



Full wwPDB X-ray Structure Validation Report ⓘ

May 21, 2020 – 08:26 am BST

PDB ID : 1TKC
Title : SPECIFICITY OF COENZYME BINDING IN THIAMIN DIPHOSPHATE
DEPENDENT ENZYMES: CRYSTAL STRUCTURES OF YEAST TRANS-
KETOLASE IN COMPLEX WITH ANALOGS OF THIAMIN DIPHOS-
PHATE
Authors : Schneider, G.; Koenig, S.
Deposited on : 1994-02-07
Resolution : 2.70 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) : **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

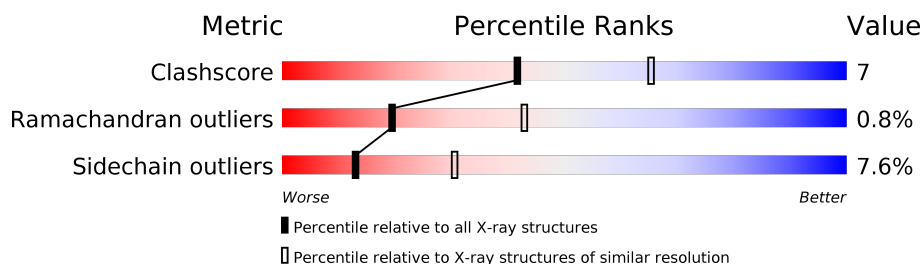
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.70 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	3122 (2.70-2.70)
Ramachandran outliers	138981	3069 (2.70-2.70)
Sidechain outliers	138945	3069 (2.70-2.70)

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 $\leq 5\%$.

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	678	
1	B	678	

2 Entry composition [i](#)

There are 3 unique types of molecules in this entry. The entry contains 10452 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.

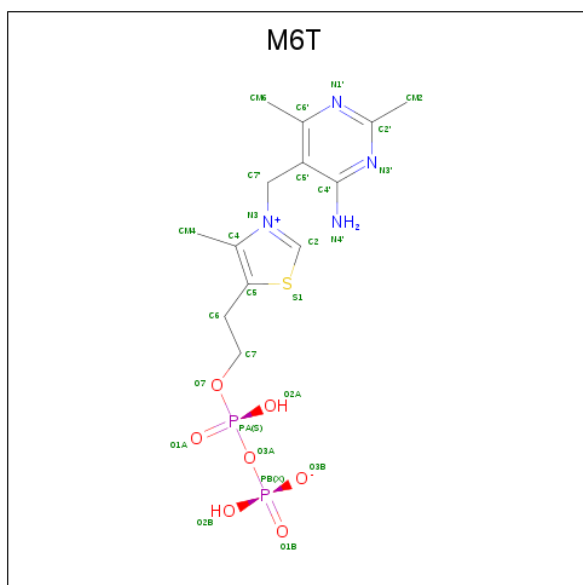
- Molecule 1 is a protein called TRANSKETOLASE.

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 6'-METHYL-THIAMIN DIPHOSPHATE (three-letter code: M6T) (formula: C₁₃H₂₀N₄O₇P₂S).



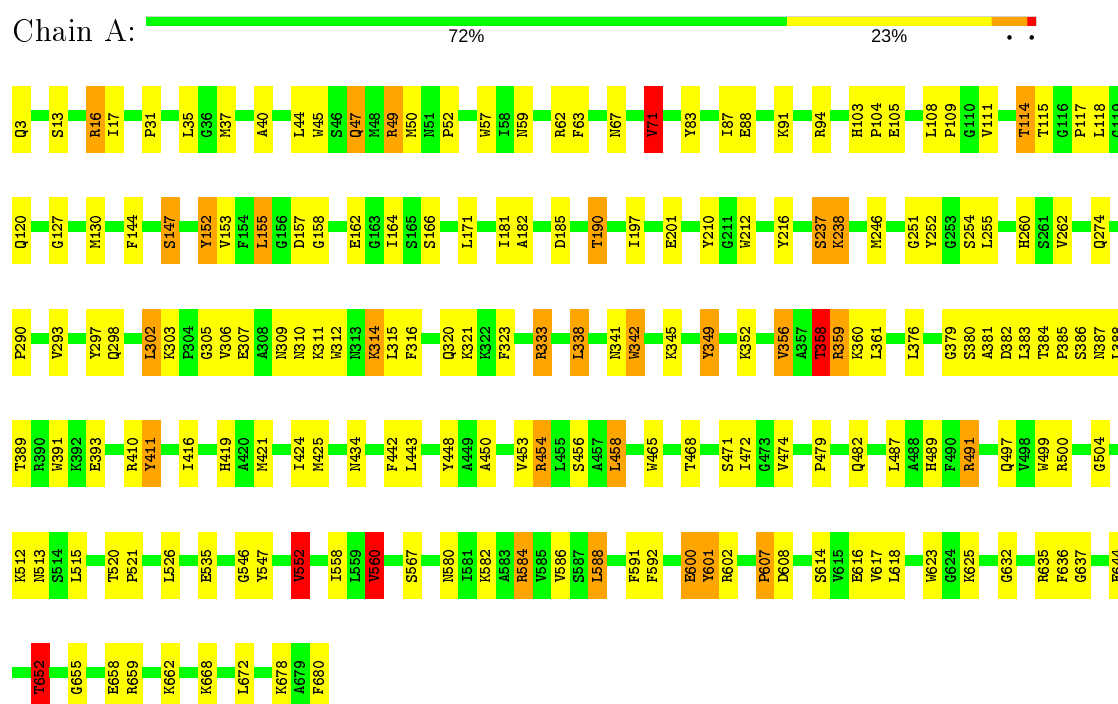
Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
3	A	1	Total	C	N	O	P	S	0	0
			27	13	4	7	2	1		
3	B	1	Total	C	N	O	P	S	0	0
			27	13	4	7	2	1		

3 Residue-property plots [i](#)

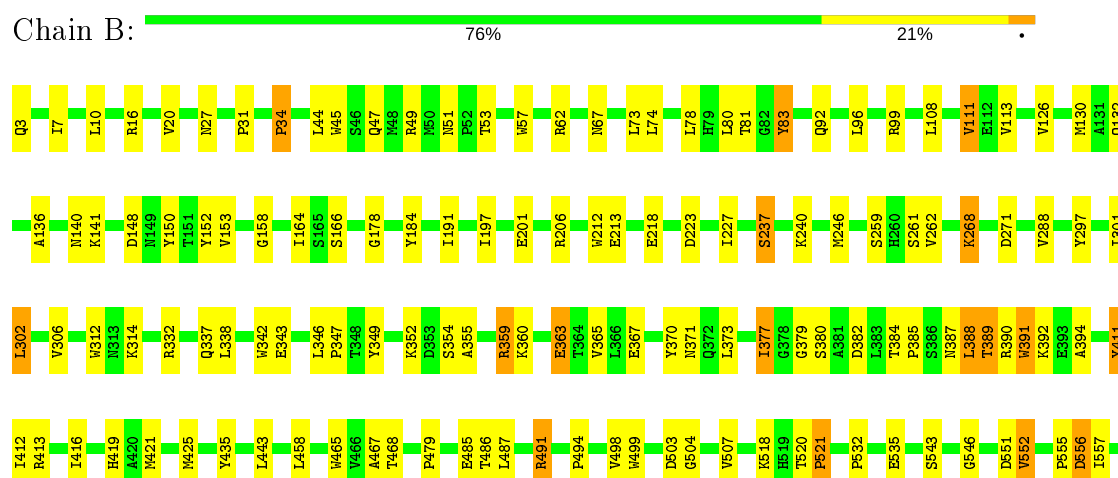
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry. Residues are color-coded according 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, α , β , γ	76.30 Å 113.30 Å 160.90 Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	15.00 – 2.70	Depositor
% Data completeness (in resolution range)	(Not available) (15.00-2.70)	Depositor
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	X-PLOR	Depositor
R, R_{free}	0.152 , (Not available)	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	10452	wwPDB-VP
Average B, all atoms (Å ²)	16.0	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, M6T

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	2/5324 (0.0%)	1.60	78/7230 (1.1%)
1	B	0.86	0/5324	1.58	68/7230 (0.9%)
All	All	0.86	2/10648 (0.0%)	1.59	146/14460 (1.0%)

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	535	GLU	CD-OE2	7.63	1.34	1.25
1	A	237	SER	CA-CB	5.73	1.61	1.52

All (146) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	491	ARG	NE-CZ-NH1	15.37	127.99	120.30
1	A	465	TRP	CD1-CG-CD2	11.85	115.78	106.30
1	B	99	ARG	NE-CZ-NH2	-10.75	114.92	120.30
1	B	465	TRP	CD1-CG-CD2	10.06	114.35	106.30
1	A	499	TRP	CD1-CG-CD2	9.66	114.03	106.30
1	A	49	ARG	NE-CZ-NH2	-9.62	115.49	120.30
1	A	358	THR	CA-CB-CG2	9.42	125.58	112.40
1	A	584	ARG	NE-CZ-NH2	-9.17	115.71	120.30
1	A	49	ARG	NE-CZ-NH1	8.98	124.79	120.30
1	A	623	TRP	CD1-CG-CD2	8.92	113.44	106.30
1	B	499	TRP	CD1-CG-CD2	8.81	113.35	106.30
1	B	342	TRP	CD1-CG-CD2	8.78	113.33	106.30
1	A	465	TRP	CG-CD1-NE1	-8.74	101.36	110.10
1	A	57	TRP	CD1-CG-CD2	8.65	113.22	106.30
1	B	83	TYR	CB-CG-CD2	-8.59	115.85	121.00
1	A	411	TYR	CB-CG-CD1	-8.55	115.87	121.00
1	A	491	ARG	NE-CZ-NH1	8.48	124.54	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	465	TRP	CE2-CD2-CG	-8.37	100.60	107.30
1	B	57	TRP	CD1-CG-CD2	8.34	112.97	106.30
1	A	465	TRP	CG-CD2-CE3	8.34	141.40	133.90
1	B	391	TRP	CD1-CG-CD2	8.13	112.80	106.30
1	A	391	TRP	CD1-CG-CD2	8.08	112.76	106.30
1	B	465	TRP	CE2-CD2-CG	-8.01	100.89	107.30
1	B	312	TRP	CD1-CG-CD2	7.97	112.68	106.30
1	A	16	ARG	NE-CZ-NH1	7.95	124.28	120.30
1	A	499	TRP	CE2-CD2-CG	-7.91	100.98	107.30
1	A	94	ARG	NE-CZ-NH1	7.89	124.24	120.30
1	B	659	ARG	NE-CZ-NH2	-7.83	116.38	120.30
1	A	312	TRP	CD1-CG-CD2	7.82	112.55	106.30
1	A	333	ARG	NE-CZ-NH2	-7.79	116.40	120.30
1	A	45	TRP	CD1-CG-CD2	7.78	112.52	106.30
1	B	659	ARG	CA-CB-CG	-7.68	96.51	113.40
1	A	448	TYR	CB-CG-CD2	-7.60	116.44	121.00
1	B	332	ARG	NE-CZ-NH1	7.54	124.07	120.30
1	B	391	TRP	CE2-CD2-CG	-7.49	101.31	107.30
1	A	391	TRP	CE2-CD2-CG	-7.48	101.32	107.30
1	B	184	TYR	CB-CG-CD2	-7.46	116.53	121.00
1	A	623	TRP	CE2-CD2-CG	-7.38	101.39	107.30
1	B	45	TRP	CG-CD2-CE3	7.37	140.53	133.90
1	B	312	TRP	CE2-CD2-CG	-7.32	101.45	107.30
1	B	367	GLU	CA-CB-CG	-7.30	97.33	113.40
1	A	342	TRP	CD1-CG-CD2	7.24	112.09	106.30
1	A	465	TRP	CB-CG-CD1	-7.22	117.61	127.00
1	A	45	TRP	CE2-CD2-CG	-7.22	101.53	107.30
1	A	57	TRP	CE2-CD2-CG	-7.18	101.56	107.30
1	A	312	TRP	CE2-CD2-CG	-7.05	101.66	107.30
1	B	623	TRP	CD1-CG-CD2	7.04	111.93	106.30
1	B	623	TRP	CE2-CD2-CG	-7.01	101.69	107.30
1	B	342	TRP	CE2-CD2-CG	-6.95	101.74	107.30
1	B	57	TRP	CE2-CD2-CG	-6.92	101.77	107.30
1	B	499	TRP	CE2-CD2-CG	-6.91	101.77	107.30
1	B	45	TRP	CD1-CG-CD2	6.83	111.77	106.30
1	A	210	TYR	CB-CG-CD2	-6.81	116.91	121.00
1	A	349	TYR	CB-CG-CD1	-6.81	116.91	121.00
1	A	342	TRP	CE2-CD2-CG	-6.76	101.89	107.30
1	B	111	VAL	CA-C-N	-6.72	102.41	117.20
1	B	297	TYR	CB-CG-CD2	-6.71	116.97	121.00
1	A	212	TRP	CD1-CG-CD2	6.67	111.64	106.30
1	B	111	VAL	O-C-N	6.67	133.37	122.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	465	TRP	CG-CD1-NE1	-6.65	103.45	110.10
1	A	356	VAL	CA-CB-CG1	-6.64	100.95	110.90
1	B	212	TRP	CE2-CD2-CG	-6.62	102.01	107.30
1	A	500	ARG	NE-CZ-NH1	6.53	123.57	120.30
1	B	312	TRP	CG-CD2-CE3	6.50	139.75	133.90
1	B	312	TRP	CB-CG-CD1	-6.50	118.55	127.00
1	B	45	TRP	CE2-CD2-CG	-6.48	102.11	107.30
1	A	83	TYR	CB-CG-CD2	-6.38	117.17	121.00
1	A	152	TYR	CB-CG-CD2	-6.38	117.17	121.00
1	A	359	ARG	NE-CZ-NH2	-6.34	117.13	120.30
1	A	212	TRP	CE2-CD2-CG	-6.32	102.25	107.30
1	A	47	GLN	N-CA-CB	-6.29	99.28	110.60
1	B	580	ASN	N-CA-C	6.25	127.88	111.00
1	A	57	TRP	CG-CD1-NE1	-6.24	103.86	110.10
1	A	237	SER	CA-CB-OG	6.20	127.93	111.20
1	A	411	TYR	CB-CG-CD2	6.19	124.72	121.00
1	B	312	TRP	CG-CD1-NE1	-6.16	103.94	110.10
1	A	238	LYS	CA-CB-CG	6.14	126.91	113.40
1	A	262	VAL	CG1-CB-CG2	-6.14	101.08	110.90
1	A	623	TRP	CG-CD1-NE1	-6.12	103.98	110.10
1	A	652	THR	CA-CB-CG2	6.12	120.96	112.40
1	A	453	VAL	CG1-CB-CG2	-6.10	101.14	110.90
1	A	252	TYR	CB-CG-CD1	-6.04	117.37	121.00
1	A	358	THR	CA-CB-OG1	-6.03	96.34	109.00
1	B	359	ARG	NE-CZ-NH1	5.98	123.29	120.30
1	B	206	ARG	NE-CZ-NH2	-5.91	117.34	120.30
1	B	212	TRP	CD1-CG-CD2	5.91	111.03	106.30
1	B	342	TRP	CG-CD1-NE1	-5.89	104.21	110.10
1	B	246	MET	CA-CB-CG	5.85	123.24	113.30
1	B	635	ARG	NE-CZ-NH2	-5.84	117.38	120.30
1	B	465	TRP	CG-CD2-CE3	5.82	139.14	133.90
1	A	499	TRP	CG-CD1-NE1	-5.81	104.29	110.10
1	A	602	ARG	NE-CZ-NH1	5.80	123.20	120.30
1	B	411	TYR	CB-CG-CD1	-5.78	117.53	121.00
1	B	45	TRP	CB-CG-CD1	-5.77	119.50	127.00
1	B	499	TRP	CG-CD1-NE1	-5.74	104.36	110.10
1	A	312	TRP	CG-CD1-NE1	-5.73	104.37	110.10
1	A	454	ARG	NE-CZ-NH1	5.71	123.16	120.30
1	A	297	TYR	CB-CG-CD2	-5.71	117.57	121.00
1	A	547	TYR	CB-CG-CD2	-5.71	117.58	121.00
1	B	413	ARG	NE-CZ-NH1	5.71	123.15	120.30
1	A	157	ASP	CB-CG-OD1	5.70	123.43	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	288	VAL	CG1-CB-CG2	-5.70	101.78	110.90
1	B	152	TYR	CB-CG-CD2	-5.68	117.59	121.00
1	A	321	LYS	CA-CB-CG	5.67	125.89	113.40
1	B	465	TRP	CB-CG-CD1	-5.62	119.69	127.00
1	A	601	TYR	CB-CG-CD1	-5.62	117.63	121.00
1	A	391	TRP	CB-CG-CD1	-5.60	119.72	127.00
1	B	377	ILE	CA-C-N	5.60	127.40	116.20
1	A	47	GLN	CA-CB-CG	5.59	125.69	113.40
1	A	652	THR	N-CA-CB	-5.58	99.69	110.30
1	A	489	HIS	CA-CB-CG	5.54	123.01	113.60
1	B	556	ASP	CB-CG-OD1	5.50	123.25	118.30
1	B	57	TRP	CG-CD1-NE1	-5.46	104.64	110.10
1	B	150	TYR	CB-CG-CD1	-5.45	117.73	121.00
1	B	153	VAL	CB-CA-C	-5.44	101.07	111.40
1	B	388	LEU	CA-CB-CG	5.42	127.77	115.30
1	B	602	ARG	NE-CZ-NH1	5.41	123.00	120.30
1	B	491	ARG	CB-CG-CD	5.38	125.60	111.60
1	A	358	THR	N-CA-CB	-5.38	100.08	110.30
1	A	391	TRP	CG-CD2-CE3	5.37	138.74	133.90
1	A	652	THR	CA-CB-OG1	-5.35	97.76	109.00
1	B	622	CYS	CA-CB-SG	5.34	123.62	114.00
1	A	130	MET	CG-SD-CE	-5.32	91.69	100.20
1	B	435	TYR	CB-CG-CD1	-5.30	117.82	121.00
1	A	274	GLN	CA-CB-CG	5.26	124.97	113.40
1	A	391	TRP	CG-CD1-NE1	-5.26	104.84	110.10
1	B	671	LYS	CA-CB-CG	5.26	124.97	113.40
1	B	342	TRP	CB-CG-CD1	-5.25	120.17	127.00
1	A	465	TRP	CD1-NE1-CE2	5.25	113.72	109.00
1	A	71	VAL	CB-CA-C	-5.25	101.43	111.40
1	A	659	ARG	NE-CZ-NH1	5.21	122.90	120.30
1	B	62	ARG	NE-CZ-NH1	5.18	122.89	120.30
1	B	543	SER	O-C-N	-5.17	114.42	122.70
1	A	552	VAL	CB-CA-C	-5.15	101.61	111.40
1	B	80	LEU	CB-CG-CD2	-5.15	102.24	111.00
1	A	560	VAL	CA-CB-CG1	-5.14	103.19	110.90
1	B	599	LEU	CA-CB-CG	5.13	127.10	115.30
1	A	216	TYR	CB-CG-CD2	-5.12	117.93	121.00
1	A	500	ARG	NE-CZ-NH2	-5.10	117.75	120.30
1	B	365	VAL	CG1-CB-CG2	-5.08	102.78	110.90
1	A	381	ALA	CA-C-N	-5.05	106.08	117.20
1	B	391	TRP	CG-CD2-CE3	5.05	138.45	133.90
1	B	45	TRP	CG-CD1-NE1	-5.04	105.06	110.10

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	373	LEU	CA-CB-CG	5.03	126.88	115.30
1	A	342	TRP	CG-CD1-NE1	-5.02	105.08	110.10
1	A	345	LYS	CA-CB-CG	-5.00	102.39	113.40

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	5198	0	5139	85	0
1	B	5198	0	5139	64	0
2	A	1	0	0	0	0
2	B	1	0	0	0	0
3	A	27	0	18	4	0
3	B	27	0	18	2	0
All	All	10452	0	10314	143	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 7.

All (143) 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:51:ASN:HD21	1:B:53:THR:HB	1.42	0.84
1:A:105:GLU:HA	1:A:114:THR:HB	1.70	0.72
1:B:51:ASN:ND2	1:B:53:THR:HB	2.05	0.71
1:B:164:ILE:HD12	1:B:419:HIS:CD2	2.28	0.69
1:B:546:GLY:HA3	1:B:588:LEU:HD12	1.75	0.68
1:A:644:GLU:HB3	1:B:96:LEU:HD22	1.75	0.67
1:B:387:ASN:HA	1:B:468:THR:HG21	1.75	0.67
1:A:552:VAL:HG11	1:A:582:LYS:HB3	1.76	0.67
1:A:108:LEU:HD12	1:A:109:PRO:HD2	1.77	0.66
1:A:361:LEU:HD13	1:A:504:GLY:HA2	1.78	0.66
1:A:358:THR:HG22	1:A:526:LEU:HA	1.78	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:190:THR:HG22	3:A:681:M6T:O7	1.96	0.65
1:A:155:LEU:HD21	1:A:182:ALA:HB1	1.79	0.65
1:A:152:TYR:CE1	1:A:181:ILE:HD12	2.33	0.63
1:B:613:MET:HA	1:B:629:GLN:O	1.99	0.63
1:A:298:GLN:HE21	1:A:303:LYS:HE3	1.64	0.62
1:B:487:LEU:O	1:B:491:ARG:HG3	2.00	0.62
1:B:302:LEU:O	1:B:306:VAL:HG23	2.00	0.61
1:A:164:ILE:HD12	1:A:419:HIS:CD2	2.36	0.60
1:A:118:LEU:HD13	1:A:158:GLY:HA3	1.84	0.59
1:A:37:MET:SD	1:A:185:ASP:HB2	2.43	0.59
1:A:118:LEU:H	3:A:681:M6T:HM21	1.68	0.57
1:B:487:LEU:HD22	1:B:498:VAL:CG1	2.35	0.56
1:B:421:MET:O	1:B:425:MET:HG3	2.06	0.56
1:A:342:TRP:HH2	1:A:512:LYS:HA	1.71	0.56
1:A:416:ILE:HD13	1:B:158:GLY:HA2	1.86	0.56
1:A:349:TYR:CD1	1:A:504:GLY:HA3	2.41	0.55
1:B:552:VAL:HG23	1:B:555:PRO:HB3	1.87	0.55
1:B:74:LEU:HD21	1:B:111:VAL:HG22	1.86	0.55
1:A:379:GLY:HA2	1:A:411:TYR:CE1	2.41	0.55
1:A:472:ILE:HA	1:A:482:GLN:HG2	1.87	0.55
1:A:50:MET:O	1:A:305:GLY:HA3	2.07	0.55
1:A:652:THR:HG22	1:A:655:GLY:H	1.72	0.54
1:B:635:ARG:HD2	1:B:636:PHE:O	2.07	0.54
1:B:379:GLY:HA2	1:B:411:TYR:CE1	2.43	0.54
1:B:443:LEU:HA	1:B:467:ALA:HB1	1.90	0.54
1:A:359:ARG:HG2	1:A:388:LEU:HD12	1.90	0.54
1:A:560:VAL:HG11	1:A:588:LEU:HD12	1.90	0.53
1:A:40:ALA:HB2	1:A:246:MET:HE1	1.90	0.53
1:A:497:GLN:HG2	1:A:592:PHE:CD2	2.43	0.53
1:A:421:MET:O	1:A:425:MET:HG3	2.09	0.53
1:A:63:PHE:HA	1:A:152:TYR:O	2.09	0.53
1:A:311:LYS:O	1:A:314:LYS:HG3	2.09	0.52
1:B:391:TRP:CD1	1:B:394:ALA:HB2	2.44	0.52
1:B:551:ASP:HA	1:B:584:ARG:HG3	1.92	0.52
1:A:302:LEU:O	1:A:306:VAL:HG23	2.10	0.52
1:A:71:VAL:HG13	1:A:104:PRO:HD3	1.92	0.52
1:A:382:ASP:CB	1:A:416:ILE:HG13	2.39	0.51
1:A:127:GLY:HA2	1:A:424:ILE:HG23	1.92	0.51
1:A:380:SER:HB2	1:A:389:THR:HG21	1.93	0.51
1:A:44:LEU:HD11	1:A:152:TYR:CG	2.45	0.50
1:B:377:ILE:HD11	1:B:412:ILE:HD11	1.92	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:491:ARG:HD2	1:B:591:PHE:CD2	2.45	0.50
1:A:316:PHE:O	1:A:320:GLN:HG3	2.11	0.50
1:A:162:GLU:OE2	3:A:681:M6T:HM23	2.12	0.50
1:B:380:SER:HB2	1:B:389:THR:OG1	2.11	0.50
1:A:479:PRO:HB2	1:B:458:LEU:HD11	1.94	0.50
1:A:59:ASN:OD1	1:A:147:SER:HA	2.11	0.50
1:B:108:LEU:HD23	1:B:111:VAL:HG21	1.93	0.49
1:B:503:ASP:O	1:B:507:VAL:HG23	2.11	0.49
1:B:34:PRO:HA	1:B:73:LEU:HD12	1.94	0.49
1:A:118:LEU:HD12	1:B:416:ILE:HG21	1.95	0.49
1:A:314:LYS:HE2	1:A:315:LEU:HB2	1.94	0.49
1:B:44:LEU:HD12	1:B:47:GLN:NE2	2.27	0.49
1:B:213:GLU:HB2	1:B:240:LYS:HD3	1.95	0.49
1:B:268:LYS:O	1:B:271:ASP:HB3	2.13	0.49
1:A:560:VAL:HG13	1:A:586:VAL:HB	1.95	0.49
1:B:259:SER:O	1:B:262:VAL:HG22	2.13	0.49
1:A:152:TYR:HE1	1:A:181:ILE:HD12	1.74	0.48
1:A:382:ASP:HB3	1:A:416:ILE:HG13	1.94	0.48
1:A:387:ASN:HA	1:A:468:THR:HG21	1.95	0.48
1:A:558:ILE:CD1	1:A:607:PRO:HD2	2.44	0.48
1:A:560:VAL:O	1:A:614:SER:HA	2.14	0.48
1:A:384:THR:HA	1:A:389:THR:HG22	1.96	0.48
1:B:346:LEU:HA	1:B:347:PRO:HD3	1.74	0.47
1:A:636:PHE:CE2	1:B:494:PRO:HB2	2.49	0.47
3:B:681:M6T:HM61	3:B:681:M6T:H7'1	1.68	0.47
1:A:458:LEU:HD11	1:B:479:PRO:HB2	1.97	0.47
1:B:359:ARG:HG2	1:B:388:LEU:HG	1.96	0.47
1:A:251:GLY:O	1:A:254:SER:HB3	2.15	0.46
1:B:178:GLY:HA2	1:B:240:LYS:O	2.14	0.46
1:A:290:PRO:HB2	1:A:293:VAL:HG23	1.98	0.46
1:A:16:ARG:HB3	1:A:35:LEU:HD23	1.96	0.46
1:B:552:VAL:CG2	1:B:555:PRO:HB3	2.46	0.46
1:A:49:ARG:HH21	1:A:59:ASN:ND2	2.14	0.46
1:B:390:ARG:NE	1:B:394:ALA:HB3	2.31	0.46
1:A:384:THR:N	1:A:385:PRO:HD2	2.31	0.45
1:A:384:THR:HA	1:A:389:THR:CG2	2.47	0.45
1:B:629:GLN:HG3	1:B:663:THR:HG23	1.98	0.45
1:A:108:LEU:HD23	1:A:111:VAL:HG21	1.98	0.45
1:A:443:LEU:HD21	1:A:487:LEU:HD21	1.99	0.45
1:A:117:PRO:HB2	1:A:120:GLN:HG3	1.99	0.45
1:A:62:ARG:HG3	1:A:62:ARG:HH11	1.82	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:16:ARG:O	1:B:20:VAL:HG23	2.16	0.45
1:B:487:LEU:HD22	1:B:498:VAL:HG11	1.98	0.45
1:A:108:LEU:HA	1:A:109:PRO:HD3	1.78	0.45
1:B:570:VAL:O	1:B:574:LYS:HD2	2.16	0.45
1:B:191:ILE:HG13	3:B:681:M6T:H62	1.98	0.45
1:A:546:GLY:HA2	1:A:588:LEU:HA	2.00	0.44
1:B:349:TYR:CD1	1:B:504:GLY:HA3	2.53	0.44
1:A:103:HIS:HB3	1:A:115:THR:O	2.17	0.44
1:A:389:THR:HG23	1:A:411:TYR:OH	2.17	0.44
1:A:144:PHE:CD1	1:A:323:PHE:HE2	2.35	0.44
1:A:3:GLN:OE1	1:A:3:GLN:N	2.51	0.44
1:A:658:GLU:O	1:A:662:LYS:HG2	2.18	0.44
1:A:342:TRP:CH2	1:A:512:LYS:HA	2.52	0.43
1:A:680:PHE:CG	1:B:659:ARG:HG2	2.53	0.43
1:A:512:LYS:HG3	1:A:513:ASN:N	2.33	0.43
1:B:78:LEU:O	1:B:83:TYR:HB2	2.18	0.43
1:A:13:SER:O	1:A:17:ILE:HG13	2.18	0.43
1:A:491:ARG:HD2	1:A:591:PHE:CD2	2.54	0.43
1:A:600:GLU:HG2	1:A:601:TYR:N	2.33	0.43
1:B:384:THR:N	1:B:385:PRO:HD2	2.33	0.43
1:A:616:GLU:O	1:A:632:GLY:HA2	2.18	0.43
1:A:454:ARG:NH1	1:B:485:GLU:OE1	2.52	0.43
1:B:360:LYS:O	1:B:363:GLU:HB3	2.19	0.43
1:A:338:LEU:HD21	1:A:515:LEU:O	2.18	0.43
1:B:556:ASP:N	1:B:582:LYS:O	2.50	0.43
1:B:126:VAL:O	1:B:130:MET:HG3	2.19	0.42
1:B:355:ALA:HA	1:B:532:PRO:HA	2.01	0.42
1:A:171:LEU:HD23	1:A:424:ILE:CD1	2.50	0.42
1:A:87:ILE:O	1:A:91:LYS:HG3	2.20	0.42
3:A:681:M6T:HM61	3:A:681:M6T:H7'1	1.73	0.42
1:B:360:LYS:HA	1:B:388:LEU:HD12	2.01	0.42
1:A:333:ARG:O	1:A:434:ASN:HB2	2.20	0.42
1:B:647:LYS:HB3	1:B:647:LYS:HE2	1.72	0.42
1:B:363:GLU:HB2	1:B:388:LEU:HB2	2.02	0.41
1:B:390:ARG:HD3	1:B:411:TYR:CG	2.55	0.41
1:B:81:THR:HG22	1:B:301:ILE:HD12	2.02	0.41
1:B:7:ILE:HD12	1:B:10:LEU:HD23	2.02	0.41
1:B:197:ILE:HD12	1:B:197:ILE:HA	1.93	0.41
1:B:223:ASP:O	1:B:227:ILE:HG13	2.20	0.41
1:A:482:GLN:OE1	1:A:637:GLY:HA3	2.21	0.41
1:A:520:THR:HA	1:A:521:PRO:HD2	1.81	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:520:THR:HA	1:B:521:PRO:HD2	1.94	0.41
1:A:471:SER:O	1:A:474:VAL:HG23	2.20	0.41
1:B:382:ASP:HB3	1:B:416:ILE:HG13	2.02	0.41
1:A:118:LEU:HA	1:A:118:LEU:HD23	1.94	0.40
1:A:52:PRO:HD2	1:A:302:LEU:HD22	2.03	0.40
1:B:136:ALA:O	1:B:140:ASN:HB2	2.21	0.40
1:B:389:THR:O	1:B:411:TYR:HE1	2.03	0.40
1:A:376:LEU:O	1:A:410:ARG:HD2	2.22	0.40
1:A:383:LEU:HD13	1:A:442:PHE:CD1	2.56	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	676/678 (100%)	627 (93%)	44 (6%)	5 (1%)	22	46
1	B	676/678 (100%)	627 (93%)	43 (6%)	6 (1%)	17	40
All	All	1352/1356 (100%)	1254 (93%)	87 (6%)	11 (1%)	19	43

All (11) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	237	SER
1	B	148	ASP
1	A	450	ALA
1	B	237	SER
1	B	580	ASN
1	A	255	LEU
1	B	31	PRO
1	A	617	VAL
1	B	617	VAL

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Mol	Chain	Res	Type
1	A	31	PRO
1	B	521	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	552/552 (100%)	507 (92%)	45 (8%)	11	26
1	B	552/552 (100%)	513 (93%)	39 (7%)	14	34
All	All	1104/1104 (100%)	1020 (92%)	84 (8%)	13	30

All (84) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	47	GLN
1	A	67	ASN
1	A	71	VAL
1	A	88	GLU
1	A	114	THR
1	A	147	SER
1	A	153	VAL
1	A	155	LEU
1	A	166	SER
1	A	190	THR
1	A	197	ILE
1	A	201	GLU
1	A	238	LYS
1	A	260	HIS
1	A	302	LEU
1	A	307	GLU
1	A	309	ASN
1	A	310	ASN
1	A	314	LYS
1	A	338	LEU
1	A	341	ASN

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Mol	Chain	Res	Type
1	A	352	LYS
1	A	356	VAL
1	A	358	THR
1	A	360	LYS
1	A	386	SER
1	A	393	GLU
1	A	456	SER
1	A	458	LEU
1	A	552	VAL
1	A	560	VAL
1	A	567	SER
1	A	580	ASN
1	A	584	ARG
1	A	588	LEU
1	A	600	GLU
1	A	607	PRO
1	A	608	ASP
1	A	618	LEU
1	A	625	LYS
1	A	635	ARG
1	A	652	THR
1	A	668	LYS
1	A	672	LEU
1	A	678	LYS
1	B	3	GLN
1	B	27	ASN
1	B	34	PRO
1	B	49	ARG
1	B	67	ASN
1	B	92	GLN
1	B	113	VAL
1	B	132	GLN
1	B	141	LYS
1	B	166	SER
1	B	201	GLU
1	B	218	GLU
1	B	237	SER
1	B	261	SER
1	B	268	LYS
1	B	302	LEU
1	B	314	LYS
1	B	337	GLN

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Mol	Chain	Res	Type
1	B	338	LEU
1	B	343	GLU
1	B	352	LYS
1	B	354	SER
1	B	363	GLU
1	B	370	TYR
1	B	371	ASN
1	B	389	THR
1	B	392	LYS
1	B	486	THR
1	B	518	LYS
1	B	535	GLU
1	B	552	VAL
1	B	557	ILE
1	B	560	VAL
1	B	574	LYS
1	B	600	GLU
1	B	610	VAL
1	B	618	LEU
1	B	668	LYS
1	B	671	LYS

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

Mol	Chain	Res	Type
1	A	3	GLN
1	A	30	HIS
1	A	120	GLN
1	A	298	GLN
1	A	341	ASN
1	A	372	GLN
1	A	387	ASN
1	A	489	HIS
1	B	51	ASN
1	B	54	ASN
1	B	67	ASN
1	B	309	ASN
1	B	489	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 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	M6T	B	681	2	22,28,28	1.98	3 (13%)	27,42,42	1.36	4 (14%)
3	M6T	A	681	2	22,28,28	1.87	3 (13%)	27,42,42	1.31	3 (11%)

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	M6T	B	681	2	-	3/16/17/17	0/2/2/2
3	M6T	A	681	2	-	3/16/17/17	0/2/2/2

All (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	681	M6T	C4-N3	-6.98	1.33	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	681	M6T	C4-N3	-6.88	1.33	1.39
3	B	681	M6T	C6-C5	-3.61	1.49	1.50
3	B	681	M6T	PB-O3B	-2.61	1.44	1.54
3	A	681	M6T	PB-O3B	-2.30	1.46	1.54
3	A	681	M6T	PB-O2B	-2.23	1.46	1.54

All (7) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	681	M6T	C5'-C7'-N3	-3.66	109.38	114.11
3	A	681	M6T	C5'-C7'-N3	-3.54	109.53	114.11
3	A	681	M6T	N3'-C2'-N1'	-2.26	121.56	125.72
3	B	681	M6T	O2B-PB-O1B	2.20	119.28	110.68
3	A	681	M6T	CM2-C2'-N3'	2.19	120.57	117.15
3	B	681	M6T	C5-C4-N3	2.13	111.83	107.57
3	B	681	M6T	CM2-C2'-N3'	2.07	120.38	117.15

There are no chirality outliers.

All (6) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	B	681	M6T	C4-C5-C6-C7
3	A	681	M6T	PB-O3A-PA-O1A
3	B	681	M6T	PB-O3A-PA-O2A
3	B	681	M6T	PB-O3A-PA-O1A
3	A	681	M6T	C7-O7-PA-O1A
3	A	681	M6T	C4-C5-C6-C7

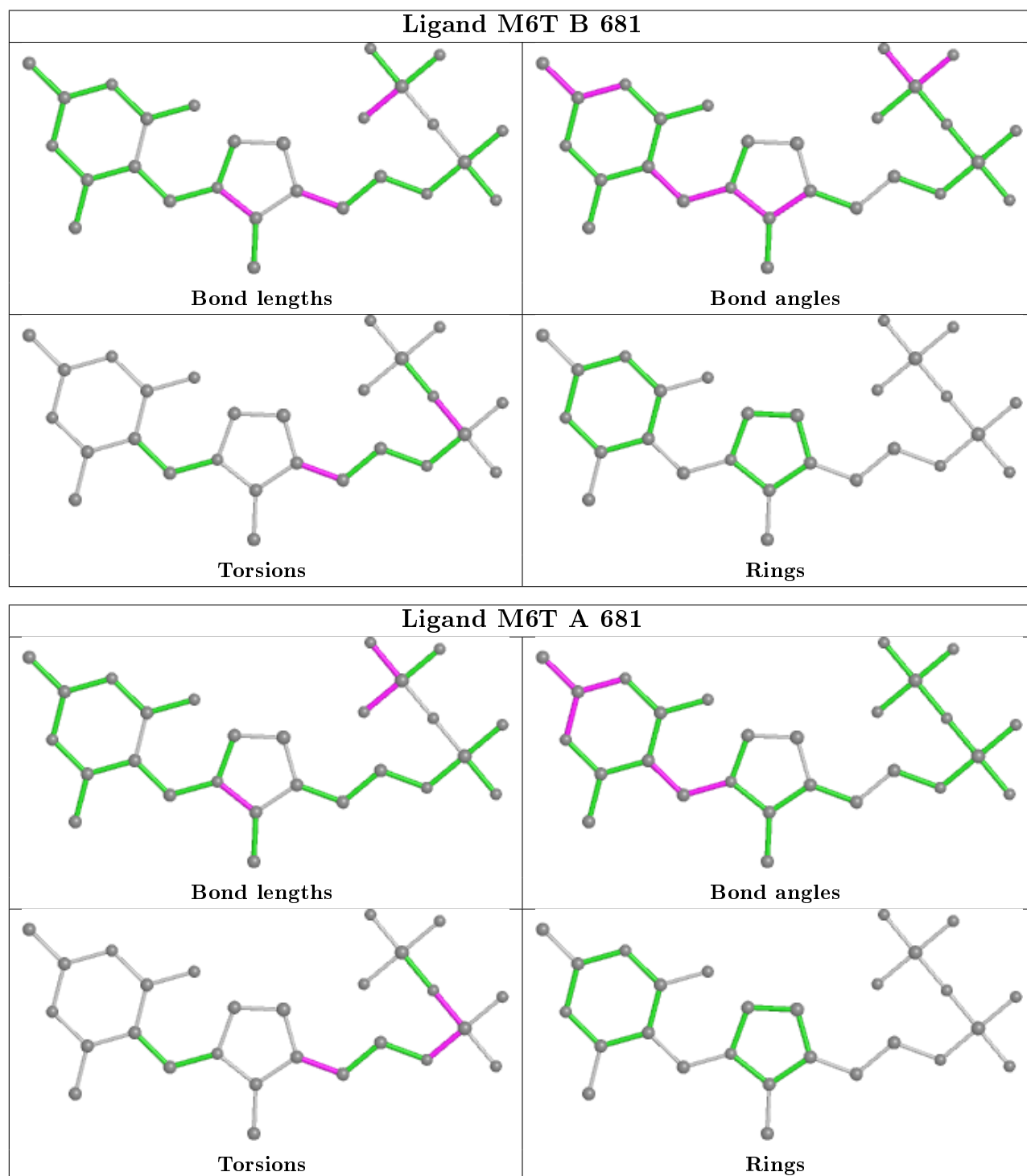
There are no ring outliers.

2 monomers are involved in 6 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	B	681	M6T	2	0
3	A	681	M6T	4	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 ⓘ

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.