



# Full wwPDB X-ray Structure Validation Report ⓘ

May 30, 2020 – 02:49 pm BST

PDB ID : 1TRK  
Title : REFINED STRUCTURE OF TRANSKETOLASE FROM SACCHAROMYCES CEREVISIAE AT 2.0 ANGSTROMS RESOLUTION  
Authors : Lindqvist, Y.; Schneider, G.; Nikkola, M.  
Deposited on : 1993-11-22  
Resolution : 2.00 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](mailto: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.

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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) : **NOT EXECUTED**  
EDS : **NOT EXECUTED**  
buster-report : 1.1.7 (2018)  
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.11

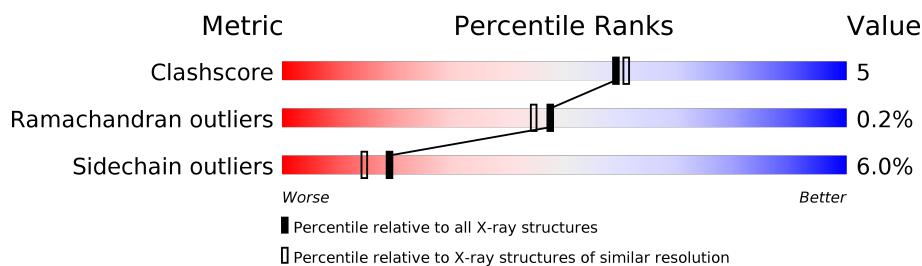
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.00 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	141614	9178 (2.00-2.00)
Ramachandran outliers	138981	9054 (2.00-2.00)
Sidechain outliers	138945	9053 (2.00-2.00)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 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  $\leq 5\%$ .

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	680	 79% 17% . .
1	B	680	 85% 11% . .

## 2 Entry composition [i](#)

There are 4 unique types of molecules in this entry. The entry contains 11471 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.

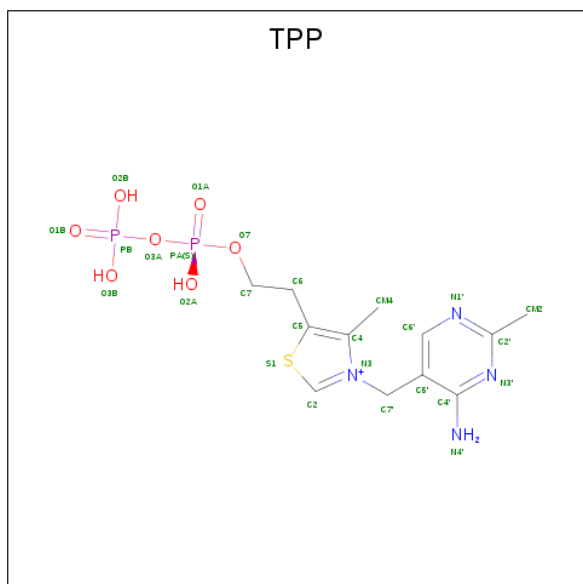
- Molecule 1 is a protein called TRANSKETOLASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	678	Total	C	N	O	S	0	0	0
			5198	3312	884	990	12			
1	B	678	Total	C	N	O	S	0	0	0
			5198	3312	884	990	12			

- Molecule 2 is CALCIUM ION (three-letter code: CA) (formula: Ca).

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

- Molecule 3 is THIAMINE DIPHOSPHATE (three-letter code: TPP) (formula: C<sub>12</sub>H<sub>19</sub>N<sub>4</sub>O<sub>7</sub>P<sub>2</sub>S).



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.

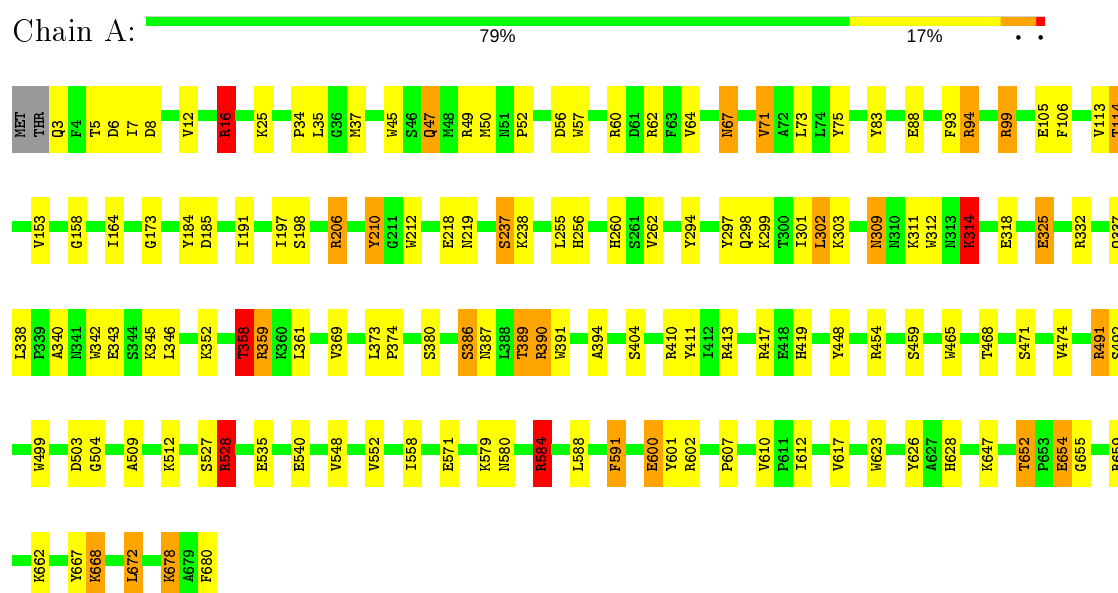
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	473	Total	O	0	0
			473	473		
4	B	548	Total	O	0	0
			548	548		

### 3 Residue-property plots [i](#)

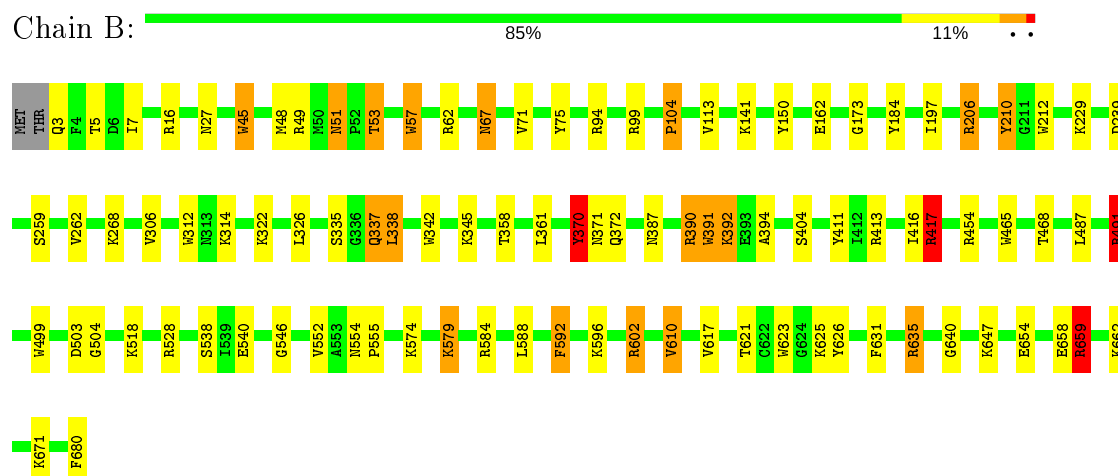
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry. Residues are color-coded according 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. 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.

Note EDS was not executed.

#### • Molecule 1: TRANSKETOLASE



#### • Molecule 1: TRANSKETOLASE



## 4 Data and refinement statistics

Xtriage (Phenix) and EDS were not executed - this section is therefore incomplete.

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	76.30 Å 113.30 Å 160.90 Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	(Not available) – 2.00	Depositor
% Data completeness (in resolution range)	(Not available) ((Not available)-2.00)	Depositor
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
Refinement program	X-PLOR	Depositor
R, $R_{free}$	0.157 , (Not available)	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	11471	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	18.0	wwPDB-VP

## 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	0.86	4/5324 (0.1%)	1.59	86/7230 (1.2%)
1	B	0.87	1/5324 (0.0%)	1.62	68/7230 (0.9%)
All	All	0.86	5/10648 (0.0%)	1.60	154/14460 (1.1%)

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	2
1	B	0	1
All	All	0	3

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	237	SER	CA-CB	7.32	1.64	1.52
1	A	237	SER	CB-OG	7.13	1.51	1.42
1	A	535	GLU	CD-OE2	7.05	1.33	1.25
1	B	540	GLU	CB-CG	-6.79	1.39	1.52
1	A	88	GLU	CA-CB	-5.06	1.42	1.53

All (154) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	491	ARG	NE-CZ-NH1	25.59	133.09	120.30
1	B	491	ARG	NE-CZ-NH2	-17.77	111.41	120.30
1	B	635	ARG	NE-CZ-NH1	16.41	128.50	120.30
1	A	16	ARG	NE-CZ-NH1	-12.50	114.05	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	659	ARG	CG-CD-NE	-11.01	88.67	111.80
1	B	659	ARG	NH1-CZ-NH2	-10.97	107.33	119.40
1	A	99	ARG	NE-CZ-NH1	10.71	125.65	120.30
1	B	417	ARG	NE-CZ-NH1	10.60	125.60	120.30
1	B	635	ARG	NE-CZ-NH2	-10.08	115.26	120.30
1	A	94	ARG	NE-CZ-NH1	9.87	125.23	120.30
1	B	391	TRP	CD1-CG-CD2	9.56	113.95	106.30
1	A	391	TRP	CD1-CG-CD2	9.34	113.77	106.30
1	A	16	ARG	NE-CZ-NH2	9.32	124.96	120.30
1	B	602	ARG	NE-CZ-NH1	9.32	124.96	120.30
1	B	623	TRP	CD1-CG-CD2	9.30	113.74	106.30
1	B	659	ARG	NE-CZ-NH1	-9.23	115.69	120.30
1	A	391	TRP	CE2-CD2-CG	-8.82	100.24	107.30
1	A	623	TRP	CD1-CG-CD2	8.77	113.32	106.30
1	A	45	TRP	CG-CD2-CE3	8.71	141.74	133.90
1	A	16	ARG	NH1-CZ-NH2	-8.54	110.00	119.40
1	B	99	ARG	NE-CZ-NH2	-8.54	116.03	120.30
1	A	359	ARG	NE-CZ-NH2	-8.48	116.06	120.30
1	B	659	ARG	CB-CG-CD	8.47	133.62	111.60
1	B	57	TRP	CD1-CG-CD2	8.28	112.92	106.30
1	A	465	TRP	CD1-CG-CD2	8.26	112.91	106.30
1	B	465	TRP	CD1-CG-CD2	8.21	112.86	106.30
1	B	626	TYR	CB-CG-CD2	-8.15	116.11	121.00
1	B	62	ARG	NE-CZ-NH1	8.14	124.37	120.30
1	A	410	ARG	NE-CZ-NH1	7.99	124.30	120.30
1	A	391	TRP	CG-CD2-CE3	7.95	141.05	133.90
1	A	342	TRP	CD1-CG-CD2	7.87	112.60	106.30
1	A	45	TRP	CE2-CD2-CG	-7.87	101.01	107.30
1	A	584	ARG	NE-CZ-NH2	-7.84	116.38	120.30
1	A	16	ARG	CG-CD-NE	-7.81	95.39	111.80
1	A	45	TRP	CD1-CG-CD2	7.75	112.50	106.30
1	A	623	TRP	CE2-CD2-CG	-7.75	101.10	107.30
1	B	391	TRP	CE2-CD2-CG	-7.75	101.10	107.30
1	B	370	TYR	CB-CG-CD1	-7.74	116.36	121.00
1	A	312	TRP	CD1-CG-CD2	7.73	112.48	106.30
1	B	465	TRP	CE2-CD2-CG	-7.64	101.19	107.30
1	B	491	ARG	CD-NE-CZ	7.64	134.30	123.60
1	B	499	TRP	CD1-CG-CD2	7.62	112.39	106.30
1	B	45	TRP	CD1-CG-CD2	7.61	112.39	106.30
1	B	342	TRP	CD1-CG-CD2	7.54	112.33	106.30
1	A	417	ARG	NE-CZ-NH1	7.50	124.05	120.30
1	A	49	ARG	CB-CG-CD	-7.43	92.29	111.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	49	ARG	NE-CZ-NH1	7.41	124.01	120.30
1	A	499	TRP	CD1-CG-CD2	7.38	112.21	106.30
1	B	57	TRP	CE2-CD2-CG	-7.32	101.44	107.30
1	A	262	VAL	CG1-CB-CG2	-7.29	99.23	110.90
1	A	332	ARG	NE-CZ-NH2	-7.26	116.67	120.30
1	A	465	TRP	CE2-CD2-CG	-7.22	101.52	107.30
1	B	491	ARG	CB-CG-CD	7.19	130.30	111.60
1	A	659	ARG	NE-CZ-NH1	7.16	123.88	120.30
1	B	342	TRP	CE2-CD2-CG	-7.13	101.59	107.30
1	B	45	TRP	CE2-CD2-CG	-7.12	101.60	107.30
1	A	499	TRP	CE2-CD2-CG	-7.11	101.61	107.30
1	A	358	THR	N-CA-CB	-7.09	96.82	110.30
1	A	184	TYR	CB-CG-CD2	-7.04	116.78	121.00
1	B	312	TRP	CD1-CG-CD2	7.02	111.91	106.30
1	B	212	TRP	CD1-CG-CD2	6.97	111.88	106.30
1	B	312	TRP	CE2-CD2-CG	-6.95	101.74	107.30
1	B	391	TRP	CG-CD1-NE1	-6.94	103.16	110.10
1	A	312	TRP	CE2-CD2-CG	-6.82	101.84	107.30
1	A	528	ARG	NE-CZ-NH1	6.82	123.71	120.30
1	B	206	ARG	NE-CZ-NH1	6.79	123.70	120.30
1	B	654	GLU	CA-CB-CG	-6.79	98.46	113.40
1	B	417	ARG	NH1-CZ-NH2	-6.78	111.95	119.40
1	A	57	TRP	CD1-CG-CD2	6.77	111.72	106.30
1	A	491	ARG	NE-CZ-NH1	6.71	123.66	120.30
1	A	237	SER	CA-CB-OG	6.69	129.26	111.20
1	B	623	TRP	CE2-CD2-CG	-6.65	101.98	107.30
1	A	206	ARG	NE-CZ-NH1	6.57	123.59	120.30
1	B	212	TRP	CE2-CD2-CG	-6.54	102.06	107.30
1	B	499	TRP	CE2-CD2-CG	-6.54	102.07	107.30
1	A	212	TRP	CD1-CG-CD2	6.48	111.49	106.30
1	A	623	TRP	CG-CD1-NE1	-6.48	103.62	110.10
1	B	454	ARG	NE-CZ-NH2	-6.42	117.09	120.30
1	B	239	ASP	CB-CG-OD1	6.41	124.07	118.30
1	B	659	ARG	NE-CZ-NH2	6.39	123.50	120.30
1	A	212	TRP	CE2-CD2-CG	-6.37	102.21	107.30
1	A	88	GLU	N-CA-CB	6.34	122.01	110.60
1	B	413	ARG	NE-CZ-NH1	6.32	123.46	120.30
1	A	57	TRP	CE2-CD2-CG	-6.30	102.26	107.30
1	A	503	ASP	CB-CG-OD1	6.29	123.96	118.30
1	B	610	VAL	CB-CA-C	-6.28	99.48	111.40
1	A	623	TRP	CG-CD2-CE3	6.27	139.54	133.90
1	A	60	ARG	NE-CZ-NH1	6.21	123.41	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	626	TYR	CB-CG-CD2	-6.20	117.28	121.00
1	A	342	TRP	CE2-CD2-CG	-6.17	102.36	107.30
1	A	94	ARG	CD-NE-CZ	6.07	132.10	123.60
1	B	623	TRP	CG-CD1-NE1	-6.06	104.04	110.10
1	A	410	ARG	NE-CZ-NH2	-6.06	117.27	120.30
1	B	584	ARG	NE-CZ-NH2	-6.04	117.28	120.30
1	B	3	GLN	N-CA-C	6.03	127.27	111.00
1	A	47	GLN	N-CA-CB	-6.02	99.77	110.60
1	A	83	TYR	CB-CG-CD2	-6.01	117.39	121.00
1	A	49	ARG	NE-CZ-NH2	-5.99	117.31	120.30
1	A	71	VAL	CB-CA-C	-5.95	100.10	111.40
1	A	337	GLN	CA-CB-CG	5.85	126.28	113.40
1	A	332	ARG	NE-CZ-NH1	5.84	123.22	120.30
1	A	47	GLN	CG-CD-NE2	5.83	130.69	116.70
1	A	389	THR	N-CA-CB	-5.82	99.24	110.30
1	B	3	GLN	CG-CD-NE2	5.78	130.57	116.70
1	A	391	TRP	CB-CG-CD1	-5.77	119.50	127.00
1	A	342	TRP	CG-CD1-NE1	-5.74	104.36	110.10
1	A	602	ARG	NE-CZ-NH2	-5.67	117.46	120.30
1	A	312	TRP	CG-CD1-NE1	-5.67	104.43	110.10
1	A	314	LYS	CA-CB-CG	5.63	125.80	113.40
1	B	592	PHE	CB-CG-CD1	-5.62	116.86	120.80
1	A	47	GLN	CA-CB-CG	5.60	125.72	113.40
1	A	294	TYR	CB-CG-CD2	-5.56	117.67	121.00
1	A	413	ARG	NE-CZ-NH2	-5.55	117.52	120.30
1	A	579	LYS	CG-CD-CE	-5.54	95.27	111.90
1	A	45	TRP	CB-CG-CD1	-5.52	119.83	127.00
1	A	62	ARG	CB-CG-CD	-5.50	97.30	111.60
1	A	345	LYS	CA-CB-CG	-5.50	101.30	113.40
1	A	153	VAL	CB-CA-C	-5.50	100.95	111.40
1	B	184	TYR	CB-CG-CD2	-5.48	117.71	121.00
1	A	99	ARG	NH1-CZ-NH2	-5.46	113.40	119.40
1	A	454	ARG	NE-CZ-NH1	5.45	123.03	120.30
1	A	309	ASN	CB-CG-ND2	5.43	129.72	116.70
1	B	75	TYR	CB-CG-CD2	-5.40	117.76	121.00
1	A	210	TYR	CB-CG-CD2	-5.39	117.77	121.00
1	B	503	ASP	CB-CG-OD1	5.37	123.13	118.30
1	B	45	TRP	CG-CD2-CE3	5.34	138.70	133.90
1	A	448	TYR	CB-CG-CD2	-5.32	117.81	121.00
1	B	579	LYS	CA-CB-CG	5.32	125.10	113.40
1	B	491	ARG	CG-CD-NE	-5.31	100.64	111.80
1	B	150	TYR	CB-CG-CD1	-5.31	117.81	121.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	64	VAL	CG1-CB-CG2	-5.30	102.42	110.90
1	B	342	TRP	CG-CD1-NE1	-5.27	104.83	110.10
1	B	53	THR	OG1-CB-CG2	5.27	122.12	110.00
1	B	16	ARG	NE-CZ-NH2	-5.25	117.68	120.30
1	B	57	TRP	CG-CD1-NE1	-5.24	104.86	110.10
1	B	338	LEU	CA-CB-CG	5.21	127.30	115.30
1	B	390	ARG	NE-CZ-NH2	-5.20	117.70	120.30
1	A	591	PHE	CB-CG-CD2	-5.19	117.17	120.80
1	A	413	ARG	NE-CZ-NH1	5.17	122.89	120.30
1	B	27	ASN	CB-CG-ND2	5.17	129.10	116.70
1	B	335	SER	CA-C-N	5.16	126.53	116.20
1	A	45	TRP	CG-CD1-NE1	-5.16	104.94	110.10
1	A	499	TRP	CG-CD2-CE3	5.16	138.54	133.90
1	A	75	TYR	CB-CG-CD2	-5.15	117.91	121.00
1	A	340	ALA	CA-C-N	-5.14	105.89	117.20
1	A	465	TRP	CG-CD1-NE1	-5.13	104.97	110.10
1	B	3	GLN	OE1-CD-NE2	-5.13	110.10	121.90
1	A	56	ASP	CB-CG-OD1	5.10	122.89	118.30
1	B	210	TYR	CB-CG-CD2	-5.09	117.94	121.00
1	B	631	PHE	CB-CG-CD2	-5.08	117.25	120.80
1	A	219	ASN	OD1-CG-ND2	-5.07	110.25	121.90
1	B	94	ARG	NE-CZ-NH1	5.07	122.83	120.30
1	A	237	SER	CA-C-N	5.05	128.31	117.20
1	B	680	PHE	N-CA-C	5.02	124.56	111.00

There are no chirality outliers.

All (3) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	16	ARG	Sidechain
1	A	99	ARG	Sidechain
1	B	659	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	5198	0	5139	64	1
1	B	5198	0	5139	39	0
2	A	1	0	0	0	0
2	B	1	0	0	0	0
3	A	26	0	16	1	0
3	B	26	0	16	2	0
4	A	473	0	0	9	2
4	B	548	0	0	5	1
All	All	11471	0	10310	98	2

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 5.

All (98) 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:164:ILE:HD12	1:A:419:HIS:CD2	2.01	0.96
1:A:652:THR:HG22	1:A:655:GLY:H	1.45	0.81
1:A:528:ARG:HD3	4:A:853:HOH:O	1.86	0.75
1:A:206:ARG:HG3	1:B:206:ARG:HG3	1.69	0.74
1:B:554:ASN:HB3	4:B:790:HOH:O	1.89	0.72
1:A:67:ASN:H	1:A:67:ASN:HD22	1.36	0.71
1:A:389:THR:HG23	1:A:411:TYR:OH	1.90	0.71
1:A:358:THR:HG21	4:A:755:HOH:O	1.94	0.67
1:B:51:ASN:HD21	1:B:53:THR:HB	1.61	0.66
1:A:298:GLN:HE21	1:A:303:LYS:HE3	1.63	0.64
1:B:51:ASN:ND2	1:B:53:THR:HB	2.13	0.63
1:A:647:LYS:NZ	1:A:647:LYS:HB3	2.14	0.62
1:A:198:SER:O	1:B:417:ARG:NH2	2.33	0.62
1:A:652:THR:HG22	1:A:655:GLY:N	2.13	0.61
1:A:358:THR:HG22	1:A:527:SER:H	1.65	0.61
1:A:164:ILE:HD12	1:A:419:HIS:NE2	2.16	0.60
1:A:106:PHE:H	1:A:114:THR:HG22	1.66	0.59
1:B:392:LYS:HA	1:B:392:LYS:NZ	2.17	0.59
1:B:392:LYS:HA	1:B:392:LYS:HZ2	1.67	0.59
1:A:311:LYS:O	1:A:314:LYS:HG3	2.03	0.59
1:B:49:ARG:HE	1:B:57:TRP:HH2	1.51	0.58
1:A:105:GLU:HA	1:A:114:THR:HB	1.86	0.57
1:B:67:ASN:H	1:B:67:ASN:HD22	1.53	0.56
1:A:67:ASN:ND2	1:A:67:ASN:H	2.01	0.56
1:B:370:TYR:HE2	4:B:1146:HOH:O	1.89	0.56
1:B:5:THR:OG1	1:B:7:ILE:HG22	2.06	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:260:HIS:HD2	4:A:724:HOH:O	1.89	0.55
1:A:667:TYR:HB3	1:A:672:LEU:HD11	1.89	0.54
1:A:387:ASN:HA	1:A:468:THR:HG21	1.87	0.54
1:B:546:GLY:HA3	1:B:588:LEU:HD12	1.91	0.53
1:B:391:TRP:CD1	1:B:394:ALA:HB2	2.43	0.53
1:A:612:ILE:H	1:A:628:HIS:HD2	1.57	0.53
1:B:259:SER:O	1:B:262:VAL:HG22	2.09	0.52
1:B:67:ASN:H	1:B:67:ASN:ND2	2.08	0.52
1:B:658:GLU:O	1:B:662:LYS:HG2	2.11	0.51
1:B:337:GLN:HG2	4:B:1128:HOH:O	2.10	0.51
1:B:538:SER:HB2	4:B:1160:HOH:O	2.11	0.51
1:B:345:LYS:CE	1:B:372:GLN:HB2	2.42	0.50
1:A:548:VAL:HG13	1:A:584:ARG:HD2	1.94	0.49
1:A:256:HIS:HE1	4:A:716:HOH:O	1.94	0.49
1:B:487:LEU:O	1:B:491:ARG:HG2	2.12	0.48
1:A:67:ASN:N	1:A:67:ASN:HD22	2.08	0.48
1:B:387:ASN:HA	1:B:468:THR:HG21	1.96	0.48
1:A:34:PRO:HB3	1:A:73:LEU:HB2	1.96	0.48
1:B:345:LYS:NZ	1:B:372:GLN:HB2	2.30	0.47
1:A:380:SER:HB2	1:A:389:THR:HG21	1.97	0.47
1:A:158:GLY:HA2	1:B:416:ILE:HD13	1.97	0.46
1:A:678:LYS:HB3	1:A:678:LYS:NZ	2.31	0.46
1:A:5:THR:OG1	1:A:7:ILE:HG22	2.16	0.46
1:B:361:LEU:HD13	1:B:504:GLY:HA2	1.97	0.46
1:B:552:VAL:HG23	1:B:555:PRO:HB3	1.98	0.45
1:B:51:ASN:HD21	1:B:306:VAL:HG22	1.82	0.45
1:A:52:PRO:HD2	1:A:302:LEU:HD13	1.98	0.45
1:A:16:ARG:HD3	1:A:35:LEU:O	2.17	0.44
1:A:359:ARG:HD2	1:A:386:SER:O	2.17	0.44
1:A:358:THR:CG2	1:A:527:SER:H	2.30	0.44
1:A:512:LYS:HE3	1:A:512:LYS:HB2	1.70	0.44
1:A:25:LYS:HB3	4:A:1110:HOH:O	2.17	0.44
1:B:358:THR:HA	1:B:361:LEU:HD12	1.99	0.44
1:A:471:SER:O	1:A:474:VAL:HG23	2.18	0.43
1:A:260:HIS:CD2	4:A:724:HOH:O	2.69	0.43
1:A:558:ILE:CD1	1:A:607:PRO:HD2	2.49	0.43
1:B:173:GLY:HA3	1:B:210:TYR:O	2.19	0.43
1:A:361:LEU:HD13	1:A:504:GLY:HA2	2.00	0.43
1:A:647:LYS:HZ2	1:A:647:LYS:HB3	1.82	0.43
1:A:359:ARG:HD3	4:A:751:HOH:O	2.18	0.42
1:A:390:ARG:NH1	1:A:394:ALA:HB3	2.33	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:346:LEU:HD11	1:A:512:LYS:HB3	2.01	0.42
1:A:8:ASP:O	1:A:12:VAL:HG23	2.18	0.42
1:A:600:GLU:HG2	1:A:601:TYR:N	2.35	0.42
1:A:191:ILE:HG13	3:A:682:TPP:H62	2.01	0.42
1:A:94:ARG:O	1:B:640:GLY:HA2	2.19	0.42
1:A:297:TYR:CD1	1:A:301:ILE:HD12	2.55	0.42
1:A:419:HIS:HD2	1:A:419:HIS:O	2.02	0.42
1:A:654:GLU:CD	1:A:654:GLU:H	2.22	0.42
1:B:602:ARG:NH1	4:B:803:HOH:O	2.49	0.42
1:B:390:ARG:HG2	1:B:411:TYR:CZ	2.55	0.41
1:A:260:HIS:H	1:A:260:HIS:CD2	2.36	0.41
1:A:668:LYS:HB3	1:A:668:LYS:HE3	1.75	0.41
1:A:369:VAL:HG12	4:A:1091:HOH:O	2.21	0.41
1:A:492:SER:HA	1:B:621:THR:HG21	2.03	0.41
1:A:37:MET:SD	1:A:185:ASP:HB2	2.60	0.41
1:A:359:ARG:HE	1:A:359:ARG:HB3	1.77	0.41
1:A:373:LEU:HA	1:A:374:PRO:HD2	1.85	0.41
1:B:71:VAL:HG23	1:B:104:PRO:HG3	2.02	0.41
4:A:746:HOH:O	3:B:682:TPP:H2	2.21	0.41
1:A:173:GLY:HA3	1:A:210:TYR:O	2.21	0.41
1:A:93:PHE:CD2	1:A:94:ARG:HG3	2.56	0.41
1:A:680:PHE:CD2	1:B:659:ARG:HD3	2.56	0.41
1:B:162:GLU:OE2	3:B:682:TPP:HM23	2.21	0.41
1:A:491:ARG:HD3	1:A:591:PHE:CD2	2.56	0.41
1:A:540:GLU:CD	1:A:540:GLU:H	2.24	0.40
1:B:592:PHE:CE2	1:B:596:LYS:HE3	2.56	0.40
1:B:67:ASN:N	1:B:67:ASN:HD22	2.17	0.40
1:A:325:GLU:H	1:A:325:GLU:HG2	1.58	0.40
1:B:647:LYS:HB3	1:B:647:LYS:HE2	1.79	0.40
1:A:509:ALA:HA	1:A:512:LYS:HG2	2.03	0.40
1:B:45:TRP:HA	1:B:48:MET:HE3	2.03	0.40

All (2) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:A:794:HOH:O	4:B:865:HOH:O[3_545]	0.47	1.73
1:A:662:LYS:NZ	4:A:922:HOH:O[3_555]	1.62	0.58

## 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	676/680 (99%)	653 (97%)	21 (3%)	2 (0%)	41	37
1	B	676/680 (99%)	654 (97%)	21 (3%)	1 (0%)	51	49
All	All	1352/1360 (99%)	1307 (97%)	42 (3%)	3 (0%)	47	44

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	237	SER
1	B	617	VAL
1	A	617	VAL

### 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	552/554 (100%)	513 (93%)	39 (7%)	14	10
1	B	552/554 (100%)	525 (95%)	27 (5%)	25	21
All	All	1104/1108 (100%)	1038 (94%)	66 (6%)	19	14

All (66) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	3	GLN
1	A	6	ASP
1	A	47	GLN

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Mol	Chain	Res	Type
1	A	50	MET
1	A	67	ASN
1	A	71	VAL
1	A	113	VAL
1	A	114	THR
1	A	197	ILE
1	A	218	GLU
1	A	238	LYS
1	A	255	LEU
1	A	299	LYS
1	A	302	LEU
1	A	309	ASN
1	A	314	LYS
1	A	318	GLU
1	A	325	GLU
1	A	338	LEU
1	A	343	GLU
1	A	352	LYS
1	A	358	THR
1	A	386	SER
1	A	390	ARG
1	A	404	SER
1	A	459	SER
1	A	528	ARG
1	A	552	VAL
1	A	571	GLU
1	A	580	ASN
1	A	584	ARG
1	A	588	LEU
1	A	600	GLU
1	A	610	VAL
1	A	652	THR
1	A	654	GLU
1	A	668	LYS
1	A	672	LEU
1	A	678	LYS
1	B	51	ASN
1	B	67	ASN
1	B	104	PRO
1	B	113	VAL
1	B	141	LYS
1	B	197	ILE

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Mol	Chain	Res	Type
1	B	229	LYS
1	B	268	LYS
1	B	314	LYS
1	B	322	LYS
1	B	326	LEU
1	B	337	GLN
1	B	338	LEU
1	B	370	TYR
1	B	371	ASN
1	B	392	LYS
1	B	404	SER
1	B	417	ARG
1	B	491	ARG
1	B	518	LYS
1	B	528	ARG
1	B	574	LYS
1	B	579	LYS
1	B	610	VAL
1	B	625	LYS
1	B	635	ARG
1	B	671	LYS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (14) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	67	ASN
1	A	120	GLN
1	A	256	HIS
1	A	260	HIS
1	A	298	GLN
1	A	341	ASN
1	A	398	GLN
1	A	580	ASN
1	A	628	HIS
1	B	51	ASN
1	B	54	ASN
1	B	67	ASN
1	B	233	GLN
1	B	309	ASN

### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

## 5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

## 5.6 Ligand geometry ⓘ

Of 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	682	2	22,27,27	1.82	2 (9%)	29,40,40	1.48	5 (17%)
3	TPP	B	682	2	22,27,27	1.80	3 (13%)	29,40,40	1.39	2 (6%)

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	682	2	-	2/16/17/17	0/2/2/2
3	TPP	B	682	2	-	5/16/17/17	0/2/2/2

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	682	TPP	C4-N3	-6.53	1.34	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	682	TPP	C4-N3	-6.53	1.34	1.39
3	A	682	TPP	C7'-N3	2.78	1.53	1.48
3	B	682	TPP	C7'-N3	2.54	1.53	1.48
3	B	682	TPP	PB-O3B	-2.10	1.46	1.54

All (7) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	682	TPP	C5'-C7'-N3	-3.35	107.70	113.28
3	B	682	TPP	O3A-PB-O1B	-3.04	94.30	111.19
3	A	682	TPP	C6-C5-C4	-2.95	125.07	127.43
3	A	682	TPP	C6'-N1'-C2'	2.74	120.62	115.96
3	A	682	TPP	C5-C4-N3	2.42	112.41	107.57
3	B	682	TPP	C5-C4-N3	2.15	111.88	107.57
3	A	682	TPP	C5'-C6'-N1'	-2.15	120.24	123.82

There are no chirality outliers.

All (7) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	682	TPP	C7-O7-PA-O3A
3	B	682	TPP	C5-C6-C7-O7
3	B	682	TPP	C7-O7-PA-O1A
3	B	682	TPP	C7-O7-PA-O2A
3	B	682	TPP	C7-O7-PA-O3A
3	A	682	TPP	C4-C5-C6-C7
3	B	682	TPP	C4-C5-C6-C7

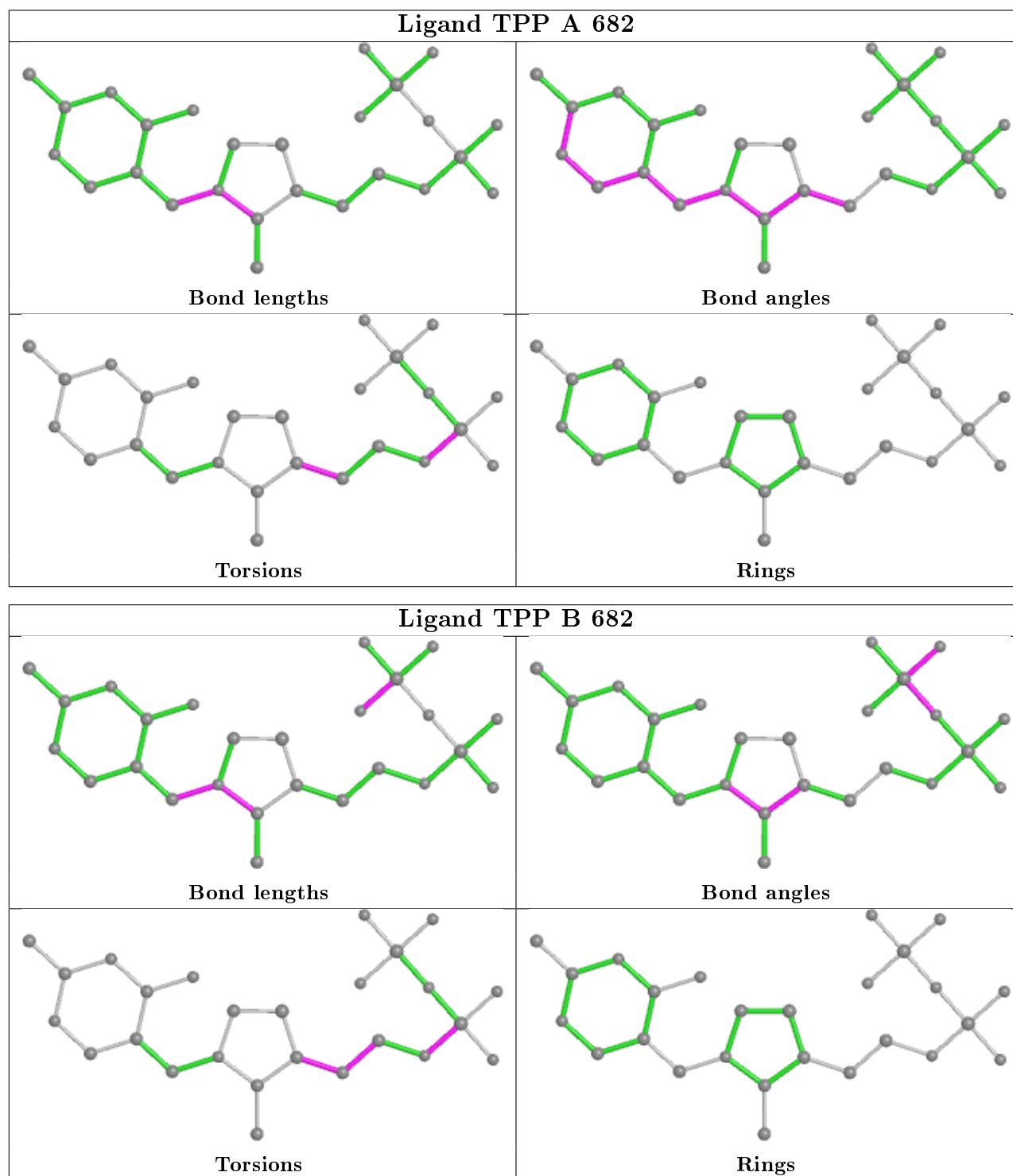
There are no ring outliers.

2 monomers are involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	682	TPP	1	0
3	B	682	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

EDS was not executed - this section is therefore empty.

### 6.2 Non-standard residues in protein, DNA, RNA chains

EDS was not executed - this section is therefore empty.

### 6.3 Carbohydrates

EDS was not executed - this section is therefore empty.

### 6.4 Ligands

EDS was not executed - this section is therefore empty.

### 6.5 Other polymers

EDS was not executed - this section is therefore empty.