



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 10, 2026 – 08:04 AM UTC

PDB ID : 1TKA / pdb_00001tka
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)
Xtriage (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

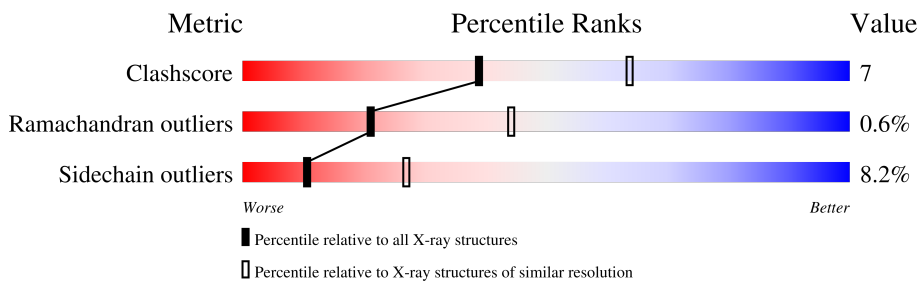
1 Overall quality at a glance

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	 64% 29% 6%
1	B	678	 67% 28%

2 Entry composition [i](#)

There are 3 unique types of molecules in this entry. The entry contains 10450 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.

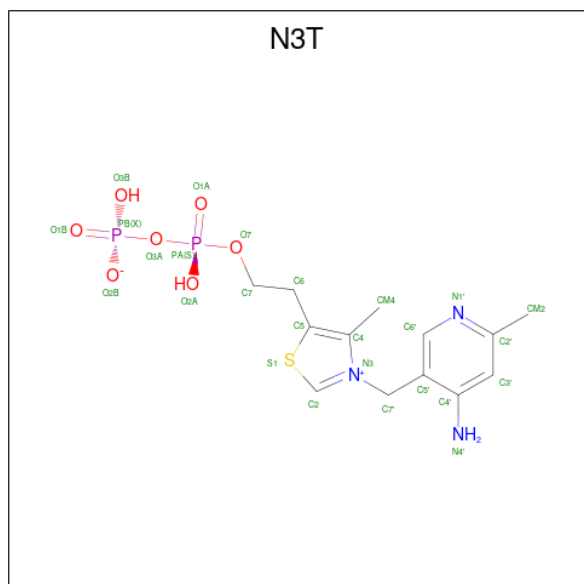
- Molecule 1 is a protein called TRANSKETOLASE.

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 (CCD ID: CA) (formula: Ca).

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

- Molecule 3 is 3'-DEAZO-THIAMIN DIPHOSPHATE (CCD ID: N3T) (formula: C₁₃H₁₉N₃O₇P₂S).



Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
3	A	1	Total	C	N	O	P	S	0	0
			26	13	3	7	2	1		
3	B	1	Total	C	N	O	P	S	0	0
			26	13	3	7	2	1		

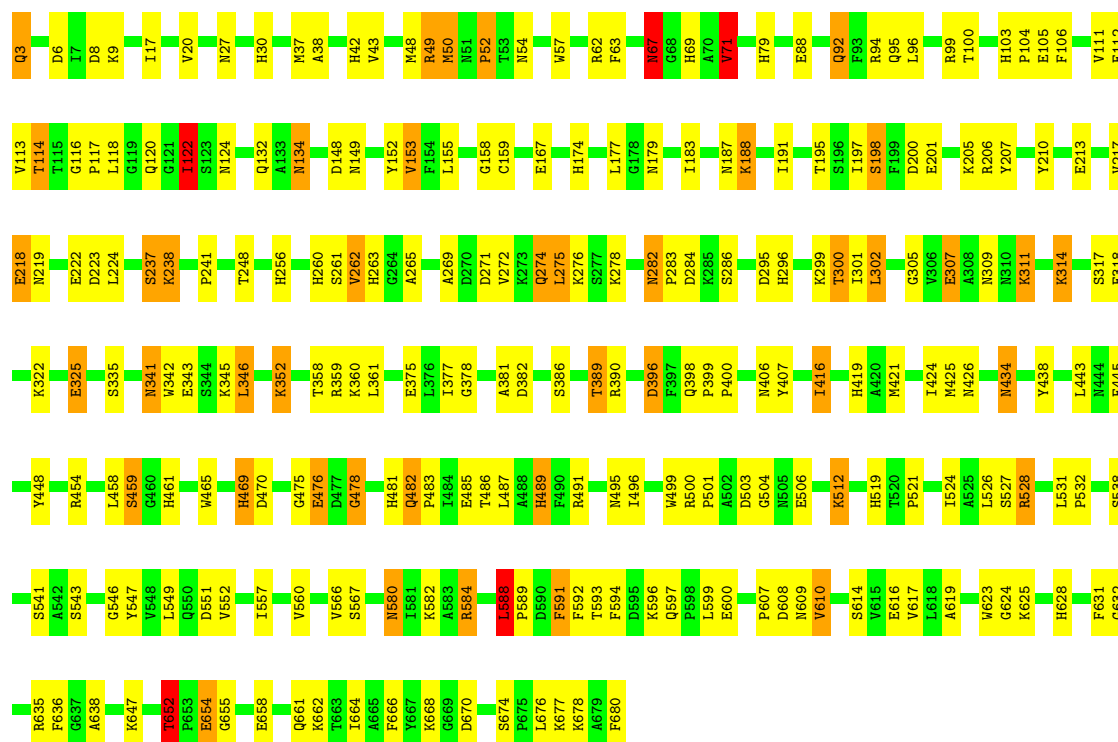
3 Residue-property plots [i](#)

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

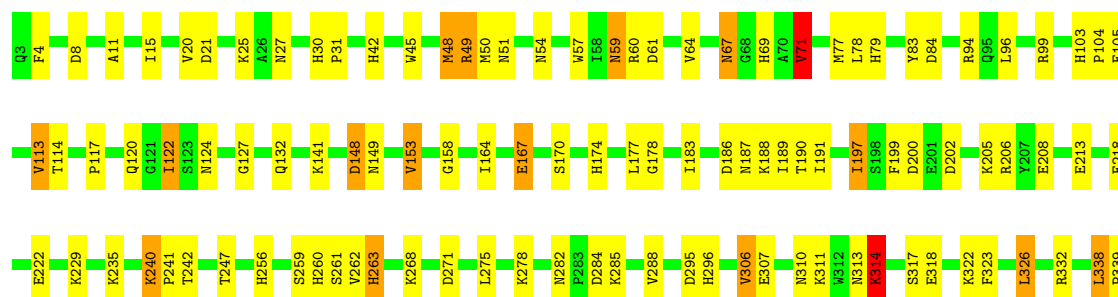
• Molecule 1: TRANSKETOLASE

Chain A:  64% 29% 6% .



• Molecule 1: TRANSKETOLASE

Chain B:  67% 28% . .





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	76.30Å 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}	0.158 , (Not available)	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	10450	wwPDB-VP
Average B, all atoms (Å ²)	10.0	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: N3T, 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	1.11	26/5324 (0.5%)	1.97	168/7230 (2.3%)
1	B	1.12	24/5324 (0.5%)	1.93	134/7230 (1.9%)
All	All	1.12	50/10648 (0.5%)	1.95	302/14460 (2.1%)

All (50) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	122	ILE	CA-CB	7.78	1.64	1.54
1	B	489	HIS	CD2-NE2	-6.99	1.30	1.37
1	A	263	HIS	CD2-NE2	-6.97	1.30	1.37
1	A	296	HIS	CD2-NE2	-6.94	1.30	1.37
1	B	419	HIS	CD2-NE2	-6.93	1.30	1.37
1	A	114	THR	CA-CB	6.88	1.63	1.53
1	B	484	ILE	CA-CB	6.87	1.63	1.54
1	A	489	HIS	CD2-NE2	-6.82	1.30	1.37
1	B	263	HIS	CD2-NE2	-6.77	1.30	1.37
1	A	628	HIS	CD2-NE2	-6.71	1.30	1.37
1	B	260	HIS	CD2-NE2	-6.68	1.30	1.37
1	A	79	HIS	CD2-NE2	-6.64	1.30	1.37
1	B	498	VAL	CA-CB	6.61	1.60	1.53
1	A	260	HIS	CD2-NE2	-6.59	1.30	1.37
1	B	79	HIS	CD2-NE2	-6.56	1.30	1.37
1	B	69	HIS	CD2-NE2	-6.45	1.30	1.37
1	B	628	HIS	CD2-NE2	-6.39	1.30	1.37
1	A	256	HIS	CD2-NE2	-6.37	1.30	1.37
1	B	174	HIS	CD2-NE2	-6.37	1.30	1.37
1	B	461	HIS	CD2-NE2	-6.34	1.30	1.37
1	B	469	HIS	CD2-NE2	-6.29	1.30	1.37
1	B	30	HIS	CD2-NE2	-6.29	1.30	1.37
1	A	174	HIS	CD2-NE2	-6.24	1.30	1.37
1	B	481	HIS	CD2-NE2	-6.23	1.30	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	461	HIS	CD2-NE2	-6.19	1.31	1.37
1	A	481	HIS	CD2-NE2	-6.19	1.31	1.37
1	A	419	HIS	CD2-NE2	-6.14	1.31	1.37
1	A	69	HIS	CD2-NE2	-6.14	1.31	1.37
1	A	377	ILE	CA-CB	6.11	1.61	1.54
1	B	256	HIS	CD2-NE2	-5.99	1.31	1.37
1	B	103	HIS	CD2-NE2	-5.98	1.31	1.37
1	B	42	HIS	CD2-NE2	-5.96	1.31	1.37
1	A	30	HIS	CD2-NE2	-5.88	1.31	1.37
1	A	519	HIS	CD2-NE2	-5.87	1.31	1.37
1	A	103	HIS	CD2-NE2	-5.69	1.31	1.37
1	B	519	HIS	CD2-NE2	-5.67	1.31	1.37
1	B	189	ILE	C-O	5.63	1.29	1.24
1	B	296	HIS	CD2-NE2	-5.61	1.31	1.37
1	A	524	ILE	CA-CB	5.39	1.60	1.53
1	A	419	HIS	CB-CG	5.34	1.57	1.50
1	A	469	HIS	CD2-NE2	-5.30	1.32	1.37
1	A	183	ILE	CA-CB	5.29	1.61	1.54
1	A	42	HIS	CD2-NE2	-5.23	1.32	1.37
1	B	208	GLU	CA-CB	-5.23	1.44	1.53
1	A	167	GLU	CA-CB	-5.21	1.45	1.53
1	B	263	HIS	CG-ND1	-5.17	1.32	1.38
1	B	79	HIS	CG-ND1	-5.12	1.32	1.38
1	B	122	ILE	CA-CB	5.08	1.60	1.54
1	A	248	THR	CA-CB	5.06	1.61	1.53
1	A	263	HIS	CG-ND1	-5.05	1.32	1.38

All (302) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	295	ASP	CA-CB-CG	11.41	124.01	112.60
1	B	67	ASN	OD1-CG-ND2	-11.04	111.56	122.60
1	B	187	ASN	CA-CB-CG	10.13	122.73	112.60
1	A	148	ASP	CA-CB-CG	10.02	122.62	112.60
1	A	389	THR	N-CA-CB	-9.46	96.07	110.73
1	A	179	ASN	OD1-CG-ND2	-9.40	113.19	122.60
1	B	27	ASN	CA-CB-CG	-9.40	103.20	112.60
1	B	424	ILE	N-CA-C	-9.33	101.76	110.53
1	B	8	ASP	CA-CB-CG	-9.12	103.48	112.60
1	B	470	ASP	N-CA-C	8.85	123.49	112.87
1	A	187	ASN	CA-CB-CG	8.66	121.26	112.60
1	B	486	THR	N-CA-C	8.57	120.23	111.07

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	591	PHE	CA-CB-CG	8.46	122.26	113.80
1	B	406	ASN	OD1-CG-ND2	-8.29	114.31	122.60
1	A	71	VAL	CB-CA-C	-8.22	97.80	111.29
1	B	529	GLN	N-CA-C	8.18	121.59	110.55
1	A	260	HIS	CB-CG-CD2	-8.10	120.66	131.20
1	B	392	LYS	N-CA-C	8.06	120.15	111.36
1	B	124	ASN	OD1-CG-ND2	-8.04	114.56	122.60
1	B	69	HIS	CA-CB-CG	7.94	121.74	113.80
1	A	580	ASN	N-CA-C	7.92	122.38	112.24
1	B	489	HIS	CA-CB-CG	7.89	121.69	113.80
1	B	67	ASN	CB-CG-ND2	7.84	128.16	116.40
1	A	67	ASN	CB-CG-ND2	7.78	128.07	116.40
1	A	54	ASN	OD1-CG-ND2	-7.73	114.87	122.60
1	A	120	GLN	OE1-CD-NE2	-7.62	114.97	122.60
1	A	434	ASN	OD1-CG-ND2	-7.61	114.99	122.60
1	B	580	ASN	N-CA-C	7.57	121.84	111.54
1	A	179	ASN	CA-CB-CG	7.46	120.06	112.60
1	B	418	GLU	N-CA-C	7.46	119.41	111.28
1	A	67	ASN	OD1-CG-ND2	-7.44	115.16	122.60
1	A	389	THR	CB-CA-C	7.38	123.20	110.72
1	A	465	TRP	CG-CD2-CE3	7.36	141.26	133.90
1	A	476	GLU	N-CA-C	7.33	121.48	112.54
1	B	476	GLU	N-CA-C	7.28	121.07	111.75
1	A	531	LEU	CA-C-N	7.27	127.25	119.76
1	A	531	LEU	C-N-CA	7.27	127.25	119.76
1	B	398	GLN	OE1-CD-NE2	-7.26	115.33	122.60
1	A	200	ASP	CA-CB-CG	7.25	119.85	112.60
1	A	503	ASP	CA-CB-CG	7.21	119.81	112.60
1	A	223	ASP	CA-CB-CG	7.20	119.80	112.60
1	B	497	GLN	OE1-CD-NE2	-7.19	115.41	122.60
1	B	84	ASP	CA-CB-CG	7.15	119.75	112.60
1	B	659	ARG	CA-CB-CG	-7.13	99.84	114.10
1	A	217	VAL	N-CA-C	-7.13	97.34	107.75
1	A	149	ASN	N-CA-C	7.11	120.15	110.55
1	B	503	ASP	CA-CB-CG	7.11	119.70	112.60
1	B	628	HIS	CB-CG-CD2	-7.09	121.98	131.20
1	B	391	TRP	N-CA-C	-7.07	101.01	110.55
1	A	475	GLY	N-CA-C	6.95	118.06	111.67
1	A	398	GLN	O-C-N	-6.92	116.60	121.65
1	B	4	PHE	N-CA-C	-6.91	98.94	109.85
1	A	426	ASN	OD1-CG-ND2	-6.87	115.73	122.60
1	A	470	ASP	N-CA-C	6.83	122.79	113.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	481	HIS	CB-CG-CD2	-6.82	122.34	131.20
1	B	99	ARG	N-CA-C	-6.76	104.77	113.16
1	A	307	GLU	CA-CB-CG	6.75	127.59	114.10
1	A	419	HIS	CA-CB-CG	6.73	120.53	113.80
1	A	286	SER	N-CA-C	6.70	119.35	109.24
1	B	188	LYS	N-CA-C	6.69	121.20	113.38
1	A	609	ASN	CA-CB-CG	6.68	119.28	112.60
1	A	677	LYS	N-CA-C	6.67	119.39	109.59
1	A	262	VAL	N-CA-CB	-6.64	100.93	112.08
1	A	381	ALA	CA-C-N	6.62	131.81	122.08
1	A	381	ALA	C-N-CA	6.62	131.81	122.08
1	A	295	ASP	CA-CB-CG	6.60	119.20	112.60
1	B	408	SER	CA-CB-OG	6.57	124.23	111.10
1	A	309	ASN	CB-CG-ND2	6.55	126.23	116.40
1	B	235	LYS	CA-CB-CG	-6.55	101.01	114.10
1	B	271	ASP	CA-CB-CG	6.54	119.14	112.60
1	A	94	ARG	CA-CB-CG	-6.54	101.02	114.10
1	A	478	GLY	CA-C-N	6.51	125.95	118.85
1	A	478	GLY	C-N-CA	6.51	125.95	118.85
1	A	434	ASN	CB-CG-ND2	6.51	126.16	116.40
1	A	566	VAL	N-CA-C	-6.49	104.43	110.53
1	B	340	ALA	CA-C-O	6.47	128.14	120.70
1	A	260	HIS	CB-CG-ND1	6.46	132.39	122.70
1	B	645	VAL	CG1-CB-CG2	-6.46	96.60	110.80
1	A	608	ASP	CA-CB-CG	6.45	119.05	112.60
1	B	373	LEU	CA-C-N	6.42	126.11	119.82
1	B	373	LEU	C-N-CA	6.42	126.11	119.82
1	A	322	LYS	N-CA-C	6.38	118.24	111.28
1	A	470	ASP	CA-CB-CG	6.38	118.98	112.60
1	B	670	ASP	CA-CB-CG	6.37	118.97	112.60
1	A	262	VAL	O-C-N	-6.36	115.97	122.14
1	A	406	ASN	OD1-CG-ND2	-6.34	116.26	122.60
1	B	580	ASN	OD1-CG-ND2	-6.34	116.26	122.60
1	B	491	ARG	CB-CG-CD	6.33	125.87	111.30
1	B	446	VAL	N-CA-C	-6.32	103.19	111.09
1	B	199	PHE	CA-CB-CG	6.29	120.09	113.80
1	A	399	PRO	CA-C-N	6.28	127.69	119.84
1	A	399	PRO	C-N-CA	6.28	127.69	119.84
1	B	178	GLY	O-C-N	-6.28	115.58	122.68
1	A	177	LEU	CA-C-N	6.28	128.04	120.13
1	A	177	LEU	C-N-CA	6.28	128.04	120.13
1	B	148	ASP	CA-CB-CG	6.26	118.86	112.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	371	ASN	OD1-CG-ND2	-6.26	116.34	122.60
1	A	424	ILE	N-CA-C	-6.25	104.41	110.72
1	A	628	HIS	CB-CG-CD2	-6.25	123.08	131.20
1	A	132	GLN	OE1-CD-NE2	-6.22	116.38	122.60
1	A	92	GLN	OE1-CD-NE2	-6.22	116.38	122.60
1	A	489	HIS	CA-CB-CG	6.21	120.01	113.80
1	A	461	HIS	CB-CG-CD2	-6.21	123.13	131.20
1	A	551	ASP	CA-CB-CG	6.20	118.80	112.60
1	B	132	GLN	OE1-CD-NE2	-6.20	116.40	122.60
1	A	105	GLU	CA-CB-CG	6.20	126.50	114.10
1	B	513	ASN	OD1-CG-ND2	-6.18	116.42	122.60
1	A	674	SER	CA-C-N	6.17	125.86	119.56
1	A	674	SER	C-N-CA	6.17	125.86	119.56
1	A	112	GLU	N-CA-C	6.17	120.01	112.23
1	B	149	ASN	N-CA-C	6.17	118.52	110.43
1	B	495	ASN	CB-CG-ND2	6.16	125.65	116.40
1	A	300	THR	CA-CB-OG1	-6.15	100.37	109.60
1	A	296	HIS	CB-CG-CD2	-6.15	123.21	131.20
1	A	482	GLN	OE1-CD-NE2	-6.15	116.45	122.60
1	A	27	ASN	CA-CB-CG	-6.12	106.48	112.60
1	B	434	ASN	OD1-CG-ND2	-6.12	116.48	122.60
1	B	42	HIS	CB-CG-CD2	-6.09	123.28	131.20
1	A	459	SER	CA-CB-OG	6.08	123.27	111.10
1	B	406	ASN	CB-CG-ND2	6.08	125.52	116.40
1	A	299	LYS	CA-CB-CG	6.07	126.24	114.10
1	A	116	GLY	CA-C-N	6.07	126.27	119.90
1	A	116	GLY	C-N-CA	6.07	126.27	119.90
1	B	564	SER	CA-CB-OG	6.05	123.21	111.10
1	B	306	VAL	CA-C-O	-6.03	114.68	120.95
1	B	314	LYS	CG-CD-CE	6.03	125.17	111.30
1	A	124	ASN	OD1-CG-ND2	-6.03	116.57	122.60
1	B	307	GLU	CB-CG-CD	6.01	122.82	112.60
1	A	269	ALA	N-CA-C	5.98	118.56	111.33
1	B	191	ILE	N-CA-C	5.97	117.43	110.62
1	A	500	ARG	CA-C-N	5.97	125.91	119.76
1	A	500	ARG	C-N-CA	5.97	125.91	119.76
1	B	197	ILE	CA-CB-CG1	-5.97	100.25	110.40
1	A	654	GLU	CA-CB-CG	5.96	126.03	114.10
1	B	408	SER	N-CA-C	-5.96	105.50	112.89
1	A	30	HIS	CA-C-N	5.94	127.27	119.84
1	A	30	HIS	C-N-CA	5.94	127.27	119.84
1	B	398	GLN	CG-CD-NE2	5.93	125.29	116.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	495	ASN	N-CA-C	5.93	119.74	111.74
1	A	396	ASP	CA-CB-CG	5.90	118.50	112.60
1	B	444	ASN	CA-CB-CG	-5.89	106.71	112.60
1	A	406	ASN	CA-CB-CG	5.89	118.49	112.60
1	A	652	THR	CA-C-N	5.88	125.58	119.05
1	A	652	THR	C-N-CA	5.88	125.58	119.05
1	B	200	ASP	CA-C-O	5.88	125.63	119.51
1	B	574	LYS	N-CA-C	-5.87	104.80	111.14
1	B	481	HIS	CB-CG-CD2	-5.87	123.57	131.20
1	B	61	ASP	CA-CB-CG	5.86	118.46	112.60
1	B	652	THR	CA-C-N	5.86	125.06	118.97
1	B	652	THR	C-N-CA	5.86	125.06	118.97
1	B	426	ASN	OD1-CG-ND2	-5.85	116.75	122.60
1	B	59	ASN	OD1-CG-ND2	-5.83	116.77	122.60
1	B	450	ALA	N-CA-C	5.83	118.38	111.33
1	A	532	PRO	N-CA-C	5.83	120.23	111.14
1	B	21	ASP	CA-C-N	5.82	128.56	120.29
1	B	21	ASP	C-N-CA	5.82	128.56	120.29
1	B	443	LEU	O-C-N	-5.82	115.95	122.12
1	A	191	ILE	N-CA-C	5.82	116.00	110.42
1	A	8	ASP	CA-CB-CG	-5.79	106.81	112.60
1	B	284	ASP	CA-CB-CG	5.78	118.38	112.60
1	B	49	ARG	CB-CG-CD	-5.77	98.04	111.30
1	A	346	LEU	CA-C-N	5.76	125.72	119.78
1	A	346	LEU	C-N-CA	5.76	125.72	119.78
1	A	309	ASN	OD1-CG-ND2	-5.76	116.84	122.60
1	A	426	ASN	CB-CG-ND2	5.75	125.03	116.40
1	A	654	GLU	CB-CG-CD	5.75	122.38	112.60
1	A	174	HIS	CB-CG-CD2	-5.74	123.74	131.20
1	B	42	HIS	CA-CB-CG	-5.71	108.09	113.80
1	B	197	ILE	CA-CB-CG2	5.70	120.18	110.50
1	B	674	SER	CA-CB-OG	5.69	122.48	111.10
1	A	670	ASP	CA-CB-CG	5.69	118.29	112.60
1	B	469	HIS	CB-CG-CD2	-5.68	123.82	131.20
1	B	202	ASP	CA-CB-CG	5.68	118.28	112.60
1	A	159	CYS	N-CA-C	-5.67	105.24	111.82
1	B	310	ASN	OD1-CG-ND2	-5.67	116.93	122.60
1	B	256	HIS	CB-CG-CD2	-5.67	123.83	131.20
1	B	20	VAL	CG1-CB-CG2	-5.67	98.34	110.80
1	B	48	MET	N-CA-C	-5.66	102.11	110.48
1	A	134	ASN	OD1-CG-ND2	-5.65	116.95	122.60
1	A	256	HIS	CB-CG-CD2	-5.65	123.85	131.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	461	HIS	CB-CG-ND1	5.65	131.17	122.70
1	B	313	ASN	OD1-CG-ND2	-5.65	116.95	122.60
1	B	580	ASN	CB-CG-ND2	5.65	124.87	116.40
1	A	99	ARG	N-CA-C	-5.64	106.16	113.16
1	B	149	ASN	CB-CG-ND2	5.64	124.86	116.40
1	A	260	HIS	CA-CB-CG	5.63	119.44	113.80
1	A	103	HIS	CB-CG-CD2	-5.63	123.88	131.20
1	A	528	ARG	N-CA-C	-5.63	104.53	111.40
1	A	588	LEU	CA-C-N	5.63	126.00	119.47
1	A	588	LEU	C-N-CA	5.63	126.00	119.47
1	A	237	SER	O-C-N	-5.62	115.12	122.59
1	B	49	ARG	CB-CA-C	5.61	119.39	110.19
1	B	365	VAL	N-CA-C	-5.61	105.26	110.53
1	B	656	VAL	N-CA-C	-5.60	105.26	110.53
1	B	25	LYS	CA-CB-CG	5.59	125.29	114.10
1	A	311	LYS	N-CA-C	-5.59	105.26	111.36
1	B	21	ASP	N-CA-C	5.57	118.28	111.82
1	B	623	TRP	N-CA-C	5.57	120.08	113.28
1	A	69	HIS	CA-CB-CG	5.57	119.37	113.80
1	A	600	GLU	N-CA-CB	-5.56	101.72	110.06
1	A	335	SER	N-CA-C	-5.56	106.50	113.28
1	A	38	ALA	CA-C-N	5.55	125.01	119.24
1	A	38	ALA	C-N-CA	5.55	125.01	119.24
1	B	392	LYS	CG-CD-CE	5.55	124.07	111.30
1	B	174	HIS	CB-CG-CD2	-5.54	124.00	131.20
1	A	241	PRO	CB-CA-C	5.54	118.21	110.95
1	B	124	ASN	CA-CB-CG	5.54	118.14	112.60
1	B	170	SER	N-CA-C	-5.53	105.16	111.14
1	A	317	SER	CA-CB-OG	-5.53	100.04	111.10
1	B	574	LYS	CB-CG-CD	5.53	124.01	111.30
1	A	111	VAL	O-C-N	5.52	129.62	122.77
1	A	284	ASP	CA-CB-CG	5.52	118.12	112.60
1	B	49	ARG	NE-CZ-NH2	-5.52	114.23	119.20
1	B	591	PHE	CA-CB-CG	5.50	119.30	113.80
1	A	619	ALA	N-CA-C	5.50	118.33	110.24
1	A	465	TRP	CB-CG-CD1	-5.48	118.68	126.90
1	B	59	ASN	CA-C-O	5.47	126.41	119.95
1	B	242	THR	N-CA-C	5.45	117.78	108.90
1	A	485	GLU	CB-CG-CD	5.42	121.82	112.60
1	A	584	ARG	N-CA-C	-5.42	100.86	109.76
1	A	543	SER	CA-CB-OG	-5.42	100.27	111.10
1	A	341	ASN	OD1-CG-ND2	-5.41	117.19	122.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	187	ASN	CB-CG-ND2	-5.40	108.30	116.40
1	A	187	ASN	CB-CG-OD1	5.38	131.57	120.80
1	A	623	TRP	CG-CD1-NE1	-5.38	103.21	110.20
1	A	636	PHE	CA-CB-CG	5.38	119.18	113.80
1	B	222	GLU	O-C-N	-5.38	116.23	121.93
1	A	416	ILE	CB-CG1-CD1	5.37	125.07	113.80
1	B	113	VAL	CA-C-O	-5.37	116.07	121.49
1	A	262	VAL	N-CA-C	-5.37	107.52	112.83
1	B	323	PHE	CA-C-N	5.36	124.82	119.24
1	B	323	PHE	C-N-CA	5.36	124.82	119.24
1	A	282	ASN	CA-CB-CG	5.36	117.96	112.60
1	B	465	TRP	CG-CD2-CE3	5.36	139.25	133.90
1	B	528	ARG	N-CA-C	-5.35	104.87	111.40
1	B	296	HIS	CB-CG-CD2	-5.35	124.25	131.20
1	B	500	ARG	CA-C-N	5.33	125.25	119.76
1	B	500	ARG	C-N-CA	5.33	125.25	119.76
1	B	69	HIS	CB-CG-CD2	-5.33	124.28	131.20
1	A	282	ASN	CA-C-N	5.32	126.49	119.84
1	A	282	ASN	C-N-CA	5.32	126.49	119.84
1	B	167	GLU	CA-C-N	5.30	127.33	120.44
1	B	167	GLU	C-N-CA	5.30	127.33	120.44
1	A	197	ILE	N-CA-CB	-5.29	101.60	110.65
1	A	519	HIS	CB-CG-CD2	-5.29	124.32	131.20
1	B	600	GLU	CB-CG-CD	5.29	121.60	112.60
1	B	628	HIS	CB-CG-ND1	5.29	130.64	122.70
1	A	465	TRP	CE2-CD2-CG	-5.29	100.85	107.20
1	A	610	VAL	N-CA-CB	5.29	118.61	111.21
1	A	666	PHE	CA-CB-CG	5.29	119.09	113.80
1	A	599	LEU	CA-C-N	5.27	127.61	120.38
1	A	599	LEU	C-N-CA	5.27	127.61	120.38
1	A	638	ALA	N-CA-C	5.25	116.51	108.42
1	A	635	ARG	N-CA-C	-5.24	101.79	109.81
1	A	238	LYS	CA-CB-CG	5.24	124.57	114.10
1	B	235	LYS	CB-CG-CD	5.23	123.32	111.30
1	A	263	HIS	CB-CG-CD2	-5.22	124.41	131.20
1	A	580	ASN	OD1-CG-ND2	-5.21	117.39	122.60
1	B	478	GLY	CA-C-N	5.20	124.81	119.56
1	B	478	GLY	C-N-CA	5.20	124.81	119.56
1	A	282	ASN	OD1-CG-ND2	-5.20	117.40	122.60
1	B	71	VAL	N-CA-C	5.20	120.15	109.34
1	B	406	ASN	CA-CB-CG	5.20	117.80	112.60
1	A	300	THR	CA-CB-CG2	5.18	119.30	110.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	482	GLN	CA-C-N	5.17	124.93	119.76
1	B	482	GLN	C-N-CA	5.17	124.93	119.76
1	A	238	LYS	CB-CG-CD	5.16	123.17	111.30
1	A	652	THR	O-C-N	-5.16	118.41	121.71
1	A	631	PHE	N-CA-C	-5.16	100.12	108.52
1	A	201	GLU	N-CA-C	5.15	116.98	110.33
1	B	417	ARG	NE-CZ-NH1	5.15	126.65	121.50
1	A	469	HIS	CB-CG-ND1	5.14	130.41	122.70
1	B	42	HIS	CB-CG-ND1	5.14	130.41	122.70
1	B	54	ASN	CA-CB-CG	-5.13	107.47	112.60
1	A	274	GLN	CA-CB-CG	5.13	124.36	114.10
1	B	54	ASN	OD1-CG-ND2	-5.12	117.48	122.60
1	B	461	HIS	CB-CG-CD2	-5.12	124.54	131.20
1	A	607	PRO	N-CA-C	5.10	119.07	111.41
1	A	3	GLN	OE1-CD-NE2	-5.10	117.50	122.60
1	A	465	TRP	CG-CD1-NE1	-5.10	103.57	110.20
1	B	621	THR	N-CA-CB	-5.09	102.62	110.01
1	A	345	LYS	CA-CB-CG	-5.09	103.92	114.10
1	A	593	THR	CA-CB-OG1	-5.08	101.98	109.60
1	B	458	LEU	N-CA-C	5.08	116.50	110.97
1	A	469	HIS	CB-CG-CD2	-5.07	124.61	131.20
1	A	676	LEU	N-CA-C	5.07	117.54	111.71
1	A	218	GLU	CA-CB-CG	5.05	124.21	114.10
1	B	465	TRP	CE2-CD2-CG	-5.05	101.14	107.20
1	A	624	GLY	N-CA-C	-5.05	108.05	114.16
1	A	213	GLU	O-C-N	-5.05	117.14	123.04
1	A	307	GLU	N-CA-CB	-5.04	102.42	109.94
1	A	265	ALA	O-C-N	-5.04	118.30	121.88
1	A	188	LYS	N-CA-C	5.03	121.52	110.80
1	A	95	GLN	OE1-CD-NE2	-5.02	117.58	122.60
1	A	628	HIS	CB-CG-ND1	5.02	130.23	122.70
1	A	661	GLN	OE1-CD-NE2	-5.02	117.58	122.60
1	A	187	ASN	CB-CG-ND2	-5.02	108.87	116.40
1	B	495	ASN	N-CA-C	5.01	121.48	110.80
1	B	539	ILE	N-CA-C	-5.01	105.66	110.72
1	A	623	TRP	CE2-CD2-CG	-5.01	101.19	107.20
1	B	465	TRP	CG-CD1-NE1	-5.00	103.69	110.20
1	B	651	PHE	CA-CB-CG	-5.00	108.80	113.80

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	80	0
1	B	5198	0	5139	70	0
2	A	1	0	0	0	0
2	B	1	0	0	0	0
3	A	26	0	17	2	0
3	B	26	0	17	5	0
All	All	10450	0	10312	141	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 (141) 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:106:PHE:H	1:A:114:THR:HG22	1.36	0.90
1:A:652:THR:HG22	1:A:655:GLY:H	1.49	0.78
1:A:117:PRO:HA	3:A:681:N3T:H3'	1.66	0.77
1:A:118:LEU:HD12	1:B:416:ILE:HG21	1.67	0.76
1:B:105:GLU:HA	1:B:114:THR:HG23	1.72	0.72
1:A:342:TRP:HH2	1:A:512:LYS:HA	1.57	0.69
1:A:71:VAL:HG13	1:A:104:PRO:HD3	1.77	0.67
1:B:49:ARG:HH22	1:B:59:ASN:ND2	1.93	0.66
1:B:487:LEU:O	1:B:491:ARG:HG3	1.96	0.64
1:A:652:THR:HG22	1:A:655:GLY:N	2.12	0.64
1:B:635:ARG:HD2	1:B:649:PHE:HE1	1.63	0.64
1:B:117:PRO:HA	3:B:681:N3T:H3'	1.81	0.63
1:A:206:ARG:HG3	1:B:206:ARG:HG3	1.80	0.61
1:B:48:MET:HB2	1:B:50:MET:HE2	1.82	0.61
1:A:361:LEU:HD13	1:A:504:GLY:HA2	1.82	0.61
1:A:375:GLU:HG3	1:A:434:ASN:O	2.00	0.61
1:A:67:ASN:H	1:A:67:ASN:HD22	1.49	0.61
1:A:311:LYS:O	1:A:314:LYS:HG3	2.02	0.59
1:A:67:ASN:H	1:A:67:ASN:ND2	2.01	0.59
1:A:358:THR:HG22	1:A:526:LEU:HD23	1.85	0.58
1:B:358:THR:HA	1:B:361:LEU:HD12	1.86	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:377:ILE:HD11	1:B:412:ILE:HD11	1.86	0.57
1:B:658:GLU:O	1:B:662:LYS:HG2	2.04	0.57
1:A:680:PHE:CG	1:B:659:ARG:HG2	2.41	0.56
1:A:478:GLY:O	1:A:482:GLN:HG3	2.05	0.56
1:A:358:THR:HB	1:A:527:SER:H	1.71	0.56
1:A:358:THR:HG21	1:A:501:PRO:HG2	1.89	0.55
1:B:259:SER:O	1:B:262:VAL:HG22	2.07	0.55
1:A:592:PHE:CE2	1:A:596:LYS:HD2	2.42	0.55
1:A:219:ASN:HD21	1:A:222:GLU:HB2	1.72	0.55
1:B:57:TRP:O	1:B:60:ARG:HD3	2.08	0.54
1:B:11:ALA:O	1:B:15:ILE:HG13	2.08	0.54
1:B:51:ASN:ND2	1:B:306:VAL:HG22	2.22	0.54
1:B:613:MET:HA	1:B:629:GLN:O	2.08	0.53
1:B:71:VAL:HB	1:B:104:PRO:HD3	1.90	0.53
1:A:421:MET:O	1:A:425:MET:HG3	2.09	0.52
1:B:117:PRO:HB2	1:B:120:GLN:HG3	1.90	0.52
1:B:570:VAL:O	1:B:574:LYS:HD2	2.09	0.52
1:A:158:GLY:HA2	1:B:416:ILE:HD13	1.91	0.52
1:B:392:LYS:HA	1:B:392:LYS:NZ	2.25	0.52
1:B:378:GLY:HA3	1:B:438:TYR:CZ	2.45	0.51
1:A:106:PHE:N	1:A:114:THR:HG22	2.16	0.51
1:A:359:ARG:HD2	1:A:386:SER:O	2.11	0.50
1:B:49:ARG:NH2	1:B:59:ASN:ND2	2.59	0.50
1:A:52:PRO:HD2	1:A:302:LEU:HD13	1.93	0.50
1:B:282:ASN:ND2	1:B:285:LYS:HD3	2.26	0.50
1:A:300:THR:HG22	1:A:301:ILE:HG13	1.93	0.50
1:A:382:ASP:OD2	3:B:681:N3T:H62	2.12	0.50
1:B:314:LYS:O	1:B:318:GLU:HG2	2.11	0.50
1:A:50:MET:O	1:A:305:GLY:HA3	2.12	0.50
1:A:114:THR:HG23	1:A:459:SER:OG	2.11	0.50
1:B:556:ASP:HB2	1:B:581:ILE:HG23	1.93	0.50
1:A:96:LEU:HA	1:B:639:SER:O	2.12	0.49
1:A:476:GLU:HB3	1:B:94:ARG:HD3	1.94	0.49
1:A:48:MET:HE3	1:A:152:TYR:HD2	1.77	0.49
1:B:357:ALA:HA	1:B:529:GLN:O	2.13	0.49
1:B:186:ASP:HB3	1:B:247:THR:HA	1.93	0.49
1:B:599:LEU:HG	1:B:603:LEU:HD12	1.94	0.48
1:B:15:ILE:HD13	1:B:77:MET:SD	2.53	0.48
1:A:271:ASP:O	1:A:274:GLN:HG3	2.13	0.48
1:A:541:SER:HB3	1:A:547:TYR:CG	2.48	0.48
1:B:361:LEU:HD13	1:B:504:GLY:HA2	1.95	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:552:VAL:HG21	1:A:582:LYS:HB3	1.95	0.48
1:A:483:PRO:HB3	1:A:486:THR:OG1	2.13	0.48
1:B:45:TRP:HA	1:B:48:MET:HE3	1.96	0.48
1:A:358:THR:HG22	1:A:526:LEU:CD2	2.43	0.48
1:B:437:PRO:HG2	1:B:463:VAL:HG12	1.95	0.48
1:A:546:GLY:HA2	1:A:588:LEU:HA	1.97	0.47
1:B:164:ILE:HD12	1:B:419:HIS:CD2	2.49	0.47
1:A:62:ARG:HH11	1:A:62:ARG:HG3	1.80	0.47
1:A:496:ILE:HG13	1:A:521:PRO:HG2	1.96	0.47
1:A:198:SER:HB2	1:B:417:ARG:HH21	1.79	0.46
1:A:49:ARG:HD3	1:A:57:TRP:CH2	2.50	0.46
1:A:378:GLY:HA3	1:A:438:TYR:CE1	2.50	0.46
1:A:487:LEU:O	1:A:491:ARG:HG3	2.16	0.46
1:A:352:LYS:HE2	1:A:352:LYS:HB2	1.78	0.45
1:B:356:VAL:HG12	1:B:360:LYS:HB3	1.99	0.45
1:A:658:GLU:O	1:A:662:LYS:HG2	2.17	0.45
1:A:560:VAL:O	1:A:614:SER:HA	2.17	0.45
1:B:275:LEU:O	1:B:278:LYS:HB3	2.17	0.45
1:B:332:ARG:NH1	1:B:339:PRO:HD3	2.32	0.45
1:A:346:LEU:HD11	1:A:512:LYS:HB3	1.99	0.45
1:B:493:LEU:HD12	1:B:494:PRO:HD2	1.99	0.45
1:A:17:ILE:HG21	1:A:276:LYS:HG2	1.99	0.44
1:A:205:LYS:HD3	1:B:205:LYS:HG2	1.97	0.44
1:A:476:GLU:HG2	1:B:94:ARG:O	2.16	0.44
1:B:190:THR:HA	3:B:681:N3T:H71	1.99	0.44
1:A:616:GLU:O	1:A:632:GLY:HA2	2.17	0.44
1:B:346:LEU:HA	1:B:347:PRO:HD3	1.68	0.44
1:A:469:HIS:CD2	1:A:528:ARG:HD3	2.52	0.44
3:B:681:N3T:H7'1	3:B:681:N3T:HM43	1.82	0.44
1:B:167:GLU:HB3	1:B:420:ALA:HB2	1.99	0.44
1:B:345:LYS:NZ	1:B:372:GLN:HB2	2.32	0.44
1:B:78:LEU:O	1:B:83:TYR:HB2	2.18	0.44
1:A:207:TYR:HA	1:A:210:TYR:CD2	2.52	0.44
1:A:594:PHE:O	1:A:597:GLN:HG2	2.18	0.44
1:B:177:LEU:O	1:B:241:PRO:HB3	2.17	0.44
1:B:378:GLY:HA3	1:B:438:TYR:CE2	2.54	0.43
1:A:325:GLU:H	1:A:325:GLU:CD	2.26	0.43
1:A:361:LEU:HD13	1:A:504:GLY:CA	2.46	0.43
1:B:64:VAL:HB	1:B:153:VAL:HG13	1.99	0.43
1:B:213:GLU:HB2	1:B:240:LYS:HD3	1.99	0.43
1:A:342:TRP:CH2	1:A:512:LYS:HA	2.45	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:445:PHE:O	1:A:448:TYR:HB2	2.18	0.43
1:B:552:VAL:HG21	1:B:582:LYS:HB3	2.01	0.43
1:A:219:ASN:ND2	1:A:222:GLU:HB2	2.33	0.43
1:B:546:GLY:HA3	1:B:588:LEU:HD12	2.00	0.43
1:A:282:ASN:HA	1:A:283:PRO:HD2	1.71	0.43
1:A:48:MET:HE1	1:A:63:PHE:HB2	2.00	0.43
1:A:454:ARG:NH1	1:B:485:GLU:OE1	2.52	0.42
1:B:263:HIS:ND1	3:B:681:N3T:O3B	2.50	0.42
1:B:114:THR:HG21	1:B:458:LEU:HD22	2.02	0.42
3:A:681:N3T:H7'1	3:A:681:N3T:HM43	1.82	0.42
1:B:390:ARG:HG2	1:B:411:TYR:CZ	2.54	0.42
1:A:416:ILE:HD13	1:B:158:GLY:HA2	2.01	0.42
1:A:664:ILE:HG21	1:A:664:ILE:HD13	1.79	0.42
1:B:546:GLY:HA2	1:B:589:PRO:HD2	2.01	0.42
1:B:51:ASN:HD21	1:B:306:VAL:HG22	1.85	0.42
1:A:118:LEU:HD13	1:A:158:GLY:HA3	2.01	0.41
1:A:443:LEU:HD23	1:A:483:PRO:HG2	2.02	0.41
1:A:63:PHE:HA	1:A:152:TYR:O	2.20	0.41
1:A:67:ASN:HD22	1:A:67:ASN:N	2.15	0.41
1:A:275:LEU:HA	1:A:278:LYS:HB3	2.02	0.41
1:B:531:LEU:HD21	1:B:564:SER:HB3	2.03	0.41
1:A:43:VAL:HG23	1:A:224:LEU:HD22	2.03	0.41
1:A:48:MET:HE3	1:A:152:TYR:CD2	2.56	0.41
1:A:6:ASP:HA	1:A:9:LYS:HE3	2.01	0.41
1:A:272:VAL:O	1:A:275:LEU:HD23	2.20	0.41
1:B:127:GLY:HA2	1:B:424:ILE:HG23	2.02	0.41
1:A:122:ILE:HA	1:A:153:VAL:HG11	2.03	0.41
1:A:307:GLU:O	1:A:311:LYS:HG2	2.20	0.41
1:A:390:ARG:NH1	1:A:396:ASP:OD1	2.54	0.41
1:B:565:GLU:OE1	1:B:617:VAL:HG22	2.21	0.41
1:B:285:LYS:HB3	1:B:288:VAL:HG21	2.03	0.41
1:A:491:ARG:HD2	1:A:591:PHE:CD2	2.56	0.40
1:B:457:ALA:HB1	1:B:494:PRO:O	2.20	0.40
1:A:134:ASN:HA	1:A:407:TYR:O	2.21	0.40
1:A:499:TRP:CE3	1:A:589:PRO:HB2	2.57	0.40
1:B:326:LEU:HD12	1:B:326:LEU:HA	1.91	0.40
1:B:338:LEU:HD12	1:B:338:LEU:HA	1.90	0.40
1:B:359:ARG:HD2	1:B:386:SER:O	2.21	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%)	637 (94%)	35 (5%)	4 (1%)	21	44
1	B	676/678 (100%)	633 (94%)	39 (6%)	4 (1%)	21	44
All	All	1352/1356 (100%)	1270 (94%)	74 (6%)	8 (1%)	21	44

All (8) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	237	SER
1	A	400	PRO
1	A	188	LYS
1	B	148	ASP
1	B	617	VAL
1	B	71	VAL
1	A	617	VAL
1	B	31	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%)	503 (91%)	49 (9%)	9	23
1	B	552/552 (100%)	510 (92%)	42 (8%)	12	30
All	All	1104/1104 (100%)	1013 (92%)	91 (8%)	10	27

All (91) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	3	GLN
1	A	20	VAL
1	A	37	MET
1	A	49	ARG
1	A	50	MET
1	A	52	PRO
1	A	67	ASN
1	A	71	VAL
1	A	88	GLU
1	A	92	GLN
1	A	100	THR
1	A	113	VAL
1	A	122	ILE
1	A	153	VAL
1	A	155	LEU
1	A	195	THR
1	A	198	SER
1	A	218	GLU
1	A	238	LYS
1	A	261	SER
1	A	262	VAL
1	A	275	LEU
1	A	302	LEU
1	A	314	LYS
1	A	318	GLU
1	A	325	GLU
1	A	341	ASN
1	A	343	GLU
1	A	352	LYS
1	A	360	LYS
1	A	389	THR
1	A	458	LEU
1	A	489	HIS
1	A	506	GLU
1	A	512	LYS
1	A	538	SER
1	A	549	LEU
1	A	557	ILE
1	A	567	SER
1	A	580	ASN
1	A	584	ARG
1	A	588	LEU
1	A	610	VAL

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Mol	Chain	Res	Type
1	A	625	LYS
1	A	647	LYS
1	A	652	THR
1	A	654	GLU
1	A	668	LYS
1	A	678	LYS
1	B	67	ASN
1	B	96	LEU
1	B	113	VAL
1	B	122	ILE
1	B	141	LYS
1	B	153	VAL
1	B	183	ILE
1	B	197	ILE
1	B	218	GLU
1	B	229	LYS
1	B	240	LYS
1	B	261	SER
1	B	268	LYS
1	B	311	LYS
1	B	314	LYS
1	B	317	SER
1	B	322	LYS
1	B	326	LEU
1	B	338	LEU
1	B	343	GLU
1	B	348	THR
1	B	354	SER
1	B	356	VAL
1	B	358	THR
1	B	371	ASN
1	B	377	ILE
1	B	389	THR
1	B	392	LYS
1	B	393	GLU
1	B	401	SER
1	B	404	SER
1	B	518	LYS
1	B	535	GLU
1	B	564	SER
1	B	574	LYS
1	B	581	ILE

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Mol	Chain	Res	Type
1	B	582	LYS
1	B	596	LYS
1	B	635	ARG
1	B	639	SER
1	B	659	ARG
1	B	671	LYS

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

Mol	Chain	Res	Type
1	A	3	GLN
1	A	27	ASN
1	A	124	ASN
1	A	219	ASN
1	A	260	HIS
1	A	313	ASN
1	A	341	ASN
1	A	371	ASN
1	A	398	GLN
1	A	519	HIS
1	A	609	ASN
1	A	661	GLN
1	B	51	ASN
1	B	54	ASN
1	B	59	ASN
1	B	92	GLN
1	B	95	GLN
1	B	120	GLN
1	B	132	GLN
1	B	149	ASN
1	B	256	HIS
1	B	298	GLN
1	B	309	ASN
1	B	313	ASN
1	B	387	ASN
1	B	398	GLN
1	B	519	HIS
1	B	609	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 oligosaccharides in this entry.

5.6 Ligand geometry ⓘ

Of 4 ligands modelled in this entry, 2 are monoatomic - leaving 2 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
3	N3T	B	681	2	26,27,27	1.44	4 (15%)	35,40,40	1.31	5 (14%)
3	N3T	A	681	2	26,27,27	1.40	6 (23%)	35,40,40	1.26	5 (14%)

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	N3T	B	681	2	-	4/17/17/17	0/2/2/2
3	N3T	A	681	2	-	4/17/17/17	0/2/2/2

All (10) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	681	N3T	C4-N3	-3.36	1.33	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	681	N3T	C4-N3	-3.31	1.33	1.39
3	B	681	N3T	C7'-N3	2.94	1.54	1.48
3	A	681	N3T	PA-O3A	2.69	1.62	1.59
3	B	681	N3T	C4'-N4'	-2.56	1.29	1.38
3	A	681	N3T	PB-O3B	-2.34	1.46	1.54
3	B	681	N3T	PB-O3B	-2.29	1.46	1.54
3	A	681	N3T	C4'-N4'	-2.14	1.30	1.38
3	A	681	N3T	PB-O2B	-2.05	1.47	1.54
3	A	681	N3T	C7'-N3	2.04	1.53	1.48

All (10) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	681	N3T	C6'-N1'-C2'	3.65	121.83	117.53
3	B	681	N3T	O7-C7-C6	-2.99	96.61	108.63
3	A	681	N3T	C2-S1-C5	-2.85	89.32	91.22
3	B	681	N3T	C6'-N1'-C2'	2.70	120.71	117.53
3	B	681	N3T	C2-S1-C5	-2.59	89.50	91.22
3	A	681	N3T	C7-C6-C5	2.47	120.49	112.73
3	A	681	N3T	O3A-PB-O1B	-2.20	99.48	111.04
3	B	681	N3T	C5'-C6'-N1'	-2.16	120.32	123.83
3	B	681	N3T	C3'-C2'-N1'	-2.16	119.50	121.61
3	A	681	N3T	C3'-C2'-N1'	-2.08	119.58	121.61

There are no chirality outliers.

All (8) torsion outliers are listed below:

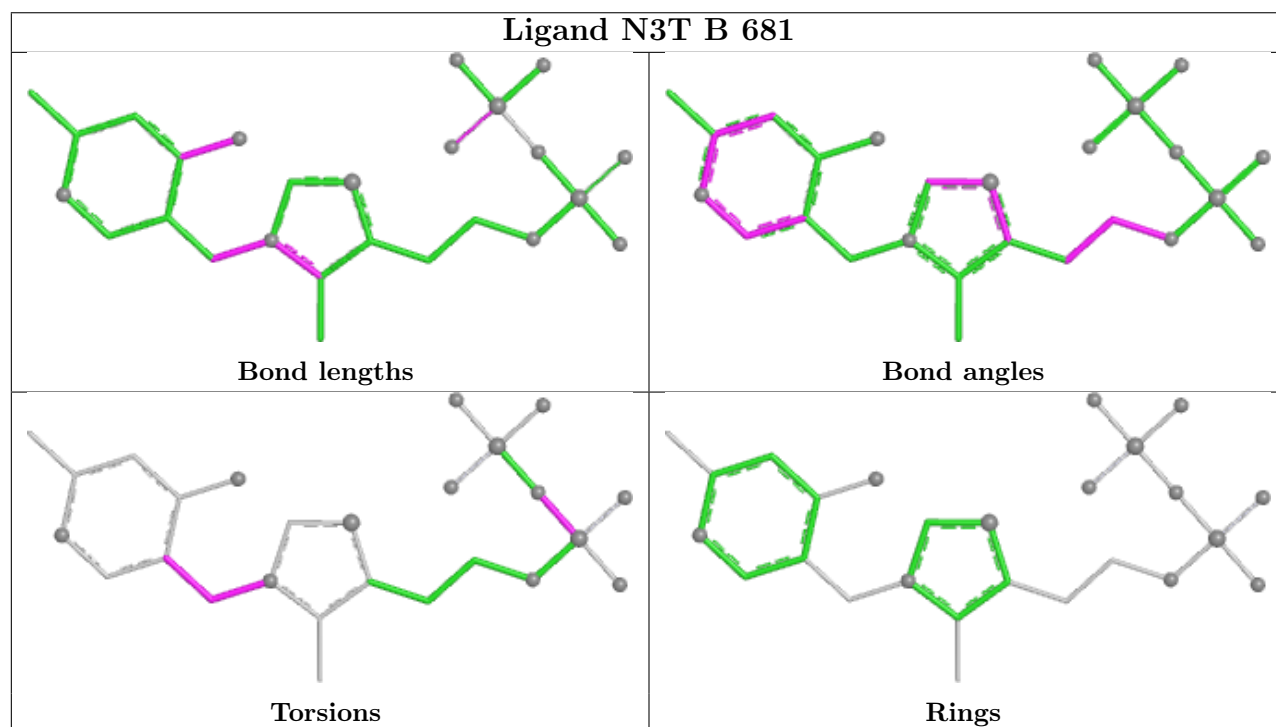
Mol	Chain	Res	Type	Atoms
3	B	681	N3T	C6'-C5'-C7'-N3
3	A	681	N3T	PB-O3A-PA-O2A
3	A	681	N3T	C7-O7-PA-O3A
3	B	681	N3T	PB-O3A-PA-O2A
3	A	681	N3T	C4-C5-C6-C7
3	B	681	N3T	C5'-C7'-N3-C2
3	B	681	N3T	PB-O3A-PA-O1A
3	A	681	N3T	S1-C5-C6-C7

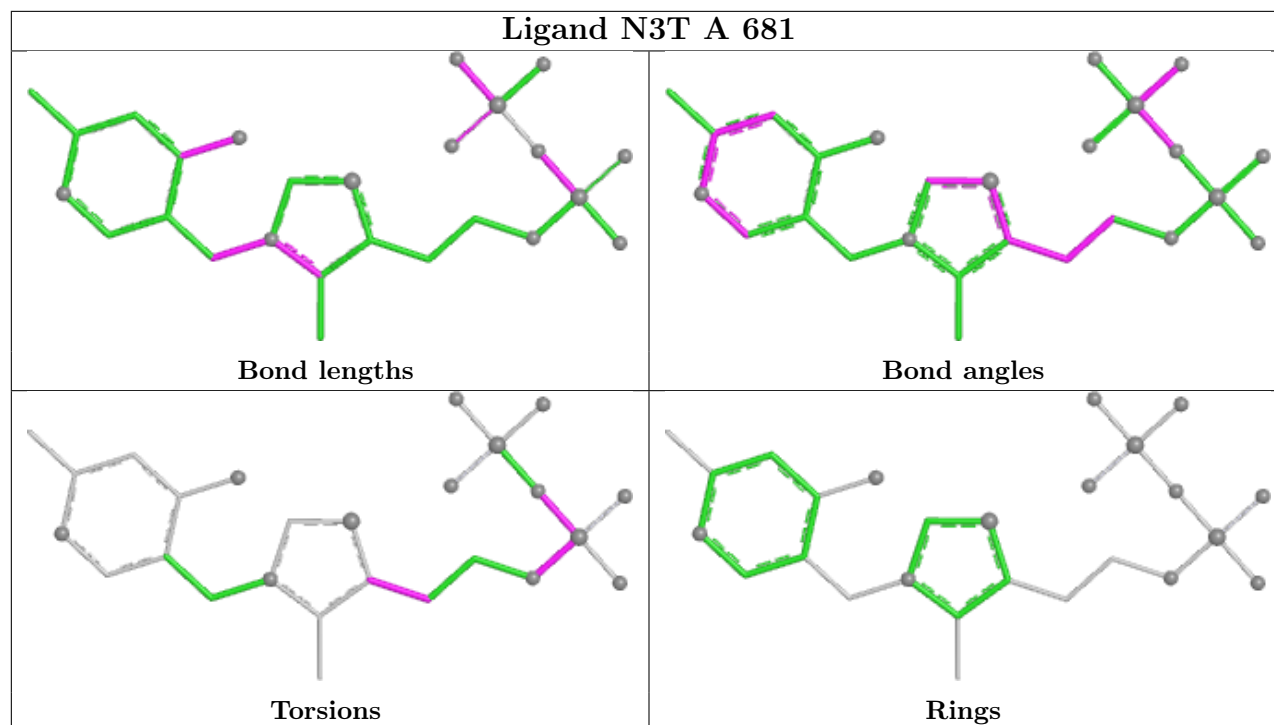
There are no ring outliers.

2 monomers are involved in 7 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	B	681	N3T	5	0
3	A	681	N3T	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.