L334	I337	A338	D339	Y344	K345	P346	V347	A348	V349	T353	N356
A357	A358	V359	L365	E368	W371	N372	Q373	G389	T390	S391	A392	F393	G394	I395	N402	N403	T404	Y405	G406	V410	L411	W412	L423	A426	F427	K435	V438	I439	L440	F441	L447	Q448	V451	Q452	E453	T456	M457	L462	N471	T475	L476	E477	K478				
L479	I480	H481	G482	P483	K484	W493	D494	H495	L496	S497	L498	L499	P500	Y507	E508	T509	V512	A513	T514	T515	D519	Q523	T533	R534	W535	I536	P541	D544	Q547	N548	L549	V550	E551	Q552	L555	T556	ALA	ALA	THR	ASN	ALA	LYS	GLN				

4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	145.05Å 119.70Å 81.28Å 90.00° 120.21° 90.00°	Depositor
Resolution (Å)	15.00 – 2.40 15.00 – 2.40	Depositor EDS
% Data completeness (in resolution range)	89.0 (15.00-2.40) 90.7 (15.00-2.40)	Depositor EDS
R_{merge}	0.11	Depositor
R_{sym}	0.09	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.40 (at 2.39Å)	Xtriage
Refinement program	CNS 3.8	Depositor
R, R_{free}	0.233 , 0.287 0.242 , (Not available)	Depositor DCC
R_{free} test set	No test flags present.	wwPDB-VP
Wilson B-factor (Å ²)	29.3	Xtriage
Anisotropy	0.208	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.30 , 27.6	EDS
L-test for twinning ²	$\langle L \rangle = 0.45$, $\langle L^2 \rangle = 0.27$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	8757	wwPDB-VP
Average B, all atoms (Å ²)	35.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.40% 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: TPP, MG, PYM

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	0.51	0/4366	1.00	19/5937 (0.3%)
1	B	0.48	1/4366 (0.0%)	0.97	10/5937 (0.2%)
All	All	0.49	1/8732 (0.0%)	0.98	29/11874 (0.2%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	406	GLY	CA-C	5.30	1.57	1.52

The worst 5 of 29 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	451	VAL	N-CA-C	9.47	120.31	110.36
1	A	542	VAL	N-CA-C	7.94	118.48	110.23
1	B	410	VAL	N-CA-C	7.24	118.03	110.72
1	A	326	MET	N-CA-C	7.02	118.58	111.07
1	A	18	ASN	N-CA-C	6.88	120.97	112.58

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts ⓘ

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	4275	0	4287	224	0
1	B	4275	0	4287	186	0
2	A	26	0	16	1	0
2	B	26	0	16	2	0
3	A	1	0	0	0	0
3	B	1	0	0	0	0
4	A	6	0	5	0	0
4	B	6	0	5	1	0
5	A	85	0	0	8	0
5	B	56	0	0	3	0
All	All	8757	0	8616	395	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 23.

The worst 5 of 395 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:533:ILE:HD12	1:B:533:ILE:H	1.22	1.04
1:B:267:LEU:HD21	1:B:552:GLN:HB3	1.37	1.04
1:A:533:ILE:HD12	1:A:533:ILE:H	1.24	1.01
1:A:454:ILE:HA	1:A:457:MET:HE3	1.47	0.97
1:B:496:LEU:HD22	1:B:509:THR:HB	1.51	0.92

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	553/563 (98%)	493 (89%)	46 (8%)	14 (2%)	4	5
1	B	553/563 (98%)	489 (88%)	56 (10%)	8 (1%)	9	13
All	All	1106/1126 (98%)	982 (89%)	102 (9%)	22 (2%)	6	7

5 of 22 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	356	ASN
1	B	358	ALA
1	A	75	GLY
1	A	103	SER
1	A	346	PRO

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	462/467 (99%)	431 (93%)	31 (7%)	15	26
1	B	462/467 (99%)	420 (91%)	42 (9%)	9	14
All	All	924/934 (99%)	851 (92%)	73 (8%)	11	19

5 of 73 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	349	VAL
1	B	547	GLN
1	B	365	LEU
1	B	471	ASN
1	A	476	ILE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 32 such sidechains are listed below:

Mol	Chain	Res	Type
1	B	486	GLN
1	B	523	GLN
1	A	488	ASN
1	A	481	HIS
1	B	547	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry ⓘ

Of 6 ligands modelled in this entry, 2 are monoatomic - leaving 4 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
4	PYM	B	602	-	5,5,5	6.13	3 (60%)	4,6,6	6.74	3 (75%)
2	TPP	B	600	3	26,27,27	1.82	11 (42%)	38,40,40	1.56	8 (21%)
4	PYM	A	602	-	5,5,5	5.30	3 (60%)	4,6,6	6.73	3 (75%)
2	TPP	A	600	3	26,27,27	1.55	8 (30%)	38,40,40	1.65	7 (18%)

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
4	PYM	B	602	-	-	0/1/4/4	-
2	TPP	B	600	3	-	2/17/17/17	0/2/2/2
4	PYM	A	602	-	-	0/1/4/4	-
2	TPP	A	600	3	-	0/17/17/17	0/2/2/2

The worst 5 of 25 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	B	602	PYM	C1-C2	-10.76	1.40	1.54
4	A	602	PYM	C1-C2	-8.72	1.43	1.54
4	B	602	PYM	C3-C2	-8.08	1.34	1.50
4	A	602	PYM	C3-C2	-7.69	1.35	1.50
2	A	600	TPP	C5'-C4'	3.08	1.48	1.42

The worst 5 of 21 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	B	602	PYM	C3-C2-C1	8.82	131.70	117.91
4	A	602	PYM	C3-C2-C1	8.21	130.74	117.91
4	B	602	PYM	O2-C2-C3	-7.86	102.16	119.77
4	A	602	PYM	O2-C2-C3	-7.82	102.25	119.77
4	A	602	PYM	O2-C2-C1	7.16	127.00	118.98

There are no chirality outliers.

All (2) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	B	600	TPP	C5-C6-C7-O7
2	B	600	TPP	PB-O3A-PA-O2A

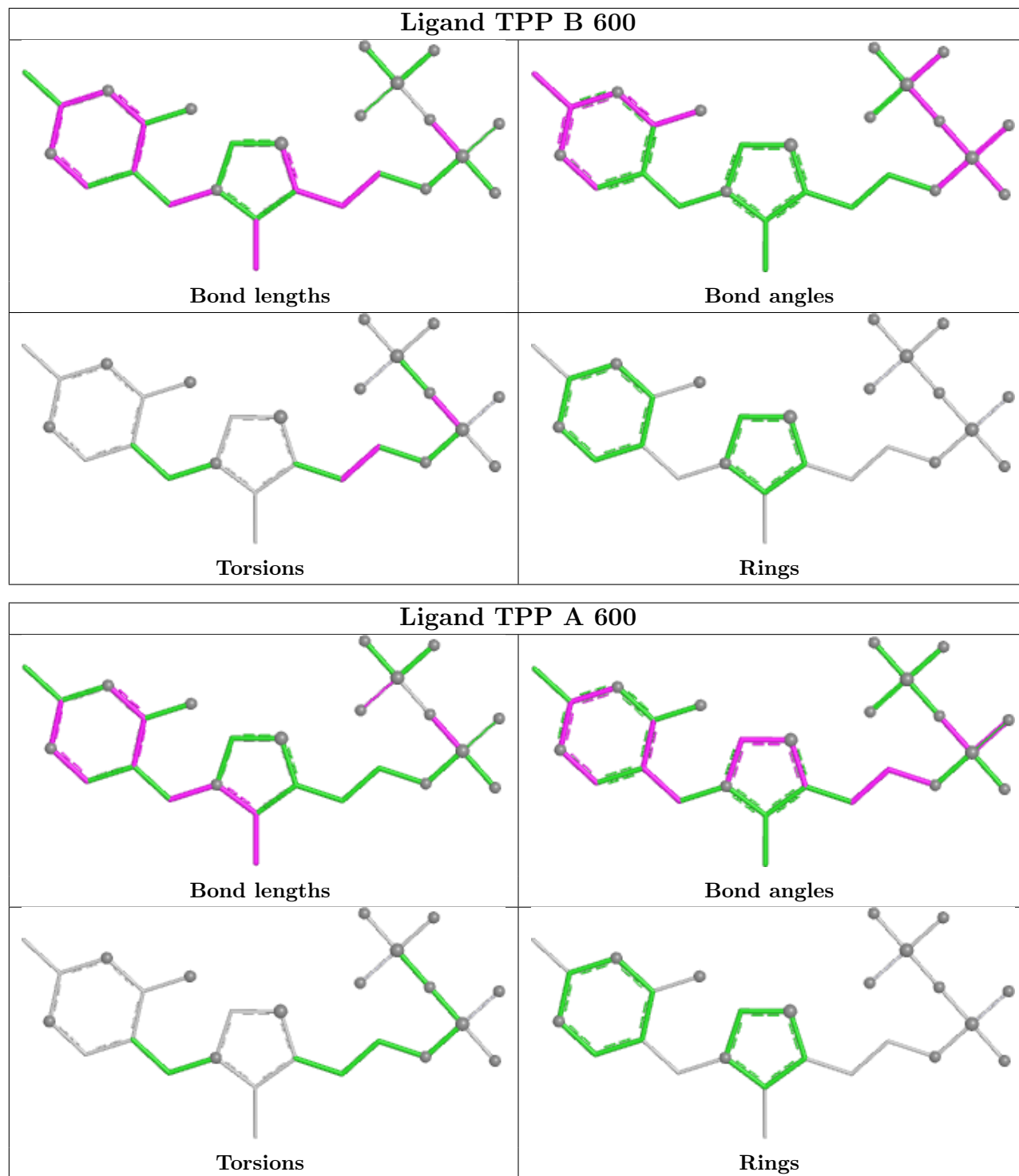
There are no ring outliers.

3 monomers are involved in 4 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	B	602	PYM	1	0
2	B	600	TPP	2	0
2	A	600	TPP	1	0

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

equivalents in the CSD to analyse the geometry.



5.7 Other polymers ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

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	545/563 (96%)	-1.75	0 100 100	10, 31, 53, 68	0
1	B	540/563 (95%)	-1.72	0 100 100	10, 34, 64, 98	1 (0%)
All	All	1085/1126 (96%)	-1.73	0 100 100	10, 32, 60, 98	1 (0%)

There are no RSRZ outliers to report.

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](#)

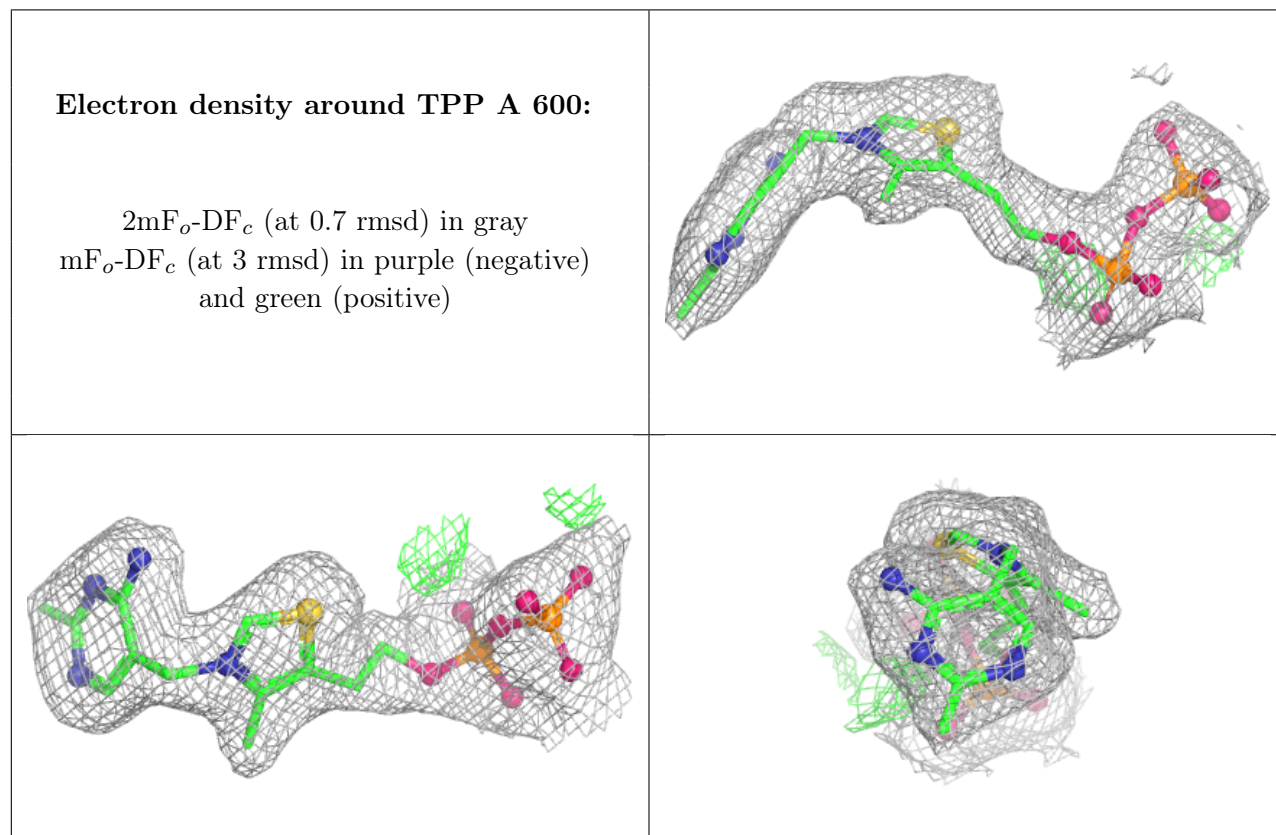
There are no oligosaccharides in this entry.

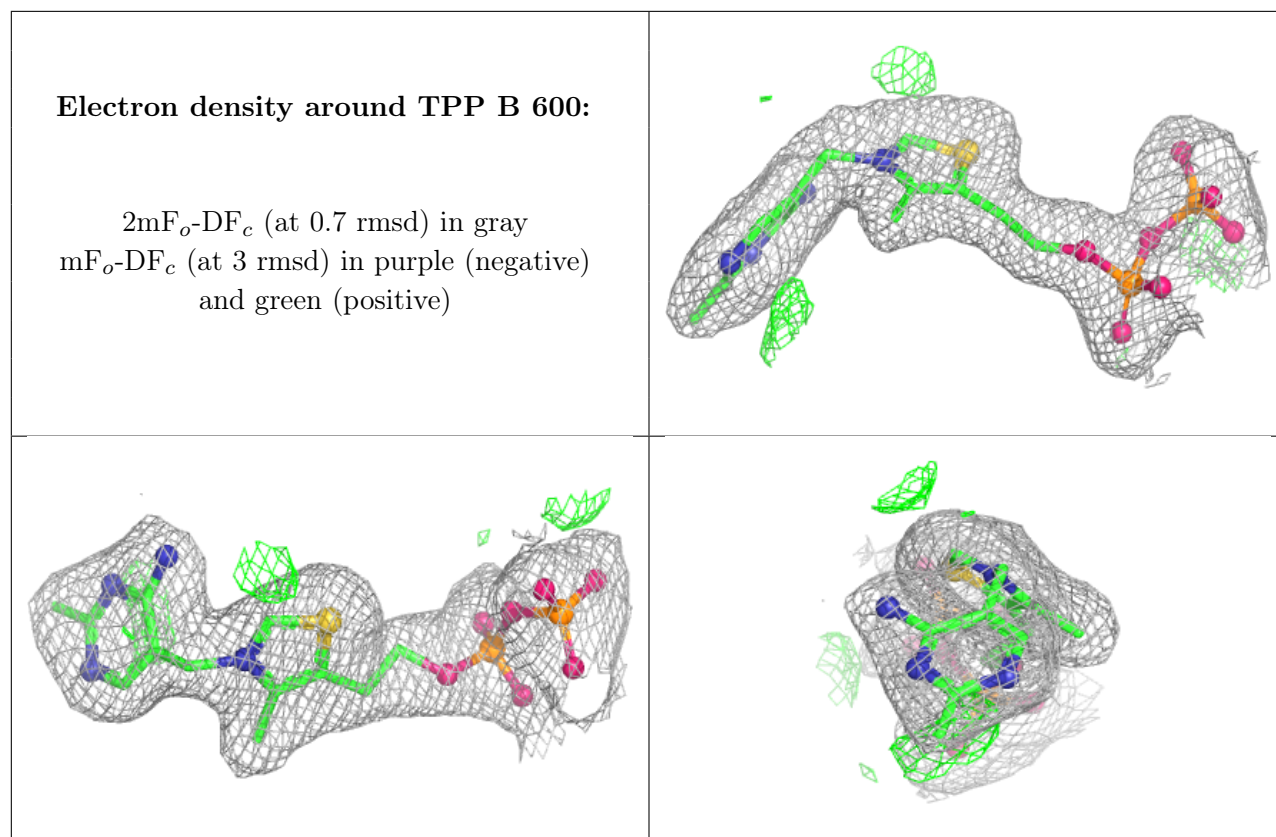
6.4 Ligands [i](#)

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
4	PYM	B	602	6/6	0.98	0.05	44,46,46,46	0
4	PYM	A	602	6/6	0.99	0.04	50,52,54,54	0
3	MG	A	601	1/1	1.00	0.01	26,26,26,26	0
3	MG	B	601	1/1	1.00	0.03	71,71,71,71	0
2	TPP	A	600	26/26	1.00	0.01	18,24,27,28	0
2	TPP	B	600	26/26	1.00	0.01	11,18,22,23	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.





6.5 Other polymers [i](#)

There are no such residues in this entry.