



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 4, 2026 – 06:14 PM UTC

PDB ID : 1TRK / pdb_00001trk
Title : REFINED STRUCTURE OF TRANSKETOLASE FROM SACCHAROMYCES CEREVISIAE AT 2.0 ANGSTROMS RESOLUTION
Authors : Lindqvist, Y.; Schneider, G.; Nikkola, M.
Deposited on : 1993-11-22
Resolution : 2.00 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

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

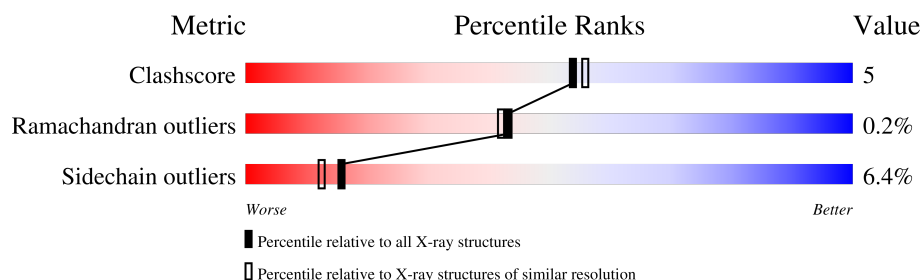
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.00 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
Clashscore	190562	11152 (2.00-2.00)
Ramachandran outliers	187476	11031 (2.00-2.00)
Sidechain outliers	187428	11029 (2.00-2.00)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments 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	680	 70% 25% . .
1	B	680	 74% 21% . .

2 Entry composition [i](#)

There are 4 unique types of molecules in this entry. The entry contains 11471 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

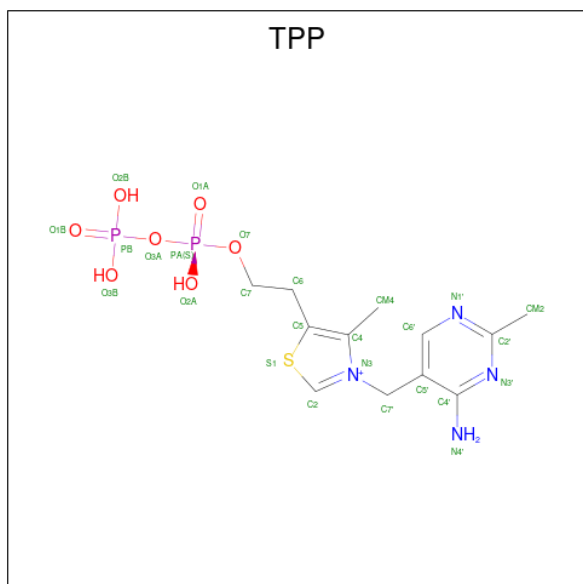
- Molecule 1 is a protein called TRANSKETOLASE.

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

- Molecule 2 is CALCIUM ION (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 THIAMINE DIPHOSPHATE (CCD ID: TPP) (formula: C₁₂H₁₉N₄O₇P₂S).



Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
3	A	1	Total	C	N	O	P	S	0	0
			26	12	4	7	2	1		
3	B	1	Total	C	N	O	P	S	0	0
			26	12	4	7	2	1		

- Molecule 4 is water.

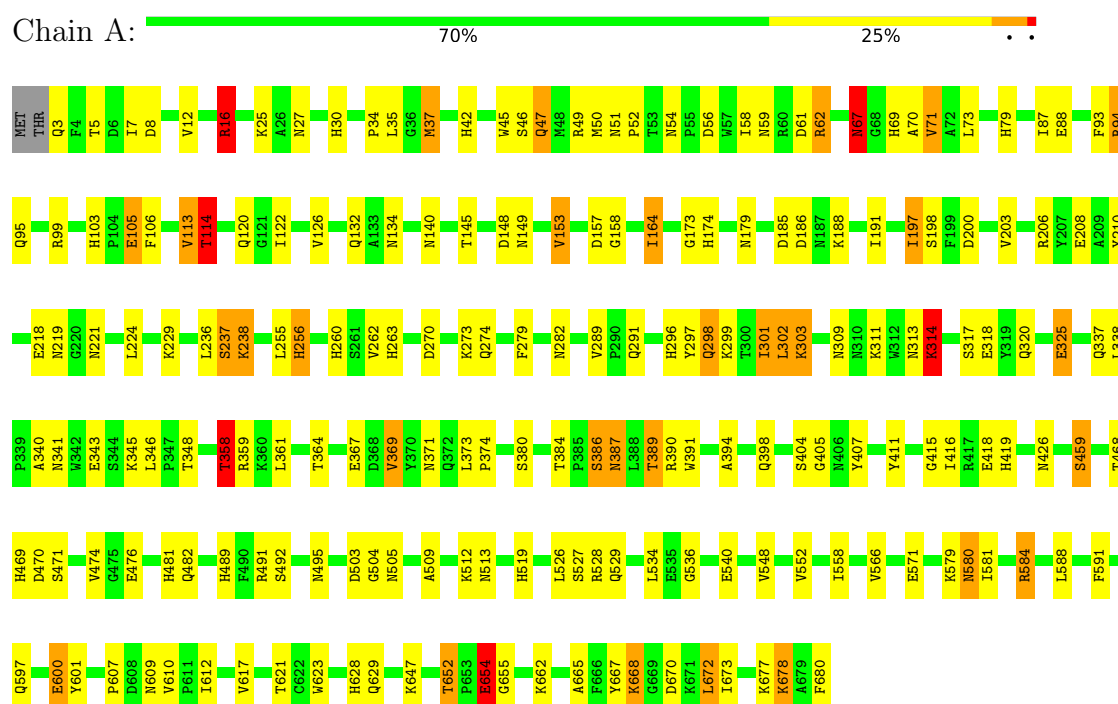
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	473	Total	O	0	0
			473	473		
4	B	548	Total	O	0	0
			548	548		

3 Residue-property plots

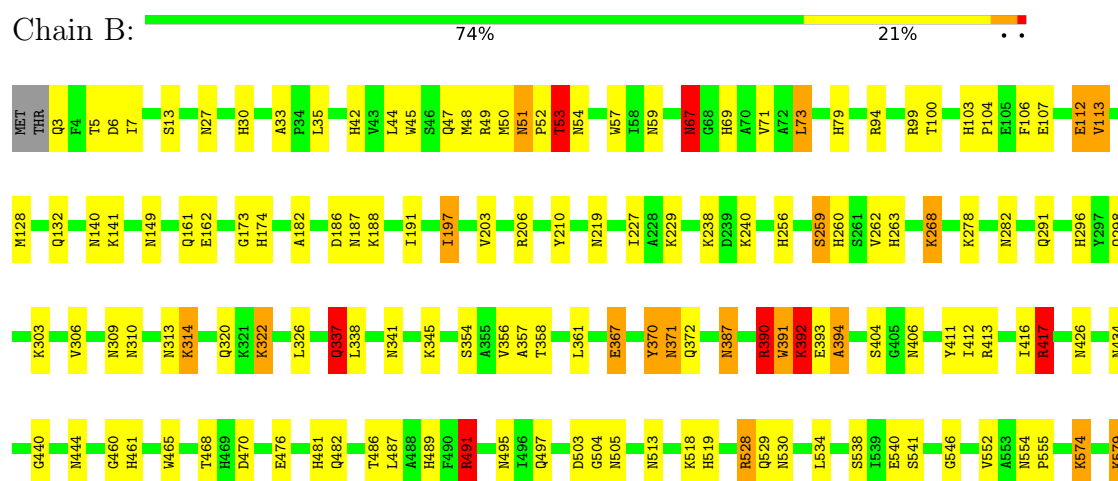
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry. Residues are color-coded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



• Molecule 1: TRANSKETOLASE





4 Data and refinement statistics

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

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

5 Model quality

5.1 Standard geometry

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

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	A	1.10	23/5324 (0.4%)	1.97	154/7230 (2.1%)
1	B	1.12	18/5324 (0.3%)	1.95	162/7230 (2.2%)
All	All	1.11	41/10648 (0.4%)	1.96	316/14460 (2.2%)

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	A	0	2
1	B	0	1
All	All	0	3

All (41) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	263	HIS	CD2-NE2	-7.50	1.29	1.37
1	B	296	HIS	CD2-NE2	-7.32	1.29	1.37
1	B	174	HIS	CD2-NE2	-7.25	1.29	1.37
1	B	489	HIS	CD2-NE2	-7.16	1.29	1.37
1	B	481	HIS	CD2-NE2	-6.92	1.30	1.37
1	A	384	THR	CA-CB	6.72	1.61	1.53
1	A	88	GLU	CA-CB	-6.72	1.42	1.53
1	A	42	HIS	CD2-NE2	-6.49	1.30	1.37
1	A	79	HIS	CD2-NE2	-6.40	1.30	1.37
1	A	69	HIS	CD2-NE2	-6.36	1.30	1.37
1	B	227	ILE	CA-CB	6.32	1.61	1.54
1	B	260	HIS	CD2-NE2	-6.24	1.30	1.37
1	A	256	HIS	CD2-NE2	-6.22	1.31	1.37
1	A	237	SER	CA-CB	6.19	1.64	1.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	174	HIS	CD2-NE2	-6.17	1.31	1.37
1	B	30	HIS	CD2-NE2	-6.17	1.31	1.37
1	B	103	HIS	CD2-NE2	-6.12	1.31	1.37
1	A	263	HIS	CD2-NE2	-6.09	1.31	1.37
1	B	69	HIS	CD2-NE2	-6.08	1.31	1.37
1	A	489	HIS	CD2-NE2	-6.07	1.31	1.37
1	B	42	HIS	CD2-NE2	-6.03	1.31	1.37
1	B	656	VAL	CA-CB	5.98	1.61	1.54
1	A	519	HIS	CD2-NE2	-5.92	1.31	1.37
1	B	296	HIS	CG-ND1	-5.86	1.31	1.38
1	B	628	HIS	CD2-NE2	-5.84	1.31	1.37
1	A	164	ILE	CA-CB	5.78	1.61	1.54
1	A	30	HIS	CD2-NE2	-5.73	1.31	1.37
1	B	256	HIS	CD2-NE2	-5.70	1.31	1.37
1	B	461	HIS	CG-ND1	-5.65	1.32	1.38
1	A	296	HIS	CD2-NE2	-5.61	1.31	1.37
1	A	481	HIS	CD2-NE2	-5.52	1.31	1.37
1	A	122	ILE	CA-CB	5.47	1.61	1.54
1	A	87	ILE	CA-CB	5.38	1.61	1.54
1	B	413	ARG	CD-NE	-5.33	1.38	1.46
1	B	42	HIS	CG-ND1	-5.31	1.32	1.38
1	A	489	HIS	CG-ND1	-5.23	1.32	1.38
1	A	301	ILE	CA-CB	5.19	1.59	1.55
1	A	126	VAL	CA-CB	5.11	1.60	1.54
1	A	114	THR	CA-CB	5.09	1.60	1.53
1	A	69	HIS	CG-ND1	-5.08	1.32	1.38
1	A	174	HIS	CG-ND1	-5.05	1.32	1.38

All (316) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	3	GLN	OE1-CD-NE2	-12.50	110.10	122.60
1	A	219	ASN	OD1-CG-ND2	-12.35	110.25	122.60
1	A	309	ASN	OD1-CG-ND2	-11.68	110.92	122.60
1	B	491	ARG	NE-CZ-NH1	11.60	133.09	121.50
1	B	27	ASN	OD1-CG-ND2	-11.09	111.51	122.60
1	B	67	ASN	OD1-CG-ND2	-11.03	111.57	122.60
1	B	629	GLN	OE1-CD-NE2	-10.64	111.95	122.60
1	B	659	ARG	CG-CD-NE	-10.60	88.67	112.00
1	B	495	ASN	OD1-CG-ND2	-10.06	112.54	122.60
1	B	394	ALA	N-CA-C	9.85	124.13	110.24
1	B	313	ASN	OD1-CG-ND2	-9.83	112.77	122.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	134	ASN	OD1-CG-ND2	-9.72	112.88	122.60
1	B	659	ARG	CB-CG-CD	9.70	133.62	111.30
1	A	47	GLN	CG-CD-NE2	9.52	130.69	116.40
1	A	597	GLN	OE1-CD-NE2	-9.48	113.12	122.60
1	A	609	ASN	N-CA-C	9.46	124.41	112.86
1	B	3	GLN	CG-CD-NE2	9.45	130.57	116.40
1	B	54	ASN	OD1-CG-ND2	-9.42	113.18	122.60
1	A	47	GLN	OE1-CD-NE2	-9.23	113.37	122.60
1	A	27	ASN	OD1-CG-ND2	-9.23	113.37	122.60
1	B	659	ARG	NH1-CZ-NH2	-9.21	107.33	119.30
1	A	71	VAL	CB-CA-C	-9.11	100.10	112.04
1	A	237	SER	CA-CB-OG	9.08	129.26	111.10
1	A	309	ASN	CB-CG-ND2	8.88	129.72	116.40
1	B	371	ASN	OD1-CG-ND2	-8.87	113.73	122.60
1	A	371	ASN	OD1-CG-ND2	-8.77	113.83	122.60
1	B	491	ARG	NE-CZ-NH2	-8.65	111.41	119.20
1	B	387	ASN	OD1-CG-ND2	-8.61	113.99	122.60
1	B	282	ASN	OD1-CG-ND2	-8.57	114.03	122.60
1	A	67	ASN	OD1-CG-ND2	-8.54	114.06	122.60
1	B	219	ASN	OD1-CG-ND2	-8.50	114.10	122.60
1	B	27	ASN	CB-CG-ND2	8.46	129.10	116.40
1	A	49	ARG	CB-CG-CD	-8.27	92.29	111.30
1	B	491	ARG	CB-CG-CD	8.26	130.30	111.30
1	A	120	GLN	OE1-CD-NE2	-8.23	114.36	122.60
1	B	309	ASN	OD1-CG-ND2	-8.22	114.38	122.60
1	A	358	THR	N-CA-CB	-8.17	96.82	110.39
1	B	187	ASN	OD1-CG-ND2	-8.15	114.45	122.60
1	A	88	GLU	N-CA-CB	8.09	122.01	110.12
1	A	629	GLN	OE1-CD-NE2	-8.09	114.51	122.60
1	A	54	ASN	OD1-CG-ND2	-8.03	114.57	122.60
1	A	320	GLN	OE1-CD-NE2	-7.84	114.76	122.60
1	B	628	HIS	CB-CG-CD2	-7.84	121.01	131.20
1	A	45	TRP	CG-CD2-CE3	7.84	141.74	133.90
1	B	654	GLU	CA-CB-CG	-7.82	98.46	114.10
1	A	341	ASN	OD1-CG-ND2	-7.79	114.81	122.60
1	B	444	ASN	OD1-CG-ND2	-7.79	114.81	122.60
1	B	354	SER	N-CA-C	7.78	120.80	110.53
1	A	389	THR	N-CA-CB	-7.76	99.24	110.65
1	A	238	LYS	N-CA-C	7.73	120.60	111.71
1	B	371	ASN	CA-CB-CG	-7.72	104.88	112.60
1	B	52	PRO	CA-C-N	7.66	131.30	120.28
1	B	52	PRO	C-N-CA	7.66	131.30	120.28

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	274	GLN	OE1-CD-NE2	-7.64	114.96	122.60
1	A	621	THR	N-CA-C	7.57	121.44	111.75
1	A	670	ASP	CA-CB-CG	7.56	120.16	112.60
1	B	434	ASN	OD1-CG-ND2	-7.55	115.05	122.60
1	A	16	ARG	CG-CD-NE	-7.55	95.39	112.00
1	B	541	SER	N-CA-C	7.52	119.12	111.07
1	A	134	ASN	CB-CG-ND2	7.51	127.67	116.40
1	A	529	GLN	OE1-CD-NE2	-7.47	115.13	122.60
1	A	337	GLN	OE1-CD-NE2	-7.46	115.14	122.60
1	A	16	ARG	NE-CZ-NH1	-7.45	114.05	121.50
1	A	426	ASN	OD1-CG-ND2	-7.45	115.15	122.60
1	A	313	ASN	OD1-CG-ND2	-7.39	115.21	122.60
1	B	426	ASN	OD1-CG-ND2	-7.37	115.23	122.60
1	B	112	GLU	N-CA-C	7.33	121.47	112.23
1	A	179	ASN	OD1-CG-ND2	-7.33	115.27	122.60
1	B	676	LEU	N-CA-C	7.29	120.09	111.71
1	B	434	ASN	CB-CG-ND2	7.28	127.32	116.40
1	B	310	ASN	OD1-CG-ND2	-7.28	115.32	122.60
1	A	298	GLN	OE1-CD-NE2	-7.25	115.35	122.60
1	A	389	THR	CA-C-O	7.23	127.00	119.05
1	A	47	GLN	N-CA-CB	-7.22	99.77	110.53
1	B	298	GLN	CG-CD-NE2	7.19	127.18	116.40
1	A	149	ASN	N-CA-C	7.17	120.00	110.53
1	A	16	ARG	NH1-CZ-NH2	-7.15	110.00	119.30
1	A	391	TRP	CG-CD2-CE3	7.15	141.05	133.90
1	B	298	GLN	OE1-CD-NE2	-7.14	115.46	122.60
1	B	322	LYS	N-CA-C	7.14	119.06	111.28
1	B	67	ASN	CB-CG-ND2	7.12	127.08	116.40
1	B	282	ASN	CA-CB-CG	7.12	119.72	112.60
1	B	491	ARG	CD-NE-CZ	7.07	134.30	124.40
1	B	623	TRP	N-CA-C	7.02	121.67	113.18
1	B	519	HIS	CB-CG-CD2	-7.01	122.09	131.20
1	B	635	ARG	NE-CZ-NH1	7.00	128.50	121.50
1	B	191	ILE	N-CA-C	7.00	117.14	110.42
1	A	341	ASN	CB-CG-ND2	6.98	126.87	116.40
1	A	579	LYS	CG-CD-CE	-6.97	95.27	111.30
1	A	470	ASP	N-CA-C	6.95	121.46	113.19
1	A	103	HIS	O-C-N	-6.92	116.97	121.88
1	B	51	ASN	OD1-CG-ND2	-6.92	115.68	122.60
1	A	282	ASN	CA-C-N	6.87	126.50	119.56
1	A	282	ASN	C-N-CA	6.87	126.50	119.56
1	A	157	ASP	N-CA-C	6.85	118.40	111.07

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	628	HIS	CB-CG-ND1	6.79	132.89	122.70
1	B	629	GLN	CG-CD-NE2	6.76	126.54	116.40
1	B	595	ASP	N-CA-C	6.76	119.48	111.71
1	A	148	ASP	CA-CB-CG	6.75	119.34	112.60
1	B	59	ASN	OD1-CG-ND2	-6.74	115.86	122.60
1	A	105	GLU	N-CA-C	6.70	120.16	109.24
1	B	470	ASP	N-CA-C	6.70	121.05	113.01
1	A	665	ALA	N-CA-C	6.66	118.19	111.07
1	A	398	GLN	O-C-N	-6.64	117.46	121.71
1	B	505	ASN	OD1-CG-ND2	-6.64	115.96	122.60
1	A	3	GLN	OE1-CD-NE2	-6.59	116.01	122.60
1	A	629	GLN	CG-CD-NE2	6.55	126.23	116.40
1	B	530	ASN	OD1-CG-ND2	-6.55	116.05	122.60
1	B	481	HIS	CB-CG-CD2	-6.55	122.69	131.20
1	B	610	VAL	CB-CA-C	-6.53	99.48	111.36
1	B	610	VAL	N-CA-CB	6.47	120.26	111.21
1	A	67	ASN	CB-CG-ND2	6.45	126.07	116.40
1	A	59	ASN	OD1-CG-ND2	-6.44	116.16	122.60
1	A	153	VAL	CB-CA-C	-6.42	100.95	110.33
1	B	390	ARG	N-CA-C	6.41	118.74	108.41
1	B	53	THR	OG1-CB-CG2	6.41	122.12	109.30
1	A	345	LYS	CA-CB-CG	-6.40	101.30	114.10
1	A	673	ILE	O-C-N	-6.40	115.70	122.81
1	A	16	ARG	NE-CZ-NH2	6.40	124.96	119.20
1	B	495	ASN	CB-CG-ND2	6.40	126.00	116.40
1	B	238	LYS	N-CA-C	6.39	120.33	112.54
1	A	289	VAL	CA-C-N	6.37	126.74	119.93
1	A	289	VAL	C-N-CA	6.37	126.74	119.93
1	A	46	SER	CA-C-O	6.35	127.19	119.38
1	B	197	ILE	N-CA-C	6.33	121.00	111.89
1	B	583	ALA	N-CA-C	6.32	119.24	109.07
1	A	145	THR	CA-CB-OG1	-6.29	100.17	109.60
1	A	580	ASN	OD1-CG-ND2	-6.28	116.32	122.60
1	B	6	ASP	N-CA-C	6.27	118.92	111.33
1	B	263	HIS	CB-CG-CD2	-6.27	123.06	131.20
1	B	140	ASN	OD1-CG-ND2	-6.25	116.34	122.60
1	A	459	SER	CA-CB-OG	6.24	123.58	111.10
1	B	482	GLN	OE1-CD-NE2	-6.24	116.36	122.60
1	A	219	ASN	CB-CG-ND2	6.24	125.76	116.40
1	A	513	ASN	OD1-CG-ND2	-6.23	116.37	122.60
1	A	566	VAL	N-CA-C	-6.22	104.79	110.82
1	B	161	GLN	OE1-CD-NE2	-6.17	116.43	122.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	296	HIS	CB-CG-CD2	-6.15	123.21	131.20
1	A	416	ILE	CA-C-O	6.14	127.97	122.63
1	B	371	ASN	CB-CG-ND2	6.11	125.57	116.40
1	A	407	TYR	N-CA-C	6.11	120.20	112.87
1	A	27	ASN	CA-CB-CG	-6.10	106.50	112.60
1	A	62	ARG	CB-CG-CD	-6.09	97.30	111.30
1	A	337	GLN	CA-CB-CG	6.09	126.28	114.10
1	B	260	HIS	CB-CG-CD2	-6.07	123.31	131.20
1	B	636	PHE	CA-CB-CG	-6.05	107.75	113.80
1	A	505	ASN	OD1-CG-ND2	-6.03	116.57	122.60
1	A	132	GLN	OE1-CD-NE2	-6.02	116.58	122.60
1	B	203	VAL	N-CA-C	6.01	116.19	110.42
1	B	513	ASN	OD1-CG-ND2	-6.00	116.59	122.60
1	A	27	ASN	CB-CG-ND2	6.00	125.40	116.40
1	A	495	ASN	OD1-CG-ND2	-5.99	116.61	122.60
1	A	58	ILE	N-CA-C	5.99	116.73	110.62
1	B	132	GLN	OE1-CD-NE2	-5.99	116.61	122.60
1	B	188	LYS	N-CA-C	5.97	120.15	112.86
1	A	371	ASN	CB-CG-ND2	5.97	125.35	116.40
1	B	580	ASN	N-CA-C	5.95	119.63	111.54
1	A	519	HIS	CB-CG-CD2	-5.91	123.52	131.20
1	A	291	GLN	CG-CD-NE2	5.88	125.22	116.40
1	A	415	GLY	O-C-N	-5.88	116.99	123.05
1	A	238	LYS	CA-C-O	5.86	126.72	120.10
1	A	476	GLU	N-CA-C	5.86	118.45	111.71
1	B	149	ASN	OD1-CG-ND2	-5.86	116.74	122.60
1	A	314	LYS	CA-CB-CG	5.85	125.80	114.10
1	B	263	HIS	CB-CG-ND1	5.83	131.45	122.70
1	B	659	ARG	NE-CZ-NH1	-5.81	115.69	121.50
1	A	47	GLN	CA-CB-CG	5.81	125.72	114.10
1	B	3	GLN	N-CA-C	5.81	127.27	111.00
1	A	391	TRP	CE2-CD2-CG	-5.80	100.24	107.20
1	A	426	ASN	CB-CG-ND2	5.79	125.09	116.40
1	B	341	ASN	OD1-CG-ND2	-5.79	116.81	122.60
1	B	35	LEU	N-CA-C	5.79	117.59	111.28
1	B	476	GLU	N-CA-C	5.79	118.37	111.71
1	B	54	ASN	CB-CG-ND2	5.79	125.08	116.40
1	A	291	GLN	OE1-CD-NE2	-5.74	116.86	122.60
1	A	120	GLN	N-CA-C	5.73	117.21	110.97
1	A	186	ASP	CA-CB-CG	5.72	118.32	112.60
1	B	593	THR	CA-CB-OG1	-5.72	101.02	109.60
1	B	412	ILE	N-CA-C	5.71	116.53	108.36

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	71	VAL	N-CA-CB	5.69	117.59	110.47
1	A	418	GLU	N-CA-C	5.68	117.47	111.28
1	A	237	SER	O-C-N	-5.68	115.04	122.59
1	A	416	ILE	N-CA-CB	-5.68	106.60	112.28
1	B	303	LYS	CA-C-N	5.68	125.14	119.24
1	B	303	LYS	C-N-CA	5.68	125.14	119.24
1	B	417	ARG	NH1-CZ-NH2	-5.66	111.95	119.30
1	A	481	HIS	CB-CG-CD2	-5.65	123.86	131.20
1	A	224	LEU	N-CA-C	5.64	117.43	111.28
1	A	387	ASN	CA-CB-CG	5.64	118.24	112.60
1	A	623	TRP	CG-CD2-CE3	5.64	139.54	133.90
1	B	444	ASN	CB-CG-ND2	5.63	124.85	116.40
1	A	459	SER	N-CA-C	5.62	119.86	112.89
1	A	16	ARG	CB-CG-CD	5.61	124.20	111.30
1	B	674	SER	CA-C-N	5.61	125.97	119.47
1	B	674	SER	C-N-CA	5.61	125.97	119.47
1	B	574	LYS	CB-CG-CD	5.60	124.19	111.30
1	B	320	GLN	OE1-CD-NE2	-5.59	117.00	122.60
1	B	503	ASP	CA-CB-CG	5.59	118.19	112.60
1	B	440	GLY	CA-C-O	5.58	126.14	121.11
1	A	482	GLN	OE1-CD-NE2	-5.57	117.03	122.60
1	B	519	HIS	CB-CG-ND1	5.57	131.06	122.70
1	B	268	LYS	CA-C-O	-5.57	114.92	121.16
1	B	291	GLN	OE1-CD-NE2	-5.57	117.03	122.60
1	B	107	GLU	CB-CG-CD	5.56	122.05	112.60
1	B	149	ASN	N-CA-C	5.54	117.85	110.53
1	B	53	THR	N-CA-CB	-5.53	101.70	110.22
1	A	389	THR	CB-CA-C	5.53	118.83	109.55
1	B	673	ILE	O-C-N	-5.53	116.90	123.03
1	B	367	GLU	O-C-N	-5.51	116.28	122.12
1	B	579	LYS	CA-CB-CG	5.50	125.10	114.10
1	A	94	ARG	CD-NE-CZ	5.50	132.10	124.40
1	B	426	ASN	CB-CG-ND2	5.50	124.65	116.40
1	B	79	HIS	CA-CB-CG	-5.50	108.30	113.80
1	B	642	ALA	N-CA-C	5.50	120.39	113.25
1	B	652	THR	CA-C-N	5.47	124.93	119.24
1	B	652	THR	C-N-CA	5.47	124.93	119.24
1	B	182	ALA	O-C-N	-5.47	117.09	123.27
1	B	529	GLN	OE1-CD-NE2	-5.46	117.14	122.60
1	B	609	ASN	OD1-CG-ND2	-5.46	117.14	122.60
1	A	197	ILE	N-CA-C	5.46	117.87	111.05
1	A	200	ASP	CA-CB-CG	5.44	118.04	112.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	56	ASP	N-CA-C	5.44	120.02	113.17
1	B	314	LYS	CB-CG-CD	5.44	123.80	111.30
1	B	391	TRP	CG-CD1-NE1	-5.42	103.16	110.20
1	A	369	VAL	N-CA-C	5.39	120.56	109.34
1	B	174	HIS	CB-CG-CD2	-5.39	124.19	131.20
1	B	679	ALA	N-CA-C	5.39	119.86	113.28
1	A	95	GLN	OE1-CD-NE2	-5.38	117.22	122.60
1	A	317	SER	CB-CA-C	-5.37	102.44	110.88
1	B	73	LEU	CD1-CG-CD2	-5.37	98.99	110.80
1	B	337	GLN	CA-CB-CG	-5.36	103.37	114.10
1	A	529	GLN	N-CA-C	5.36	118.42	110.48
1	B	609	ASN	N-CA-C	5.36	119.10	112.24
1	B	486	THR	N-CA-C	5.36	117.12	111.28
1	B	69	HIS	CB-CG-CD2	-5.35	124.25	131.20
1	B	392	LYS	N-CA-C	5.32	117.98	111.82
1	A	621	THR	O-C-N	-5.31	116.14	122.20
1	B	406	ASN	CA-CB-CG	5.31	117.91	112.60
1	B	313	ASN	CB-CG-ND2	5.31	124.37	116.40
1	A	113	VAL	CA-C-N	-5.30	114.71	122.19
1	A	113	VAL	C-N-CA	-5.30	114.71	122.19
1	A	503	ASP	CA-CB-CG	5.30	117.91	112.60
1	B	186	ASP	CA-CB-CG	5.30	117.90	112.60
1	B	497	GLN	OE1-CD-NE2	-5.29	117.31	122.60
1	A	188	LYS	N-CA-C	5.29	121.75	113.72
1	A	221	ASN	OD1-CG-ND2	-5.29	117.31	122.60
1	B	580	ASN	OD1-CG-ND2	-5.28	117.32	122.60
1	A	405	GLY	O-C-N	-5.28	118.86	123.88
1	A	340	ALA	CA-C-O	5.28	126.50	120.80
1	A	367	GLU	CB-CA-C	-5.27	102.60	110.88
1	A	42	HIS	CA-CB-CG	-5.27	108.53	113.80
1	A	262	VAL	CG1-CB-CG2	-5.26	99.23	110.80
1	B	106	PHE	CA-CB-CG	5.26	119.06	113.80
1	A	364	THR	CA-CB-OG1	-5.26	101.72	109.60
1	B	528	ARG	CD-NE-CZ	-5.23	117.08	124.40
1	A	677	LYS	N-CA-C	5.22	117.27	109.59
1	A	51	ASN	O-C-N	-5.22	116.28	121.19
1	B	99	ARG	CA-CB-CG	-5.22	103.65	114.10
1	B	303	LYS	CA-CB-CG	-5.22	103.66	114.10
1	B	529	GLN	N-CA-C	5.22	117.42	110.53
1	B	240	LYS	O-C-N	-5.22	116.37	121.38
1	A	273	LYS	N-CA-C	5.21	117.38	111.02
1	A	70	ALA	CA-C-N	5.21	127.87	120.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	70	ALA	C-N-CA	5.21	127.87	120.53
1	B	259	SER	N-CA-C	5.21	118.60	110.32
1	A	37	MET	N-CA-C	5.19	119.61	113.28
1	A	495	ASN	CA-C-O	5.18	127.71	121.65
1	A	495	ASN	N-CA-C	5.18	118.77	111.52
1	B	461	HIS	O-C-N	-5.18	116.58	121.35
1	A	270	ASP	CA-CB-CG	-5.18	107.42	112.60
1	B	186	ASP	N-CA-CB	-5.17	103.59	110.57
1	A	303	LYS	CA-CB-CG	-5.17	103.76	114.10
1	B	624	GLY	O-C-N	-5.17	116.76	122.24
1	B	534	LEU	N-CA-C	5.17	117.97	109.76
1	B	621	THR	CA-CB-OG1	-5.16	101.86	109.60
1	A	45	TRP	CE2-CD2-CG	-5.16	101.01	107.20
1	B	491	ARG	CG-CD-NE	-5.16	100.64	112.00
1	A	61	ASP	CA-CB-CG	5.16	117.76	112.60
1	B	679	ALA	CA-C-N	-5.16	112.41	121.70
1	B	679	ALA	C-N-CA	-5.16	112.41	121.70
1	B	33	ALA	CA-C-N	5.15	124.60	119.24
1	B	33	ALA	C-N-CA	5.15	124.60	119.24
1	A	238	LYS	CB-CG-CD	5.15	123.14	111.30
1	A	654	GLU	CA-CB-CG	5.14	124.39	114.10
1	A	236	LEU	CA-C-N	5.14	131.35	121.54
1	A	236	LEU	C-N-CA	5.14	131.35	121.54
1	B	94	ARG	CA-CB-CG	-5.12	103.86	114.10
1	A	262	VAL	O-C-N	-5.12	116.18	122.57
1	B	13	SER	CB-CA-C	-5.12	102.16	110.85
1	B	357	ALA	O-C-N	-5.11	116.58	122.87
1	A	534	LEU	N-CA-C	5.11	117.89	109.76
1	B	387	ASN	CB-CG-ND2	5.11	124.07	116.40
1	B	460	GLY	O-C-N	-5.11	116.36	122.34
1	A	597	GLN	CG-CD-NE2	5.11	124.06	116.40
1	A	279	PHE	N-CA-C	5.10	119.49	113.16
1	A	263	HIS	N-CA-C	5.10	116.64	111.14
1	A	140	ASN	OD1-CG-ND2	-5.09	117.51	122.60
1	A	623	TRP	CE2-CD2-CG	-5.08	101.10	107.20
1	B	391	TRP	CE2-CD2-CG	-5.08	101.10	107.20
1	A	536	GLY	CA-C-O	5.07	124.81	119.03
1	A	203	VAL	N-CA-C	5.07	115.68	110.36
1	B	51	ASN	CA-C-N	5.06	124.67	119.05
1	B	51	ASN	C-N-CA	5.06	124.67	119.05
1	A	623	TRP	CG-CD1-NE1	-5.06	103.62	110.20
1	B	393	GLU	CB-CG-CD	5.06	121.20	112.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	526	LEU	N-CA-C	5.06	117.65	109.40
1	B	540	GLU	O-C-N	5.06	127.28	122.07
1	B	47	GLN	OE1-CD-NE2	-5.06	117.54	122.60
1	B	113	VAL	CA-C-O	-5.06	116.94	121.09
1	A	79	HIS	CB-CG-CD2	-5.05	124.64	131.20
1	A	469	HIS	CB-CG-CD2	-5.04	124.64	131.20
1	B	30	HIS	CB-CG-CD2	-5.04	124.64	131.20
1	B	100	THR	N-CA-C	5.04	118.15	108.97
1	A	208	GLU	O-C-N	-5.04	116.78	122.12
1	B	238	LYS	CA-C-O	5.02	125.56	119.38
1	B	465	TRP	CE2-CD2-CG	-5.01	101.19	107.20

There are no chirality outliers.

All (3) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	16	ARG	Sidechain
1	A	99	ARG	Sidechain
1	B	659	ARG	Sidechain

5.2 Too-close contacts ⓘ

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	5198	0	5139	64	1
1	B	5198	0	5139	43	0
2	A	1	0	0	0	0
2	B	1	0	0	0	0
3	A	26	0	16	1	0
3	B	26	0	16	2	0
4	A	473	0	0	9	2
4	B	548	0	0	5	1
All	All	11471	0	10310	102	2

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 5.

All (102) close contacts within the same asymmetric unit are listed below, sorted by their clash

magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:164:ILE:HD12	1:A:419:HIS:CD2	2.01	0.96
1:A:652:THR:HG22	1:A:655:GLY:H	1.45	0.81
1:A:528:ARG:HD3	4:A:853:HOH:O	1.86	0.75
1:A:206:ARG:HG3	1:B:206:ARG:HG3	1.69	0.74
1:B:554:ASN:HB3	4:B:790:HOH:O	1.89	0.72
1:A:67:ASN:H	1:A:67:ASN:HD22	1.36	0.71
1:A:389:THR:HG23	1:A:411:TYR:OH	1.90	0.71
1:B:48:MET:HB2	1:B:50:MET:HE2	1.75	0.69
1:B:392:LYS:HZ2	1:B:392:LYS:HA	1.58	0.68
1:A:358:THR:HG21	4:A:755:HOH:O	1.94	0.67
1:B:51:ASN:HD21	1:B:53:THR:HB	1.61	0.66
1:A:298:GLN:HE21	1:A:303:LYS:HE3	1.63	0.64
1:B:51:ASN:ND2	1:B:53:THR:HB	2.13	0.63
1:B:45:TRP:HA	1:B:48:MET:HE3	1.80	0.63
1:A:647:LYS:HB3	1:A:647:LYS:NZ	2.14	0.62
1:A:198:SER:O	1:B:417:ARG:NH2	2.33	0.62
1:A:652:THR:HG22	1:A:655:GLY:N	2.13	0.61
1:A:358:THR:HG22	1:A:527:SER:H	1.65	0.61
1:B:44:LEU:HG	1:B:48:MET:HE2	1.83	0.61
1:A:164:ILE:HD12	1:A:419:HIS:NE2	2.16	0.60
1:A:106:PHE:H	1:A:114:THR:HG22	1.66	0.59
1:B:392:LYS:HA	1:B:392:LYS:NZ	2.17	0.59
1:A:311:LYS:O	1:A:314:LYS:HG3	2.03	0.59
1:B:49:ARG:HE	1:B:57:TRP:HH2	1.51	0.58
1:A:105:GLU:HA	1:A:114:THR:HB	1.86	0.57
1:B:67:ASN:HD22	1:B:67:ASN:H	1.53	0.56
1:A:67:ASN:H	1:A:67:ASN:ND2	2.01	0.56
1:B:370:TYR:HE2	4:B:1146:HOH:O	1.89	0.56
1:B:5:THR:OG1	1:B:7:ILE:HG22	2.06	0.55
1:A:260:HIS:HD2	4:A:724:HOH:O	1.89	0.55
1:A:667:TYR:HB3	1:A:672:LEU:HD11	1.89	0.54
1:A:387:ASN:HA	1:A:468:THR:HG21	1.87	0.54
1:B:546:GLY:HA3	1:B:588:LEU:HD12	1.91	0.53
1:B:391:TRP:CD1	1:B:394:ALA:HB2	2.43	0.53
1:A:612:ILE:H	1:A:628:HIS:HD2	1.57	0.53
1:B:259:SER:O	1:B:262:VAL:HG22	2.09	0.52
1:B:67:ASN:H	1:B:67:ASN:ND2	2.08	0.52
1:B:658:GLU:O	1:B:662:LYS:HG2	2.11	0.51
1:B:337:GLN:HG2	4:B:1128:HOH:O	2.10	0.51
1:B:538:SER:HB2	4:B:1160:HOH:O	2.11	0.51
1:B:345:LYS:CE	1:B:372:GLN:HB2	2.42	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:548:VAL:HG13	1:A:584:ARG:HD2	1.94	0.49
1:A:256:HIS:HE1	4:A:716:HOH:O	1.94	0.49
1:B:487:LEU:O	1:B:491:ARG:HG2	2.12	0.48
1:A:67:ASN:HD22	1:A:67:ASN:N	2.08	0.48
1:B:387:ASN:HA	1:B:468:THR:HG21	1.96	0.48
1:A:34:PRO:HB3	1:A:73:LEU:HB2	1.96	0.48
1:B:112:GLU:HB3	1:B:128:MET:HE1	1.96	0.48
1:B:345:LYS:NZ	1:B:372:GLN:HB2	2.30	0.47
1:A:380:SER:HB2	1:A:389:THR:HG21	1.97	0.47
1:A:654:GLU:H	1:A:654:GLU:CD	2.22	0.47
1:A:540:GLU:CD	1:A:540:GLU:H	2.24	0.46
1:A:158:GLY:HA2	1:B:416:ILE:HD13	1.97	0.46
1:A:678:LYS:NZ	1:A:678:LYS:HB3	2.31	0.46
1:A:5:THR:OG1	1:A:7:ILE:HG22	2.16	0.46
1:B:361:LEU:HD13	1:B:504:GLY:HA2	1.97	0.46
1:B:552:VAL:HG23	1:B:555:PRO:HB3	1.98	0.45
1:B:51:ASN:HD21	1:B:306:VAL:HG22	1.82	0.45
1:A:52:PRO:HD2	1:A:302:LEU:HD13	1.98	0.45
1:A:16:ARG:HD3	1:A:35:LEU:O	2.17	0.44
1:A:359:ARG:HD2	1:A:386:SER:O	2.17	0.44
1:A:358:THR:CG2	1:A:527:SER:H	2.30	0.44
1:A:512:LYS:HE3	1:A:512:LYS:HB2	1.70	0.44
1:A:25:LYS:HB3	4:A:1110:HOH:O	2.17	0.44
1:B:358:THR:HA	1:B:361:LEU:HD12	1.99	0.44
1:A:471:SER:O	1:A:474:VAL:HG23	2.18	0.43
1:A:260:HIS:CD2	4:A:724:HOH:O	2.69	0.43
1:A:558:ILE:CD1	1:A:607:PRO:HD2	2.49	0.43
1:B:173:GLY:HA3	1:B:210:TYR:O	2.19	0.43
1:A:361:LEU:HD13	1:A:504:GLY:HA2	2.00	0.43
1:A:647:LYS:HB3	1:A:647:LYS:HZ2	1.82	0.43
1:A:359:ARG:HD3	4:A:751:HOH:O	2.18	0.42
1:A:390:ARG:NH1	1:A:394:ALA:HB3	2.33	0.42
1:A:346:LEU:HD11	1:A:512:LYS:HB3	2.01	0.42
1:A:8:ASP:O	1:A:12:VAL:HG23	2.18	0.42
1:A:600:GLU:HG2	1:A:601:TYR:N	2.35	0.42
1:A:94:ARG:O	1:B:640:GLY:HA2	2.19	0.42
1:A:191:ILE:HG13	3:A:682:TPP:H62	2.01	0.42
1:A:297:TYR:CD1	1:A:301:ILE:HD12	2.55	0.42
1:A:419:HIS:O	1:A:419:HIS:HD2	2.02	0.42
1:B:602:ARG:NH1	4:B:803:HOH:O	2.49	0.42
1:B:390:ARG:HG2	1:B:411:TYR:CZ	2.55	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:260:HIS:CD2	1:A:260:HIS:H	2.36	0.41
1:A:668:LYS:HB3	1:A:668:LYS:HE3	1.75	0.41
1:B:345:LYS:HZ3	1:B:372:GLN:HB2	1.85	0.41
1:A:369:VAL:HG12	4:A:1091:HOH:O	2.21	0.41
1:A:492:SER:HA	1:B:621:THR:HG21	2.03	0.41
1:A:37:MET:SD	1:A:185:ASP:HB2	2.60	0.41
1:A:359:ARG:HE	1:A:359:ARG:HB3	1.77	0.41
1:A:373:LEU:HA	1:A:374:PRO:HD2	1.85	0.41
1:B:71:VAL:HG23	1:B:104:PRO:HG3	2.02	0.41
4:A:746:HOH:O	3:B:682:TPP:H2	2.21	0.41
1:A:93:PHE:CD2	1:A:94:ARG:HG3	2.56	0.41
1:A:173:GLY:HA3	1:A:210:TYR:O	2.21	0.41
1:A:680:PHE:CD2	1:B:659:ARG:HD3	2.56	0.41
1:B:162:GLU:OE2	3:B:682:TPP:HM23	2.21	0.41
1:A:491:ARG:HD3	1:A:591:PHE:CD2	2.56	0.41
1:B:67:ASN:HD22	1:B:67:ASN:N	2.17	0.40
1:B:592:PHE:CE2	1:B:596:LYS:HE3	2.56	0.40
1:A:325:GLU:H	1:A:325:GLU:HG2	1.58	0.40
1:B:647:LYS:HE2	1:B:647:LYS:HB3	1.79	0.40
1:A:509:ALA:HA	1:A:512:LYS:HG2	2.03	0.40

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

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

5.3 Torsion angles

5.3.1 Protein backbone

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	676/680 (99%)	653 (97%)	21 (3%)	2 (0%)	36	35
1	B	676/680 (99%)	654 (97%)	21 (3%)	1 (0%)	48	46
All	All	1352/1360 (99%)	1307 (97%)	42 (3%)	3 (0%)	43	42

All (3) Ramachandran outliers are listed below:

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

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	552/554 (100%)	514 (93%)	38 (7%)	14	11
1	B	552/554 (100%)	519 (94%)	33 (6%)	17	14
All	All	1104/1108 (100%)	1033 (94%)	71 (6%)	16	12

All (71) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	47	GLN
1	A	50	MET
1	A	62	ARG
1	A	67	ASN
1	A	71	VAL
1	A	113	VAL
1	A	114	THR
1	A	153	VAL
1	A	197	ILE
1	A	218	GLU
1	A	229	LYS
1	A	238	LYS
1	A	255	LEU

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Mol	Chain	Res	Type
1	A	299	LYS
1	A	302	LEU
1	A	314	LYS
1	A	318	GLU
1	A	325	GLU
1	A	338	LEU
1	A	343	GLU
1	A	348	THR
1	A	358	THR
1	A	386	SER
1	A	404	SER
1	A	459	SER
1	A	552	VAL
1	A	571	GLU
1	A	580	ASN
1	A	581	ILE
1	A	584	ARG
1	A	588	LEU
1	A	600	GLU
1	A	610	VAL
1	A	652	THR
1	A	654	GLU
1	A	668	LYS
1	A	672	LEU
1	A	678	LYS
1	B	53	THR
1	B	67	ASN
1	B	73	LEU
1	B	113	VAL
1	B	141	LYS
1	B	197	ILE
1	B	229	LYS
1	B	268	LYS
1	B	278	LYS
1	B	314	LYS
1	B	322	LYS
1	B	326	LEU
1	B	337	GLN
1	B	338	LEU
1	B	356	VAL
1	B	367	GLU
1	B	370	TYR

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Mol	Chain	Res	Type
1	B	371	ASN
1	B	390	ARG
1	B	392	LYS
1	B	404	SER
1	B	417	ARG
1	B	491	ARG
1	B	518	LYS
1	B	528	ARG
1	B	574	LYS
1	B	579	LYS
1	B	596	LYS
1	B	610	VAL
1	B	625	LYS
1	B	635	ARG
1	B	647	LYS
1	B	671	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (24) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	54	ASN
1	A	67	ASN
1	A	124	ASN
1	A	134	ASN
1	A	233	GLN
1	A	256	HIS
1	A	260	HIS
1	A	298	GLN
1	A	313	ASN
1	A	320	GLN
1	A	398	GLN
1	A	580	ASN
1	A	597	GLN
1	A	628	HIS
1	A	661	GLN
1	B	51	ASN
1	B	54	ASN
1	B	67	ASN
1	B	120	GLN
1	B	309	ASN
1	B	434	ASN
1	B	519	HIS

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Mol	Chain	Res	Type
1	B	580	ASN
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	TPP	A	682	2	26,27,27	1.29	2 (7%)	38,40,40	1.26	5 (13%)
3	TPP	B	682	2	26,27,27	1.39	4 (15%)	38,40,40	1.44	4 (10%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	TPP	A	682	2	-	4/17/17/17	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	TPP	B	682	2	-	4/17/17/17	0/2/2/2

All (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	682	TPP	PA-O3A	3.22	1.63	1.59
3	A	682	TPP	C4-N3	-2.85	1.34	1.39
3	B	682	TPP	C4-N3	-2.84	1.34	1.39
3	A	682	TPP	C7'-N3	2.40	1.53	1.48
3	B	682	TPP	C7'-N3	2.20	1.53	1.48
3	B	682	TPP	PB-O3B	-2.16	1.46	1.54

All (9) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	682	TPP	C2-S1-C5	-4.41	88.30	91.22
3	B	682	TPP	O3A-PB-O1B	-3.18	94.30	111.04
3	A	682	TPP	C2-S1-C5	-3.04	89.20	91.22
3	A	682	TPP	C6'-N1'-C2'	2.77	120.62	116.07
3	A	682	TPP	C5'-C7'-N3	-2.45	107.70	112.97
3	A	682	TPP	C7-C6-C5	2.34	120.08	112.73
3	A	682	TPP	C5'-C6'-N1'	-2.21	120.24	123.83
3	B	682	TPP	O3A-PA-O1A	2.05	116.88	110.70
3	B	682	TPP	N1'-C2'-N3'	-2.04	122.13	125.53

There are no chirality outliers.

All (8) torsion outliers are listed below:

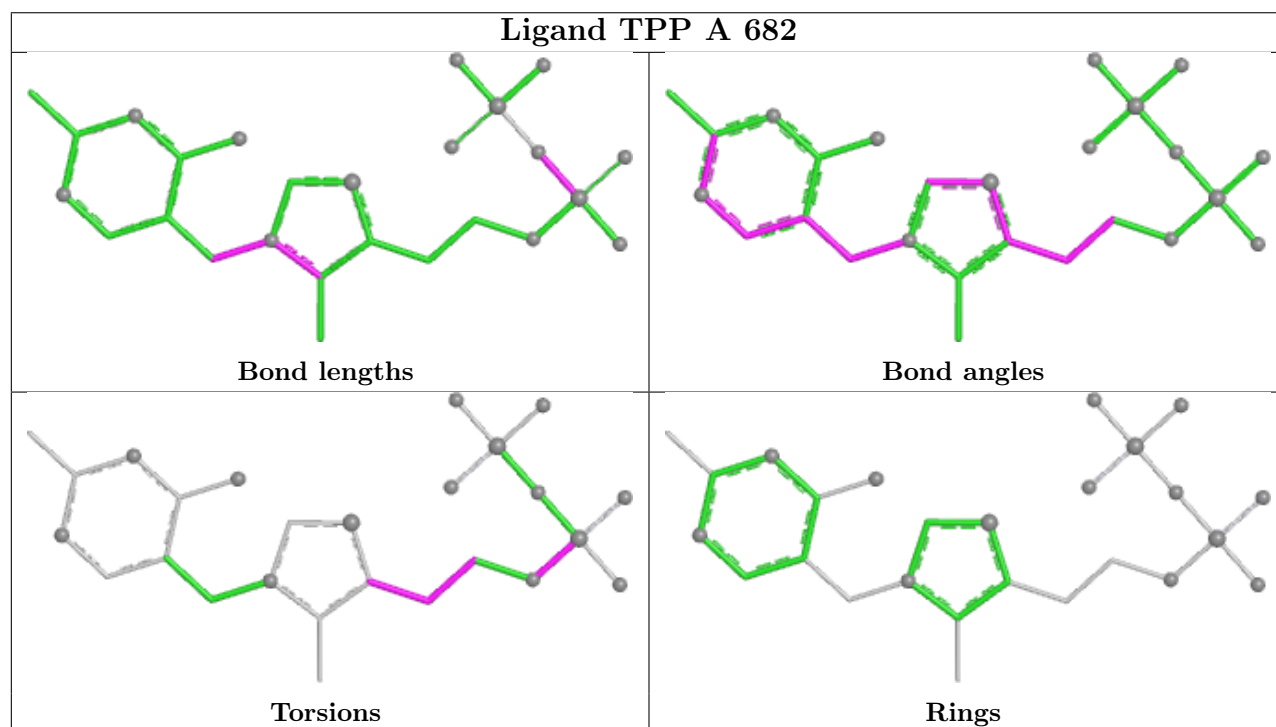
Mol	Chain	Res	Type	Atoms
3	A	682	TPP	C7-O7-PA-O3A
3	B	682	TPP	C5-C6-C7-O7
3	B	682	TPP	C7-O7-PA-O1A
3	B	682	TPP	C7-O7-PA-O2A
3	B	682	TPP	C7-O7-PA-O3A
3	A	682	TPP	C4-C5-C6-C7
3	A	682	TPP	S1-C5-C6-C7
3	A	682	TPP	C5-C6-C7-O7

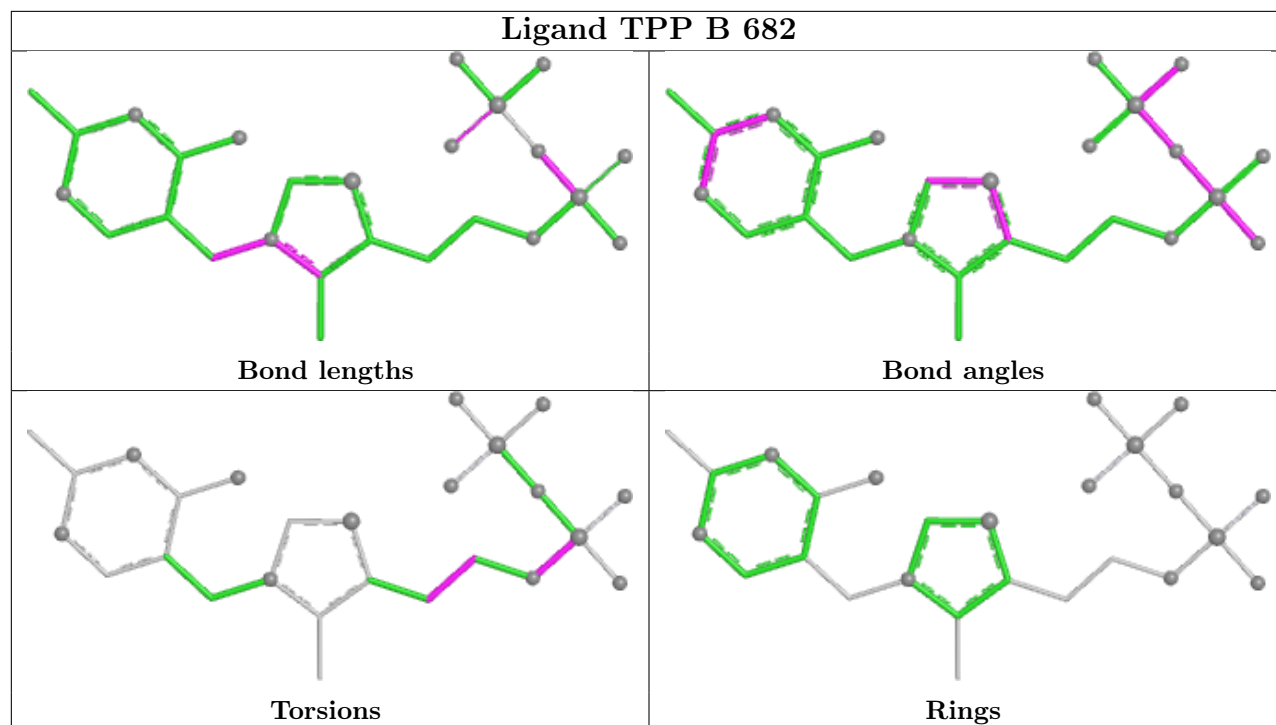
There are no ring outliers.

2 monomers are involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	682	TPP	1	0
3	B	682	TPP	2	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.





5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

EDS was not executed - this section is therefore empty.

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

EDS was not executed - this section is therefore empty.

6.3 Carbohydrates

EDS was not executed - this section is therefore empty.

6.4 Ligands

EDS was not executed - this section is therefore empty.

6.5 Other polymers

EDS was not executed - this section is therefore empty.