



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 11:11 AM UTC

PDB ID : 1TKC / pdb_00001tkc
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 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)
Xtrriage (Phenix) : **NOT EXECUTED**
EDS : **NOT EXECUTED**
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

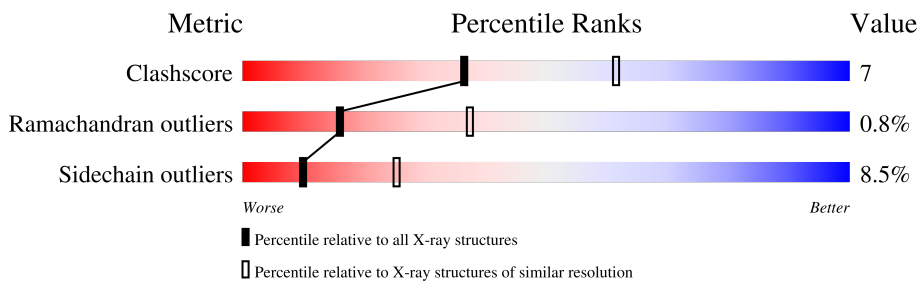
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.70 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	190562	3843 (2.70-2.70)
Ramachandran outliers	187476	3778 (2.70-2.70)
Sidechain outliers	187428	3778 (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 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 $\leq 5\%$

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.

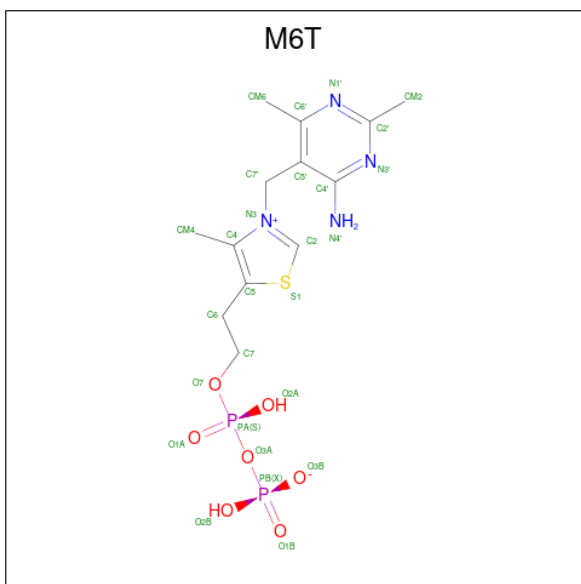
- Molecule 1 is a protein called TRANSKETOLASE.

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

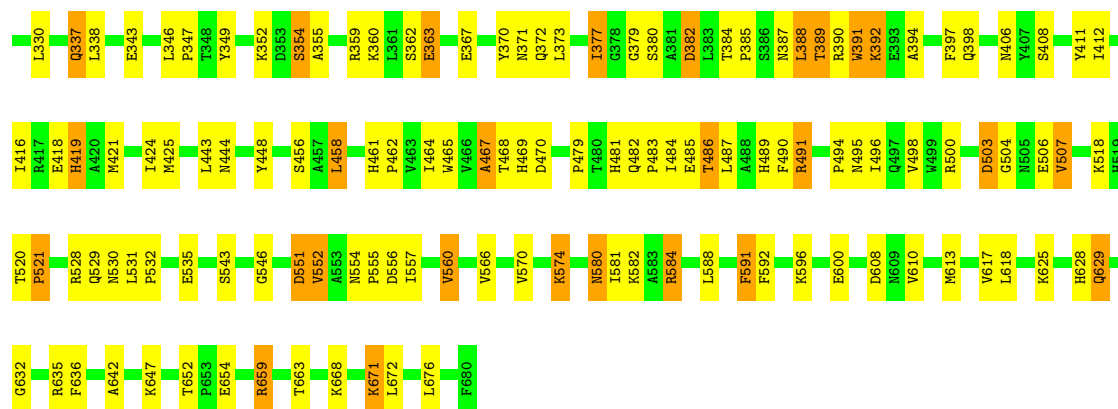
- Molecule 2 is CALCIUM ION (CCD ID: CA) (formula: Ca).

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

- Molecule 3 is 6'-METHYL-THIAMIN DIPHOSPHATE (CCD ID: M6T) (formula: C₁₃H₂₀N₄O₇P₂S).



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



4 Data and refinement statistics

Xtrriage (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	76.30Å 113.30Å 160.90Å 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.	Xtrriage
Total number of atoms	10452	wwPDB-VP
Average B, all atoms (Å ²)	16.0	wwPDB-VP

5 Model quality [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: M6T, CA

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	1.09	28/5324 (0.5%)	1.96	165/7230 (2.3%)
1	B	1.10	23/5324 (0.4%)	1.96	171/7230 (2.4%)
All	All	1.10	51/10648 (0.5%)	1.96	336/14460 (2.3%)

All (51) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	296	HIS	CD2-NE2	-7.30	1.29	1.37
1	B	174	HIS	CD2-NE2	-6.78	1.30	1.37
1	B	79	HIS	CD2-NE2	-6.75	1.30	1.37
1	B	42	HIS	CD2-NE2	-6.72	1.30	1.37
1	A	122	ILE	CA-CB	6.71	1.62	1.54
1	B	263	HIS	CD2-NE2	-6.68	1.30	1.37
1	A	69	HIS	CD2-NE2	-6.66	1.30	1.37
1	A	250	ILE	CA-CB	6.61	1.61	1.54
1	A	260	HIS	CD2-NE2	-6.61	1.30	1.37
1	A	628	HIS	CD2-NE2	-6.59	1.30	1.37
1	A	174	HIS	CD2-NE2	-6.47	1.30	1.37
1	A	263	HIS	CD2-NE2	-6.43	1.30	1.37
1	A	30	HIS	CD2-NE2	-6.42	1.30	1.37
1	A	469	HIS	CD2-NE2	-6.42	1.30	1.37
1	B	461	HIS	CD2-NE2	-6.41	1.30	1.37
1	B	469	HIS	CD2-NE2	-6.40	1.30	1.37
1	A	481	HIS	CD2-NE2	-6.37	1.30	1.37
1	A	103	HIS	CD2-NE2	-6.37	1.30	1.37
1	A	42	HIS	CD2-NE2	-6.28	1.30	1.37
1	B	30	HIS	CD2-NE2	-6.20	1.31	1.37
1	A	256	HIS	CD2-NE2	-6.09	1.31	1.37
1	B	628	HIS	CD2-NE2	-6.08	1.31	1.37
1	B	103	HIS	CD2-NE2	-6.07	1.31	1.37
1	B	489	HIS	CD2-NE2	-6.01	1.31	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	489	HIS	CD2-NE2	-6.01	1.31	1.37
1	B	481	HIS	CD2-NE2	-5.96	1.31	1.37
1	B	42	HIS	CG-ND1	-5.87	1.31	1.38
1	B	419	HIS	CD2-NE2	-5.78	1.31	1.37
1	B	189	ILE	C-O	5.78	1.29	1.24
1	B	260	HIS	CD2-NE2	-5.77	1.31	1.37
1	A	461	HIS	CD2-NE2	-5.74	1.31	1.37
1	A	296	HIS	CD2-NE2	-5.73	1.31	1.37
1	B	263	HIS	CG-ND1	-5.71	1.31	1.38
1	A	114	THR	CA-CB	5.70	1.62	1.53
1	B	69	HIS	CD2-NE2	-5.68	1.31	1.37
1	A	377	ILE	CA-CB	5.64	1.61	1.54
1	B	69	HIS	CG-ND1	-5.56	1.32	1.38
1	B	256	HIS	CD2-NE2	-5.52	1.31	1.37
1	A	419	HIS	CD2-NE2	-5.50	1.31	1.37
1	A	174	HIS	CG-ND1	-5.48	1.32	1.38
1	A	248	THR	CA-CB	5.48	1.62	1.53
1	B	424	ILE	CA-CB	5.41	1.61	1.54
1	A	164	ILE	CA-CB	5.40	1.61	1.54
1	A	558	ILE	CA-CB	5.38	1.61	1.54
1	A	30	HIS	CG-ND1	-5.37	1.32	1.38
1	A	79	HIS	CD2-NE2	-5.22	1.32	1.37
1	A	359	ARG	CA-CB	-5.11	1.45	1.53
1	A	519	HIS	CD2-NE2	-5.08	1.32	1.37
1	B	79	HIS	CG-ND1	-5.08	1.32	1.38
1	A	167	GLU	CA-CB	-5.02	1.45	1.53
1	B	483	PRO	CA-CB	-5.00	1.47	1.53

All (336) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	185	ASP	CA-CB-CG	11.51	124.11	112.60
1	B	191	ILE	N-CA-C	10.15	120.17	110.42
1	B	372	GLN	N-CA-C	-9.99	101.59	113.88
1	B	187	ASN	CA-CB-CG	9.83	122.43	112.60
1	B	424	ILE	N-CA-C	-9.80	101.32	110.82
1	A	200	ASP	CA-CB-CG	9.26	121.86	112.60
1	A	489	HIS	CA-CB-CG	9.21	123.01	113.80
1	B	27	ASN	OD1-CG-ND2	-8.93	113.67	122.60
1	A	358	THR	CA-CB-CG2	8.87	125.58	110.50
1	A	358	THR	CA-CB-OG1	-8.84	96.34	109.60
1	B	659	ARG	CA-CB-CG	-8.79	96.51	114.10

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	111	VAL	O-C-N	8.78	133.37	123.10
1	B	470	ASP	N-CA-C	8.54	123.25	113.01
1	A	260	HIS	CB-CG-CD2	-8.46	120.21	131.20
1	B	54	ASN	OD1-CG-ND2	-8.45	114.15	122.60
1	A	237	SER	CA-CB-OG	8.41	127.93	111.10
1	B	367	GLU	CA-CB-CG	-8.38	97.33	114.10
1	A	461	HIS	CA-CB-CG	8.22	122.02	113.80
1	A	71	VAL	CB-CA-C	-8.10	101.43	112.04
1	A	187	ASN	CA-CB-CG	8.07	120.67	112.60
1	B	188	LYS	N-CA-C	8.05	122.69	112.86
1	B	580	ASN	N-CA-C	8.02	127.88	110.80
1	A	426	ASN	OD1-CG-ND2	-8.02	114.58	122.60
1	A	503	ASP	CA-CB-CG	8.01	120.61	112.60
1	A	652	THR	CA-CB-OG1	-7.90	97.76	109.60
1	B	295	ASP	CA-CB-CG	7.84	120.44	112.60
1	A	406	ASN	CA-CB-CG	7.83	120.44	112.60
1	B	495	ASN	CB-CG-ND2	7.79	128.08	116.40
1	A	124	ASN	OD1-CG-ND2	-7.77	114.83	122.60
1	A	221	ASN	OD1-CG-ND2	-7.77	114.83	122.60
1	A	486	THR	N-CA-C	7.70	120.35	111.11
1	A	424	ILE	N-CA-C	-7.68	102.96	110.72
1	B	486	THR	N-CA-C	7.62	120.26	111.11
1	A	112	GLU	N-CA-C	7.61	121.81	112.23
1	B	67	ASN	OD1-CG-ND2	-7.60	115.00	122.60
1	A	309	ASN	OD1-CG-ND2	-7.56	115.04	122.60
1	A	47	GLN	N-CA-CB	-7.50	99.28	110.61
1	A	465	TRP	CG-CD2-CE3	7.50	141.40	133.90
1	B	584	ARG	N-CA-C	-7.42	97.64	109.59
1	A	188	LYS	N-CA-C	7.41	122.05	113.38
1	B	282	ASN	OD1-CG-ND2	-7.40	115.20	122.60
1	B	202	ASP	CA-CB-CG	7.38	119.97	112.60
1	B	27	ASN	CB-CG-ND2	7.33	127.39	116.40
1	B	469	HIS	CB-CG-CD2	-7.25	121.78	131.20
1	B	199	PHE	CA-CB-CG	7.23	121.03	113.80
1	B	628	HIS	CB-CG-CD2	-7.19	121.85	131.20
1	A	629	GLN	OE1-CD-NE2	-7.17	115.43	122.60
1	B	67	ASN	CB-CG-ND2	7.13	127.10	116.40
1	A	591	PHE	CA-CB-CG	7.06	120.86	113.80
1	A	270	ASP	CA-CB-CG	-7.04	105.56	112.60
1	B	187	ASN	CB-CG-ND2	-7.02	105.87	116.40
1	B	200	ASP	CA-C-O	7.01	126.44	119.08
1	A	418	GLU	N-CA-C	6.97	118.53	111.07

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	313	ASN	OD1-CG-ND2	-6.93	115.67	122.60
1	B	111	VAL	N-CA-C	-6.91	97.78	107.80
1	A	465	TRP	CG-CD1-NE1	-6.80	101.36	110.20
1	B	632	GLY	CA-C-O	-6.80	114.95	121.41
1	A	382	ASP	CA-CB-CG	6.80	119.40	112.60
1	A	310	ASN	OD1-CG-ND2	-6.77	115.83	122.60
1	B	337	GLN	OE1-CD-NE2	-6.76	115.84	122.60
1	B	444	ASN	CA-CB-CG	-6.75	105.85	112.60
1	A	531	LEU	CA-C-N	6.74	126.68	120.21
1	A	531	LEU	C-N-CA	6.74	126.68	120.21
1	B	489	HIS	CA-CB-CG	6.67	120.47	113.80
1	B	53	THR	CA-CB-OG1	-6.66	99.61	109.60
1	A	481	HIS	CB-CG-CD2	-6.63	122.57	131.20
1	B	45	TRP	CG-CD2-CE3	6.63	140.53	133.90
1	A	148	ASP	CA-CB-CG	6.62	119.22	112.60
1	B	608	ASP	CA-CB-CG	6.59	119.19	112.60
1	B	260	HIS	CB-CG-CD2	-6.57	122.66	131.20
1	A	145	THR	CA-CB-OG1	-6.55	99.78	109.60
1	B	503	ASP	CA-CB-CG	6.54	119.14	112.60
1	B	391	TRP	N-CA-C	-6.53	98.75	109.40
1	B	32	GLY	N-CA-C	6.51	120.05	112.50
1	A	109	PRO	N-CA-C	6.49	120.69	110.50
1	B	89	ASP	N-CA-C	-6.49	104.29	111.36
1	B	491	ARG	NE-CZ-NH1	6.49	127.99	121.50
1	A	461	HIS	CB-CG-CD2	-6.42	122.85	131.20
1	A	238	LYS	CA-CB-CG	6.40	126.91	114.10
1	A	554	ASN	CA-C-N	6.40	126.31	119.85
1	A	554	ASN	C-N-CA	6.40	126.31	119.85
1	A	377	ILE	O-C-N	-6.39	116.36	123.26
1	A	652	THR	N-CA-CB	-6.38	99.69	111.18
1	A	157	ASP	CA-CB-CG	6.38	118.98	112.60
1	A	358	THR	N-CA-CB	-6.36	100.08	110.14
1	A	165	SER	N-CA-C	-6.33	104.47	111.82
1	A	221	ASN	CA-CB-CG	6.32	118.92	112.60
1	A	191	ILE	N-CA-C	6.31	116.79	110.23
1	B	461	HIS	CB-CG-ND1	6.31	132.16	122.70
1	B	495	ASN	OD1-CG-ND2	-6.30	116.30	122.60
1	A	187	ASN	CB-CG-ND2	-6.28	106.98	116.40
1	B	8	ASP	N-CA-C	-6.27	104.53	111.36
1	B	551	ASP	CA-CB-CG	6.26	118.86	112.60
1	A	478	GLY	CA-C-N	6.22	125.92	119.64
1	A	478	GLY	C-N-CA	6.22	125.92	119.64

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	223	ASP	N-CA-C	6.22	118.94	109.62
1	B	491	ARG	CB-CG-CD	6.22	125.60	111.30
1	B	406	ASN	CA-CB-CG	6.19	118.79	112.60
1	A	465	TRP	CB-CG-CD1	-6.19	117.61	126.90
1	B	461	HIS	CB-CG-CD2	-6.17	123.17	131.20
1	B	54	ASN	CB-CG-ND2	6.16	125.64	116.40
1	B	481	HIS	CB-CG-CD2	-6.16	123.19	131.20
1	A	652	THR	CA-CB-CG2	6.15	120.96	110.50
1	A	27	ASN	OD1-CG-ND2	-6.14	116.46	122.60
1	B	179	ASN	OD1-CG-ND2	-6.14	116.46	122.60
1	B	216	TYR	O-C-N	-6.12	115.27	123.23
1	B	107	GLU	CB-CG-CD	6.12	123.00	112.60
1	A	461	HIS	CB-CG-ND1	6.11	131.87	122.70
1	A	482	GLN	CA-C-N	6.10	126.42	119.83
1	A	482	GLN	C-N-CA	6.10	126.42	119.83
1	B	392	LYS	N-CA-C	6.10	120.45	112.89
1	A	260	HIS	CB-CG-ND1	6.09	131.84	122.70
1	B	500	ARG	CA-C-N	6.08	125.84	119.76
1	B	500	ARG	C-N-CA	6.08	125.84	119.76
1	A	202	ASP	CA-CB-CG	6.08	118.68	112.60
1	A	393	GLU	N-CA-CB	-6.08	101.65	110.70
1	A	628	HIS	CB-CG-CD2	-6.06	123.32	131.20
1	B	629	GLN	OE1-CD-NE2	-6.06	116.54	122.60
1	A	51	ASN	OD1-CG-ND2	-6.05	116.55	122.60
1	A	495	ASN	N-CA-C	6.04	119.90	111.74
1	A	179	ASN	OD1-CG-ND2	-6.03	116.57	122.60
1	B	372	GLN	OE1-CD-NE2	-6.03	116.57	122.60
1	B	543	SER	O-C-N	-6.02	114.42	122.43
1	A	552	VAL	CA-C-N	-6.00	114.45	122.72
1	A	552	VAL	C-N-CA	-6.00	114.45	122.72
1	A	177	LEU	CA-C-N	5.99	127.63	120.14
1	A	177	LEU	C-N-CA	5.99	127.63	120.14
1	B	298	GLN	OE1-CD-NE2	-5.96	116.64	122.60
1	B	628	HIS	CB-CG-ND1	5.95	131.62	122.70
1	A	234	ALA	N-CA-C	-5.95	104.80	111.28
1	B	94	ARG	N-CA-C	5.93	120.32	113.38
1	B	282	ASN	CA-CB-CG	5.93	118.53	112.60
1	A	465	TRP	CD1-CG-CD2	5.93	115.78	106.30
1	A	469	HIS	CB-CG-CD2	-5.92	123.50	131.20
1	A	61	ASP	CA-CB-CG	5.92	118.52	112.60
1	A	581	ILE	N-CA-C	-5.91	99.90	108.17
1	B	141	LYS	O-C-N	-5.90	116.95	121.55

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	321	LYS	CA-CB-CG	5.89	125.89	114.10
1	A	389	THR	N-CA-CB	-5.89	101.50	111.27
1	B	296	HIS	CB-CG-CD2	-5.88	123.55	131.20
1	B	67	ASN	CA-CB-CG	5.88	118.48	112.60
1	B	496	ILE	O-C-N	-5.87	116.28	123.09
1	A	239	ASP	CA-CB-CG	5.86	118.46	112.60
1	A	345	LYS	CA-CB-CG	-5.86	102.39	114.10
1	B	312	TRP	CG-CD2-CE3	5.85	139.75	133.90
1	A	27	ASN	CA-CB-CG	-5.82	106.78	112.60
1	A	64	VAL	O-C-N	-5.81	117.04	123.20
1	B	458	LEU	CD1-CG-CD2	-5.81	98.01	110.80
1	A	459	SER	CB-CA-C	-5.81	100.97	110.85
1	B	591	PHE	O-C-N	-5.80	115.97	122.12
1	A	69	HIS	CA-CB-CG	5.80	119.60	113.80
1	A	47	GLN	CA-CB-CG	5.79	125.69	114.10
1	A	483	PRO	N-CA-CB	5.79	108.48	103.27
1	A	313	ASN	CB-CG-ND2	5.77	125.05	116.40
1	B	299	LYS	N-CA-C	5.76	117.25	110.97
1	A	500	ARG	O-C-N	-5.73	116.65	121.12
1	A	313	ASN	CA-C-O	-5.73	114.35	120.42
1	A	554	ASN	OD1-CG-ND2	-5.72	116.88	122.60
1	B	73	LEU	N-CA-C	-5.72	105.12	111.36
1	A	444	ASN	OD1-CG-ND2	-5.71	116.89	122.60
1	A	174	HIS	CB-CG-CD2	-5.71	123.78	131.20
1	A	236	LEU	CA-C-N	5.70	132.43	121.54
1	A	236	LEU	C-N-CA	5.70	132.43	121.54
1	B	59	ASN	OD1-CG-ND2	-5.69	116.91	122.60
1	A	185	ASP	CA-CB-CG	5.68	118.28	112.60
1	A	529	GLN	CB-CG-CD	5.68	122.25	112.60
1	B	47	GLN	OE1-CD-NE2	-5.65	116.95	122.60
1	B	408	SER	N-CA-C	-5.65	106.39	113.28
1	B	30	HIS	N-CA-C	-5.64	99.73	109.15
1	B	154	PHE	CA-CB-CG	5.64	119.44	113.80
1	B	174	HIS	CB-CG-CD2	-5.64	123.87	131.20
1	B	51	ASN	OD1-CG-ND2	-5.63	116.97	122.60
1	B	676	LEU	N-CA-C	5.63	118.19	111.71
1	A	470	ASP	N-CA-C	5.63	120.01	113.20
1	B	163	GLY	O-C-N	-5.62	115.40	122.70
1	B	271	ASP	CA-CB-CG	5.61	118.21	112.60
1	A	537	SER	CA-C-O	-5.59	115.72	121.87
1	B	85	LEU	N-CA-C	-5.59	99.14	108.32
1	A	609	ASN	CA-CB-CG	5.59	118.19	112.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	510	ALA	N-CA-C	-5.59	105.09	111.07
1	A	310	ASN	CA-CB-CG	5.58	118.18	112.60
1	B	153	VAL	CB-CA-C	-5.58	101.07	110.71
1	A	500	ARG	CA-C-N	5.57	125.85	119.83
1	A	500	ARG	C-N-CA	5.57	125.85	119.83
1	B	312	TRP	CB-CG-CD1	-5.57	118.55	126.90
1	A	341	ASN	OD1-CG-ND2	-5.56	117.04	122.60
1	A	356	VAL	CA-CB-CG1	-5.56	100.95	110.40
1	B	194	ALA	N-CA-C	5.56	118.34	110.50
1	A	426	ASN	CB-CG-ND2	5.56	124.74	116.40
1	B	21	ASP	N-CA-C	5.56	117.42	111.36
1	A	653	PRO	N-CA-C	-5.54	105.54	113.47
1	A	309	ASN	CB-CG-ND2	5.54	124.72	116.40
1	A	111	VAL	N-CA-C	-5.53	97.93	106.72
1	A	244	ILE	N-CA-C	-5.53	99.19	107.37
1	A	341	ASN	CA-CB-CG	5.51	118.11	112.60
1	A	289	VAL	CA-C-N	5.50	126.72	119.84
1	A	289	VAL	C-N-CA	5.50	126.72	119.84
1	A	465	TRP	CE2-CD2-CG	-5.50	100.60	107.20
1	A	623	TRP	N-CA-C	5.49	119.82	113.18
1	A	652	THR	CB-CA-C	5.48	118.70	109.32
1	B	232	ALA	CA-C-N	5.48	127.56	120.44
1	B	232	ALA	C-N-CA	5.48	127.56	120.44
1	B	490	PHE	CA-CB-CG	-5.47	108.33	113.80
1	B	507	VAL	N-CA-C	-5.46	105.52	110.82
1	B	93	PHE	CA-CB-CG	5.44	119.24	113.80
1	B	108	LEU	CA-C-N	5.44	126.64	119.84
1	B	108	LEU	C-N-CA	5.44	126.64	119.84
1	A	42	HIS	CB-CG-CD2	-5.44	124.13	131.20
1	A	274	GLN	CA-CB-CG	5.44	124.97	114.10
1	B	625	LYS	N-CA-C	5.44	119.78	113.20
1	B	671	LYS	CA-CB-CG	5.44	124.97	114.10
1	B	528	ARG	CA-CB-CG	-5.42	103.27	114.10
1	B	481	HIS	CA-CB-CG	-5.41	108.39	113.80
1	A	12	VAL	O-C-N	-5.41	116.41	121.87
1	B	42	HIS	CA-CB-CG	-5.40	108.40	113.80
1	B	377	ILE	O-C-N	-5.40	117.33	123.10
1	A	303	LYS	CG-CD-CE	5.39	123.70	111.30
1	B	482	GLN	CA-C-N	5.39	125.15	119.76
1	B	482	GLN	C-N-CA	5.39	125.15	119.76
1	B	448	TYR	N-CA-C	-5.39	105.41	111.28
1	B	398	GLN	O-C-N	-5.38	116.97	121.54

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	282	ASN	CA-C-N	5.38	126.56	119.84
1	A	282	ASN	C-N-CA	5.38	126.56	119.84
1	B	156	GLY	O-C-N	-5.37	119.82	123.95
1	B	506	GLU	CA-CB-CG	-5.37	103.37	114.10
1	A	506	GLU	CA-CB-CG	-5.36	103.38	114.10
1	A	652	THR	CA-C-O	-5.36	115.57	120.50
1	B	64	VAL	O-C-N	-5.35	117.62	123.18
1	B	15	ILE	CB-CG1-CD1	-5.35	102.57	113.80
1	A	71	VAL	N-CA-CB	5.33	117.13	110.47
1	A	621	THR	CA-C-O	-5.31	114.89	120.63
1	A	466	VAL	N-CA-CB	-5.31	106.37	111.89
1	A	529	GLN	OE1-CD-NE2	-5.31	117.29	122.60
1	A	621	THR	N-CA-C	5.30	117.75	111.33
1	B	560	VAL	CB-CA-C	-5.30	103.50	110.98
1	A	392	LYS	N-CA-C	5.30	118.54	111.75
1	B	111	VAL	CA-C-N	5.30	129.65	120.58
1	B	111	VAL	C-N-CA	5.30	129.65	120.58
1	A	296	HIS	CB-CG-CD2	-5.30	124.31	131.20
1	B	238	LYS	N-CA-C	5.30	118.84	112.38
1	A	265	ALA	CA-C-N	5.29	125.21	119.76
1	A	265	ALA	C-N-CA	5.29	125.21	119.76
1	B	354	SER	N-CA-C	5.29	117.97	110.50
1	A	187	ASN	N-CA-C	5.29	119.43	112.92
1	B	530	ASN	OD1-CG-ND2	-5.28	117.32	122.60
1	B	654	GLU	CA-CB-CG	-5.28	103.55	114.10
1	A	595	ASP	CA-CB-CG	5.26	117.86	112.60
1	B	592	PHE	N-CA-C	5.26	116.87	111.03
1	A	295	ASP	CA-CB-CG	5.25	117.86	112.60
1	B	465	TRP	CE2-CD2-CG	-5.25	100.89	107.20
1	B	212	TRP	N-CA-C	-5.25	101.61	109.95
1	A	100	THR	N-CA-CB	-5.24	102.71	110.99
1	B	465	TRP	CG-CD2-CE3	5.24	139.14	133.90
1	A	459	SER	CA-CB-OG	5.23	121.56	111.10
1	A	341	ASN	CB-CG-ND2	5.22	124.23	116.40
1	A	93	PHE	CA-CB-CG	5.21	119.01	113.80
1	A	482	GLN	CA-C-O	-5.21	114.80	119.59
1	B	642	ALA	N-CA-C	5.21	120.69	113.45
1	B	531	LEU	CA-C-O	-5.20	115.51	120.97
1	B	397	PHE	N-CA-C	-5.20	100.61	108.67
1	B	382	ASP	CA-CB-CG	5.20	117.80	112.60
1	B	672	LEU	N-CA-C	5.19	118.21	109.95
1	A	560	VAL	N-CA-CB	5.19	118.31	111.25

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	465	TRP	CG-CD1-NE1	-5.19	103.45	110.20
1	B	529	GLN	CB-CG-CD	5.19	121.42	112.60
1	A	499	TRP	CE2-CD2-CG	-5.19	100.98	107.20
1	B	377	ILE	N-CA-C	-5.19	100.73	108.46
1	A	263	HIS	CB-CG-CD2	-5.17	124.48	131.20
1	B	165	SER	N-CA-C	-5.17	105.82	111.82
1	A	54	ASN	CA-C-N	5.17	126.30	119.84
1	A	54	ASN	C-N-CA	5.17	126.30	119.84
1	B	187	ASN	CB-CG-OD1	5.15	131.10	120.80
1	B	246	MET	CA-C-O	-5.15	115.25	120.71
1	B	288	VAL	CA-C-N	-5.15	117.58	123.25
1	B	288	VAL	C-N-CA	-5.15	117.58	123.25
1	A	189	ILE	O-C-N	5.15	128.87	123.00
1	B	15	ILE	CB-CA-C	-5.15	105.12	112.22
1	B	444	ASN	N-CA-C	5.14	117.55	111.33
1	B	462	PRO	N-CA-C	5.14	123.07	112.47
1	B	464	ILE	O-C-N	-5.14	116.18	122.97
1	B	337	GLN	CG-CD-NE2	5.14	124.11	116.40
1	B	69	HIS	CB-CG-CD2	-5.14	124.52	131.20
1	B	298	GLN	CG-CD-NE2	5.14	124.11	116.40
1	B	362	SER	N-CA-C	-5.13	105.60	111.14
1	B	116	GLY	CA-C-N	5.12	125.41	119.93
1	B	116	GLY	C-N-CA	5.12	125.41	119.93
1	A	310	ASN	CB-CG-ND2	5.12	124.08	116.40
1	B	298	GLN	N-CA-C	-5.12	105.59	111.07
1	A	677	LYS	CB-CG-CD	-5.12	99.52	111.30
1	B	53	THR	N-CA-CB	-5.12	102.34	110.28
1	B	554	ASN	CA-C-N	5.12	124.88	119.76
1	B	554	ASN	C-N-CA	5.12	124.88	119.76
1	A	174	HIS	CB-CG-ND1	5.11	130.36	122.70
1	B	330	LEU	CA-C-O	-5.11	115.46	120.82
1	B	215	LEU	CA-C-O	-5.11	115.39	121.16
1	A	566	VAL	CA-C-N	5.10	127.43	120.54
1	A	566	VAL	C-N-CA	5.10	127.43	120.54
1	A	631	PHE	N-CA-C	-5.10	100.20	108.52
1	B	148	ASP	CA-CB-CG	5.10	117.70	112.60
1	A	67	ASN	CB-CG-ND2	5.10	124.04	116.40
1	B	112	GLU	CA-CB-CG	5.10	124.29	114.10
1	B	177	LEU	CA-C-N	5.09	126.55	120.13
1	B	177	LEU	C-N-CA	5.09	126.55	120.13
1	B	456	SER	N-CA-C	-5.09	105.62	111.07
1	A	552	VAL	CB-CA-C	-5.08	101.61	110.71

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	492	SER	N-CA-C	-5.08	107.13	113.38
1	B	104	PRO	O-C-N	-5.07	116.72	123.01
1	B	629	GLN	CG-CD-NE2	5.07	124.01	116.40
1	A	83	TYR	N-CA-C	-5.07	103.35	110.35
1	A	232	ALA	N-CA-C	5.07	116.81	111.28
1	A	485	GLU	CB-CG-CD	5.07	121.22	112.60
1	A	535	GLU	N-CA-C	-5.07	100.52	108.63
1	B	42	HIS	CB-CG-CD2	-5.07	124.61	131.20
1	B	461	HIS	N-CA-C	-5.07	101.34	109.04
1	A	580	ASN	N-CA-C	5.06	118.37	111.39
1	A	381	ALA	O-C-N	5.06	128.00	122.64
1	A	607	PRO	N-CA-C	5.05	120.03	111.03
1	B	8	ASP	CA-C-O	-5.05	115.06	120.42
1	A	3	GLN	OE1-CD-NE2	-5.05	117.55	122.60
1	B	467	ALA	O-C-N	-5.05	115.44	122.41
1	B	93	PHE	N-CA-C	-5.05	103.48	110.35
1	B	265	ALA	CA-C-N	5.04	125.03	119.89
1	B	265	ALA	C-N-CA	5.04	125.03	119.89
1	B	566	VAL	CA-C-O	-5.04	115.51	120.85
1	B	58	ILE	CA-C-O	-5.04	115.81	121.05
1	B	465	TRP	CD1-CG-CD2	5.03	114.35	106.30
1	A	192	ASP	CA-CB-CG	5.02	117.62	112.60
1	A	358	THR	CB-CA-C	5.02	120.20	110.46
1	B	408	SER	CA-CB-OG	5.02	121.14	111.10
1	B	418	GLU	N-CA-C	5.01	116.75	111.28
1	A	243	LEU	N-CA-C	-5.01	101.00	109.07
1	B	652	THR	CA-C-N	5.01	126.11	119.84
1	B	652	THR	C-N-CA	5.01	126.11	119.84
1	B	212	TRP	CA-CB-CG	5.01	123.12	113.60
1	A	609	ASN	O-C-N	-5.00	116.31	122.57
1	B	214	VAL	O-C-N	-5.00	117.25	123.10

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	88	0
1	B	5198	0	5139	67	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	1	0
All	All	10452	0	10314	148	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 (148) 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
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:48:MET:HB2	1:A:50:MET:HE2	1.82	0.60
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:48:MET:HB2	1:B:50:MET:HE2	1.86	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:B:44:LEU:HG	1:B:48:MET:HE2	1.89	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: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
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:A:479:PRO:HB2	1:B:458:LEU:HD11	1.94	0.50
1:B:380:SER:HB2	1:B:389:THR:OG1	2.11	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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:130:MET:HE3	1:A:175:LEU:HD13	1.97	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:62:ARG:HH11	1:A:62:ARG:HG3	1.82	0.45
1:A:117:PRO:HB2	1:A:120:GLN:HG3	1.99	0.45
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:191:ILE:HG13	3:B:681:M6T:H62	1.98	0.45
1:B:570:VAL:O	1:B:574:LYS:HD2	2.16	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:3:GLN:OE1	1:A:3:GLN:N	2.51	0.44
1:A:144:PHE:CD1	1:A:323:PHE:HE2	2.35	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:40:ALA:HB2	1:A:246:MET:HE1	2.00	0.43
1:A:616:GLU:O	1:A:632:GLY:HA2	2.18	0.43
1:B:45:TRP:HA	1:B:48:MET:HE3	2.00	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:87:ILE:O	1:A:91:LYS:HG3	2.20	0.42
1:A:171:LEU:HD23	1:A:424:ILE:CD1	2.50	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:HE2	1:B:647:LYS:HB3	1.72	0.42
1:B:81:THR:HG22	1:B:301:ILE:HD12	2.02	0.41
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: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
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:HD23	1:A:118:LEU:HA	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
1:A:540:GLU:H	1:A:540:GLU:CD	2.29	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	676/678 (100%)	627 (93%)	44 (6%)	5 (1%)	18	41
1	B	676/678 (100%)	627 (93%)	43 (6%)	6 (1%)	14	35
All	All	1352/1356 (100%)	1254 (93%)	87 (6%)	11 (1%)	16	37

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
1	A	31	PRO
1	B	521	PRO

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	552/552 (100%)	503 (91%)	49 (9%)	9	23
1	B	552/552 (100%)	507 (92%)	45 (8%)	10	27

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
All	All	1104/1104 (100%)	1010 (92%)	94 (8%)	10	25

All (94) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	3	GLN
1	A	47	GLN
1	A	60	ARG
1	A	67	ASN
1	A	71	VAL
1	A	88	GLU
1	A	92	GLN
1	A	114	THR
1	A	117	PRO
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	310	ASN
1	A	314	LYS
1	A	338	LEU
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	486	THR
1	A	518	LYS
1	A	552	VAL
1	A	560	VAL
1	A	567	SER
1	A	580	ASN

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Mol	Chain	Res	Type
1	A	584	ARG
1	A	588	LEU
1	A	600	GLU
1	A	607	PRO
1	A	608	ASP
1	A	615	VAL
1	A	618	LEU
1	A	652	THR
1	A	654	GLU
1	A	668	LYS
1	A	672	LEU
1	A	678	LYS
1	B	3	GLN
1	B	34	PRO
1	B	62	ARG
1	B	67	ASN
1	B	92	GLN
1	B	109	PRO
1	B	113	VAL
1	B	122	ILE
1	B	141	LYS
1	B	166	SER
1	B	197	ILE
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
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	373	LEU
1	B	388	LEU
1	B	389	THR
1	B	392	LYS

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Mol	Chain	Res	Type
1	B	484	ILE
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	581	ILE
1	B	596	LYS
1	B	600	GLU
1	B	610	VAL
1	B	618	LEU
1	B	668	LYS
1	B	671	LYS

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	3	GLN
1	A	27	ASN
1	A	30	HIS
1	A	54	ASN
1	A	132	GLN
1	A	179	ASN
1	A	219	ASN
1	A	298	GLN
1	A	341	ASN
1	A	387	ASN
1	A	489	HIS
1	A	597	GLN
1	A	661	GLN
1	B	51	ASN
1	B	54	ASN
1	B	124	ASN
1	B	282	ASN
1	B	309	ASN
1	B	313	ASN
1	B	489	HIS
1	B	513	ASN
1	B	530	ASN

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 oligosaccharides 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	M6T	B	681	2	27,28,28	1.54	4 (14%)	38,42,42	1.04	3 (7%)
3	M6T	A	681	2	27,28,28	1.22	3 (11%)	38,42,42	1.13	3 (7%)

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	-	3/17/17/17	0/2/2/2
3	M6T	A	681	2	-	4/17/17/17	0/2/2/2

All (7) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	681	M6T	PA-O3A	4.55	1.64	1.59

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	681	M6T	C4-N3	-3.04	1.33	1.39
3	A	681	M6T	C4-N3	-2.99	1.33	1.39
3	B	681	M6T	PB-O3B	-2.69	1.44	1.54
3	A	681	M6T	PB-O3B	-2.37	1.46	1.54
3	A	681	M6T	PB-O2B	-2.31	1.46	1.54
3	B	681	M6T	C5'-C4'	2.26	1.44	1.41

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	681	M6T	C2-S1-C5	-3.84	88.67	91.22
3	B	681	M6T	C7-C6-C5	-2.44	105.08	112.73
3	A	681	M6T	N3'-C2'-N1'	-2.38	121.56	125.77
3	A	681	M6T	CM2-C2'-N3'	2.30	120.57	117.13
3	B	681	M6T	CM2-C2'-N3'	2.17	120.38	117.13
3	B	681	M6T	O2B-PB-O1B	2.17	119.28	110.83

There are no chirality outliers.

All (7) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	681	M6T	PB-O3A-PA-O1A
3	B	681	M6T	PB-O3A-PA-O2A
3	A	681	M6T	C7-O7-PA-O1A
3	A	681	M6T	S1-C5-C6-C7
3	B	681	M6T	PB-O3A-PA-O1A
3	B	681	M6T	C6'-C5'-C7'-N3
3	A	681	M6T	PB-O3A-PA-O2A

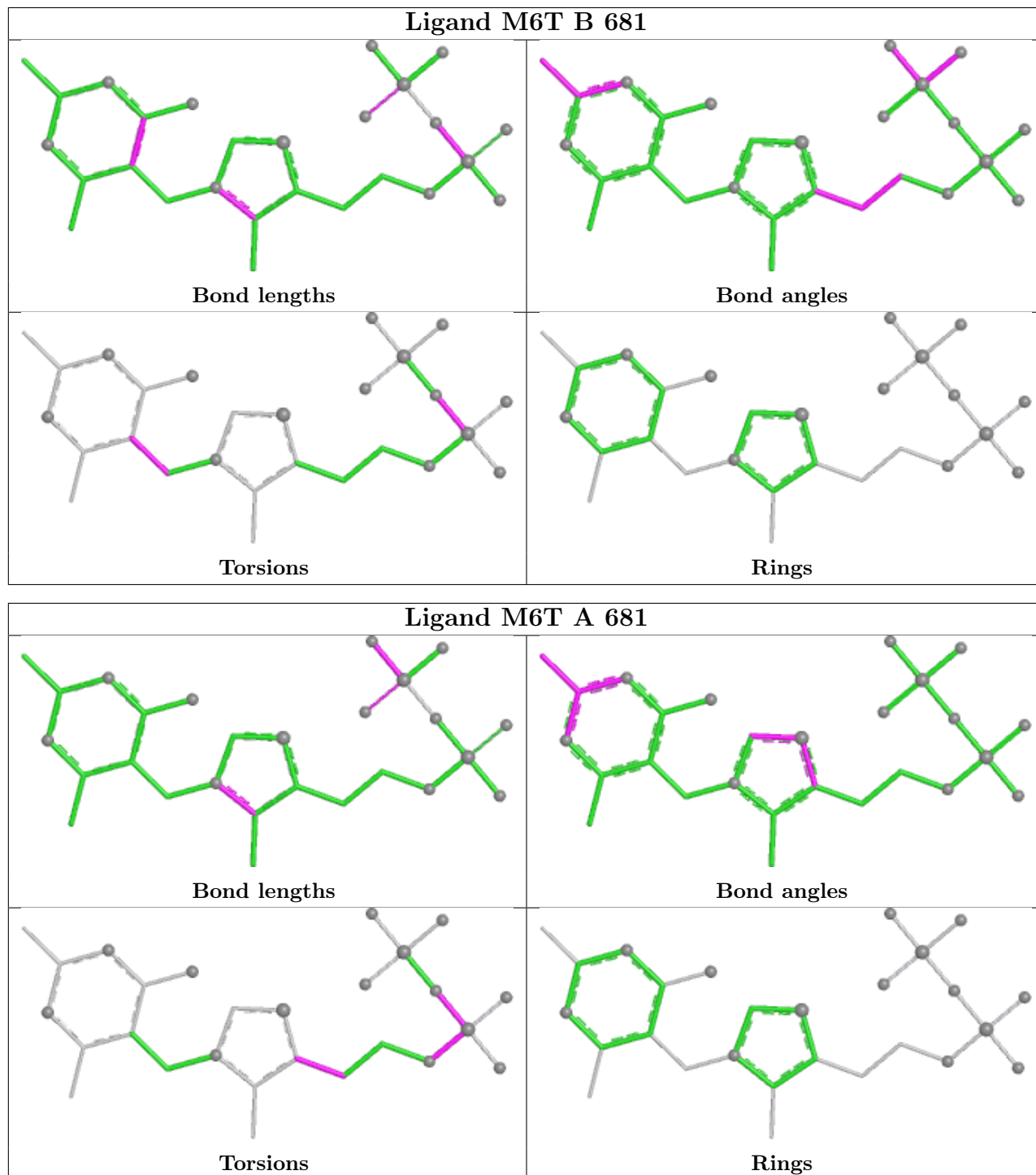
There are no ring outliers.

2 monomers are involved in 5 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	B	681	M6T	1	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 [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](#)

EDS was not executed - this section is therefore empty.

6.2 Non-standard residues in protein, DNA, RNA chains [i](#)

EDS was not executed - this section is therefore empty.

6.3 Carbohydrates [i](#)

EDS was not executed - this section is therefore empty.

6.4 Ligands [i](#)

EDS was not executed - this section is therefore empty.

6.5 Other polymers [i](#)

EDS was not executed - this section is therefore empty.