



Full wwPDB X-ray Structure Validation Report ⓘ

May 21, 2020 – 02:55 am BST

PDB ID : 5ND5
Title : Crystal structure of transketolase from Chlamydomonas reinhardtii in complex with TPP and Mg²⁺
Authors : Fermani, S.; Zaffagnini, M.; Francia, F.; Pasquini, M.
Deposited on : 2017-03-07
Resolution : 1.74 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

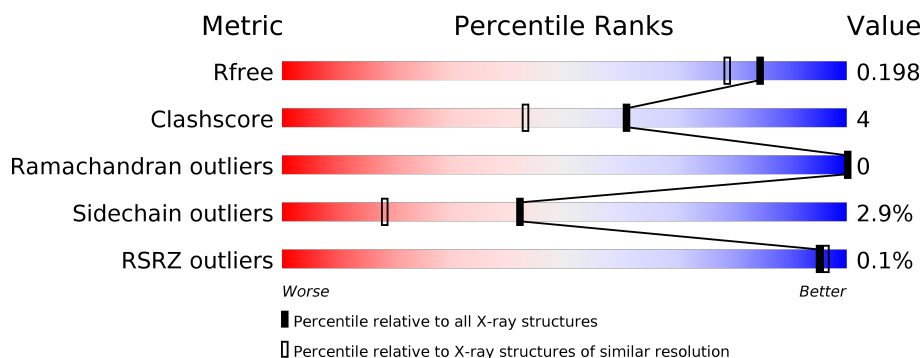
1 Overall quality at a glance ⓘ

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.74 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	3764 (1.76-1.72)
Clashscore	141614	3923 (1.76-1.72)
Ramachandran outliers	138981	3878 (1.76-1.72)
Sidechain outliers	138945	3878 (1.76-1.72)
RSRZ outliers	127900	3705 (1.76-1.72)

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	692	
1	B	692	

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 10992 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 Transketolase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	669	Total	C	N	O	S	0	3	0
			5123	3245	883	962	33			
1	B	669	Total	C	N	O	S	0	2	0
			5117	3242	883	959	33			

There are 18 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	27	MET	-	initiating methionine	UNP A8IAN1
A	28	HIS	-	expression tag	UNP A8IAN1
A	29	HIS	-	expression tag	UNP A8IAN1
A	30	HIS	-	expression tag	UNP A8IAN1
A	31	HIS	-	expression tag	UNP A8IAN1
A	32	HIS	-	expression tag	UNP A8IAN1
A	33	HIS	-	expression tag	UNP A8IAN1
A	34	HIS	-	expression tag	UNP A8IAN1
A	35	MET	-	expression tag	UNP A8IAN1
B	27	MET	-	initiating methionine	UNP A8IAN1
B	28	HIS	-	expression tag	UNP A8IAN1
B	29	HIS	-	expression tag	UNP A8IAN1
B	30	HIS	-	expression tag	UNP A8IAN1
B	31	HIS	-	expression tag	UNP A8IAN1
B	32	HIS	-	expression tag	UNP A8IAN1
B	33	HIS	-	expression tag	UNP A8IAN1
B	34	HIS	-	expression tag	UNP A8IAN1
B	35	MET	-	expression tag	UNP A8IAN1

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

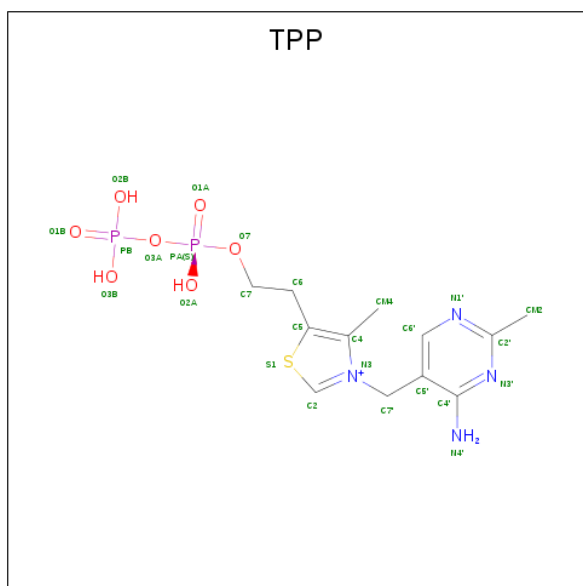
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	B	1	Total	Mg	0	0
			1	1		

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	1	Total	Mg	0	0
			1	1		

- Molecule 3 is THIAMINE DIPHOSPHATE (three-letter code: TPP) (formula: C₁₂H₁₉N₄O₇P₂S).



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


- Molecule 4 is water.

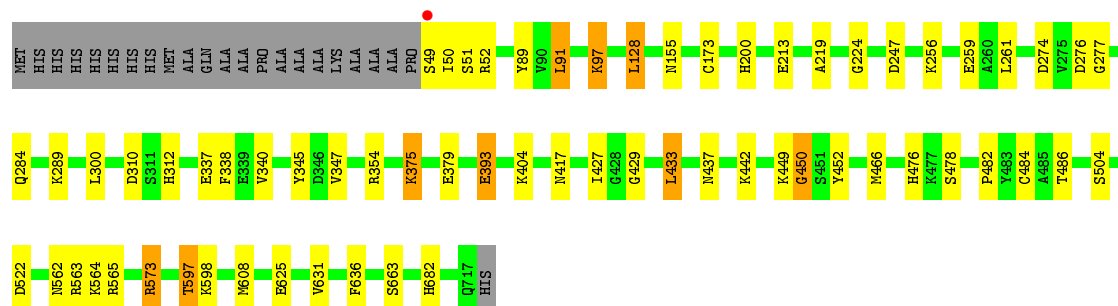
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	338	Total	O	0	0
			338	338		
4	B	360	Total	O	0	0
			360	360		

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.

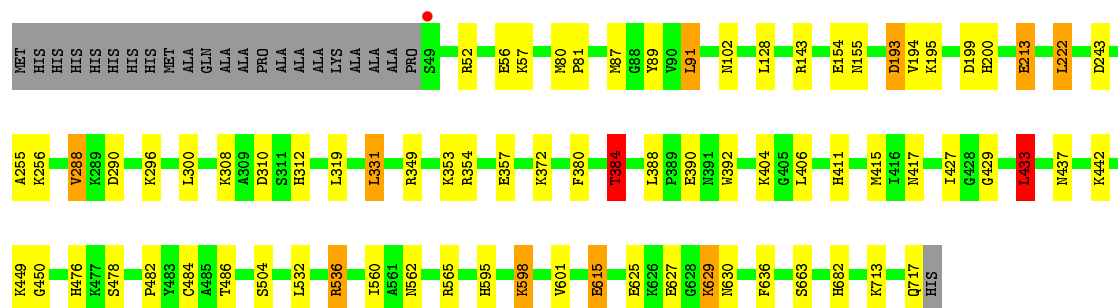
• Molecule 1: Transketolase

Chain A: 



• Molecule 1: Transketolase

Chain B: 



4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	201.49Å 75.93Å 103.76Å 90.00° 109.99° 90.00°	Depositor
Resolution (Å)	97.51 – 1.74 48.88 – 1.74	Depositor EDS
% Data completeness (in resolution range)	75.9 (97.51-1.74) 75.9 (48.88-1.74)	Depositor EDS
R_{merge}	0.05	Depositor
R_{sym}	0.05	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.67 (at 1.74Å)	Xtriage
Refinement program	REFMAC 5.8.0073	Depositor
R, R_{free}	0.145 , 0.186 0.157 , 0.198	Depositor DCC
R_{free} test set	5757 reflections (5.01%)	wwPDB-VP
Wilson B-factor (Å ²)	15.9	Xtriage
Anisotropy	0.030	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 43.9	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.97	EDS
Total number of atoms	10992	wwPDB-VP
Average B, all atoms (Å ²)	17.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.34% 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: 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	0.97	3/5258 (0.1%)	0.93	10/7134 (0.1%)
1	B	0.96	4/5249 (0.1%)	1.02	18/7122 (0.3%)
All	All	0.96	7/10507 (0.1%)	0.98	28/14256 (0.2%)

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	3

All (7) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	379	GLU	CD-OE2	7.61	1.34	1.25
1	B	450	GLY	N-CA	6.98	1.56	1.46
1	A	450	GLY	N-CA	6.62	1.55	1.46
1	B	615	GLU	CD-OE1	5.89	1.32	1.25
1	B	213	GLU	CD-OE2	5.53	1.31	1.25
1	A	452	TYR	CZ-OH	5.18	1.46	1.37
1	B	154	GLU	CD-OE2	-5.11	1.20	1.25

All (28) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	536	ARG	NE-CZ-NH1	20.88	130.74	120.30
1	B	536	ARG	NE-CZ-NH2	-16.93	111.84	120.30
1	B	536	ARG	CB-CG-CD	9.70	136.82	111.60
1	A	91	LEU	CB-CG-CD1	8.83	126.00	111.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	290	ASP	CB-CG-OD1	7.49	125.04	118.30
1	B	222	LEU	CB-CG-CD1	7.33	123.47	111.00
1	A	573	ARG	NE-CZ-NH2	-7.17	116.72	120.30
1	B	449	LYS	C-N-CA	-6.60	108.44	122.30
1	B	87	MET	CB-CA-C	6.49	123.38	110.40
1	B	143	ARG	NE-CZ-NH2	6.30	123.45	120.30
1	B	536	ARG	CD-NE-CZ	6.10	132.14	123.60
1	B	331	LEU	CB-CG-CD1	6.07	121.31	111.00
1	A	247	ASP	CB-CG-OD1	6.06	123.76	118.30
1	B	193	ASP	CB-CA-C	-6.04	98.31	110.40
1	B	91	LEU	CB-CG-CD1	6.03	121.26	111.00
1	A	128	LEU	CA-CB-CG	6.00	129.11	115.30
1	A	128	LEU	CB-CG-CD1	5.87	120.98	111.00
1	B	87	MET	CA-CB-CG	5.64	122.88	113.30
1	B	615	GLU	OE1-CD-OE2	5.56	129.98	123.30
1	A	608	MET	CA-CB-CG	5.50	122.65	113.30
1	B	433	LEU	CB-CG-CD1	5.38	120.14	111.00
1	B	384	THR	N-CA-CB	-5.32	100.20	110.30
1	A	449	LYS	C-N-CA	-5.26	111.25	122.30
1	B	199	ASP	CB-CG-OD1	5.24	123.02	118.30
1	A	276	ASP	CB-CG-OD1	5.07	122.86	118.30
1	A	433	LEU	CB-CG-CD2	5.06	119.60	111.00
1	A	522	ASP	CB-CG-OD1	5.02	122.82	118.30
1	B	243	ASP	CB-CG-OD1	5.02	122.82	118.30

There are no chirality outliers.

All (3) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	289	LYS	Peptide
1	A	450	GLY	Peptide
1	A	89	TYR	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	5123	0	5034	43	0
1	B	5117	0	5027	52	0
2	A	1	0	0	0	0
2	B	1	0	0	0	0
3	A	26	0	16	3	0
3	B	26	0	16	2	0
4	A	338	0	0	4	0
4	B	360	0	0	7	0
All	All	10992	0	10093	91	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 4.

All (91) 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:259[B]:GLU:OE2	1:B:256:LYS:NZ	1.92	1.01
3:A:801:TPP:H2	4:B:1193:HOH:O	1.63	0.96
1:B:598:LYS:HG3	1:B:601:VAL:HG11	1.53	0.90
1:B:300:LEU:HD11	1:B:310:ASP:HB2	1.56	0.87
1:A:259[B]:GLU:CD	1:B:256:LYS:NZ	2.31	0.83
1:A:597:THR:CG2	1:A:631:VAL:H	1.91	0.82
1:B:194:VAL:HG12	4:B:1054:HOH:O	1.80	0.82
1:A:155:ASN:HD21	1:A:504[A]:SER:HB2	1.44	0.81
1:B:128:LEU:O	1:B:349:ARG:NH1	2.17	0.77
1:A:476:HIS:HD2	1:A:478[A]:SER:OG	1.68	0.76
1:A:476:HIS:CD2	1:A:478[A]:SER:OG	2.40	0.75
1:B:536:ARG:HD3	4:B:982:HOH:O	1.86	0.75
1:A:50:ILE:HG22	1:A:51:SER:H	1.50	0.74
1:A:259[B]:GLU:CD	1:B:256:LYS:HZ3	1.90	0.74
1:A:300:LEU:HD11	1:A:310:ASP:HB2	1.69	0.73
1:B:380:PHE:O	1:B:384:THR:HB	1.88	0.73
1:B:595:HIS:HE1	1:B:625:GLU:OE2	1.72	0.73
1:B:56[B]:GLU:OE1	4:B:901:HOH:O	2.10	0.70
1:A:393:GLU:OE2	4:A:901:HOH:O	2.10	0.68
1:B:404:LYS:HD2	1:B:406:LEU:HD21	1.75	0.68
1:A:597:THR:HB	1:A:625:GLU:OE2	1.94	0.67
1:B:562:ASN:HD21	1:B:565:ARG:HH11	1.43	0.66
1:B:52:ARG:NE	1:B:56[A]:GLU:OE2	2.25	0.66
1:A:597:THR:HG23	1:A:631:VAL:H	1.60	0.66
1:B:615:GLU:OE2	4:B:902:HOH:O	2.14	0.65
1:A:300:LEU:CD1	1:A:310:ASP:HB2	2.28	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:52:ARG:NH1	4:B:903:HOH:O	2.31	0.63
1:A:375:LYS:HD3	4:A:1140:HOH:O	1.98	0.63
1:A:259[B]:GLU:CD	1:B:256:LYS:HZ1	2.03	0.62
1:B:598:LYS:HG3	1:B:601:VAL:CG1	2.29	0.62
1:B:476:HIS:HD2	1:B:478:SER:OG	1.81	0.61
1:B:417:ASN:HD21	1:B:442:LYS:H	1.48	0.61
1:A:417:ASN:HD21	1:A:442:LYS:H	1.49	0.60
1:A:476:HIS:HD2	1:A:478[B]:SER:OG	1.83	0.60
1:B:194:VAL:CG1	4:B:1054:HOH:O	2.45	0.59
1:B:194:VAL:HG12	1:B:195:LYS:N	2.20	0.57
1:A:437:ASN:HD21	1:A:486:THR:HA	1.72	0.55
1:B:155:ASN:HD21	1:B:504[A]:SER:HB2	1.72	0.55
1:B:417:ASN:ND2	1:B:442:LYS:H	2.05	0.54
1:B:598:LYS:O	1:B:601:VAL:HG12	2.07	0.54
1:A:259[B]:GLU:HB3	1:B:256:LYS:HE2	1.90	0.53
1:A:417:ASN:ND2	1:A:442:LYS:H	2.05	0.53
1:A:663:SER:OG	1:A:682:HIS:HD2	1.92	0.53
1:A:337:GLU:HG2	1:A:338:PHE:CD2	2.45	0.52
1:A:564:LYS:HE2	1:A:564:LYS:HA	1.91	0.51
1:A:155:ASN:HD21	1:A:504[A]:SER:CB	2.19	0.51
1:A:375:LYS:CD	4:A:1140:HOH:O	2.57	0.51
1:B:532:LEU:O	1:B:536:ARG:HG3	2.11	0.50
1:B:194:VAL:HG12	1:B:195:LYS:H	1.77	0.50
1:A:155:ASN:ND2	1:A:504[A]:SER:HB2	2.22	0.50
1:A:50:ILE:HG22	1:A:51:SER:N	2.23	0.50
1:B:200:HIS:NE2	1:B:476:HIS:HE1	2.10	0.49
1:A:256:LYS:HG3	1:B:256:LYS:HE3	1.95	0.48
1:A:50:ILE:CG2	1:A:51:SER:H	2.22	0.48
1:B:300:LEU:CD1	1:B:310:ASP:HB2	2.36	0.48
1:A:340:VAL:HB	1:A:345:TYR:CE2	2.49	0.47
1:A:284:GLN:NE2	4:A:905:HOH:O	2.44	0.47
1:B:627:GLU:OE2	1:B:629:LYS:NZ	2.48	0.46
1:B:193:ASP:HB3	1:B:194:VAL:HG23	1.96	0.46
1:A:562:ASN:HD21	1:A:565:ARG:HH11	1.64	0.46
1:A:466:MET:SD	1:A:484:CYS:HB2	2.56	0.46
1:B:372:LYS:O	1:B:372:LYS:HG3	2.15	0.46
1:B:255:ALA:HB2	1:B:296:LYS:HE3	1.98	0.46
1:B:437:ASN:HD21	1:B:486:THR:HA	1.81	0.46
1:A:50:ILE:HD12	1:A:347:VAL:HG22	1.98	0.46
1:B:89:TYR:CD1	1:B:89:TYR:C	2.88	0.46
1:A:200:HIS:NE2	1:A:476:HIS:HE1	2.14	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:308:LYS:NZ	1:B:319:LEU:O	2.49	0.45
1:B:80:MET:HB3	1:B:81:PRO:HD3	1.98	0.45
1:B:598:LYS:HE3	1:B:630:ASN:OD1	2.16	0.45
1:B:155:ASN:HD21	1:B:504[B]:SER:HB3	1.79	0.45
1:B:663:SER:OG	1:B:682:HIS:HD2	2.00	0.44
1:B:429:GLY:O	1:B:484:CYS:HA	2.18	0.44
1:B:213:GLU:OE2	3:B:801:TPP:HM23	2.17	0.44
1:B:427:ILE:O	1:B:482:PRO:HA	2.17	0.43
1:A:427:ILE:O	1:A:482:PRO:HA	2.18	0.43
1:B:128:LEU:C	1:B:349:ARG:NH1	2.71	0.43
1:A:274:ASP:OD2	1:A:277:GLY:HA3	2.19	0.43
1:B:627:GLU:OE2	1:B:713:LYS:HE2	2.19	0.42
3:B:801:TPP:HM41	3:B:801:TPP:H61	1.85	0.42
1:A:97:LYS:HG3	1:A:97:LYS:O	2.19	0.42
1:A:213:GLU:OE2	3:A:801:TPP:HM23	2.20	0.42
1:A:429:GLY:O	1:A:484:CYS:HA	2.20	0.42
1:A:224:GLY:HA3	1:A:261:LEU:O	2.20	0.41
1:B:411:HIS:O	1:B:415:MET:HG2	2.21	0.41
1:A:563:ARG:C	1:A:564:LYS:HD2	2.41	0.41
1:B:392:TRP:CH2	1:B:560:ILE:HB	2.56	0.41
1:B:353:LYS:O	1:B:357:GLU:HG3	2.21	0.40
1:B:288:VAL:O	1:B:288:VAL:HG12	2.21	0.40
3:A:801:TPP:HM43	1:B:433:LEU:HD13	2.03	0.40
1:A:173:CYS:SG	1:A:219:ALA:HB2	2.62	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	670/692 (97%)	650 (97%)	20 (3%)	0	100 100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	B	669/692 (97%)	653 (98%)	16 (2%)	0	100	100
All	All	1339/1384 (97%)	1303 (97%)	36 (3%)	0	100	100

There are no Ramachandran outliers to report.

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	537/548 (98%)	522 (97%)	15 (3%)	43	19
1	B	535/548 (98%)	519 (97%)	16 (3%)	41	17
All	All	1072/1096 (98%)	1041 (97%)	31 (3%)	42	18

All (31) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	49	SER
1	A	52	ARG
1	A	91	LEU
1	A	97	LYS
1	A	128	LEU
1	A	312	HIS
1	A	354	ARG
1	A	375	LYS
1	A	393	GLU
1	A	404	LYS
1	A	433	LEU
1	A	573	ARG
1	A	597	THR
1	A	598	LYS
1	A	636	PHE
1	B	57	LYS
1	B	91	LEU
1	B	102	ASN

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Mol	Chain	Res	Type
1	B	222	LEU
1	B	288	VAL
1	B	312	HIS
1	B	331	LEU
1	B	354	ARG
1	B	384	THR
1	B	388	LEU
1	B	390	GLU
1	B	433	LEU
1	B	598	LYS
1	B	629	LYS
1	B	636	PHE
1	B	717	GLN

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (28) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	102	ASN
1	A	155	ASN
1	A	284	GLN
1	A	307	ASN
1	A	417	ASN
1	A	437	ASN
1	A	464	HIS
1	A	471	ASN
1	A	476	HIS
1	A	496	ASN
1	A	562	ASN
1	A	630	ASN
1	A	682	HIS
1	A	717	GLN
1	B	102	ASN
1	B	141	GLN
1	B	155	ASN
1	B	284	GLN
1	B	307	ASN
1	B	417	ASN
1	B	437	ASN
1	B	464	HIS
1	B	471	ASN
1	B	476	HIS
1	B	496	ASN

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Mol	Chain	Res	Type
1	B	562	ASN
1	B	595	HIS
1	B	682	HIS

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 carbohydrates in this entry.

5.6 Ligand geometry [i](#)

Of 4 ligands modelled in this entry, 2 are monoatomic - leaving 2 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	B	801	2	22,27,27	2.11	4 (18%)	29,40,40	2.33	10 (34%)
3	TPP	A	801	2	22,27,27	2.07	5 (22%)	29,40,40	1.85	10 (34%)

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	B	801	2	-	1/16/17/17	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	TPP	A	801	2	-	2/16/17/17	0/2/2/2

All (9) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	801	TPP	C4-N3	-7.57	1.33	1.39
3	A	801	TPP	C4-N3	-5.48	1.34	1.39
3	A	801	TPP	C5'-C4'	3.89	1.49	1.42
3	A	801	TPP	C6-C5	-3.53	1.49	1.50
3	B	801	TPP	C5'-C4'	3.46	1.48	1.42
3	B	801	TPP	C7'-N3	-2.76	1.43	1.48
3	B	801	TPP	C6-C5	2.68	1.52	1.50
3	A	801	TPP	PB-O2B	-2.67	1.44	1.54
3	A	801	TPP	PB-O1B	2.56	1.58	1.50

All (20) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	801	TPP	C6-C5-C4	-7.50	121.42	127.43
3	B	801	TPP	CM4-C4-N3	5.27	129.25	122.53
3	B	801	TPP	CM4-C4-C5	-4.33	118.13	127.60
3	A	801	TPP	O3B-PB-O2B	3.55	121.22	107.64
3	A	801	TPP	C2'-N3'-C4'	3.35	123.31	118.08
3	A	801	TPP	N1'-C2'-N3'	-3.21	120.02	125.54
3	A	801	TPP	CM4-C4-N3	2.97	126.32	122.53
3	A	801	TPP	CM4-C4-C5	-2.81	121.46	127.60
3	B	801	TPP	C7'-N3-C2	2.56	129.98	125.35
3	B	801	TPP	N1'-C2'-N3'	-2.52	121.21	125.54
3	A	801	TPP	O3A-PB-O1B	-2.49	97.39	111.19
3	A	801	TPP	C7'-N3-C2	2.46	129.80	125.35
3	A	801	TPP	CM2-C2'-N1'	2.44	119.82	117.14
3	B	801	TPP	C5-C4-N3	2.36	112.29	107.57
3	A	801	TPP	PA-O7-C7	-2.30	110.27	121.59
3	A	801	TPP	C5-C4-N3	2.24	112.05	107.57
3	B	801	TPP	PA-O7-C7	-2.23	110.59	121.59
3	B	801	TPP	C6'-N1'-C2'	2.14	119.60	115.96
3	B	801	TPP	N4'-C4'-N3'	2.13	120.04	117.03
3	B	801	TPP	CM2-C2'-N3'	2.01	120.29	117.15

There are no chirality outliers.

All (3) torsion outliers are listed below:

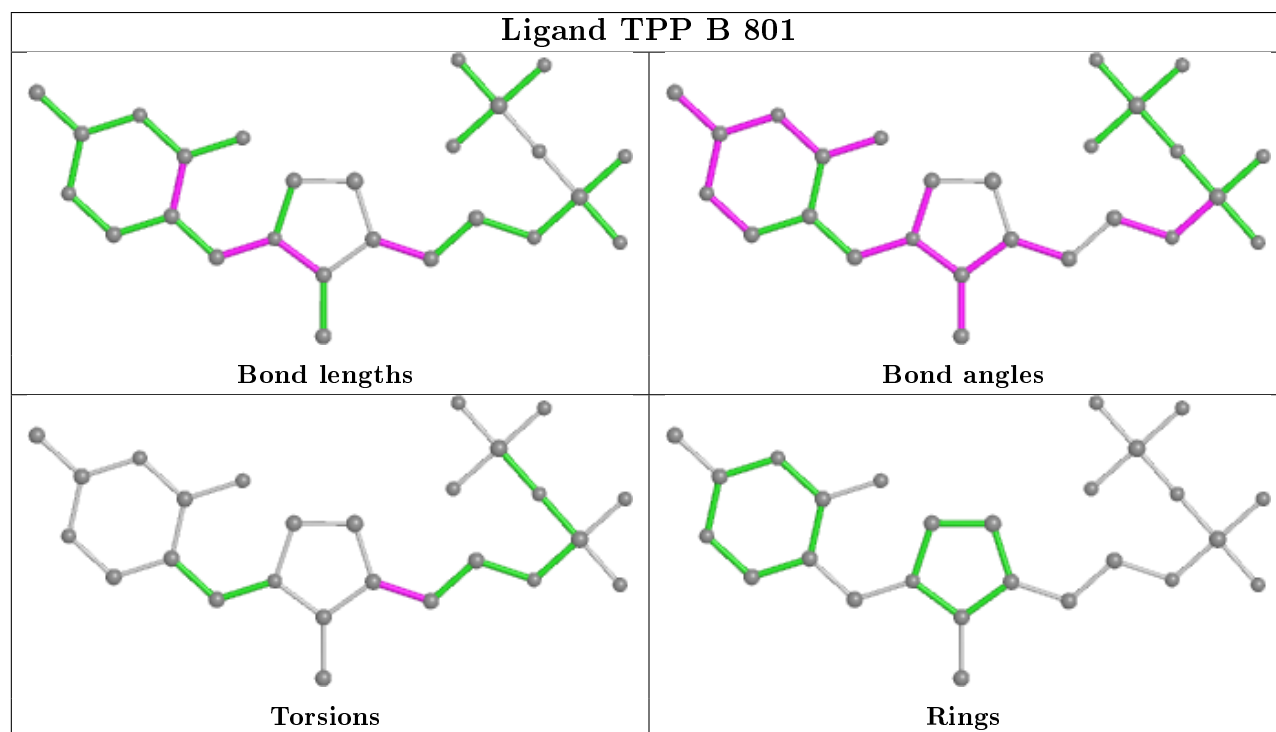
Mol	Chain	Res	Type	Atoms
3	B	801	TPP	C4-C5-C6-C7
3	A	801	TPP	PB-O3A-PA-O1A
3	A	801	TPP	PB-O3A-PA-O2A

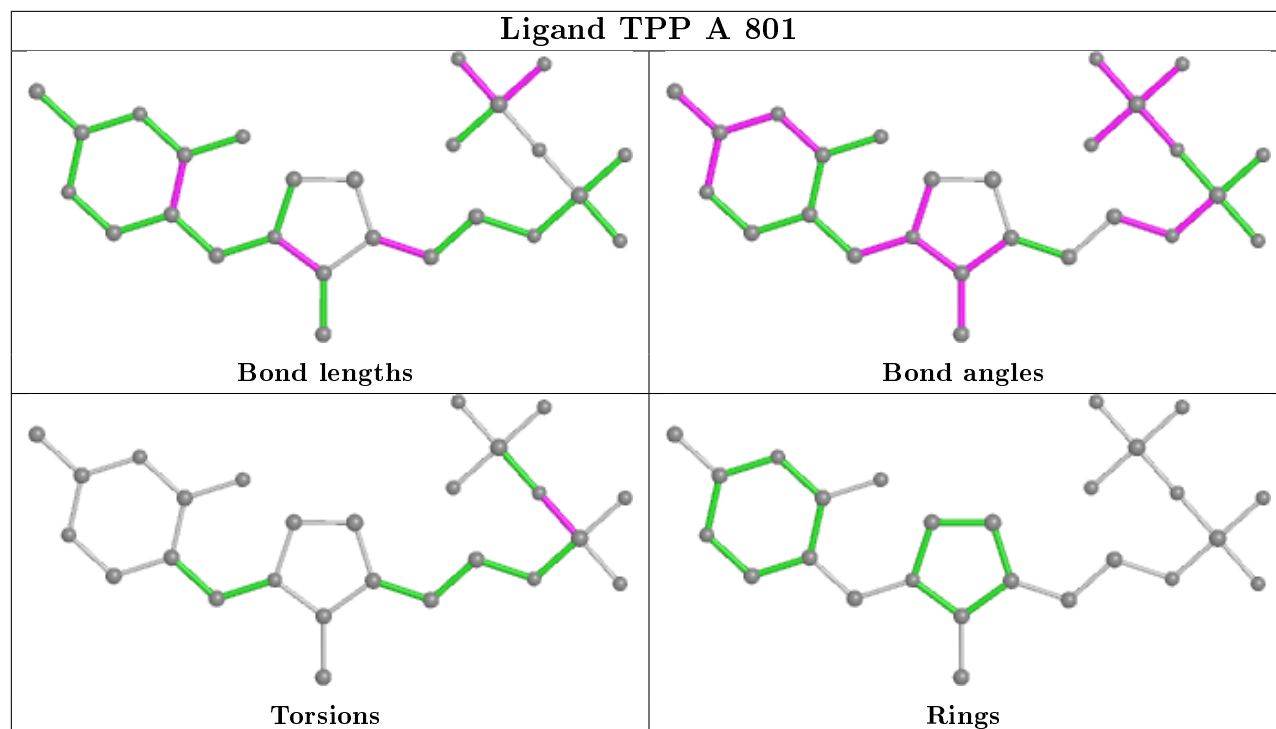
There are no ring outliers.

2 monomers are involved in 5 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	B	801	TPP	2	0
3	A	801	TPP	3	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	669/692 (96%)	-0.71	1 (0%) 95 96	10, 16, 30, 58	0
1	B	669/692 (96%)	-0.60	1 (0%) 95 96	10, 15, 29, 55	0
All	All	1338/1384 (96%)	-0.66	2 (0%) 95 96	10, 15, 30, 58	0

All (2) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	49	SER	4.2
1	B	49	SER	2.5

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 carbohydrates in this entry.

6.4 Ligands [i](#)

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
3	TPP	B	801	26/26	0.98	0.06	12,15,20,25	0
3	TPP	A	801	26/26	0.98	0.06	11,15,20,27	0
2	MG	A	800	1/1	0.99	0.03	14,14,14,14	0

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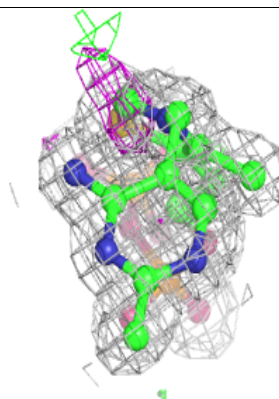
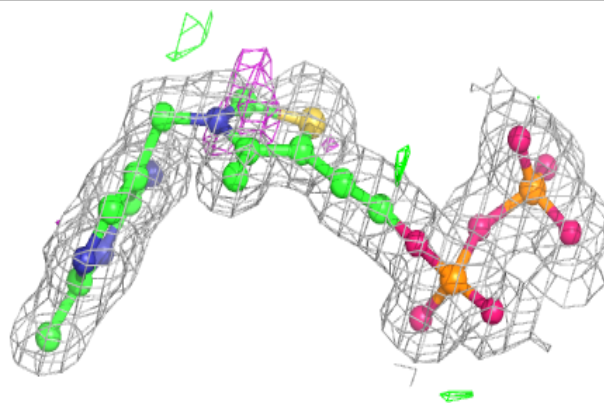
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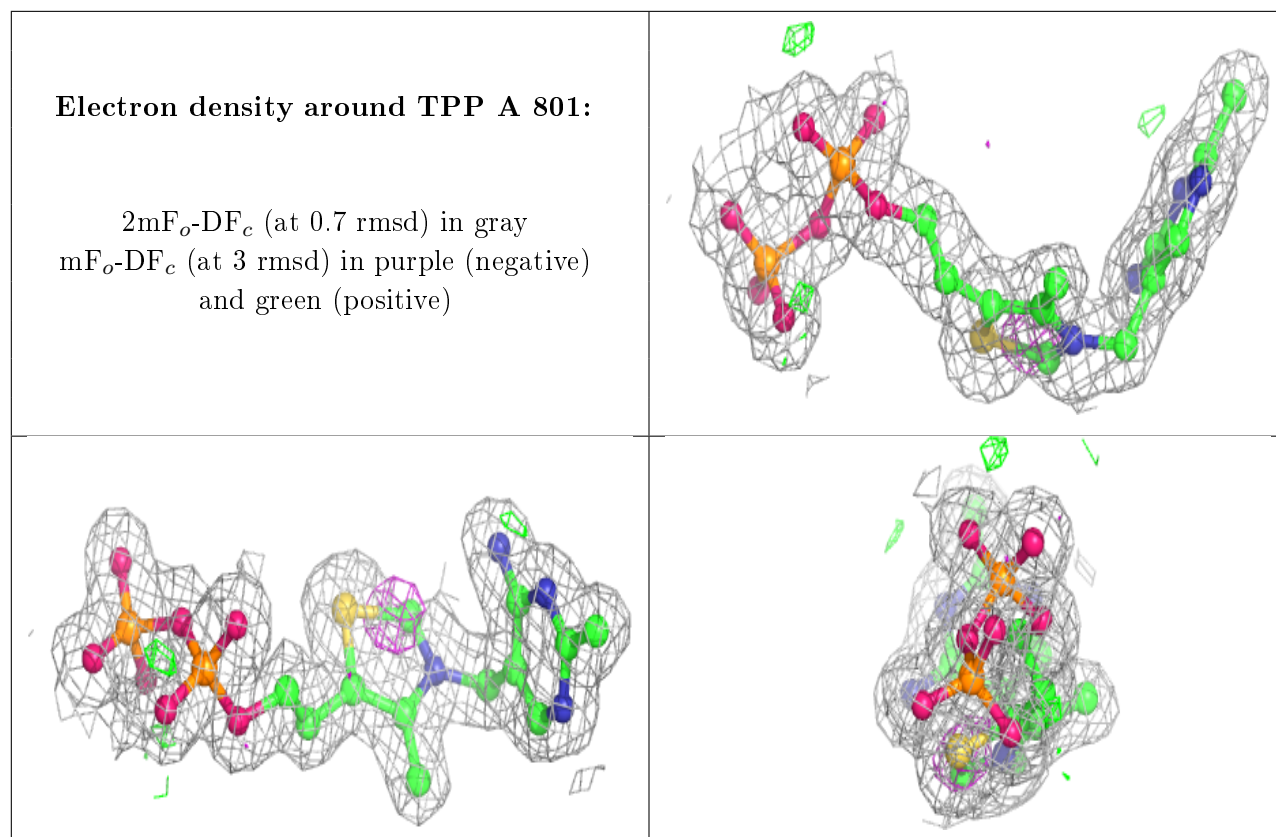
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
2	MG	B	800	1/1	1.00	0.04	13,13,13,13	0

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 B 801:

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.