



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 8, 2026 – 04:10 AM UTC

PDB ID : 1R9J / pdb_00001r9j
Title : Transketolase from Leishmania mexicana
Authors : Veitch, N.J.; Mauger, D.A.; Cazzulo, J.J.; Lindqvist, Y.; Barrett, M.P.
Deposited on : 2003-10-30
Resolution : 2.22 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

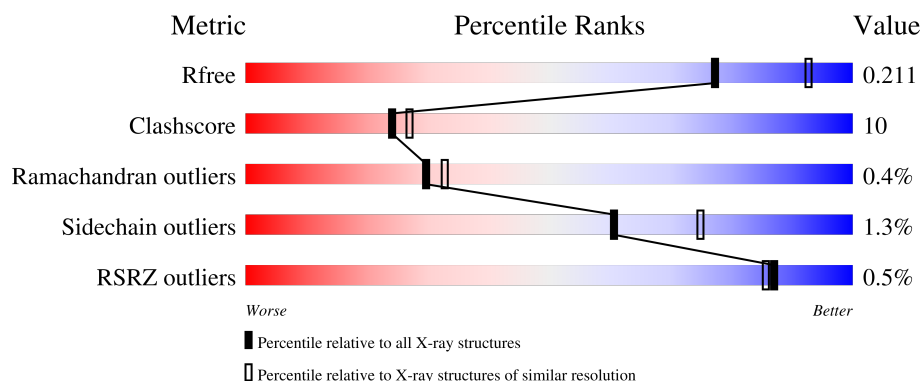
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.22 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	7682 (2.24-2.20)
Clashscore	190562	8402 (2.24-2.20)
Ramachandran outliers	187476	8303 (2.24-2.20)
Sidechain outliers	187428	8304 (2.24-2.20)
RSRZ outliers	180081	7683 (2.24-2.20)

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	673	82% 16% .
1	B	673	78% 19% .

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 11050 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	670	Total	C	N	O	S	0	0	0
			5037	3171	878	958	30			
1	B	671	Total	C	N	O	S	0	0	0
			5048	3177	882	959	30			

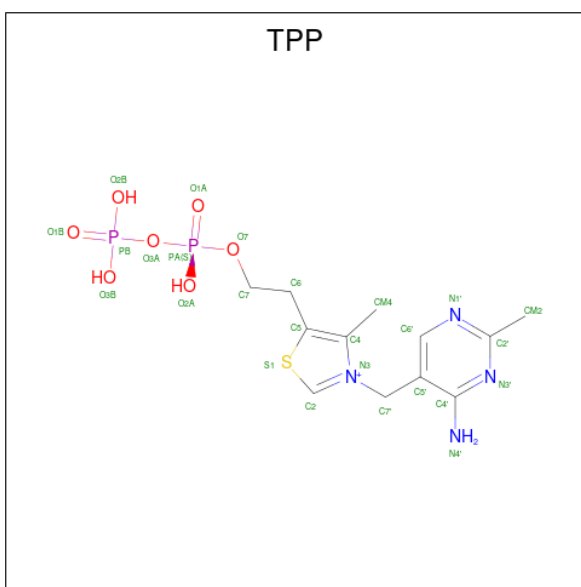
There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-1	ARG	-	expression tag	UNP Q8MPM3
A	0	HIS	-	expression tag	UNP Q8MPM3
B	-1	ARG	-	expression tag	UNP Q8MPM3
B	0	HIS	-	expression tag	UNP Q8MPM3

- Molecule 2 is CALCIUM ION (CCD ID: CA) (formula: Ca).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	1	Total	Ca	0	0
			1	1		
2	B	1	Total	Ca	0	0
			1	1		

- Molecule 3 is THIAMINE DIPHOSPHATE (CCD ID: TPP) (formula: C₁₂H₁₉N₄O₇P₂S).



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

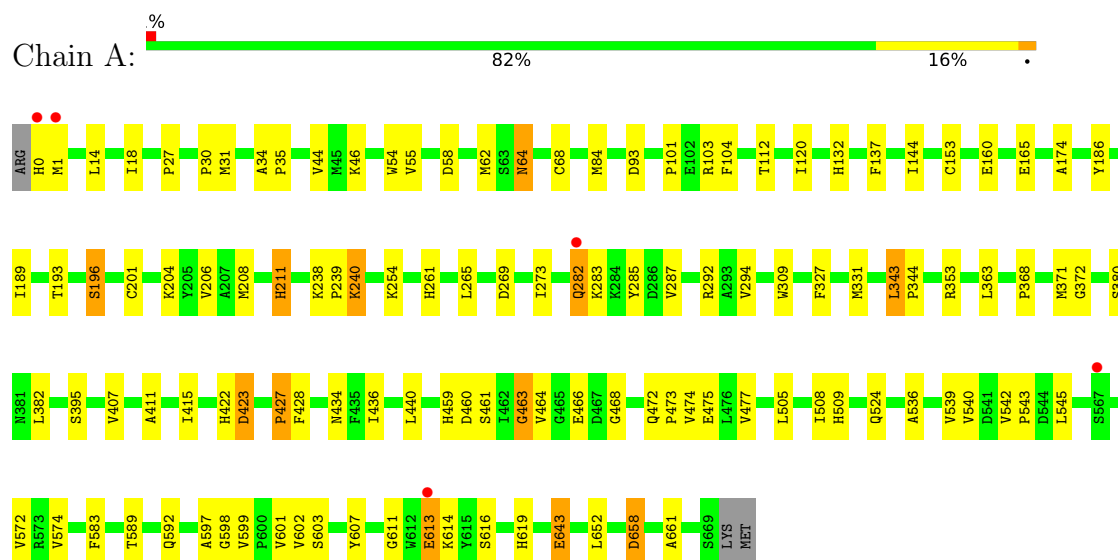
- Molecule 4 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	473	Total O 473 473	0	0
4	B	438	Total O 438 438	0	0

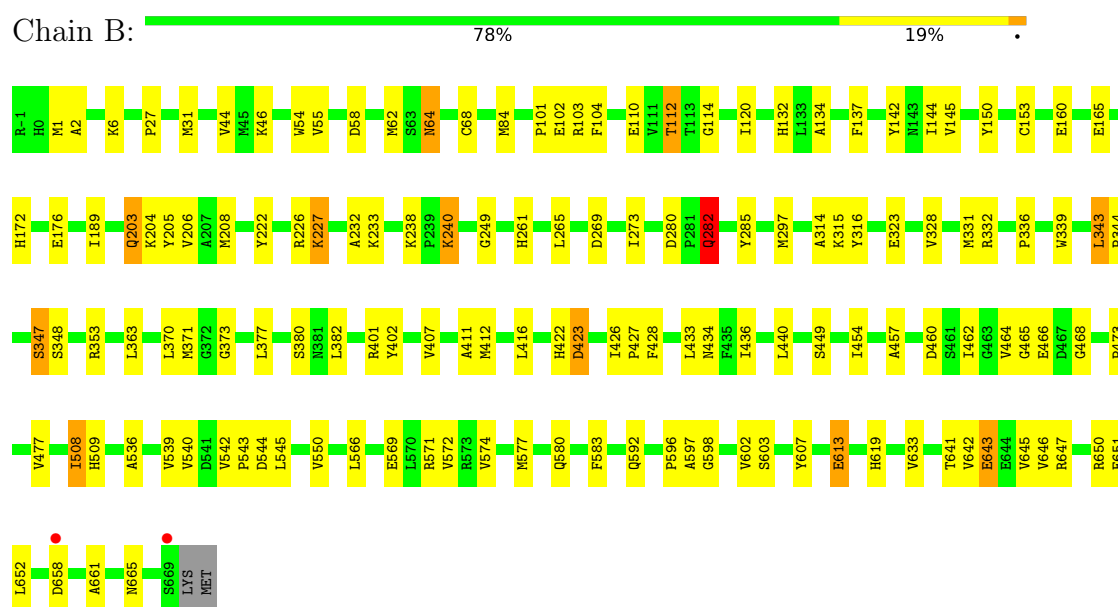
3 Residue-property plots

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: transketolase



• Molecule 1: transketolase



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	76.80Å 120.44Å 139.15Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	25.00 – 2.22 25.00 – 2.22	Depositor EDS
% Data completeness (in resolution range)	(Not available) (25.00-2.22) 95.3 (25.00-2.22)	Depositor EDS
R_{merge}	0.11	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.24 (at 2.22Å)	Xtriage
Refinement program	CNS	Depositor
R, R_{free}	0.170 , 0.213 0.171 , 0.211	Depositor DCC
R_{free} test set	3096 reflections (5.03%)	wwPDB-VP
Wilson B-factor (Å ²)	19.7	Xtriage
Anisotropy	0.460	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.37 , 47.2	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	11050	wwPDB-VP
Average B, all atoms (Å ²)	21.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.10% 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: CA, 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	0.40	0/5148	0.93	18/6988 (0.3%)
1	B	0.40	0/5159	0.93	19/7002 (0.3%)
All	All	0.40	0/10307	0.93	37/13990 (0.3%)

There are no bond length outliers.

All (37) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	44	VAL	N-CA-C	10.30	120.42	111.56
1	B	44	VAL	N-CA-C	9.22	118.91	111.62
1	A	436	ILE	N-CA-C	-8.04	100.79	112.04
1	B	436	ILE	N-CA-C	-7.60	101.40	112.04
1	B	466	GLU	N-CA-C	7.34	121.15	111.75
1	A	466	GLU	N-CA-C	7.31	121.10	111.75
1	B	460	ASP	N-CA-C	7.21	121.93	113.20
1	A	468	GLY	CA-C-N	7.00	127.59	119.47
1	A	468	GLY	C-N-CA	7.00	127.59	119.47
1	B	426	ILE	N-CA-C	-6.97	101.25	108.15
1	B	539	VAL	N-CA-C	-6.41	105.92	113.42
1	B	465	GLY	N-CA-C	6.40	119.03	111.35
1	A	572	VAL	N-CA-C	6.34	117.61	108.48
1	B	343	LEU	CA-C-N	6.12	126.09	120.03
1	B	343	LEU	C-N-CA	6.12	126.09	120.03
1	A	539	VAL	N-CA-C	-5.97	106.93	113.43
1	A	460	ASP	N-CA-C	5.96	120.41	113.20
1	A	474	VAL	N-CA-C	-5.91	108.09	113.71
1	A	343	LEU	CA-C-N	5.75	125.73	120.03
1	A	343	LEU	C-N-CA	5.75	125.73	120.03
1	B	468	GLY	CA-C-N	5.72	125.84	119.32
1	B	468	GLY	C-N-CA	5.72	125.84	119.32

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	463	GLY	N-CA-C	-5.64	107.34	114.16
1	B	110	GLU	N-CA-C	5.54	117.40	111.36
1	A	206	VAL	N-CA-C	-5.45	105.21	110.72
1	A	58	ASP	N-CA-C	-5.38	102.92	110.50
1	B	363	LEU	N-CA-C	5.37	117.21	111.36
1	A	211	HIS	N-CA-C	-5.30	99.14	108.20
1	B	114	GLY	N-CA-C	-5.26	101.60	112.34
1	B	282	GLN	N-CA-C	-5.25	107.42	113.88
1	A	427	PRO	N-CA-C	5.23	120.42	111.68
1	A	239	PRO	N-CA-C	-5.23	103.57	111.41
1	B	206	VAL	N-CA-C	-5.20	105.47	110.72
1	B	508	ILE	N-CA-C	5.07	117.39	111.05
1	B	572	VAL	N-CA-C	5.04	115.84	108.53
1	A	201	CYS	N-CA-C	5.04	117.43	111.33
1	B	58	ASP	N-CA-C	-5.01	103.44	110.50

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	5037	0	4964	98	0
1	B	5048	0	4977	114	0
2	A	1	0	0	0	0
2	B	1	0	0	0	0
3	A	26	0	16	2	0
3	B	26	0	16	2	0
4	A	473	0	0	12	0
4	B	438	0	0	9	0
All	All	11050	0	9973	201	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 10.

All (201) 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:440:LEU:HD12	1:B:440:LEU:HD12	1.33	1.06
1:B:282:GLN:NE2	1:B:282:GLN:HA	1.84	0.90
1:B:103:ARG:H	1:B:112:THR:HG22	1.36	0.90
1:B:592:GLN:HE22	1:B:597:ALA:H	1.20	0.90
1:A:592:GLN:HE22	1:A:597:ALA:H	1.11	0.89
1:B:592:GLN:NE2	1:B:597:ALA:H	1.70	0.88
1:A:64:ASN:HD22	1:A:64:ASN:H	1.18	0.88
1:B:227:LYS:HA	1:B:227:LYS:HE3	1.53	0.86
1:B:203:GLN:HE21	1:B:203:GLN:HA	1.40	0.86
1:A:282:GLN:NE2	1:A:282:GLN:HA	1.93	0.84
1:B:282:GLN:HA	1:B:282:GLN:HE21	1.42	0.83
1:B:64:ASN:H	1:B:64:ASN:HD22	1.26	0.80
1:A:602:VAL:HG22	1:A:652:LEU:HD12	1.62	0.80
1:A:353:ARG:HG2	1:A:382:LEU:HD12	1.65	0.79
1:A:592:GLN:NE2	1:A:597:ALA:H	1.81	0.79
1:B:602:VAL:HG22	1:B:652:LEU:HD12	1.67	0.77
1:A:64:ASN:H	1:A:64:ASN:ND2	1.81	0.76
1:A:254:LYS:HE2	4:A:1822:HOH:O	1.84	0.76
1:B:64:ASN:H	1:B:64:ASN:ND2	1.84	0.76
1:B:112:THR:HG23	1:B:449:SER:OG	1.85	0.75
1:A:613:GLU:HB2	4:A:2093:HOH:O	1.88	0.72
1:B:353:ARG:HD2	1:B:380:SER:O	1.88	0.72
1:B:64:ASN:HD22	1:B:64:ASN:N	1.83	0.70
1:B:602:VAL:CG2	1:B:652:LEU:HD12	2.21	0.69
1:A:120:ILE:HD11	1:A:153:CYS:HB3	1.74	0.69
1:A:64:ASN:HD22	1:A:64:ASN:N	1.80	0.68
1:A:282:GLN:HA	1:A:282:GLN:HE21	1.58	0.67
1:A:353:ARG:HD2	1:A:380:SER:O	1.96	0.66
1:A:602:VAL:CG2	1:A:652:LEU:HD12	2.25	0.66
1:B:204:LYS:HE2	1:B:208:MET:HE1	1.78	0.65
1:A:0:HIS:HA	4:A:2028:HOH:O	1.97	0.65
1:B:204:LYS:HG2	1:B:208:MET:HE2	1.79	0.64
1:A:204:LYS:HE2	1:A:208:MET:HE1	1.80	0.63
1:A:27:PRO:HB2	1:A:31:MET:HE2	1.80	0.63
1:B:46:LYS:HD3	1:B:54:TRP:CH2	2.34	0.62
1:A:84:MET:HG2	4:A:1981:HOH:O	1.99	0.62
1:A:611:GLY:O	1:A:614:LYS:HG2	1.98	0.62
1:B:204:LYS:HE2	1:B:208:MET:CE	2.30	0.62
1:A:613:GLU:OE1	1:B:613:GLU:O	2.18	0.62
1:B:238:LYS:O	1:B:240:LYS:HE2	1.99	0.62
1:A:46:LYS:HD3	1:A:54:TRP:CH2	2.35	0.62
1:A:440:LEU:HD12	1:B:440:LEU:CD1	2.21	0.62

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:641:THR:O	1:B:645:VAL:HG23	2.00	0.61
1:B:31:MET:HE3	1:B:249:GLY:HA2	1.82	0.61
1:B:204:LYS:HG2	1:B:208:MET:CE	2.31	0.60
1:B:27:PRO:HB2	1:B:31:MET:HE2	1.85	0.59
1:B:227:LYS:HE3	1:B:227:LYS:CA	2.31	0.59
1:A:174:ALA:HB3	1:A:395:SER:HB3	1.85	0.59
1:A:440:LEU:CD1	1:B:440:LEU:HD12	2.22	0.59
1:B:422:HIS:O	1:B:423:ASP:HB2	2.02	0.58
1:A:0:HIS:CD2	1:A:1:MET:H	2.21	0.58
1:B:647:ARG:NH1	1:B:651:GLU:OE1	2.37	0.58
1:A:643:GLU:H	1:A:643:GLU:CD	2.11	0.57
1:A:524:GLN:HB3	4:A:2087:HOH:O	2.05	0.57
1:B:592:GLN:HE22	1:B:597:ALA:N	1.96	0.57
1:B:102:GLU:HA	1:B:112:THR:HB	1.86	0.56
1:B:569:GLU:OE2	1:B:650:ARG:NH1	2.38	0.56
1:B:592:GLN:HG2	4:B:2900:HOH:O	2.05	0.56
1:A:545:LEU:HD13	1:A:599:VAL:HG11	1.88	0.56
1:B:545:LEU:HD23	1:B:545:LEU:H	1.69	0.56
1:A:103:ARG:O	1:A:104:PHE:HB2	2.06	0.56
1:B:544:ASP:HB3	4:B:3030:HOH:O	2.06	0.56
1:A:422:HIS:O	1:A:423:ASP:HB2	2.05	0.56
1:A:204:LYS:HE2	1:A:208:MET:CE	2.35	0.55
1:B:566:LEU:HD21	1:B:646:VAL:HG13	1.89	0.55
1:B:540:VAL:HB	1:B:574:VAL:HB	1.89	0.55
1:B:643:GLU:H	1:B:643:GLU:CD	2.16	0.54
1:B:62:MET:HG3	1:B:64:ASN:ND2	2.22	0.54
1:A:34:ALA:HB3	1:A:35:PRO:HD3	1.89	0.54
1:A:363:LEU:HD13	1:A:505:LEU:HD11	1.90	0.53
1:A:536:ALA:HB3	1:A:583:PHE:CD1	2.44	0.53
1:B:103:ARG:O	1:B:104:PHE:HB2	2.07	0.53
1:A:64:ASN:ND2	1:A:64:ASN:N	2.48	0.53
1:B:536:ALA:HB3	1:B:583:PHE:CD1	2.45	0.52
1:A:137:PHE:HB3	1:A:144:ILE:HD11	1.91	0.52
1:B:353:ARG:HG2	1:B:382:LEU:HD12	1.91	0.52
1:A:1:MET:HE1	1:A:294:VAL:HA	1.91	0.52
1:B:314:ALA:HB3	4:B:3096:HOH:O	2.08	0.52
1:B:508:ILE:HG13	1:B:509:HIS:CD2	2.44	0.52
1:A:196:SER:HA	1:B:172:HIS:CD2	2.45	0.52
1:A:540:VAL:HB	1:A:574:VAL:HB	1.92	0.52
1:B:137:PHE:HB3	1:B:144:ILE:HD11	1.91	0.51
1:A:603:SER:OG	1:A:619:HIS:HD2	1.93	0.51

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:120:ILE:HD11	1:B:153:CYS:HB3	1.92	0.51
1:B:545:LEU:HD23	1:B:545:LEU:N	2.25	0.51
1:A:204:LYS:HG2	1:A:208:MET:CE	2.41	0.51
1:A:31:MET:HE1	1:A:265:LEU:HD11	1.93	0.51
1:B:31:MET:CE	1:B:265:LEU:HD11	2.41	0.50
1:A:62:MET:HG3	1:A:64:ASN:ND2	2.27	0.50
1:A:14:LEU:O	1:A:18:ILE:HG13	2.12	0.50
1:A:292:ARG:HD2	4:A:1974:HOH:O	2.11	0.50
1:B:428:PHE:HA	1:B:454:ILE:O	2.11	0.50
1:A:132:HIS:HE1	4:A:1830:HOH:O	1.95	0.50
1:A:211:HIS:HB3	1:A:240:LYS:HG3	1.94	0.49
1:A:269:ASP:O	1:A:273:ILE:HG13	2.13	0.49
1:B:46:LYS:HE3	4:B:2757:HOH:O	2.12	0.49
1:B:371:MET:O	1:B:427:PRO:HA	2.13	0.49
1:A:68:CYS:HB3	1:A:101:PRO:HD3	1.93	0.49
1:A:461:SER:C	1:A:463:GLY:H	2.20	0.49
1:A:592:GLN:HG2	4:A:1860:HOH:O	2.12	0.49
1:B:142:TYR:CE2	1:B:315:LYS:HE3	2.48	0.49
1:B:477:VAL:HG21	1:B:607:TYR:CE1	2.47	0.49
1:B:542:VAL:HG13	1:B:543:PRO:HD2	1.93	0.49
1:A:508:ILE:HG13	1:A:509:HIS:ND1	2.28	0.48
1:B:328:VAL:HG12	1:B:332:ARG:CZ	2.42	0.48
1:A:428:PHE:CD1	1:A:428:PHE:C	2.92	0.48
1:A:613:GLU:HG2	1:B:665:ASN:ND2	2.29	0.48
1:B:508:ILE:HG12	4:B:3102:HOH:O	2.13	0.48
1:A:31:MET:CE	1:A:265:LEU:HD11	2.42	0.48
1:A:84:MET:SD	1:A:285:TYR:HB3	2.54	0.48
1:A:459:HIS:HB3	1:A:464:VAL:HG22	1.94	0.48
1:A:282:GLN:NE2	1:A:282:GLN:CA	2.70	0.47
1:B:373:GLY:HA2	1:B:402:TYR:CE1	2.49	0.47
1:B:545:LEU:H	1:B:545:LEU:CD2	2.27	0.47
1:B:545:LEU:HD22	4:B:3090:HOH:O	2.14	0.47
1:B:603:SER:OG	1:B:619:HIS:HD2	1.97	0.47
1:A:46:LYS:HE3	4:A:1709:HOH:O	2.14	0.47
1:A:475:GLU:OE1	1:A:475:GLU:N	2.46	0.47
1:B:112:THR:CG2	1:B:449:SER:OG	2.59	0.47
1:B:269:ASP:O	1:B:273:ILE:HG13	2.13	0.47
1:B:422:HIS:O	1:B:423:ASP:CB	2.61	0.47
1:A:1:MET:HE3	1:A:294:VAL:HG22	1.97	0.47
1:A:189:ILE:HD12	1:B:377:LEU:HD23	1.97	0.47
1:A:545:LEU:O	1:A:545:LEU:HD12	2.15	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:412:MET:O	1:B:416:LEU:HG	2.15	0.47
1:B:282:GLN:NE2	1:B:282:GLN:CA	2.66	0.47
1:A:238:LYS:O	1:A:240:LYS:HE2	2.15	0.46
1:B:336:PRO:O	1:B:339:TRP:HD1	1.98	0.46
1:B:232:ALA:O	1:B:240:LYS:HD2	2.15	0.46
1:A:27:PRO:C	1:A:30:PRO:HD2	2.41	0.46
1:A:204:LYS:HG2	1:A:208:MET:HE2	1.98	0.46
1:B:323:GLU:OE2	1:B:323:GLU:N	2.44	0.46
1:A:589:THR:HG23	4:A:1944:HOH:O	2.16	0.46
1:B:1:MET:HE2	1:B:297:MET:SD	2.56	0.46
1:B:203:GLN:HE21	1:B:203:GLN:CA	2.17	0.46
1:A:422:HIS:O	1:A:423:ASP:CB	2.64	0.46
1:B:347:SER:OG	1:B:348:SER:N	2.43	0.46
1:A:461:SER:C	1:A:463:GLY:N	2.72	0.45
1:B:176:GLU:O	1:B:240:LYS:NZ	2.46	0.45
1:A:283:LYS:NZ	4:A:1940:HOH:O	2.50	0.45
1:A:411:ALA:O	1:A:415:ILE:HG13	2.17	0.45
1:B:370:LEU:O	1:B:401:ARG:HD2	2.17	0.45
1:B:150:TYR:OH	1:B:233:LYS:HD3	2.17	0.45
1:B:577:MET:SD	1:B:580:GLN:HG2	2.57	0.45
1:A:186:TYR:C	1:A:193:THR:HG23	2.41	0.45
1:A:372:GLY:HA3	1:A:428:PHE:CE2	2.52	0.45
1:A:372:GLY:HA3	1:A:428:PHE:CZ	2.51	0.44
1:B:261:HIS:CE1	3:B:2671:TPP:H71	2.53	0.44
1:B:434:ASN:HB2	1:B:473:PRO:HG3	2.00	0.44
1:B:165:GLU:HB2	1:B:411:ALA:HB2	2.00	0.44
1:B:205:TYR:CD2	1:B:208:MET:HE3	2.53	0.44
1:A:434:ASN:HB2	1:A:473:PRO:HG3	1.99	0.44
1:B:68:CYS:HB3	1:B:101:PRO:HD3	1.99	0.44
1:B:132:HIS:HE1	4:B:2869:HOH:O	2.00	0.44
1:A:1:MET:HE3	1:A:1:MET:HA	2.00	0.43
3:A:1671:TPP:H7'1	1:B:377:LEU:HD21	2.00	0.43
1:A:407:VAL:HG12	1:B:160:GLU:OE2	2.17	0.43
1:B:642:VAL:HG23	4:B:2777:HOH:O	2.18	0.43
1:A:101:PRO:O	1:A:112:THR:HG23	2.18	0.43
1:B:222:TYR:O	1:B:226:ARG:HG3	2.19	0.43
1:B:280:ASP:OD1	1:B:282:GLN:HB2	2.18	0.43
1:A:261:HIS:ND1	3:A:1671:TPP:O3B	2.49	0.43
1:B:31:MET:HE1	1:B:265:LEU:HD11	2.00	0.43
1:B:189:ILE:HG13	3:B:2671:TPP:H62	2.00	0.43
1:B:144:ILE:HG13	1:B:145:VAL:HG23	2.00	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:31:MET:HE1	1:A:265:LEU:HD21	1.99	0.43
1:B:2:ALA:HB1	1:B:6:LYS:HD3	2.01	0.43
1:B:428:PHE:C	1:B:428:PHE:CD1	2.96	0.43
1:A:371:MET:O	1:A:427:PRO:HA	2.18	0.43
1:A:598:GLY:C	1:A:661:ALA:HB3	2.44	0.42
1:A:601:VAL:HB	1:A:616:SER:HA	2.01	0.42
1:B:134:ALA:HA	1:B:145:VAL:HB	2.01	0.42
1:B:592:GLN:NE2	1:B:596:PRO:HA	2.34	0.42
1:A:440:LEU:HD23	1:A:440:LEU:HA	1.84	0.42
1:B:84:MET:SD	1:B:285:TYR:HB3	2.59	0.42
1:A:343:LEU:HA	1:A:344:PRO:HD3	1.79	0.42
1:B:566:LEU:CD2	1:B:646:VAL:HG13	2.50	0.42
1:B:598:GLY:C	1:B:661:ALA:HB3	2.44	0.42
1:A:165:GLU:HB2	1:A:411:ALA:HB2	2.02	0.42
1:A:614:LYS:HA	1:B:613:GLU:OE2	2.20	0.41
1:B:433:LEU:HA	1:B:457:ALA:HB1	2.02	0.41
1:A:93:ASP:HB2	1:B:633:VAL:HG11	2.02	0.41
1:A:472:GLN:HA	1:A:473:PRO:HD3	1.92	0.41
1:B:343:LEU:HA	1:B:344:PRO:HD3	1.80	0.41
1:B:462:ILE:C	1:B:464:VAL:N	2.77	0.41
1:A:160:GLU:OE2	1:B:407:VAL:HG12	2.20	0.41
1:A:542:VAL:HG13	1:A:543:PRO:HD2	2.03	0.41
1:A:287:VAL:HG12	1:A:292:ARG:HG3	2.02	0.41
1:B:227:LYS:HA	1:B:227:LYS:CE	2.37	0.41
1:A:55:VAL:HG22	1:A:309:TRP:CH2	2.55	0.41
1:B:27:PRO:O	1:B:31:MET:HG3	2.21	0.41
1:A:327:PHE:O	1:A:331:MET:HG2	2.21	0.41
1:A:459:HIS:HB3	1:A:464:VAL:CG2	2.51	0.40
1:B:101:PRO:HB2	4:B:2786:HOH:O	2.20	0.40
1:B:328:VAL:HG12	1:B:332:ARG:NH2	2.36	0.40
1:B:550:VAL:O	1:B:603:SER:HA	2.21	0.40
1:B:55:VAL:HB	1:B:331:MET:HE2	2.01	0.40
1:A:368:PRO:HG2	4:A:1829:HOH:O	2.20	0.40
1:A:477:VAL:HG21	1:A:607:TYR:CE1	2.57	0.40
1:B:142:TYR:CE2	1:B:316:TYR:HA	2.56	0.40
1:B:571:ARG:HG3	1:B:571:ARG:HH11	1.86	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	668/673 (99%)	639 (96%)	26 (4%)	3 (0%)	30	33
1	B	669/673 (99%)	642 (96%)	24 (4%)	3 (0%)	30	33
All	All	1337/1346 (99%)	1281 (96%)	50 (4%)	6 (0%)	30	33

All (6) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	423	ASP
1	A	658	ASP
1	B	423	ASP
1	B	658	ASP
1	A	196	SER
1	B	347	SER

5.3.2 Protein sidechains [i](#)

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	530/533 (99%)	524 (99%)	6 (1%)	65	78
1	B	531/533 (100%)	523 (98%)	8 (2%)	57	71
All	All	1061/1066 (100%)	1047 (99%)	14 (1%)	61	75

All (14) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	64	ASN
1	A	240	LYS
1	A	282	GLN
1	A	613	GLU
1	A	643	GLU
1	A	658	ASP
1	B	64	ASN
1	B	112	THR
1	B	203	GLN
1	B	227	LYS
1	B	240	LYS
1	B	282	GLN
1	B	613	GLU
1	B	643	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (22) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	0	HIS
1	A	64	ASN
1	A	132	HIS
1	A	282	GLN
1	A	330	GLN
1	A	434	ASN
1	A	450	HIS
1	A	487	GLN
1	A	520	ASN
1	A	592	GLN
1	A	619	HIS
1	B	64	ASN
1	B	71	GLN
1	B	122	ASN
1	B	203	GLN
1	B	282	GLN
1	B	330	GLN
1	B	358	ASN
1	B	487	GLN
1	B	509	HIS
1	B	592	GLN
1	B	619	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 oligosaccharides in this entry.

5.6 Ligand geometry ⓘ

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	A	1671	2	26,27,27	1.71	7 (26%)	38,40,40	1.61	9 (23%)
3	TPP	B	2671	2	26,27,27	1.75	7 (26%)	38,40,40	1.61	10 (26%)

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	1671	2	-	6/17/17/17	0/2/2/2
3	TPP	B	2671	2	-	6/17/17/17	0/2/2/2

All (14) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	2671	TPP	C4'-N3'	4.39	1.40	1.35

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	1671	TPP	C4'-N3'	4.34	1.40	1.35
3	A	1671	TPP	C4-N3	-3.08	1.33	1.39
3	B	2671	TPP	C7'-N3	2.82	1.54	1.48
3	B	2671	TPP	C4-N3	-2.73	1.34	1.39
3	B	2671	TPP	PA-O3A	2.68	1.62	1.59
3	A	1671	TPP	C6'-N1'	2.59	1.39	1.34
3	B	2671	TPP	C6'-N1'	2.52	1.39	1.34
3	A	1671	TPP	C7'-N3	2.48	1.53	1.48
3	B	2671	TPP	PA-O2A	-2.29	1.44	1.55
3	A	1671	TPP	PA-O2A	-2.19	1.45	1.55
3	A	1671	TPP	PA-O3A	2.19	1.61	1.59
3	B	2671	TPP	PB-O2B	-2.10	1.47	1.54
3	A	1671	TPP	PB-O2B	-2.05	1.47	1.54

All (19) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	1671	TPP	O2A-PA-O3A	-3.54	97.71	107.27
3	B	2671	TPP	O3A-PB-O1B	-3.27	93.85	111.04
3	B	2671	TPP	O2A-PA-O3A	-3.21	98.61	107.27
3	A	1671	TPP	O3A-PB-O1B	-3.06	94.95	111.04
3	A	1671	TPP	C2-S1-C5	-2.97	89.25	91.22
3	B	2671	TPP	N1'-C2'-N3'	-2.91	120.69	125.53
3	A	1671	TPP	N1'-C2'-N3'	-2.91	120.69	125.53
3	B	2671	TPP	O2A-PA-O7	-2.79	94.92	107.57
3	A	1671	TPP	O2A-PA-O7	-2.70	95.35	107.57
3	B	2671	TPP	C6'-N1'-C2'	2.68	120.48	116.07
3	A	1671	TPP	C6'-N1'-C2'	2.65	120.42	116.07
3	B	2671	TPP	C2-S1-C5	-2.52	89.55	91.22
3	A	1671	TPP	O7-PA-O1A	2.36	118.28	108.94
3	B	2671	TPP	CM2-C2'-N3'	2.34	120.63	117.13
3	A	1671	TPP	CM2-C2'-N3'	2.29	120.56	117.13
3	B	2671	TPP	O7-PA-O1A	2.27	117.92	108.94
3	B	2671	TPP	O3B-PB-O1B	2.21	119.47	110.83
3	A	1671	TPP	O3B-PB-O1B	2.20	119.41	110.83
3	B	2671	TPP	O3B-PB-O3A	2.10	111.68	104.64

There are no chirality outliers.

All (12) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	1671	TPP	C7-O7-PA-O1A

Continued on next page...

Continued from previous page...

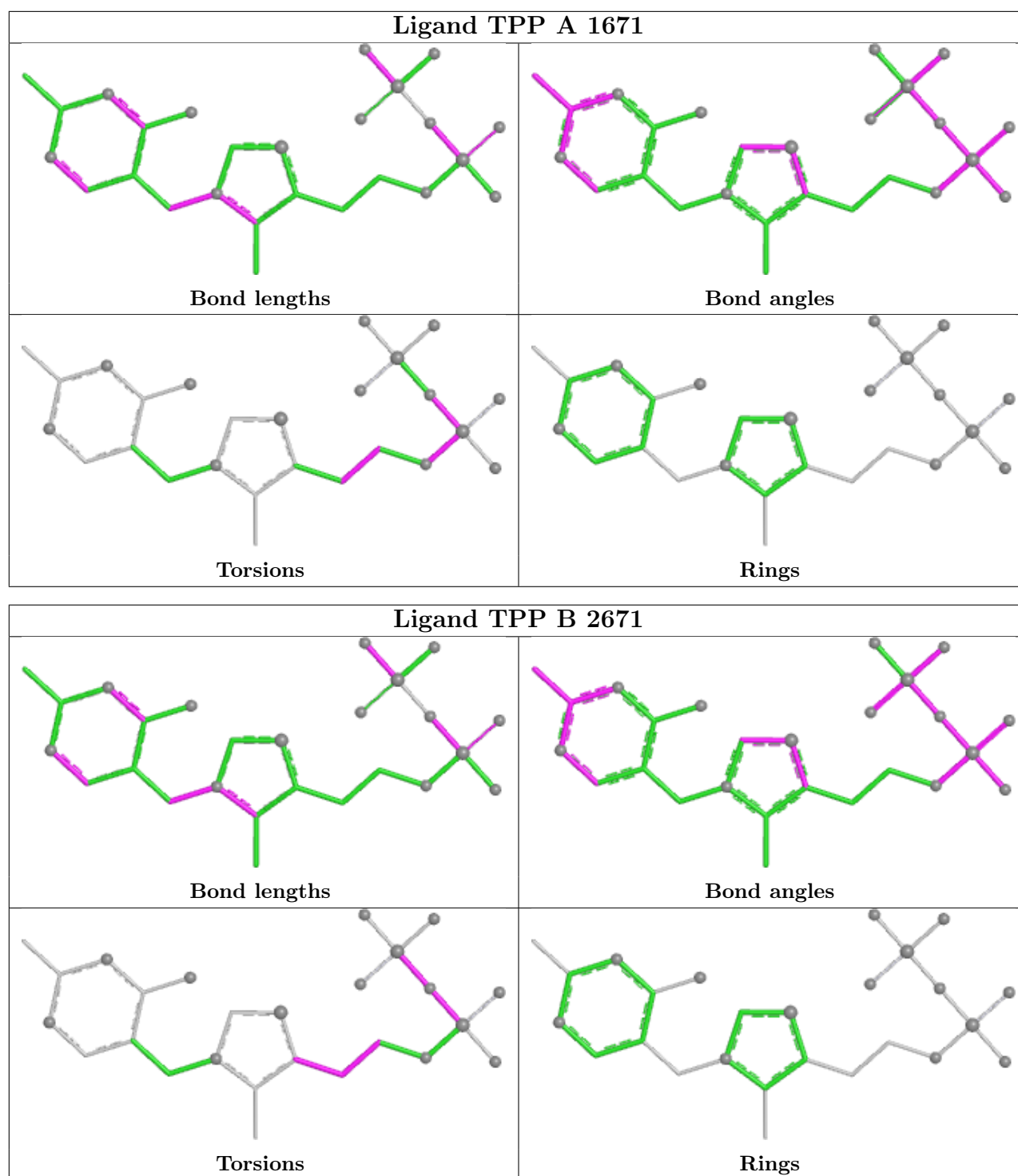
Mol	Chain	Res	Type	Atoms
3	A	1671	TPP	C7-O7-PA-O2A
3	A	1671	TPP	C7-O7-PA-O3A
3	A	1671	TPP	PB-O3A-PA-O7
3	B	2671	TPP	PA-O3A-PB-O3B
3	B	2671	TPP	PB-O3A-PA-O7
3	A	1671	TPP	C5-C6-C7-O7
3	B	2671	TPP	C5-C6-C7-O7
3	B	2671	TPP	PA-O3A-PB-O1B
3	B	2671	TPP	PB-O3A-PA-O1A
3	A	1671	TPP	PB-O3A-PA-O1A
3	B	2671	TPP	S1-C5-C6-C7

There are no ring outliers.

2 monomers are involved in 4 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	1671	TPP	2	0
3	B	2671	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 ⓘ

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	670/673 (99%)	-0.40	5 (0%)	84 83	7, 18, 35, 53	0
1	B	671/673 (99%)	-0.41	2 (0%)	90 89	9, 19, 36, 49	0
All	All	1341/1346 (99%)	-0.40	7 (0%)	87 86	7, 19, 36, 53	0

All (7) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	0	HIS	3.8
1	A	282	GLN	2.8
1	B	669	SER	2.8
1	B	658	ASP	2.4
1	A	1	MET	2.4
1	A	567	SER	2.3
1	A	613	GLU	2.2

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](#)

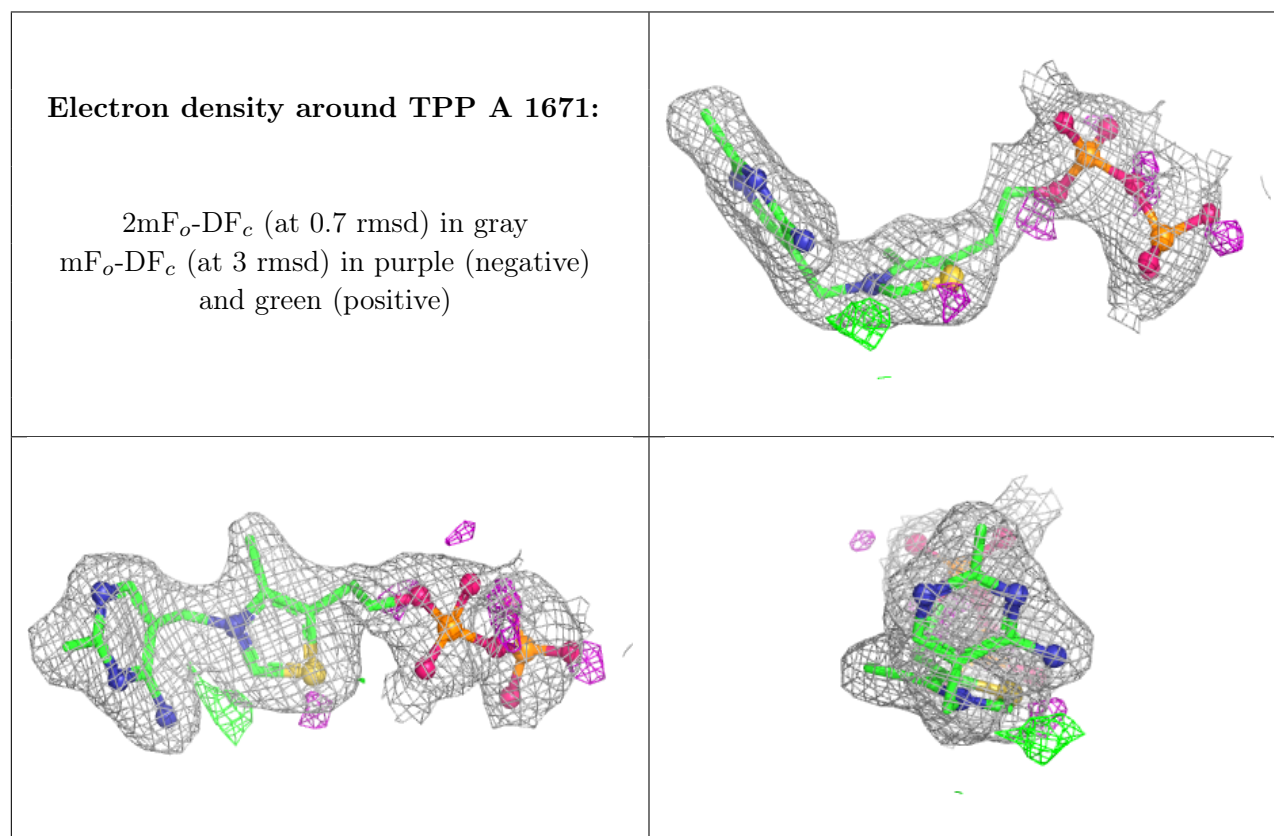
There are no oligosaccharides in this entry.

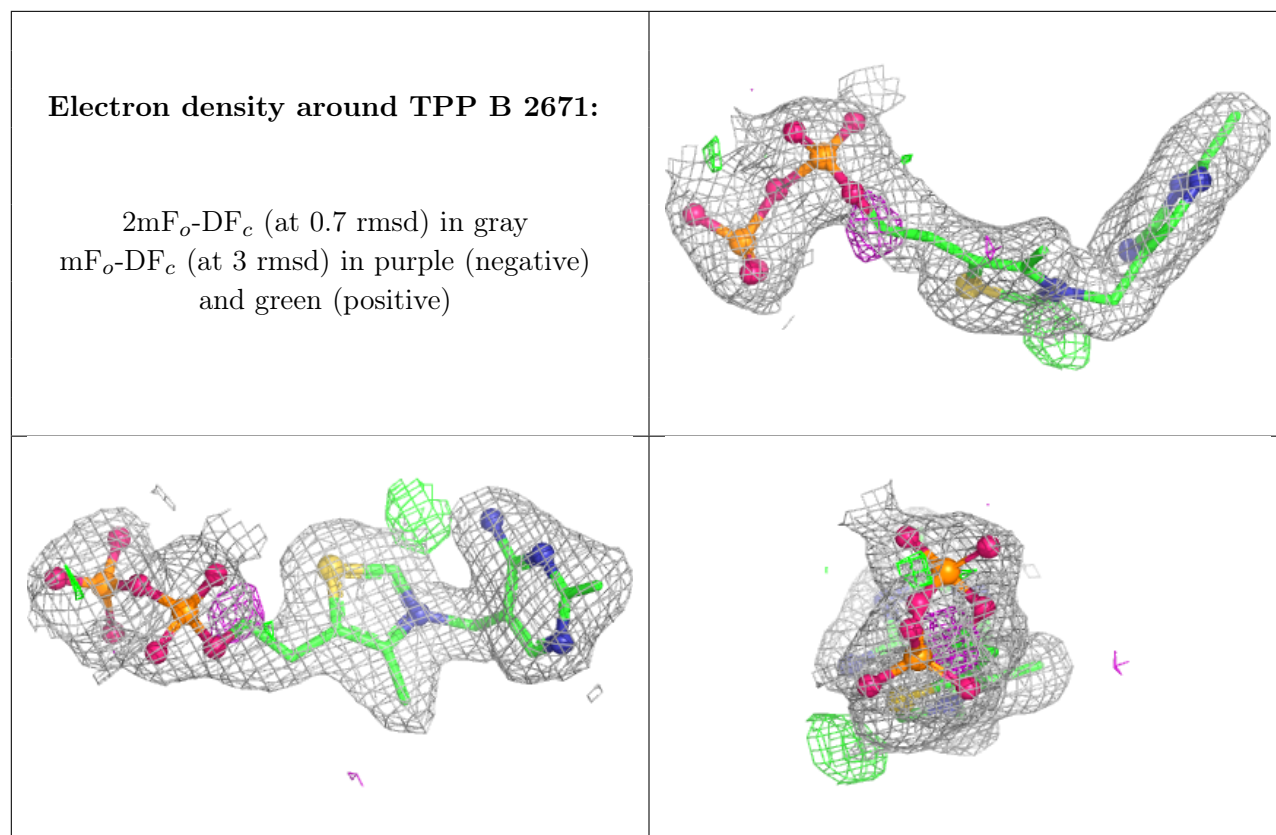
6.4 Ligands [i](#)

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($\text{\AA}^2$)	Q<0.9
2	CA	B	2670	1/1	0.89	0.07	38,38,38,38	0
3	TPP	A	1671	26/26	0.94	0.08	13,27,35,36	0
2	CA	A	1670	1/1	0.95	0.06	38,38,38,38	0
3	TPP	B	2671	26/26	0.95	0.07	15,25,31,33	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.