



Full wwPDB X-ray Structure Validation Report ⓘ

Jan 31, 2016 – 10:25 PM GMT

PDB ID : 1TKB
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 : 2.30 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
<http://wwpdb.org/validation/2016/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 : 1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix) : **NOT EXECUTED**
EDS : **NOT EXECUTED**
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : trunk26865

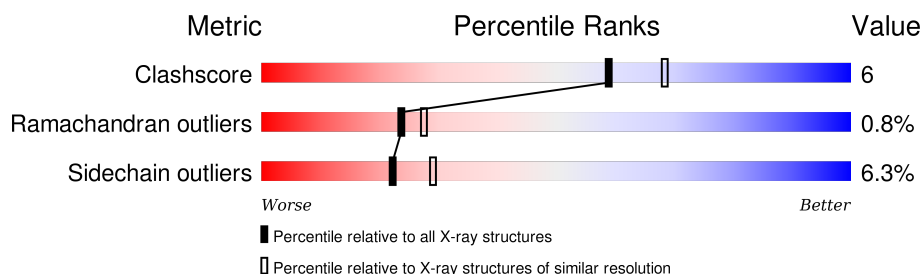
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.30 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	102246	4452 (2.30-2.30)
Ramachandran outliers	100387	4410 (2.30-2.30)
Sidechain outliers	100360	4409 (2.30-2.30)

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. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

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 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.

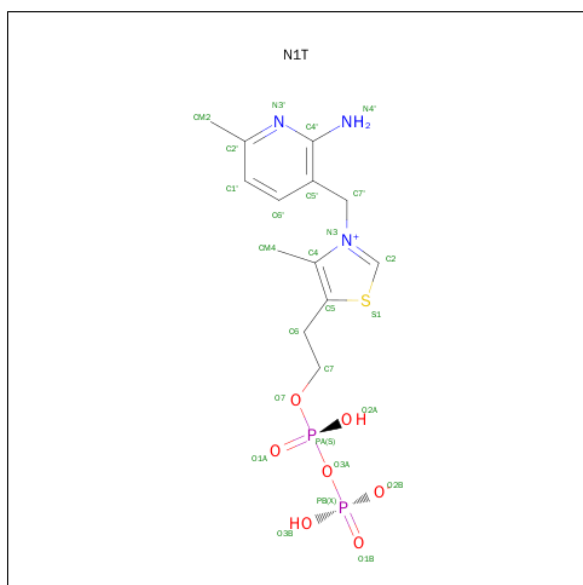
- Molecule 1 is a protein called TRANSKETOLASE.

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 (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 1'-DEAZO-THIAMIN DIPHOSPHATE (three-letter code: N1T) (formula: C₁₃H₁₉N₃O₇P₂S).



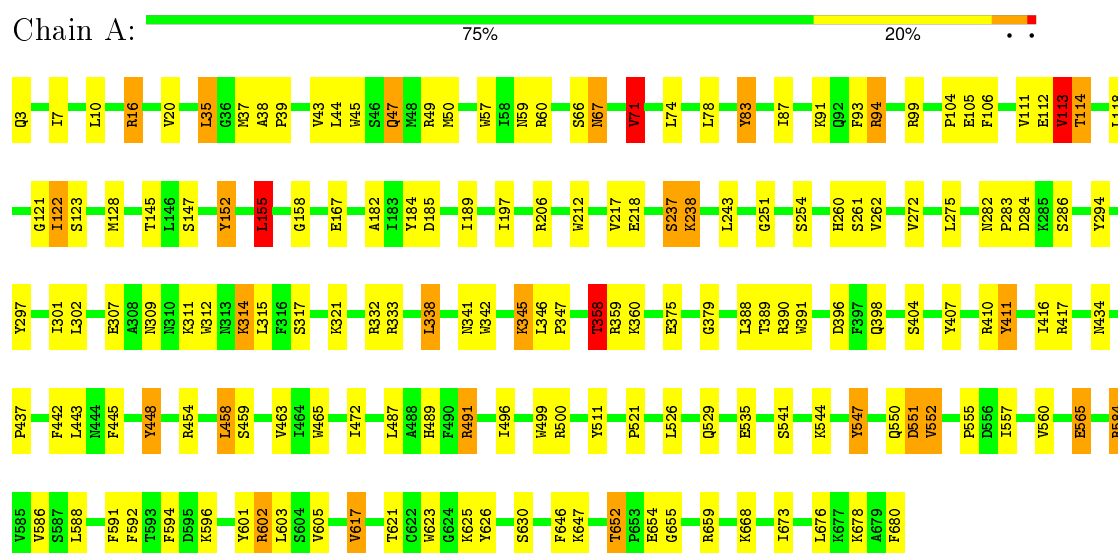
Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
3	A	1	Total	C	N	O	P	S	0	0
			26	13	3	7	2	1		
3	B	1	Total	C	N	O	P	S	0	0
			26	13	3	7	2	1		

3 Residue-property plots

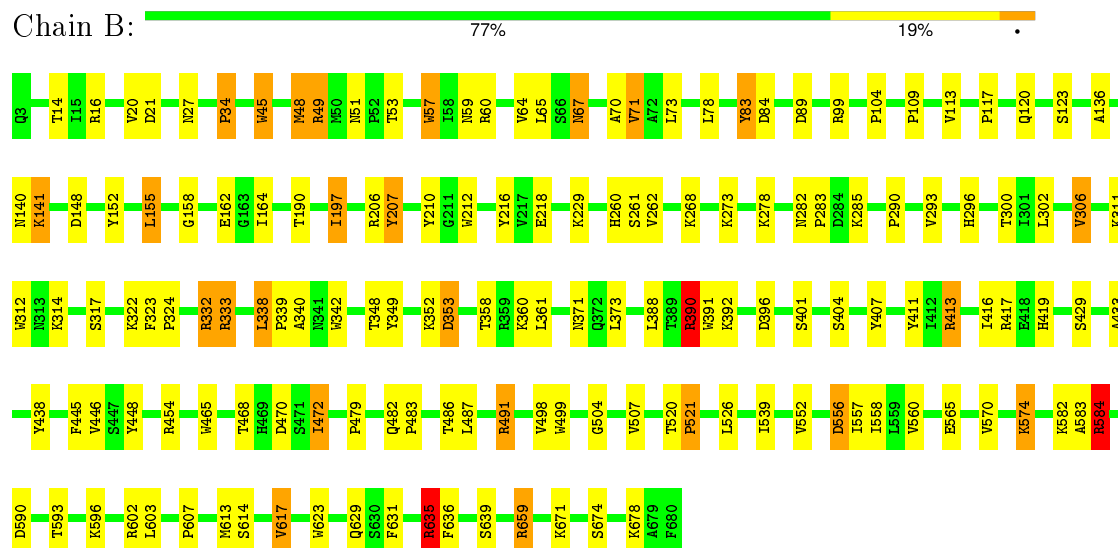
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ($RSRZ > 2$). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

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 will therefore be 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 – 2.30	Depositor
% Data completeness (in resolution range)	(Not available) (15.00-2.30)	Depositor
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	X-PLOR	Depositor
R, R_{free}	0.185 , (Not available)	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	10450	wwPDB-VP
Average B, all atoms (Å ²)	15.0	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, N1T

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	0.89	2/5324 (0.0%)	1.65	94/7230 (1.3%)
1	B	0.90	0/5324	1.64	82/7230 (1.1%)
All	All	0.90	2/10648 (0.0%)	1.64	176/14460 (1.2%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	B	0	1

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	535	GLU	CD-OE2	7.54	1.33	1.25
1	A	237	SER	CB-OG	5.39	1.49	1.42

All (176) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	491	ARG	NE-CZ-NH1	18.77	129.69	120.30
1	B	491	ARG	NE-CZ-NH2	-16.76	111.92	120.30
1	B	417	ARG	NE-CZ-NH2	-14.34	113.13	120.30
1	B	417	ARG	NE-CZ-NH1	12.96	126.78	120.30
1	A	94	ARG	NE-CZ-NH1	12.46	126.53	120.30
1	B	49	ARG	NE-CZ-NH2	-12.35	114.12	120.30
1	A	454	ARG	NE-CZ-NH1	12.19	126.39	120.30
1	A	465	TRP	CD1-CG-CD2	11.15	115.22	106.30
1	A	491	ARG	NE-CZ-NH1	10.62	125.61	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	659	ARG	NE-CZ-NH1	10.41	125.51	120.30
1	A	623	TRP	CD1-CG-CD2	10.38	114.60	106.30
1	A	94	ARG	NE-CZ-NH2	-10.12	115.24	120.30
1	A	358	THR	CA-CB-CG2	10.01	126.42	112.40
1	B	206	ARG	NE-CZ-NH2	-9.98	115.31	120.30
1	B	210	TYR	CB-CG-CD2	-9.78	115.13	121.00
1	A	49	ARG	CB-CG-CD	-9.61	86.63	111.60
1	B	465	TRP	CD1-CG-CD2	9.29	113.74	106.30
1	B	206	ARG	NE-CZ-NH1	9.28	124.94	120.30
1	B	57	TRP	CD1-CG-CD2	9.20	113.66	106.30
1	B	342	TRP	CD1-CG-CD2	9.14	113.61	106.30
1	A	57	TRP	CD1-CG-CD2	9.01	113.51	106.30
1	A	448	TYR	CB-CG-CD2	-8.94	115.63	121.00
1	A	294	TYR	CB-CG-CD2	-8.81	115.71	121.00
1	B	602	ARG	NE-CZ-NH1	8.68	124.64	120.30
1	A	465	TRP	CE2-CD2-CG	-8.67	100.36	107.30
1	A	391	TRP	CD1-CG-CD2	8.62	113.20	106.30
1	A	601	TYR	CB-CG-CD1	-8.41	115.95	121.00
1	A	499	TRP	CD1-CG-CD2	8.31	112.95	106.30
1	A	57	TRP	CE2-CD2-CG	-8.16	100.77	107.30
1	A	391	TRP	CE2-CD2-CG	-8.10	100.82	107.30
1	B	57	TRP	CE2-CD2-CG	-8.09	100.83	107.30
1	B	602	ARG	NE-CZ-NH2	-8.07	116.26	120.30
1	B	623	TRP	CD1-CG-CD2	8.06	112.75	106.30
1	A	358	THR	N-CA-CB	-8.06	94.99	110.30
1	A	500	ARG	NE-CZ-NH1	8.06	124.33	120.30
1	A	465	TRP	CG-CD2-CE3	8.01	141.11	133.90
1	A	60	ARG	NE-CZ-NH2	-7.94	116.33	120.30
1	B	212	TRP	CD1-CG-CD2	7.93	112.64	106.30
1	A	465	TRP	CG-CD1-NE1	-7.93	102.17	110.10
1	B	590	ASP	CB-CG-OD1	7.91	125.42	118.30
1	A	332	ARG	NE-CZ-NH2	-7.88	116.36	120.30
1	A	623	TRP	CE2-CD2-CG	-7.83	101.04	107.30
1	B	312	TRP	CE2-CD2-CG	-7.72	101.12	107.30
1	B	491	ARG	CG-CD-NE	-7.64	95.75	111.80
1	B	312	TRP	CD1-CG-CD2	7.63	112.40	106.30
1	B	342	TRP	CE2-CD2-CG	-7.57	101.25	107.30
1	A	45	TRP	CD1-CG-CD2	7.52	112.31	106.30
1	A	584	ARG	NE-CZ-NH2	-7.50	116.55	120.30
1	A	312	TRP	CD1-CG-CD2	7.49	112.29	106.30
1	B	584	ARG	NE-CZ-NH2	-7.45	116.58	120.30
1	A	49	ARG	NE-CZ-NH2	-7.41	116.59	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	83	TYR	CB-CG-CD1	-7.40	116.56	121.00
1	B	212	TRP	CE2-CD2-CG	-7.36	101.41	107.30
1	B	48	MET	CG-SD-CE	-7.31	88.50	100.20
1	A	45	TRP	CE2-CD2-CG	-7.30	101.46	107.30
1	B	499	TRP	CD1-CG-CD2	7.27	112.12	106.30
1	B	491	ARG	CA-CB-CG	7.20	129.24	113.40
1	A	407	TYR	CB-CG-CD2	-7.19	116.69	121.00
1	A	623	TRP	CG-CD1-NE1	-7.12	102.98	110.10
1	A	491	ARG	NE-CZ-NH2	-7.12	116.74	120.30
1	B	391	TRP	CE2-CD2-CG	-7.09	101.62	107.30
1	B	413	ARG	NE-CZ-NH1	7.08	123.84	120.30
1	A	499	TRP	CE2-CD2-CG	-7.00	101.70	107.30
1	A	391	TRP	CG-CD2-CE3	6.99	140.19	133.90
1	B	465	TRP	CE2-CD2-CG	-6.98	101.72	107.30
1	A	212	TRP	CE2-CD2-CG	-6.97	101.73	107.30
1	A	454	ARG	NE-CZ-NH2	-6.95	116.82	120.30
1	B	623	TRP	CE2-CD2-CG	-6.95	101.74	107.30
1	B	438	TYR	CB-CG-CD2	-6.94	116.84	121.00
1	A	358	THR	CA-CB-OG1	-6.93	94.45	109.00
1	B	83	TYR	CB-CG-CD2	-6.92	116.85	121.00
1	A	312	TRP	CE2-CD2-CG	-6.90	101.78	107.30
1	B	45	TRP	CE2-CD2-CG	-6.88	101.80	107.30
1	B	312	TRP	CG-CD2-CE3	6.88	140.09	133.90
1	A	626	TYR	CB-CG-CD2	-6.82	116.91	121.00
1	A	212	TRP	CG-CD2-CE3	6.80	140.02	133.90
1	B	491	ARG	CB-CG-CD	6.79	129.25	111.60
1	A	342	TRP	CD1-CG-CD2	6.78	111.72	106.30
1	A	465	TRP	CB-CG-CD1	-6.74	118.23	127.00
1	A	35	LEU	CA-C-N	6.71	129.62	116.20
1	B	45	TRP	CD1-CG-CD2	6.64	111.61	106.30
1	A	47	GLN	N-CA-CB	-6.62	98.69	110.60
1	B	197	ILE	CA-CB-CG1	-6.60	98.46	111.00
1	B	491	ARG	CD-NE-CZ	6.57	132.80	123.60
1	B	353	ASP	CB-CG-OD1	6.56	124.21	118.30
1	B	312	TRP	CB-CG-CD1	-6.54	118.50	127.00
1	A	547	TYR	CB-CG-CD2	-6.52	117.09	121.00
1	A	212	TRP	CD1-CG-CD2	6.51	111.51	106.30
1	B	390	ARG	CA-CB-CG	6.51	127.72	113.40
1	A	16	ARG	NE-CZ-NH1	6.42	123.51	120.30
1	A	57	TRP	CG-CD1-NE1	-6.42	103.68	110.10
1	B	333	ARG	NE-CZ-NH2	-6.42	117.09	120.30
1	B	21	ASP	CB-CG-OD1	6.41	124.07	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	391	TRP	CB-CG-CD1	-6.40	118.68	127.00
1	B	391	TRP	CD1-CG-CD2	6.27	111.31	106.30
1	B	390	ARG	CB-CA-C	-6.26	97.87	110.40
1	A	410	ARG	NE-CZ-NH1	6.25	123.43	120.30
1	B	216	TYR	CB-CG-CD2	-6.24	117.26	121.00
1	B	207	TYR	CB-CG-CD1	-6.22	117.27	121.00
1	A	16	ARG	NE-CZ-NH2	6.21	123.40	120.30
1	A	342	TRP	CE2-CD2-CG	-6.20	102.34	107.30
1	B	152	TYR	CB-CG-CD2	-6.15	117.31	121.00
1	A	333	ARG	NE-CZ-NH2	-6.14	117.23	120.30
1	A	71	VAL	CB-CA-C	-6.12	99.78	111.40
1	B	499	TRP	CE2-CD2-CG	-6.08	102.44	107.30
1	A	262	VAL	CG1-CB-CG2	-6.04	101.24	110.90
1	B	465	TRP	CG-CD1-NE1	-6.04	104.06	110.10
1	A	391	TRP	CG-CD1-NE1	-6.01	104.09	110.10
1	B	45	TRP	CG-CD2-CE3	6.00	139.30	133.90
1	B	206	ARG	CG-CD-NE	-5.96	99.29	111.80
1	A	99	ARG	NE-CZ-NH2	-5.94	117.33	120.30
1	A	499	TRP	CG-CD1-NE1	-5.93	104.17	110.10
1	A	113	VAL	CG1-CB-CG2	-5.91	101.44	110.90
1	A	217	VAL	CA-C-N	5.88	130.13	117.20
1	A	16	ARG	NH1-CZ-NH2	-5.87	112.94	119.40
1	A	389	THR	N-CA-CB	-5.87	99.14	110.30
1	B	89	ASP	CB-CG-OD2	5.87	123.58	118.30
1	A	294	TYR	CB-CG-CD1	5.86	124.51	121.00
1	B	659	ARG	CA-CB-CG	-5.82	100.60	113.40
1	A	47	GLN	CA-CB-CG	5.80	126.16	113.40
1	B	446	VAL	CG1-CB-CG2	-5.76	101.68	110.90
1	B	391	TRP	CB-CG-CD1	-5.76	119.52	127.00
1	A	489	HIS	CA-CB-CG	5.75	123.38	113.60
1	A	128	MET	CG-SD-CE	-5.73	91.03	100.20
1	A	602	ARG	NE-CZ-NH1	5.70	123.15	120.30
1	A	332	ARG	NE-CZ-NH1	5.69	123.14	120.30
1	B	342	TRP	CG-CD1-NE1	-5.66	104.44	110.10
1	B	507	VAL	CG1-CB-CG2	-5.65	101.86	110.90
1	B	49	ARG	CB-CG-CD	-5.61	97.02	111.60
1	A	410	ARG	NE-CZ-NH2	-5.57	117.51	120.30
1	B	623	TRP	CG-CD1-NE1	-5.56	104.54	110.10
1	A	71	VAL	CA-CB-CG1	-5.56	102.56	110.90
1	A	155	LEU	CA-CB-CG	5.55	128.07	115.30
1	B	391	TRP	CG-CD2-CE3	5.49	138.84	133.90
1	A	448	TYR	CB-CG-CD1	5.45	124.27	121.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	593	THR	CA-CB-CG2	5.44	120.02	112.40
1	A	217	VAL	O-C-N	-5.43	114.01	122.70
1	B	57	TRP	CG-CD1-NE1	-5.43	104.67	110.10
1	B	340	ALA	CA-C-N	-5.41	105.29	117.20
1	B	306	VAL	CG1-CB-CG2	-5.40	102.25	110.90
1	A	238	LYS	CA-CB-CG	5.37	125.22	113.40
1	A	442	PHE	CB-CG-CD2	-5.36	117.05	120.80
1	B	278	LYS	CA-CB-CG	5.35	125.17	113.40
1	B	631	PHE	CB-CG-CD2	-5.35	117.05	120.80
1	B	332	ARG	NE-CZ-NH1	5.35	122.97	120.30
1	A	605	VAL	CG1-CB-CG2	-5.33	102.37	110.90
1	A	411	TYR	CB-CG-CD1	-5.29	117.83	121.00
1	B	312	TRP	CG-CD1-NE1	-5.29	104.81	110.10
1	B	155	LEU	CA-CB-CG	5.28	127.45	115.30
1	A	511	TYR	CB-CG-CD2	-5.28	117.83	121.00
1	A	345	LYS	CA-CB-CG	-5.26	101.83	113.40
1	B	262	VAL	CA-CB-CG1	-5.25	103.03	110.90
1	A	123	SER	N-CA-CB	-5.23	102.65	110.50
1	A	145	THR	CA-CB-CG2	5.23	119.72	112.40
1	A	317	SER	N-CA-CB	-5.20	102.70	110.50
1	B	64	VAL	O-C-N	-5.20	114.39	122.70
1	A	206	ARG	CG-CD-NE	-5.18	100.92	111.80
1	A	57	TRP	CG-CD2-CE3	5.18	138.56	133.90
1	A	529	GLN	CA-CB-CG	5.16	124.75	113.40
1	B	373	LEU	CA-CB-CG	5.16	127.17	115.30
1	A	152	TYR	CB-CG-CD2	-5.14	117.91	121.00
1	A	591	PHE	CB-CG-CD2	-5.14	117.20	120.80
1	A	551	ASP	CB-CG-OD1	5.14	122.92	118.30
1	B	99	ARG	NE-CZ-NH2	-5.14	117.73	120.30
1	A	321	LYS	CA-CB-CG	5.13	124.70	113.40
1	B	407	TYR	CB-CG-CD2	-5.11	117.93	121.00
1	A	623	TRP	N-CA-C	5.11	124.79	111.00
1	B	470	ASP	N-CA-C	5.10	124.77	111.00
1	B	48	MET	CA-CB-CG	5.09	121.95	113.30
1	B	498	VAL	CG1-CB-CG2	-5.09	102.76	110.90
1	B	635	ARG	CA-CB-CG	5.08	124.57	113.40
1	B	454	ARG	NE-CZ-NH2	-5.05	117.77	120.30
1	B	499	TRP	CG-CD1-NE1	-5.04	105.06	110.10
1	A	338	LEU	CA-CB-CG	5.02	126.85	115.30
1	B	556	ASP	CB-CG-OD2	5.01	122.81	118.30
1	A	145	THR	CA-CB-OG1	-5.00	98.50	109.00

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	B	207	TYR	Sidechain

5.2 Too-close contacts ⓘ

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	5198	0	5139	63	0
1	B	5198	0	5139	62	0
2	A	1	0	0	0	0
2	B	1	0	0	0	0
3	A	26	0	17	1	0
3	B	26	0	17	1	0
All	All	10450	0	10312	119	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 6.

All (119) 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:416:ILE:HD13	1:B:158:GLY:HA2	1.61	0.83
1:B:51:ASN:HD21	1:B:53:THR:HB	1.47	0.79
1:A:105:GLU:HA	1:A:114:THR:HB	1.72	0.71
1:A:652:THR:HG22	1:A:655:GLY:H	1.55	0.70
1:B:34:PRO:HA	1:B:73:LEU:HD12	1.73	0.69
1:A:106:PHE:H	1:A:114:THR:HG22	1.56	0.69
1:A:311:LYS:O	1:A:314:LYS:HG3	1.97	0.65
1:B:51:ASN:ND2	1:B:53:THR:HB	2.11	0.64
1:B:358:THR:HA	1:B:361:LEU:HD12	1.80	0.64
1:A:550:GLN:O	1:A:584:ARG:HG3	1.99	0.62
1:A:158:GLY:HA2	1:B:416:ILE:HD13	1.80	0.62
1:B:78:LEU:O	1:B:83:TYR:HB2	1.99	0.62
1:B:635:ARG:HD2	1:B:636:PHE:O	1.99	0.61
1:B:117:PRO:HB2	1:B:120:GLN:HG3	1.81	0.61
1:B:49:ARG:HH22	1:B:59:ASN:HD22	1.47	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:487:LEU:O	1:B:491:ARG:HG2	2.01	0.60
1:B:49:ARG:HH22	1:B:59:ASN:ND2	2.02	0.57
1:A:552:VAL:HG23	1:A:555:PRO:HB3	1.86	0.56
1:B:348:THR:HG22	1:B:539:ILE:HD11	1.87	0.56
1:B:570:VAL:O	1:B:574:LYS:HD2	2.06	0.56
1:A:71:VAL:HG13	1:A:104:PRO:HD3	1.87	0.56
1:A:155:LEU:HD21	1:A:182:ALA:HB1	1.88	0.55
1:A:114:THR:HG23	1:A:459:SER:OG	2.07	0.55
1:A:59:ASN:OD1	1:A:147:SER:HA	2.07	0.55
1:A:496:ILE:HG13	1:A:521:PRO:HG2	1.88	0.55
1:A:647:LYS:NZ	1:A:647:LYS:HB3	2.22	0.54
1:A:375:GLU:HG3	1:A:434:ASN:O	2.07	0.54
1:A:359:ARG:HG2	1:A:388:LEU:HD12	1.88	0.54
1:B:390:ARG:HG2	1:B:411:TYR:CE1	2.43	0.53
1:B:396:ASP:OD2	1:B:413:ARG:HD2	2.08	0.53
1:B:565:GLU:OE1	1:B:617:VAL:HG22	2.09	0.52
1:B:136:ALA:O	1:B:140:ASN:HB2	2.10	0.52
1:B:67:ASN:H	1:B:67:ASN:HD22	1.58	0.52
1:B:445:PHE:O	1:B:448:TYR:HB2	2.10	0.52
1:A:416:ILE:HG22	1:B:162:GLU:OE2	2.11	0.51
1:B:14:THR:HG21	1:B:293:VAL:HG11	1.93	0.50
1:A:37:MET:SD	1:A:185:ASP:HB2	2.52	0.49
1:B:613:MET:HA	1:B:629:GLN:O	2.13	0.49
1:B:552:VAL:HG21	1:B:582:LYS:HB3	1.94	0.48
1:B:164:ILE:HD12	1:B:419:HIS:CD2	2.49	0.48
1:B:71:VAL:HB	1:B:104:PRO:HD3	1.95	0.48
1:B:560:VAL:O	1:B:614:SER:HA	2.14	0.48
1:B:16:ARG:O	1:B:20:VAL:HG23	2.13	0.48
1:B:141:LYS:HG2	1:B:323:PHE:CZ	2.49	0.48
1:B:190:THR:HB	3:B:681:N1T:H71	1.94	0.48
1:A:445:PHE:O	1:A:448:TYR:HB2	2.13	0.48
1:A:358:THR:HG22	1:A:526:LEU:HD23	1.96	0.47
1:A:458:LEU:HD11	1:B:479:PRO:HB2	1.96	0.47
1:A:680:PHE:CG	1:B:659:ARG:HG2	2.49	0.47
1:B:349:TYR:CD1	1:B:504:GLY:HA3	2.50	0.47
1:B:282:ASN:HD22	1:B:285:LYS:HD3	1.80	0.47
1:B:296:HIS:O	1:B:300:THR:HG23	2.16	0.46
1:A:541:SER:HB3	1:A:547:TYR:CD2	2.50	0.46
1:A:74:LEU:HD21	1:A:111:VAL:HG22	1.97	0.46
1:A:67:ASN:H	1:A:67:ASN:HD22	1.61	0.46
1:B:302:LEU:O	1:B:306:VAL:HG23	2.16	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:617:VAL:HG11	1:A:646:PHE:HE1	1.81	0.46
1:A:3:GLN:OE1	1:A:3:GLN:N	2.49	0.46
1:A:437:PRO:HG2	1:A:463:VAL:HG12	1.98	0.45
1:A:630:SER:H	1:B:678:LYS:NZ	2.15	0.45
1:A:93:PHE:CZ	1:A:94:ARG:HD2	2.51	0.45
1:A:398:GLN:HG3	1:A:404:SER:OG	2.17	0.45
1:B:468:THR:HA	1:B:526:LEU:HB2	1.99	0.45
1:A:487:LEU:O	1:A:491:ARG:HG3	2.16	0.45
1:A:282:ASN:HA	1:A:283:PRO:HD2	1.77	0.45
1:B:65:LEU:HD11	1:B:70:ALA:HB3	1.98	0.44
1:A:551:ASP:HA	1:A:584:ARG:HG3	1.99	0.44
1:A:443:LEU:HD21	1:A:487:LEU:HD21	1.99	0.44
1:A:184:TYR:HB2	1:A:243:LEU:HD11	1.98	0.44
1:A:592:PHE:CE2	1:A:596:LYS:HD2	2.53	0.44
1:B:390:ARG:HG2	1:B:411:TYR:CZ	2.52	0.44
1:A:155:LEU:CD2	1:A:182:ALA:HB1	2.48	0.44
1:A:87:ILE:O	1:A:91:LYS:HG3	2.18	0.44
1:A:390:ARG:NH1	1:A:396:ASP:OD1	2.50	0.44
1:B:607:PRO:O	1:B:674:SER:HB2	2.17	0.44
1:B:557:ILE:O	1:B:583:ALA:HA	2.17	0.44
1:B:338:LEU:HD12	1:B:338:LEU:HA	1.90	0.44
1:B:290:PRO:O	1:B:293:VAL:HB	2.18	0.43
1:A:44:LEU:HD11	1:A:152:TYR:CD1	2.53	0.43
1:A:16:ARG:NH1	1:A:35:LEU:O	2.52	0.43
1:A:78:LEU:O	1:A:83:TYR:HB2	2.18	0.43
1:A:314:LYS:HE2	1:A:315:LEU:HB2	1.99	0.43
1:A:38:ALA:HB3	1:A:39:PRO:HD3	1.99	0.43
1:B:558:ILE:HG12	1:B:584:ARG:HD2	2.00	0.43
1:A:112:GLU:O	1:A:113:VAL:HG13	2.17	0.43
1:A:379:GLY:HA2	1:A:411:TYR:CE1	2.53	0.43
1:A:20:VAL:HG11	1:A:272:VAL:HG13	2.00	0.43
1:B:349:TYR:CE1	1:B:504:GLY:HA3	2.53	0.43
1:B:67:ASN:H	1:B:67:ASN:ND2	2.16	0.42
1:A:297:TYR:CD1	1:A:301:ILE:HD12	2.53	0.42
1:B:45:TRP:HA	1:B:48:MET:HG3	2.01	0.42
1:A:603:LEU:HD23	1:A:676:LEU:HD12	2.01	0.42
1:A:118:LEU:H	3:A:681:N1T:HM21	1.83	0.42
1:A:565:GLU:OE1	1:A:617:VAL:HG22	2.19	0.42
1:A:346:LEU:HA	1:A:347:PRO:HD3	1.89	0.42
1:B:273:LYS:HD3	1:B:283:PRO:HB2	2.02	0.42
1:B:57:TRP:O	1:B:60:ARG:NH1	2.52	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:390:ARG:HD2	1:B:411:TYR:CG	2.56	0.41
1:A:592:PHE:O	1:A:596:LYS:HG3	2.21	0.41
1:A:251:GLY:O	1:A:254:SER:HB3	2.21	0.41
1:A:66:SER:HA	1:A:121:GLY:HA3	2.02	0.41
1:A:66:SER:OG	1:A:122:ILE:HG22	2.20	0.41
1:A:7:ILE:HD12	1:A:10:LEU:HB3	2.01	0.41
1:B:360:LYS:HA	1:B:388:LEU:HD12	2.02	0.41
1:B:67:ASN:N	1:B:67:ASN:HD22	2.17	0.41
1:A:39:PRO:O	1:A:43:VAL:HG23	2.20	0.41
1:A:167:GLU:HG2	1:A:417:ARG:HG2	2.02	0.41
1:B:556:ASP:N	1:B:582:LYS:O	2.53	0.41
1:B:482:GLN:HA	1:B:483:PRO:HD3	1.92	0.41
1:A:560:VAL:HG13	1:A:586:VAL:HB	2.01	0.41
1:B:332:ARG:NH1	1:B:339:PRO:HD3	2.36	0.41
1:B:520:THR:HA	1:B:521:PRO:HD2	1.83	0.40
1:B:603:LEU:HA	1:B:603:LEU:HD23	1.93	0.40
1:B:472:ILE:HA	1:B:482:GLN:HG2	2.03	0.40
1:B:333:ARG:HB3	1:B:433:ALA:O	2.22	0.40
1:A:594:PHE:O	1:A:602:ARG:HD2	2.22	0.40
1:B:282:ASN:ND2	1:B:285:LYS:HD3	2.36	0.40
1:B:51:ASN:ND2	1:B:306:VAL:HG22	2.37	0.40
1:A:189:ILE:HD12	1:A:260:HIS:HB3	2.03	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%)	633 (94%)	40 (6%)	3 (0%)	39	48
1	B	676/678 (100%)	638 (94%)	30 (4%)	8 (1%)	16	16
All	All	1352/1356 (100%)	1271 (94%)	70 (5%)	11 (1%)	24	27

All (11) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	237	SER
1	A	617	VAL
1	B	84	ASP
1	B	148	ASP
1	B	324	PRO
1	B	617	VAL
1	B	71	VAL
1	A	472	ILE
1	B	521	PRO
1	B	472	ILE
1	B	34	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%)	515 (93%)	37 (7%)	20	26
1	B	552/552 (100%)	519 (94%)	33 (6%)	24	31
All	All	1104/1104 (100%)	1034 (94%)	70 (6%)	22	29

All (70) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	47	GLN
1	A	50	MET
1	A	67	ASN
1	A	71	VAL
1	A	113	VAL
1	A	114	THR
1	A	122	ILE
1	A	155	LEU
1	A	197	ILE
1	A	218	GLU
1	A	238	LYS
1	A	261	SER

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Mol	Chain	Res	Type
1	A	275	LEU
1	A	284	ASP
1	A	286	SER
1	A	302	LEU
1	A	307	GLU
1	A	309	ASN
1	A	314	LYS
1	A	338	LEU
1	A	341	ASN
1	A	345	LYS
1	A	358	THR
1	A	360	LYS
1	A	458	LEU
1	A	544	LYS
1	A	552	VAL
1	A	557	ILE
1	A	565	GLU
1	A	588	LEU
1	A	621	THR
1	A	625	LYS
1	A	652	THR
1	A	654	GLU
1	A	668	LYS
1	A	673	ILE
1	A	678	LYS
1	B	27	ASN
1	B	67	ASN
1	B	109	PRO
1	B	113	VAL
1	B	123	SER
1	B	141	LYS
1	B	155	LEU
1	B	197	ILE
1	B	218	GLU
1	B	229	LYS
1	B	260	HIS
1	B	261	SER
1	B	268	LYS
1	B	311	LYS
1	B	314	LYS
1	B	317	SER
1	B	322	LYS

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Mol	Chain	Res	Type
1	B	338	LEU
1	B	352	LYS
1	B	353	ASP
1	B	371	ASN
1	B	390	ARG
1	B	392	LYS
1	B	401	SER
1	B	404	SER
1	B	429	SER
1	B	486	THR
1	B	574	LYS
1	B	584	ARG
1	B	596	LYS
1	B	635	ARG
1	B	639	SER
1	B	671	LYS

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

Mol	Chain	Res	Type
1	A	3	GLN
1	A	54	ASN
1	A	120	GLN
1	A	341	ASN
1	A	372	GLN
1	A	387	ASN
1	A	489	HIS
1	B	27	ASN
1	B	51	ASN
1	B	54	ASN
1	B	67	ASN
1	B	120	GLN
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 [i](#)

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

5.5 Carbohydrates [i](#)

There are no carbohydrates 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	N1T	A	681	2	21,27,27	2.30	6 (28%)	31,40,40	1.30	3 (9%)
3	N1T	B	681	2	21,27,27	1.92	5 (23%)	31,40,40	1.62	7 (22%)

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	N1T	A	681	2	-	0/16/17/17	0/2/2/2
3	N1T	B	681	2	-	0/16/17/17	0/2/2/2

All (11) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	681	N1T	C4-N3	-7.15	1.33	1.39
3	B	681	N1T	C4-N3	-5.60	1.34	1.39
3	A	681	N1T	C6'-C5'	-3.53	1.33	1.39
3	A	681	N1T	PB-O3B	-2.63	1.44	1.55
3	B	681	N1T	C6'-C5'	-2.23	1.35	1.39
3	B	681	N1T	PB-O3B	-2.12	1.46	1.55

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	681	N1T	PB-O3A	-2.07	1.56	1.61
3	B	681	N1T	C1'-C2'	2.00	1.44	1.39
3	A	681	N1T	C1'-C2'	2.33	1.45	1.39
3	B	681	N1T	C6'-C1'	4.07	1.46	1.38
3	A	681	N1T	C6'-C1'	4.36	1.46	1.38

All (10) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	681	N1T	O3A-PB-O1B	-4.02	95.16	107.70
3	B	681	N1T	CM4-C4-N3	-2.38	119.41	122.59
3	B	681	N1T	O7-C7-C6	-2.33	99.57	109.30
3	A	681	N1T	C5'-C7'-N3	-2.22	109.61	113.33
3	A	681	N1T	O2A-PA-O7	-2.12	97.77	108.46
3	B	681	N1T	C6'-C1'-C2'	-2.10	117.63	120.00
3	B	681	N1T	O2B-PB-O1B	2.15	125.03	114.72
3	B	681	N1T	O3A-PA-O7	2.24	108.87	102.94
3	B	681	N1T	CM2-C2'-N3'	2.80	120.93	116.59
3	A	681	N1T	CM2-C2'-N3'	3.26	121.64	116.59

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

2 monomers are involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	681	N1T	1	0
3	B	681	N1T	1	0

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

6 Fit of model and data [i](#)

6.1 Protein, DNA and RNA chains [i](#)

EDS was not executed - this section will therefore be empty.

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

EDS was not executed - this section will therefore be empty.

6.3 Carbohydrates [i](#)

EDS was not executed - this section will therefore be empty.

6.4 Ligands [i](#)

EDS was not executed - this section will therefore be empty.

6.5 Other polymers [i](#)

EDS was not executed - this section will therefore be empty.