



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 6, 2026 – 07:08 PM UTC

PDB ID : 1SER / pdb_00001ser
Title : THE 2.9 ANGSTROMS CRYSTAL STRUCTURE OF T. THERMOPHILUS
SERYL-TRNA SYNTHETASE COMPLEXED WITH TRNA SER
Authors : Biou, S.; Cusack, V.; Yaremchuk, A.; Tukalo, M.
Deposited on : 1994-02-21
Resolution : 2.90 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
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

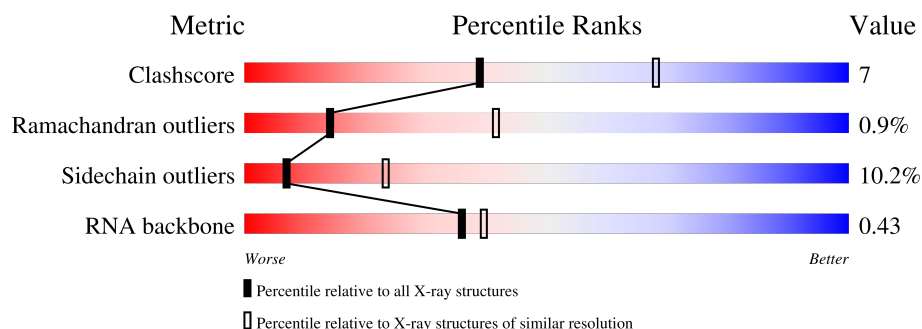
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.90 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	2690 (2.90-2.90)
Ramachandran outliers	187476	2623 (2.90-2.90)
Sidechain outliers	187428	2625 (2.90-2.90)
RNA backbone	3983	1120 (3.10-2.70)

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	T	94	
2	A	421	
2	B	421	

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 7780 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 RNA chain called TRNASER.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	T	65	Total	C	N	O	P	60	0	0
			1381	613	247	456	65			

- Molecule 2 is a protein called PROTEIN (SERYL-TRNA SYNTHETASE (E.C.6.1.1.11)).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	A	372	Total	C	N	O	S	30	0	0
			2982	1901	531	539	11			
2	B	421	Total	C	N	O	S	0	0	0
			3373	2143	606	613	11			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	208	TYR	THR	conflict	UNP P34945
B	708	TYR	THR	conflict	UNP P34945

- Molecule 3 is water.

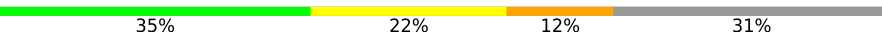
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	T	1	Total	O	0	0
			1	1		
3	A	14	Total	O	0	0
			14	14		
3	B	29	Total	O	0	0
			29	29		

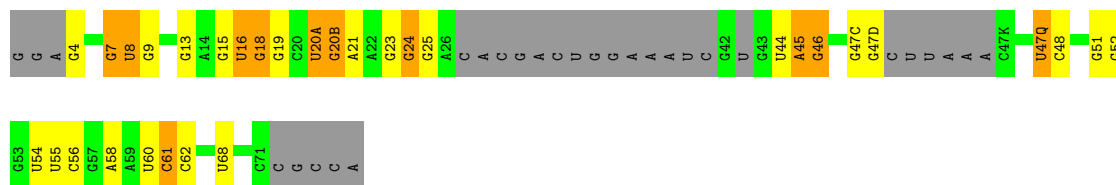
3 Residue-property plots [i](#)

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.

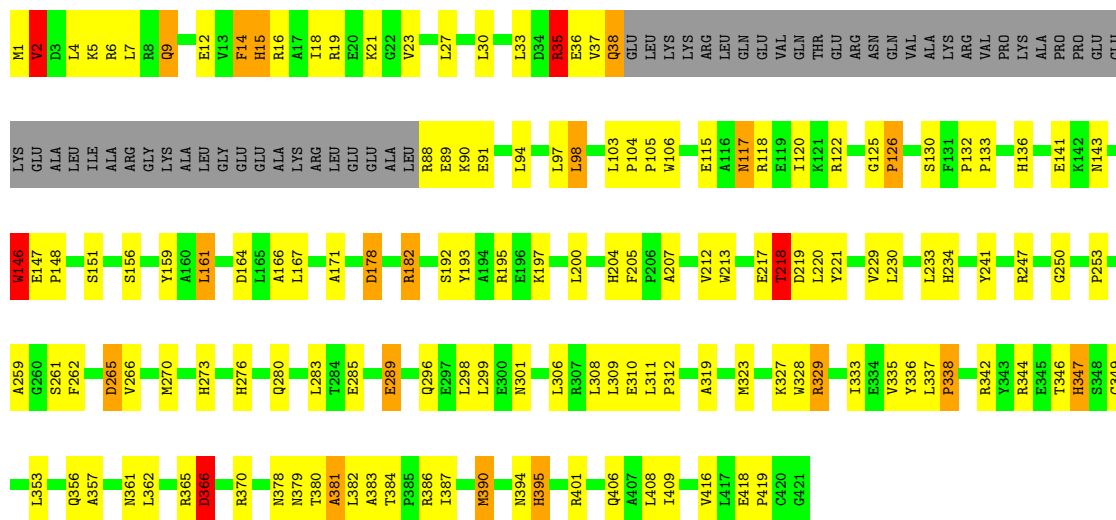
• Molecule 1: TRNASER

Chain T: 



• Molecule 2: PROTEIN (SERYL-TRNA SYNTHETASE (E.C.6.1.1.11))

Chain A: 



• Molecule 2: PROTEIN (SERYL-TRNA SYNTHETASE (E.C.6.1.1.11))

Chain B: 



E845	T846	H847	S848	C849	S850	L853	D854	W855	Q856	A857	R858	R859	A860	N861	L862	R865	D866	Y875	N878	A881	T884	F885	R886	I887	M890	L891	L892	E893	N894	H895	Q896	L897	Q898	D899	R903	V904	F905	Q906	E918	G921				
H734	E737	Y741	L746	P753	E758	S761	D765	V766	R767	Q768	L769	H773	Q774	F775	H776	K777	V778	E779	Q780	L783	E789	R793	A794	F795	Q796	L799	E800	N801	L809	L815	A819	D822	K827	W828	I833	P838	Y843	R844						
M617	R618	E619	I620	S630	F631	P632	P633	L634	D635	H636	V637	A638	L639	M640	N643	E647	S656	R657	S658	Y659	A660	L661	K662	L665	R674	F675	A676	M677	D678	P687	M688	T689	L690	Y693	F699	H704	A707	Q711	E717	T718	D719	L720	Y721	L730

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	124.50Å 128.90Å 121.20Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	10.00 – 2.90	Depositor
% Data completeness (in resolution range)	92.9 (10.00-2.90)	Depositor
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	X-PLOR	Depositor
R, R_{free}	0.194 , (Not available)	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	7780	wwPDB-VP
Average B, all atoms (Å ²)	26.0	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: H2U, 5MU, PSU

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	T	1.08	1/1472 (0.1%)	1.57	35/2290 (1.5%)
2	A	1.04	11/3053 (0.4%)	1.82	73/4138 (1.8%)
2	B	1.11	10/3448 (0.3%)	1.92	93/4667 (2.0%)
All	All	1.08	22/7973 (0.3%)	1.82	201/11095 (1.8%)

All (22) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	776	HIS	CD2-NE2	-8.11	1.28	1.37
2	A	347	HIS	CD2-NE2	-7.50	1.29	1.37
2	A	234	HIS	CD2-NE2	-7.11	1.30	1.37
2	B	904	VAL	CA-CB	6.90	1.63	1.54
2	B	773	HIS	CD2-NE2	-6.76	1.30	1.37
2	B	636	HIS	CD2-NE2	-6.65	1.30	1.37
2	A	276	HIS	CD2-NE2	-6.57	1.30	1.37
2	A	273	HIS	CD2-NE2	-6.32	1.30	1.37
2	B	847	HIS	CD2-NE2	-6.20	1.31	1.37
2	A	15	HIS	CD2-NE2	-5.96	1.31	1.37
2	A	136	HIS	CD2-NE2	-5.95	1.31	1.37
2	B	704	HIS	CD2-NE2	-5.72	1.31	1.37
2	B	515	HIS	CD2-NE2	-5.65	1.31	1.37
2	A	395	HIS	CD2-NE2	-5.64	1.31	1.37
2	B	895	HIS	CD2-NE2	-5.41	1.31	1.37
2	A	234	HIS	CG-ND1	-5.28	1.32	1.38
2	B	636	HIS	CG-ND1	-5.23	1.32	1.38
2	A	204	HIS	CD2-NE2	-5.17	1.32	1.37
2	B	734	HIS	CD2-NE2	-5.10	1.32	1.37
1	T	58	A	C5'-C4'	5.07	1.58	1.51
2	A	192	SER	CA-CB	-5.04	1.46	1.53
2	A	327	LYS	CA-CB	-5.03	1.45	1.53

All (201) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	515	HIS	CA-CB-CG	-10.21	103.59	113.80
1	T	13	G	C5'-C4'-C3'	-9.99	101.01	116.00
2	B	878	ASN	OD1-CG-ND2	-9.07	113.53	122.60
2	A	219	ASP	CA-CB-CG	9.06	121.66	112.60
2	B	854	ASP	CA-CB-CG	8.95	121.55	112.60
1	T	7	G	C5'-C4'-O4'	8.77	122.25	109.10
2	A	136	HIS	CA-CB-CG	8.39	122.19	113.80
2	A	323	MET	N-CA-C	8.23	120.33	111.36
1	T	44	U	C5'-C4'-C3'	-8.10	103.86	116.00
2	A	361	ASN	OD1-CG-ND2	-8.08	114.52	122.60
2	B	801	ASN	OD1-CG-ND2	-8.07	114.53	122.60
1	T	16	U	O4'-C1'-N1	-7.95	96.58	108.50
2	B	514	PHE	CA-CB-CG	-7.95	105.85	113.80
2	A	381	ALA	N-CA-C	-7.86	100.88	111.96
2	B	737	GLU	N-CA-CB	-7.85	98.51	110.04
2	B	707	ALA	N-CA-C	7.82	119.44	111.07
2	B	847	HIS	CA-C-O	-7.67	113.04	121.33
2	B	847	HIS	CA-CB-CG	7.65	121.45	113.80
1	T	44	U	O3'-P-O5'	-7.61	92.59	104.00
2	B	801	ASN	CB-CG-ND2	7.53	127.69	116.40
1	T	4	G	C5'-C4'-C3'	-7.48	104.77	116.00
2	B	719	ASP	CA-CB-CG	7.46	120.06	112.60
1	T	18	G	C5'-C4'-O4'	7.40	120.20	109.10
2	A	14	PHE	CA-CB-CG	-7.31	106.49	113.80
1	T	18	G	O4'-C1'-N9	7.21	119.02	108.20
2	A	229	VAL	N-CA-C	-7.20	104.19	110.74
2	A	117	ASN	OD1-CG-ND2	-7.16	115.44	122.60
2	A	394	ASN	OD1-CG-ND2	-7.15	115.45	122.60
2	B	881	ALA	N-CA-C	-7.15	103.18	112.68
2	A	266	VAL	N-CA-C	-7.04	106.21	112.12
2	B	765	ASP	N-CA-C	7.02	125.74	110.80
1	T	16	U	N1-C1'-C2'	6.96	122.44	112.00
2	B	559	PRO	N-CA-C	-6.96	100.97	111.41
2	A	418	GLU	CA-C-N	6.91	126.87	120.03
2	A	418	GLU	C-N-CA	6.91	126.87	120.03
2	B	899	ASP	CA-CB-CG	6.82	119.42	112.60
2	B	903	ARG	NE-CZ-NH2	-6.81	113.07	119.20
2	A	379	ASN	OD1-CG-ND2	-6.81	115.79	122.60
2	B	890	MET	CA-CB-CG	-6.81	100.49	114.10
2	B	898	GLN	N-CA-C	6.79	119.52	111.71
2	A	347	HIS	CB-CG-CD2	-6.79	122.38	131.20
2	B	603	LEU	N-CA-C	-6.76	101.56	110.07

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	538	GLN	OE1-CD-NE2	-6.75	115.85	122.60
2	B	662	LYS	O-C-N	-6.74	114.47	123.23
2	A	125	GLY	CA-C-N	6.74	127.32	120.38
2	A	125	GLY	C-N-CA	6.74	127.32	120.38
2	A	234	HIS	CB-CG-CD2	-6.72	122.46	131.20
2	B	856	GLN	CA-CB-CG	6.69	127.48	114.10
1	T	24	G	P-O3'-C3'	6.63	130.15	120.20
2	B	828	TRP	N-CA-C	-6.62	103.33	111.40
2	A	213	TRP	O-C-N	-6.61	115.31	123.04
2	A	283	LEU	N-CA-C	-6.52	98.27	108.90
2	B	601	VAL	CA-C-N	6.51	126.69	120.31
2	B	601	VAL	C-N-CA	6.51	126.69	120.31
2	B	773	HIS	CB-CG-CD2	-6.50	122.74	131.20
2	B	776	HIS	CB-CG-ND1	6.48	132.43	122.70
2	A	259	ALA	N-CA-C	-6.46	104.17	111.14
2	B	520	GLU	N-CA-CB	-6.43	99.60	110.41
2	A	337	LEU	CA-C-N	6.36	127.79	119.84
2	A	337	LEU	C-N-CA	6.36	127.79	119.84
2	B	617	ASN	OD1-CG-ND2	-6.36	116.24	122.60
2	B	866	ASP	CA-CB-CG	6.36	118.96	112.60
2	B	847	HIS	CB-CG-CD2	-6.35	122.94	131.20
2	B	846	THR	O-C-N	-6.30	115.43	122.10
1	T	19	G	C2'-C3'-O3'	6.29	118.93	109.50
2	B	635	ASP	CA-CB-CG	6.29	118.89	112.60
2	B	515	HIS	CB-CG-CD2	-6.26	123.06	131.20
2	B	776	HIS	CB-CG-CD2	-6.25	123.08	131.20
2	A	273	HIS	CB-CG-CD2	-6.18	123.16	131.20
2	B	767	ARG	O-C-N	-6.17	116.05	123.27
2	B	513	VAL	CB-CA-C	-6.16	103.83	112.14
2	B	903	ARG	CG-CD-NE	-6.13	98.52	112.00
2	B	775	PHE	CA-CB-CG	6.12	119.92	113.80
1	T	45	A	C2'-C3'-O3'	6.08	122.82	113.70
2	A	247	ARG	CB-CG-CD	-6.06	97.37	111.30
2	A	205	PHE	N-CA-C	-6.02	100.25	109.64
2	A	147	GLU	CA-C-N	5.99	125.87	119.28
2	A	147	GLU	C-N-CA	5.99	125.87	119.28
2	B	647	GLU	CA-C-N	5.99	125.86	119.28
2	B	647	GLU	C-N-CA	5.99	125.86	119.28
2	B	678	ASP	CA-CB-CG	5.98	118.58	112.60
2	B	796	GLN	OE1-CD-NE2	-5.97	116.63	122.60
2	B	884	THR	CB-CA-C	5.97	117.82	108.63
2	B	690	LEU	CA-C-O	-5.95	114.87	120.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	301	ASN	OD1-CG-ND2	-5.93	116.67	122.60
2	A	120	ILE	N-CA-C	-5.91	105.95	111.45
2	A	265	ASP	CA-C-N	5.91	128.97	122.77
2	A	265	ASP	C-N-CA	5.91	128.97	122.77
2	A	366	ASP	CA-CB-CG	5.91	118.51	112.60
1	T	8	U	N1-C1'-C2'	5.90	120.85	112.00
2	B	657	ARG	NE-CZ-NH2	-5.90	113.89	119.20
1	T	48	C	C4'-C3'-O3'	-5.90	100.55	109.40
2	B	859	ARG	N-CA-C	-5.89	104.27	112.45
1	T	60	U	C2'-C3'-O3'	5.85	118.27	109.50
2	A	347	HIS	CA-CB-CG	5.84	119.64	113.80
2	B	779	GLU	N-CA-C	5.83	118.90	109.40
1	T	44	U	C4'-C3'-O3'	-5.83	104.26	113.00
2	B	893	GLU	N-CA-C	5.79	118.06	111.11
2	B	822	ASP	CA-CB-CG	5.78	118.38	112.60
2	B	903	ARG	N-CA-CB	-5.77	101.01	110.41
2	B	704	HIS	CB-CG-CD2	-5.76	123.71	131.20
2	A	378	ASN	CA-CB-CG	5.76	118.36	112.60
2	A	276	HIS	CB-CG-CD2	-5.73	123.75	131.20
2	A	207	ALA	N-CA-C	5.73	119.08	111.75
2	A	349	CYS	CA-CB-SG	-5.73	101.23	114.40
2	B	878	ASN	CB-CG-ND2	5.73	124.99	116.40
1	T	13	G	N9-C1'-C2'	5.70	120.55	112.00
1	T	7	G	C1'-C2'-O2'	-5.69	103.27	111.80
1	T	16	U	C5'-C4'-C3'	-5.67	107.49	116.00
2	B	635	ASP	O-C-N	-5.67	116.32	122.79
2	B	918	GLU	CA-C-N	5.67	126.15	120.14
2	B	918	GLU	C-N-CA	5.67	126.15	120.14
2	B	848	SER	CB-CA-C	-5.66	101.43	110.14
2	A	35	ARG	N-CA-C	-5.65	98.77	110.80
2	A	383	ALA	O-C-N	-5.64	116.47	123.36
2	A	349	CYS	CA-C-O	-5.64	114.26	120.69
2	A	204	HIS	CB-CG-ND1	5.63	131.15	122.70
2	A	218	THR	N-CA-CB	-5.63	101.90	111.69
2	B	815	LEU	O-C-N	-5.62	116.77	123.06
2	A	361	ASN	CB-CG-ND2	5.60	124.80	116.40
1	T	51	G	P-O5'-C5'	-5.56	112.56	120.90
2	B	847	HIS	CB-CG-ND1	5.55	131.03	122.70
2	B	598	LEU	N-CA-CB	-5.54	100.91	110.32
2	B	801	ASN	CA-CB-CG	5.54	118.14	112.60
2	B	895	HIS	CA-CB-CG	5.53	119.33	113.80
1	T	19	G	C3'-C2'-O2'	-5.53	106.31	114.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	T	68	U	C5'-C4'-C3'	-5.52	107.72	116.00
2	A	234	HIS	CB-CG-ND1	5.51	130.97	122.70
2	B	753	PRO	CA-C-O	-5.51	115.06	121.34
1	T	47(Q)	U	O4'-C1'-N1	5.48	116.72	108.50
2	B	833	ILE	N-CA-C	-5.48	100.23	108.12
2	A	333	ILE	N-CA-C	-5.46	100.57	108.71
2	A	38	GLN	OE1-CD-NE2	-5.46	117.14	122.60
2	A	204	HIS	CB-CG-CD2	-5.46	124.10	131.20
2	A	212	VAL	N-CA-C	5.46	115.75	108.11
2	A	323	MET	CB-CA-C	-5.45	101.58	110.85
2	A	328	TRP	N-CA-C	-5.45	106.31	113.12
2	B	676	ALA	CA-C-O	-5.44	115.11	120.82
2	B	861	ASN	OD1-CG-ND2	-5.42	117.18	122.60
1	T	15	G	O4'-C1'-N9	5.41	116.62	108.50
2	B	619	GLU	CA-C-N	5.41	128.73	122.35
2	B	619	GLU	C-N-CA	5.41	128.73	122.35
2	A	380	THR	CA-CB-OG1	-5.39	101.51	109.60
1	T	7	G	C5'-C4'-C3'	5.39	123.29	115.20
2	B	643	ASN	OD1-CG-ND2	-5.39	117.21	122.60
2	A	265	ASP	CA-C-O	5.37	127.19	121.02
2	B	617	ASN	CB-CG-ND2	5.35	124.43	116.40
1	T	45	A	C4'-C3'-O3'	5.33	121.00	113.00
2	B	884	THR	N-CA-C	-5.32	102.79	110.40
2	B	704	HIS	CB-CG-ND1	5.31	130.67	122.70
2	A	395	HIS	CB-CG-CD2	-5.30	124.31	131.20
2	B	640	MET	CG-SD-CE	-5.30	89.24	100.90
2	B	855	TRP	CE2-CD2-CG	-5.28	100.86	107.20
2	B	545	GLN	OE1-CD-NE2	-5.28	117.32	122.60
2	A	312	PRO	CA-C-O	-5.28	115.59	121.23
2	A	356	GLN	CA-CB-CG	5.28	124.65	114.10
2	A	384	THR	N-CA-C	-5.27	102.86	110.40
2	B	561	ALA	CA-C-N	5.27	125.81	120.38
2	B	561	ALA	C-N-CA	5.27	125.81	120.38
2	A	296	GLN	OE1-CD-NE2	-5.26	117.34	122.60
2	B	886	ARG	O-C-N	-5.26	116.54	122.12
1	T	52	G	O4'-C1'-N9	5.26	116.38	108.50
2	B	620	ILE	CB-CG1-CD1	-5.26	102.76	113.80
2	B	658	SER	O-C-N	-5.25	116.78	123.24
2	A	347	HIS	CA-C-O	-5.25	114.08	120.54
2	A	395	HIS	CB-CG-ND1	5.25	130.57	122.70
2	A	289	GLU	N-CA-C	-5.24	105.65	111.36
1	T	47(C)	G	O4'-C1'-N9	5.24	116.35	108.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	597	LEU	N-CA-CB	-5.21	102.52	110.07
1	T	23	G	C4'-C3'-O3'	5.21	120.81	113.00
2	B	795	PHE	CA-CB-CG	5.19	118.99	113.80
2	B	789	GLU	CA-CB-CG	5.18	124.46	114.10
2	A	280	GLN	OE1-CD-NE2	-5.18	117.42	122.60
2	A	15	HIS	CB-CG-CD2	-5.17	124.48	131.20
2	B	508	ARG	N-CA-C	-5.16	105.57	111.14
2	B	843	TYR	N-CA-C	-5.15	102.07	110.20
2	B	844	ARG	CB-CG-CD	-5.14	99.47	111.30
1	T	16	U	C5'-C4'-O4'	-5.13	102.11	109.80
2	A	118	ARG	O-C-N	-5.11	117.24	123.27
2	B	606	TRP	CE2-CD2-CG	-5.09	101.09	107.20
1	T	19	G	O3'-P-O5'	-5.09	96.36	104.00
2	A	342	ARG	CA-C-O	-5.09	115.96	121.36
2	A	122	ARG	NE-CZ-NH2	-5.08	114.62	119.20
1	T	47(D)	G	N9-C1'-C2'	5.08	119.61	112.00
2	A	178	ASP	CA-CB-CG	5.08	117.67	112.60
2	B	635	ASP	N-CA-CB	-5.07	103.11	110.36
2	B	564	GLU	N-CA-C	-5.07	100.00	110.80
2	B	884	THR	N-CA-CB	-5.07	99.06	110.56
1	T	58	A	P-O5'-C5'	5.05	128.48	120.90
2	A	250	GLY	O-C-N	-5.05	119.72	123.61
2	A	233	LEU	O-C-N	-5.04	116.88	122.07
2	B	620	ILE	CB-CA-C	-5.04	105.75	111.55
1	T	19	G	O4'-C1'-N9	-5.04	100.64	108.20
1	T	16	U	P-O3'-C3'	5.03	127.75	120.20
2	A	273	HIS	N-CA-C	5.03	116.84	111.36
2	B	617	ASN	CA-CB-CG	5.03	117.62	112.60
2	A	270	MET	O-C-N	-5.02	116.55	122.32
2	A	2	VAL	CA-CB-CG2	-5.02	101.87	110.40
2	A	164	ASP	CA-CB-CG	5.02	117.62	112.60
2	A	146	TRP	CB-CG-CD2	-5.01	119.78	126.80
2	B	510	GLU	O-C-N	-5.00	116.65	121.05

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	T	1381	0	701	6	0
2	A	2982	0	2974	47	0
2	B	3373	0	3391	50	0
3	A	14	0	0	0	0
3	B	29	0	0	0	0
3	T	1	0	0	0	0
All	All	7780	0	7066	99	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 (99) 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)
2:A:21:LYS:HE3	2:A:105:PRO:HD3	1.51	0.92
2:A:36:GLU:HB3	2:A:90:LYS:HG2	1.74	0.70
2:B:550:GLU:HB3	2:B:576:LEU:HD21	1.75	0.67
2:A:382:LEU:HD21	2:A:387:ILE:HG21	1.80	0.64
2:B:558:VAL:N	2:B:559:PRO:HD2	2.13	0.64
2:B:693:TYR:HD1	2:B:720:LEU:HD22	1.64	0.62
2:A:1:MET:HE3	2:A:98:LEU:HD12	1.82	0.61
2:B:775:PHE:HB2	2:B:884:THR:O	2.01	0.61
2:B:617:ASN:ND2	2:B:819:ALA:H	1.99	0.61
2:A:16:ARG:O	2:A:19:ARG:HB3	2.03	0.59
2:B:857:ALA:HA	2:B:862:LEU:HD12	1.84	0.59
2:A:265:ASP:HB3	2:A:344:ARG:NH2	2.18	0.58
2:B:504:LEU:O	2:B:508:ARG:HG2	2.05	0.57
2:A:386:ARG:HG2	2:A:390:MET:HE2	1.87	0.56
2:A:117:ASN:ND2	2:A:319:ALA:H	2.03	0.56
2:A:7:LEU:HD11	2:A:27:LEU:HD11	1.88	0.56
2:A:171:ALA:HB2	2:B:674:ARG:HH21	1.69	0.56
2:A:15:HIS:CE1	2:A:27:LEU:HB3	2.42	0.55
1:T:20(B):G:O6	1:T:47(Q):U:H2'	2.07	0.55
2:A:366:ASP:OD1	2:A:370:ARG:HB2	2.06	0.55
1:T:56:C:H1'	2:B:558:VAL:HG21	1.90	0.54
2:B:640:MET:HE1	2:B:769:LEU:HD11	1.90	0.53
2:A:103:LEU:HD21	2:A:353:LEU:HD12	1.91	0.53
2:A:178:ASP:HB3	2:A:182:ARG:NH1	2.24	0.52
2:B:827:LYS:HD2	2:B:850:SER:HB3	1.92	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:406:GLN:HA	2:A:409:ILE:HD12	1.91	0.52
2:B:507:LEU:HD11	2:B:527:LEU:HD11	1.91	0.51
2:B:523:VAL:HG21	2:B:602:PRO:HG3	1.92	0.51
2:B:510:GLU:HB3	2:B:513:VAL:HG23	1.93	0.51
2:B:606:TRP:CD1	2:B:609:ALA:HB2	2.46	0.50
2:B:677:MET:HE2	2:B:687:PRO:HB3	1.92	0.50
2:A:37:VAL:HG21	2:A:94:LEU:HD22	1.93	0.50
2:A:218:THR:HG22	2:A:220:LEU:H	1.75	0.50
2:A:18:ILE:HG23	2:A:23:VAL:HB	1.94	0.50
2:A:30:LEU:HD12	2:A:97:LEU:HB3	1.94	0.49
2:B:502:VAL:HG21	2:B:514:PHE:HE1	1.77	0.49
2:A:159:TYR:HD2	2:A:161:LEU:HD13	1.78	0.49
2:A:166:ALA:HB1	2:B:689:THR:HG23	1.95	0.49
2:A:218:THR:CG2	2:A:220:LEU:H	2.26	0.49
2:B:502:VAL:HG21	2:B:514:PHE:CE1	2.48	0.49
2:B:523:VAL:HG21	2:B:602:PRO:CG	2.43	0.49
2:A:347:HIS:HE1	2:A:381:ALA:O	1.96	0.49
2:B:603:LEU:HD21	2:B:853:LEU:HD12	1.95	0.48
2:A:241:TYR:HB2	2:A:365:ARG:O	2.12	0.48
2:B:853:LEU:O	2:B:875:TYR:HA	2.13	0.48
1:T:46:G:P	2:B:865:ARG:HH22	2.37	0.48
2:B:690:LEU:HD11	2:B:730:LEU:HD13	1.96	0.48
2:A:366:ASP:HB3	2:A:370:ARG:O	2.14	0.47
2:B:634:LEU:HB2	2:B:639:LEU:HD13	1.95	0.47
2:A:35:ARG:O	2:A:38:GLN:HG2	2.15	0.47
2:A:106:TRP:CE2	2:A:329:ARG:HD3	2.50	0.47
2:A:346:THR:CG2	2:A:390:MET:HE3	2.45	0.47
2:B:640:MET:CE	2:B:665:LEU:HD21	2.44	0.47
2:B:777:LYS:HE2	2:B:779:GLU:OE2	2.15	0.47
1:T:61:C:H2'	1:T:62:C:H6	1.79	0.47
2:B:558:VAL:N	2:B:559:PRO:CD	2.78	0.46
2:A:197:LYS:HA	2:A:200:LEU:HD12	1.97	0.46
1:T:20(B):G:H4'	1:T:21:A:O4'	2.16	0.46
2:A:33:LEU:O	2:A:37:VAL:HG23	2.17	0.45
2:A:126:PRO:HB3	2:A:336:TYR:CE2	2.52	0.45
2:A:311:LEU:HD13	2:A:335:VAL:HG11	1.99	0.45
2:A:104:PRO:HA	2:A:105:PRO:HD2	1.89	0.45
2:B:809:LEU:HG	2:B:891:LEU:HD21	1.99	0.44
2:A:346:THR:OG1	2:A:347:HIS:HD2	2.00	0.44
2:A:401:ARG:NH1	2:A:416:VAL:HG11	2.32	0.44
2:B:780:GLN:HE22	2:B:801:ASN:HB2	1.82	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:544:LEU:HA	2:B:583:LEU:HD23	1.98	0.44
1:T:61:C:H2'	1:T:62:C:C6	2.52	0.44
2:A:6:ARG:HA	2:A:9:GLN:HB3	1.99	0.44
2:B:639:LEU:HD21	2:B:896:GLN:HB3	2.00	0.43
2:B:647:GLU:HB3	2:B:660:ALA:HB3	2.00	0.43
2:A:146:TRP:O	2:A:148:PRO:HD3	2.18	0.43
2:B:505:LYS:HD2	2:B:505:LYS:HA	1.82	0.43
2:B:758:GLU:HG3	2:B:761:SER:OG	2.19	0.43
2:B:504:LEU:HD13	2:B:598:LEU:HD11	2.01	0.43
2:A:265:ASP:HB3	2:A:344:ARG:HH21	1.84	0.42
2:B:699:PHE:CE2	2:B:721:TYR:HB2	2.54	0.42
2:A:132:PRO:HA	2:A:133:PRO:HD2	1.85	0.42
2:B:617:ASN:HD22	2:B:819:ALA:H	1.66	0.42
2:B:640:MET:HE2	2:B:665:LEU:CD2	2.50	0.42
2:A:357:ALA:HA	2:A:362:LEU:HD12	2.01	0.42
2:A:2:VAL:HG21	2:A:14:PHE:CE1	2.54	0.42
2:B:631:PHE:HD2	2:B:632:PRO:O	2.02	0.42
2:B:601:VAL:HA	2:B:602:PRO:HD3	1.74	0.42
2:A:193:TYR:HA	2:A:221:TYR:O	2.20	0.41
2:B:693:TYR:CD1	2:B:720:LEU:HD22	2.49	0.41
2:B:562:PRO:O	2:B:564:GLU:N	2.52	0.41
2:B:677:MET:HA	2:B:677:MET:HE3	2.03	0.41
2:A:310:GLU:O	2:A:395:HIS:HE1	2.03	0.41
2:B:543:ARG:HA	2:B:543:ARG:HD3	1.93	0.40
2:B:574:LYS:HE3	2:B:574:LYS:HB3	1.91	0.40
2:A:143:ASN:OD1	2:A:419:PRO:HG3	2.21	0.40
2:B:559:PRO:O	2:B:560:LYS:HB2	2.22	0.40
2:A:37:VAL:HG22	2:A:90:LYS:HB3	2.03	0.40
2:A:159:TYR:CD2	2:A:161:LEU:HD13	2.56	0.40
2:B:504:LEU:HD12	2:B:507:LEU:HD23	2.02	0.40
2:B:534:ASP:O	2:B:538:GLN:HG2	2.22	0.40
2:B:741:TYR:HB2	2:B:865:ARG:O	2.22	0.40
2:A:15:HIS:CD2	2:A:27:LEU:HD23	2.57	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	
2	A	368/421 (87%)	345 (94%)	20 (5%)	3 (1%)	16	44
2	B	419/421 (100%)	405 (97%)	10 (2%)	4 (1%)	12	39
All	All	787/842 (94%)	750 (95%)	30 (4%)	7 (1%)	14	41

All (7) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	B	765	ASP
2	A	35	ARG
2	B	564	GLU
2	A	126	PRO
2	A	338	PRO
2	B	838	PRO
2	B	563	PRO

5.3.2 Protein sidechains [i](#)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	A	307/347 (88%)	269 (88%)	38 (12%)	4	15
2	B	347/347 (100%)	318 (92%)	29 (8%)	10	31
All	All	654/694 (94%)	587 (90%)	67 (10%)	7	23

All (67) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	A	2	VAL
2	A	4	LEU
2	A	5	LYS
2	A	9	GLN
2	A	12	GLU
2	A	35	ARG
2	A	88	ARG
2	A	89	GLU
2	A	91	GLU
2	A	98	LEU
2	A	115	GLU
2	A	130	SER
2	A	141	GLU
2	A	146	TRP
2	A	151	SER
2	A	156	SER
2	A	161	LEU
2	A	167	LEU
2	A	182	ARG
2	A	195	ARG
2	A	217	GLU
2	A	218	THR
2	A	230	LEU
2	A	253	PRO
2	A	261	SER
2	A	262	PHE
2	A	285	GLU
2	A	289	GLU
2	A	298	LEU
2	A	299	LEU
2	A	306	LEU
2	A	308	LEU
2	A	309	LEU
2	A	329	ARG
2	A	338	PRO
2	A	366	ASP
2	A	390	MET
2	A	408	LEU
2	B	502	VAL
2	B	505	LYS
2	B	512	GLU
2	B	530	LEU
2	B	531	LEU

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Mol	Chain	Res	Type
2	B	539	GLU
2	B	576	LEU
2	B	583	LEU
2	B	597	LEU
2	B	630	SER
2	B	635	ASP
2	B	637	VAL
2	B	656	SER
2	B	677	MET
2	B	711	GLN
2	B	717	GLU
2	B	730	LEU
2	B	746	LEU
2	B	761	SER
2	B	783	LEU
2	B	793	ARG
2	B	799	LEU
2	B	809	LEU
2	B	815	LEU
2	B	838	PRO
2	B	884	THR
2	B	887	ILE
2	B	904	VAL
2	B	906	GLN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (20) such sidechains are listed below:

Mol	Chain	Res	Type
2	A	9	GLN
2	A	15	HIS
2	A	117	ASN
2	A	152	GLN
2	A	276	HIS
2	A	280	GLN
2	A	301	ASN
2	A	347	HIS
2	A	395	HIS
2	B	538	GLN
2	B	617	ASN
2	B	636	HIS
2	B	643	ASN
2	B	731	ASN

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Mol	Chain	Res	Type
2	B	776	HIS
2	B	780	GLN
2	B	801	ASN
2	B	856	GLN
2	B	861	ASN
2	B	894	ASN

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	T	61/94 (64%)	11 (18%)	5 (8%)

All (11) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	T	7	G
1	T	8	U
1	T	9	G
1	T	16	U
1	T	18	G
1	T	20(A)	H2U
1	T	20(B)	G
1	T	25	G
1	T	45	A
1	T	46	G
1	T	61	C

All (5) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
1	T	7	G
1	T	16	U
1	T	20(A)	H2U
1	T	24	G
1	T	45	A

5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

3 non-standard protein/DNA/RNA residues are modelled in this entry.

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$
1	5MU	T	54	1	19,22,23	0.71	0	27,32,35	1.62	5 (18%)
1	H2U	T	20(A)	1	18,21,22	1.07	2 (11%)	19,30,33	1.17	2 (10%)
1	PSU	T	55	1	18,21,22	0.79	0	21,30,33	2.29	7 (33%)

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
1	5MU	T	54	1	-	0/7/25/26	0/2/2/2
1	H2U	T	20(A)	1	-	0/7/38/39	0/2/2/2
1	PSU	T	55	1	-	1/7/25/26	0/2/2/2

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	T	20(A)	H2U	C5-C4	-2.91	1.43	1.50
1	T	20(A)	H2U	C2-N1	2.37	1.38	1.35

All (14) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	T	55	PSU	C6-C5-C4	7.51	123.24	118.17
1	T	54	5MU	C5M-C5-C6	-4.03	117.40	122.85
1	T	54	5MU	C6-C5-C4	3.48	120.89	118.02
1	T	55	PSU	N1-C2-N3	2.91	118.24	115.17
1	T	55	PSU	C5'-C4'-C3'	-2.77	105.25	115.21
1	T	54	5MU	C5M-C5-C4	2.75	121.72	118.78
1	T	55	PSU	O2-C2-N1	-2.74	119.97	122.79
1	T	20(A)	H2U	C5-C4-N3	-2.69	113.83	116.69
1	T	54	5MU	O2-C2-N1	2.58	126.16	122.80
1	T	55	PSU	O3'-C3'-C4'	2.50	118.28	111.08
1	T	20(A)	H2U	N3-C2-N1	-2.43	114.21	116.65
1	T	55	PSU	C5-C4-N3	-2.25	111.61	116.55

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	T	54	5MU	O4-C4-C5	2.17	127.40	124.92
1	T	55	PSU	O4-C4-C5	2.03	129.04	124.01

There are no chirality outliers.

All (1) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	T	55	PSU	O4'-C4'-C5'-O5'

There are no ring outliers.

No monomer is involved in short contacts.

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

There are no ligands in this entry.

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.