



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 7, 2026 – 12:27 AM UTC

PDB ID : 2AAD / pdb_00002aad
Title : THE ROLE OF HISTIDINE-40 IN RIBONUCLEASE T1 CATALYSIS:
THREE-DIMENSIONAL STRUCTURES OF THE PARTIALLY ACTIVE
HIS40LYS MUTANT
Authors : Zegers, I.; Verhelst, P.; Choe, C.W.; Steyaert, J.; Heinemann, U.; Wyns, L.;
Saenger, W.
Deposited on : 1992-09-15
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)
Xtrriage (Phenix)	:	NOT EXECUTED
EDS	:	NOT EXECUTED
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

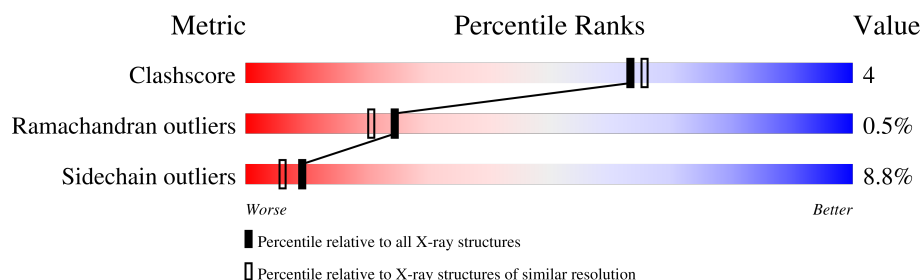
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.00 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	104	 47% 44% 7% •
1	B	104	 40% 47% 11% •

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 1849 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 RIBONUCLEASE T1 ISOZYME.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	104	Total	C	N	O	S	0	0	0
			780	480	126	170	4			
1	B	104	Total	C	N	O	S	0	0	0
			780	480	126	170	4			

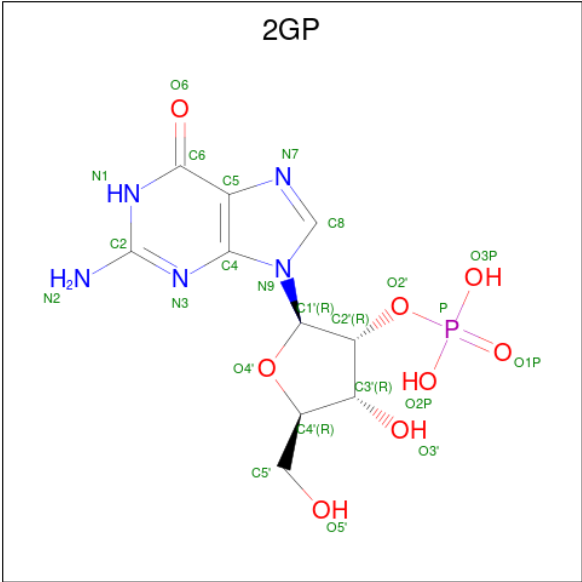
There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	25	LYS	GLN	conflict	UNP P00651
A	40	LYS	HIS	conflict	UNP P00651
B	25	LYS	GLN	conflict	UNP P00651
B	40	LYS	HIS	conflict	UNP P00651

- 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 GUANOSINE-2'-MONOPHOSPHATE (CCD ID: 2GP) (formula: C₁₀H₁₄N₅O₈P).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	A	1	Total	C	N	O	P	0	0
			24	10	5	8	1		
3	B	1	Total	C	N	O	P	0	0
			24	10	5	8	1		

- Molecule 4 is water.

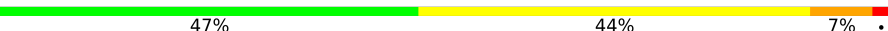
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	117	Total	O	0	0
			117	117		
4	B	122	Total	O	0	0
			122	122		

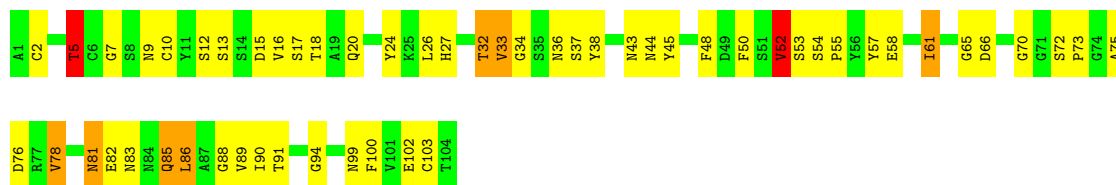
3 Residue-property plots

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.

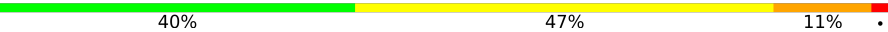
Note EDS was not executed.

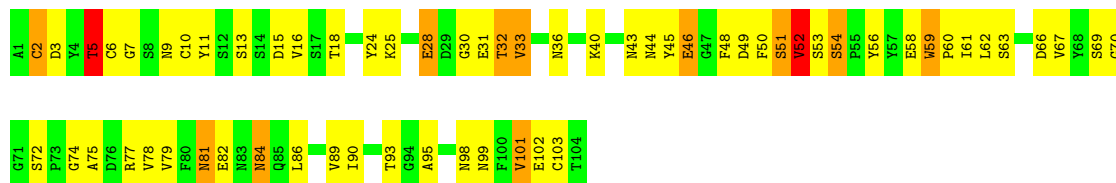
• Molecule 1: RIBONUCLEASE T1 ISOZYME

Chain A: 



• Molecule 1: RIBONUCLEASE T1 ISOZYME

Chain B: 



4 Data and refinement statistics

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

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	49.20 Å 48.19 Å 40.16 Å 90.00° 90.26° 90.00°	Depositor
Resolution (Å)	10.00 – 2.00	Depositor
% Data completeness (in resolution range)	(Not available) (10.00-2.00)	Depositor
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	PROLSQ	Depositor
R, R_{free}	0.160 , (Not available)	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	1849	wwPDB-VP
Average B, all atoms (Å ²)	19.0	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: 2GP, 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	1.69	9/800 (1.1%)	2.78	86/1088 (7.9%)
1	B	1.71	9/800 (1.1%)	2.95	89/1088 (8.2%)
All	All	1.70	18/1600 (1.1%)	2.87	175/2176 (8.0%)

All (18) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	9	ASN	N-CA	7.78	1.55	1.46
1	B	32	THR	N-CA	6.60	1.54	1.45
1	B	79	VAL	N-CA	5.89	1.53	1.46
1	A	58	GLU	N-CA	5.86	1.53	1.46
1	B	59	TRP	CA-C	5.64	1.58	1.52
1	B	7	GLY	CA-C	5.63	1.59	1.51
1	B	70	GLY	N-CA	5.57	1.50	1.45
1	A	61	ILE	C-O	5.54	1.30	1.24
1	B	90	ILE	N-CA	5.54	1.52	1.46
1	B	36	ASN	C-N	-5.48	1.27	1.33
1	A	7	GLY	N-CA	5.43	1.53	1.45
1	A	78	VAL	CA-C	5.32	1.59	1.52
1	A	33	VAL	C-O	-5.25	1.18	1.24
1	B	16	VAL	CA-C	5.16	1.59	1.52
1	A	91	THR	CB-OG1	5.10	1.51	1.43
1	A	90	ILE	C-N	-5.09	1.27	1.33
1	A	18	THR	CA-CB	5.07	1.61	1.53
1	A	32	THR	N-CA	5.07	1.52	1.45

All (175) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	36	ASN	CA-CB-CG	15.84	128.44	112.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	70	GLY	N-CA-C	-12.21	99.58	112.04
1	B	52	VAL	CB-CA-C	11.50	124.25	111.59
1	A	20	GLN	CA-C-O	-11.46	108.64	120.90
1	B	53	SER	CA-C-N	11.17	138.74	120.86
1	B	53	SER	C-N-CA	11.17	138.74	120.86
1	B	99	ASN	OD1-CG-ND2	-10.43	112.17	122.60
1	A	32	THR	N-CA-CB	-10.28	93.67	111.55
1	B	84	ASN	CB-CG-ND2	10.23	131.74	116.40
1	A	16	VAL	O-C-N	10.22	131.92	121.91
1	B	61	ILE	CB-CA-C	10.19	126.02	110.83
1	A	81	ASN	OD1-CG-ND2	-10.02	112.58	122.60
1	A	36	ASN	OD1-CG-ND2	9.87	132.47	122.60
1	A	15	ASP	CA-CB-CG	9.74	122.34	112.60
1	A	36	ASN	CA-CB-CG	9.65	122.25	112.60
1	B	99	ASN	CB-CG-ND2	9.55	130.72	116.40
1	B	51	SER	CA-C-N	9.52	134.56	120.95
1	B	51	SER	C-N-CA	9.52	134.56	120.95
1	B	98	ASN	OD1-CG-ND2	9.50	132.10	122.60
1	A	16	VAL	CA-C-O	-9.45	111.16	121.17
1	A	43	ASN	N-CA-C	9.41	124.56	112.89
1	B	81	ASN	CA-CB-CG	9.28	121.88	112.60
1	B	25	LYS	CA-C-O	-9.27	110.73	120.55
1	B	15	ASP	O-C-N	8.94	132.34	122.15
1	A	83	ASN	CA-CB-CG	8.88	121.48	112.60
1	B	77	ARG	NE-CZ-NH1	8.86	130.36	121.50
1	A	66	ASP	CA-CB-CG	8.75	121.35	112.60
1	B	52	VAL	N-CA-CB	-8.74	96.87	111.38
1	A	52	VAL	N-CA-CB	-8.70	96.43	112.43
1	B	43	ASN	N-CA-C	8.43	121.60	111.82
1	B	50	PHE	CA-CB-CG	8.40	122.20	113.80
1	B	2	CYS	CA-C-O	-8.35	111.53	121.05
1	A	27	HIS	O-C-N	8.24	130.66	122.09
1	B	10	CYS	CA-C-O	-8.08	111.57	120.38
1	B	70	GLY	O-C-N	-8.04	113.64	123.21
1	A	61	ILE	N-CA-C	-7.85	97.13	108.11
1	B	32	THR	N-CA-CB	-7.82	97.94	111.55
1	B	58	GLU	O-C-N	-7.77	113.35	123.21
1	B	58	GLU	CA-C-O	7.76	128.93	120.71
1	A	102	GLU	CB-CG-CD	7.73	125.74	112.60
1	A	27	HIS	CE1-NE2-CD2	7.64	116.64	109.00
1	A	34	GLY	O-C-N	7.61	130.59	122.60
1	B	98	ASN	CB-CG-OD1	-7.61	105.58	120.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	103	CYS	N-CA-C	-7.51	97.82	109.76
1	B	3	ASP	N-CA-C	-7.36	102.95	112.23
1	B	15	ASP	CA-C-O	-7.35	112.63	120.42
1	B	44	ASN	OD1-CG-ND2	-7.29	115.31	122.60
1	A	58	GLU	CB-CG-CD	7.27	124.95	112.60
1	A	72	SER	O-C-N	7.22	127.11	121.47
1	A	38	TYR	CA-C-O	-7.16	113.53	120.19
1	A	32	THR	CA-CB-CG2	7.15	122.66	110.50
1	A	52	VAL	CB-CA-C	7.15	121.41	111.19
1	B	77	ARG	NH1-CZ-NH2	-7.11	110.06	119.30
1	B	51	SER	CA-C-O	7.05	128.02	120.55
1	B	75	ALA	N-CA-CB	-7.01	100.02	110.61
1	A	33	VAL	CA-CB-CG1	6.99	122.28	110.40
1	A	85	GLN	CG-CD-NE2	6.93	126.80	116.40
1	A	55	PRO	CA-C-N	6.91	133.31	122.94
1	A	55	PRO	C-N-CA	6.91	133.31	122.94
1	B	66	ASP	N-CA-C	-6.91	100.29	110.52
1	B	102	GLU	CB-CG-CD	6.91	124.35	112.60
1	A	9	ASN	CA-C-N	6.87	131.90	122.77
1	A	9	ASN	C-N-CA	6.87	131.90	122.77
1	A	89	VAL	CA-C-O	-6.86	113.25	120.39
1	B	66	ASP	CA-CB-CG	6.86	119.46	112.60
1	A	24	TYR	O-C-N	6.85	129.96	122.15
1	B	48	PHE	CA-CB-CG	6.78	120.58	113.80
1	A	82	GLU	CA-CB-CG	6.76	127.62	114.10
1	A	16	VAL	CB-CA-C	6.73	120.59	111.97
1	A	75	ALA	O-C-N	6.68	131.17	122.42
1	B	61	ILE	N-CA-C	-6.68	98.81	108.17
1	B	46	GLU	CB-CG-CD	6.66	123.91	112.60
1	A	72	SER	CA-CB-OG	-6.65	97.80	111.10
1	A	86	LEU	CA-C-O	-6.65	113.11	120.69
1	B	63	SER	CA-C-O	-6.64	112.60	120.10
1	B	72	SER	O-C-N	6.61	127.89	121.28
1	B	28	GLU	CB-CG-CD	6.60	123.82	112.60
1	A	10	CYS	CA-C-O	-6.59	113.30	120.36
1	A	15	ASP	O-C-N	6.56	129.18	122.09
1	B	84	ASN	CB-CG-OD1	-6.55	107.70	120.80
1	A	103	CYS	N-CA-C	-6.54	100.81	110.48
1	A	45	TYR	CA-C-N	6.50	129.65	120.28
1	A	45	TYR	C-N-CA	6.50	129.65	120.28
1	A	66	ASP	O-C-N	6.46	130.15	122.79
1	B	13	SER	CA-C-O	6.45	127.38	120.55

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	61	ILE	N-CA-CB	6.44	120.30	111.41
1	B	24	TYR	CA-C-O	-6.42	113.61	120.42
1	B	93	THR	CA-C-O	-6.42	113.32	120.70
1	A	88	GLY	CA-C-O	-6.36	115.39	121.87
1	B	32	THR	CB-CA-C	6.33	122.78	109.79
1	B	6	CYS	CA-C-O	-6.33	113.32	121.11
1	A	48	PHE	CA-CB-CG	6.31	120.11	113.80
1	A	85	GLN	OE1-CD-NE2	-6.30	116.30	122.60
1	B	11	TYR	CA-C-O	-6.30	113.41	120.66
1	A	26	LEU	O-C-N	6.28	129.31	122.15
1	A	13	SER	CA-C-O	-6.20	113.98	120.55
1	B	11	TYR	O-C-N	6.19	130.82	123.27
1	A	90	ILE	CA-C-O	-6.17	115.38	121.67
1	A	52	VAL	CA-CB-CG1	6.16	120.88	110.40
1	B	33	VAL	CA-C-O	-6.11	114.89	121.19
1	A	27	HIS	CA-C-O	-6.11	114.37	120.90
1	A	100	PHE	CA-CB-CG	6.10	119.90	113.80
1	B	84	ASN	O-C-N	-6.08	114.44	122.47
1	A	50	PHE	CA-CB-CG	6.05	119.85	113.80
1	A	82	GLU	N-CA-C	6.04	118.66	111.71
1	A	53	SER	CA-C-N	6.04	130.69	121.03
1	A	53	SER	C-N-CA	6.04	130.69	121.03
1	B	102	GLU	N-CA-CB	6.02	120.23	110.41
1	B	5	THR	OG1-CB-CG2	-6.02	97.27	109.30
1	B	6	CYS	O-C-N	6.01	130.06	122.84
1	A	65	GLY	N-CA-C	-5.99	107.14	114.92
1	B	84	ASN	CA-CB-CG	-5.95	106.65	112.60
1	A	78	VAL	N-CA-C	-5.91	99.92	108.36
1	B	89	VAL	CA-C-N	-5.88	114.45	122.92
1	B	89	VAL	C-N-CA	-5.88	114.45	122.92
1	A	13	SER	N-CA-C	-5.88	104.87	111.28
1	A	99	ASN	CA-CB-CG	-5.85	106.75	112.60
1	B	9	ASN	CA-C-N	5.84	131.06	123.00
1	B	9	ASN	C-N-CA	5.84	131.06	123.00
1	A	17	SER	CB-CA-C	-5.84	101.10	110.79
1	B	74	GLY	N-CA-C	-5.82	101.67	112.37
1	B	67	VAL	CB-CA-C	5.79	119.15	111.21
1	A	94	GLY	O-C-N	5.78	129.63	122.41
1	B	33	VAL	CA-CB-CG1	5.75	120.17	110.40
1	A	70	GLY	CA-C-O	5.73	130.54	120.57
1	A	57	TYR	O-C-N	5.72	130.25	123.27
1	A	12	SER	O-C-N	-5.71	116.21	122.84

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	15	ASP	CA-CB-CG	5.71	118.31	112.60
1	B	30	GLY	CA-C-O	5.65	126.81	120.03
1	A	12	SER	N-CA-C	-5.65	102.10	110.46
1	B	18	THR	CA-CB-OG1	-5.62	101.17	109.60
1	B	69	SER	CA-C-O	5.62	126.05	120.32
1	A	73	PRO	CA-C-O	5.60	125.95	118.90
1	B	54	SER	N-CA-CB	-5.59	101.92	110.03
1	B	49	ASP	N-CA-CB	5.58	116.60	110.35
1	A	54	SER	CA-C-O	-5.58	114.74	120.87
1	A	76	ASP	O-C-N	5.58	129.63	123.16
1	B	61	ILE	CA-CB-CG2	5.57	119.96	110.50
1	A	44	ASN	CB-CA-C	5.54	119.17	111.63
1	B	50	PHE	CA-C-N	5.50	127.66	120.28
1	B	50	PHE	C-N-CA	5.50	127.66	120.28
1	A	13	SER	O-C-N	5.47	127.92	122.12
1	B	48	PHE	CA-C-O	-5.42	115.23	121.19
1	B	78	VAL	N-CA-C	-5.39	100.62	108.97
1	A	90	ILE	N-CA-CB	-5.39	104.98	112.52
1	A	5	THR	CB-CA-C	5.36	118.72	110.14
1	B	89	VAL	CA-C-O	-5.36	114.76	120.39
1	A	27	HIS	ND1-CE1-NE2	-5.35	103.05	108.40
1	B	82	GLU	N-CA-CB	-5.35	101.99	110.28
1	A	78	VAL	O-C-N	5.33	128.95	123.03
1	B	45	TYR	N-CA-CB	5.33	118.54	110.28
1	A	83	ASN	OD1-CG-ND2	5.32	127.92	122.60
1	A	2	CYS	CA-C-O	-5.29	115.10	120.71
1	A	36	ASN	CB-CG-OD1	-5.27	110.26	120.80
1	B	56	TYR	CA-C-O	-5.25	115.23	121.16
1	A	58	GLU	CA-C-O	5.24	126.36	120.70
1	B	82	GLU	CB-CG-CD	5.24	121.50	112.60
1	B	16	VAL	CA-CB-CG1	5.22	119.28	110.40
1	A	72	SER	CA-C-O	-5.21	115.06	119.59
1	B	99	ASN	N-CA-C	-5.21	104.01	110.41
1	A	102	GLU	CB-CA-C	-5.16	100.69	109.51
1	B	31	GLU	OE1-CD-OE2	5.15	135.26	122.90
1	A	81	ASN	CA-C-O	5.15	128.31	121.46
1	B	50	PHE	CA-C-O	5.13	126.91	121.16
1	A	12	SER	CA-C-O	5.12	128.40	121.89
1	A	45	TYR	CB-CG-CD1	5.12	128.47	120.80
1	B	5	THR	N-CA-CB	5.10	118.78	110.77
1	A	83	ASN	CA-C-O	5.10	125.32	119.35
1	A	54	SER	N-CA-CB	-5.10	102.71	110.05

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	66	ASP	N-CA-CB	5.08	117.62	110.36
1	B	24	TYR	N-CA-CB	5.08	117.68	110.16
1	B	60	PRO	CB-CA-C	-5.07	104.47	111.21
1	B	32	THR	CA-CB-CG2	5.07	119.11	110.50
1	B	101	VAL	CA-C-O	-5.04	116.38	121.67
1	B	7	GLY	O-C-N	5.03	129.24	122.70

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	780	0	684	4	0
1	B	780	0	684	6	0
2	A	1	0	0	0	0
2	B	1	0	0	0	0
3	A	24	0	10	1	0
3	B	24	0	12	1	0
4	A	117	0	0	1	0
4	B	122	0	0	3	0
All	All	1849	0	1390	12	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 4.

All (12) 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:81:ASN:HD21	1:A:85:GLN:HE21	1.42	0.68
1:B:2:CYS:HB2	1:B:5:THR:HG22	1.85	0.58
1:B:95:ALA:HB2	1:B:101:VAL:HG13	1.89	0.54
3:B:105:2GP:H3'	3:B:105:2GP:N3	2.26	0.50
1:B:62:LEU:HG	4:B:125:HOH:O	2.11	0.49
1:B:52:VAL:HG13	1:B:81:ASN:ND2	2.29	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:46:GLU:HB2	4:B:202:HOH:O	2.14	0.47
1:A:52:VAL:HG21	1:A:85:GLN:HB3	1.95	0.47
1:A:5:THR:HG22	4:A:113:HOH:O	2.15	0.46
1:B:59:TRP:HB3	4:B:124:HOH:O	2.18	0.44
1:A:61:ILE:HB	1:A:78:VAL:HG23	2.01	0.43
3:A:105:2GP:N3	3:A:105:2GP:H3'	2.37	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	102/104 (98%)	99 (97%)	2 (2%)	1 (1%)	12	8
1	B	102/104 (98%)	97 (95%)	5 (5%)	0	100	100
All	All	204/208 (98%)	196 (96%)	7 (3%)	1 (0%)	24	21

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	37	SER

5.3.2 Protein sidechains [i](#)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	85/85 (100%)	80 (94%)	5 (6%)	18	14
1	B	85/85 (100%)	75 (88%)	10 (12%)	5	3
All	All	170/170 (100%)	155 (91%)	15 (9%)	9	6

All (15) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	5	THR
1	A	32	THR
1	A	33	VAL
1	A	52	VAL
1	A	86	LEU
1	B	5	THR
1	B	28	GLU
1	B	32	THR
1	B	33	VAL
1	B	40	LYS
1	B	51	SER
1	B	52	VAL
1	B	54	SER
1	B	84	ASN
1	B	86	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (11) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	9	ASN
1	A	20	GLN
1	A	83	ASN
1	A	84	ASN
1	A	85	GLN
1	B	9	ASN
1	B	27	HIS
1	B	43	ASN
1	B	83	ASN
1	B	84	ASN
1	B	85	GLN

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 oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

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

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# $ Z > 2$	Counts	RMSZ	# $ Z > 2$
3	2GP	B	105	-	26,26,26	1.82	8 (30%)	40,40,40	2.39	16 (40%)
3	2GP	A	105	-	26,26,26	1.83	4 (15%)	40,40,40	2.93	16 (40%)

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	2GP	B	105	-	-	2/11/27/27	0/3/3/3
3	2GP	A	105	-	-	1/11/27/27	0/3/3/3

All (12) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	105	2GP	C2-N2	-5.11	1.22	1.34
3	A	105	2GP	C4-N3	4.23	1.43	1.34
3	B	105	2GP	C2-N2	-3.68	1.25	1.34
3	A	105	2GP	C6-N1	3.62	1.45	1.38
3	B	105	2GP	C6-N1	3.61	1.45	1.38
3	B	105	2GP	C2-N1	3.14	1.45	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	105	2GP	C4-N3	3.10	1.41	1.34
3	B	105	2GP	O6-C6	2.48	1.28	1.23
3	B	105	2GP	P-O2P	-2.46	1.45	1.54
3	B	105	2GP	C5-N7	-2.42	1.34	1.39
3	B	105	2GP	C3'-C2'	-2.12	1.48	1.53
3	A	105	2GP	C1'-N9	-2.08	1.41	1.47

All (32) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	105	2GP	C2-N3-C4	7.49	125.19	112.30
3	A	105	2GP	O6-C6-N1	-7.30	106.39	120.11
3	A	105	2GP	C6-C5-N7	6.72	142.51	130.29
3	A	105	2GP	C6-C5-C4	-5.92	109.93	118.83
3	B	105	2GP	C6-C5-C4	-5.91	109.94	118.83
3	A	105	2GP	N1-C2-N3	-4.74	114.64	123.32
3	B	105	2GP	C2-N3-C4	4.73	120.45	112.30
3	B	105	2GP	C5-C6-N1	4.38	124.41	113.25
3	A	105	2GP	C5-C6-N1	4.28	124.15	113.25
3	B	105	2GP	O6-C6-C5	-4.16	115.54	126.53
3	B	105	2GP	N2-C2-N3	3.83	127.15	119.67
3	B	105	2GP	C4-C5-N7	3.71	116.55	110.67
3	A	105	2GP	O3P-P-O2P	3.62	121.37	107.80
3	B	105	2GP	N1-C2-N3	-3.52	116.88	123.32
3	B	105	2GP	C2-N1-C6	-3.35	119.04	125.11
3	B	105	2GP	O3'-C3'-C4'	-3.28	101.66	111.08
3	A	105	2GP	C2'-C1'-N9	3.23	120.38	114.24
3	A	105	2GP	C4'-O4'-C1'	3.14	116.40	109.47
3	B	105	2GP	C8-N7-C5	-3.09	98.76	104.26
3	B	105	2GP	O2'-C2'-C3'	2.84	121.87	111.68
3	A	105	2GP	C5'-C4'-C3'	2.74	121.56	115.10
3	A	105	2GP	C5-C4-N3	-2.64	124.19	128.39
3	A	105	2GP	N2-C2-N1	2.62	122.29	116.76
3	B	105	2GP	O4'-C4'-C5'	2.56	114.63	109.22
3	A	105	2GP	C8-N7-C5	2.54	108.79	104.26
3	B	105	2GP	O5'-C5'-C4'	-2.54	102.68	111.33
3	A	105	2GP	O2'-C2'-C3'	2.38	120.21	111.68
3	B	105	2GP	C5'-C4'-C3'	-2.31	109.65	115.10
3	A	105	2GP	O4'-C4'-C5'	-2.17	104.63	109.22
3	B	105	2GP	O4'-C4'-C3'	-2.16	100.86	105.15
3	A	105	2GP	O3P-P-O2'	2.05	113.84	105.85
3	B	105	2GP	C1'-N9-C4	2.04	132.53	126.49

There are no chirality outliers.

All (3) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	B	105	2GP	O4'-C4'-C5'-O5'
3	A	105	2GP	C3'-C4'-C5'-O5'
3	B	105	2GP	C3'-C2'-O2'-P

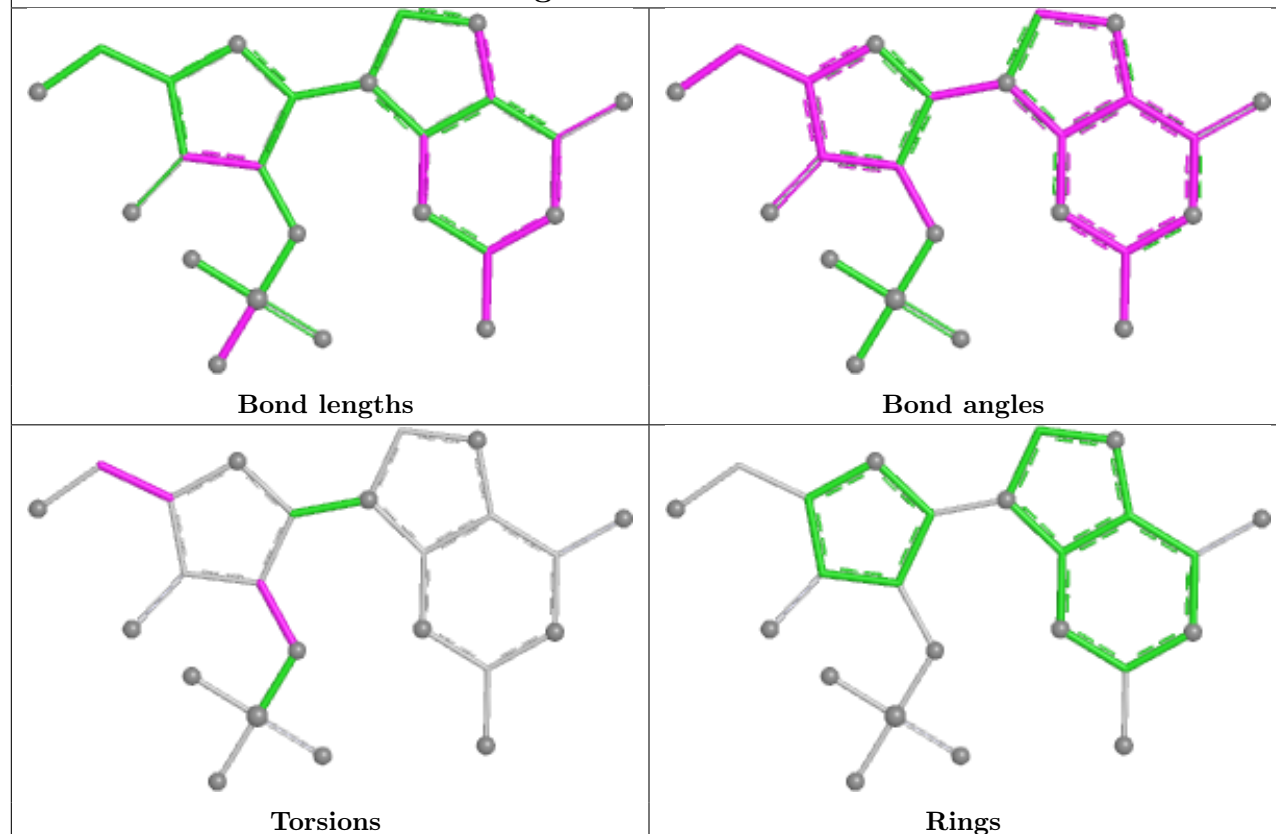
There are no ring outliers.

2 monomers are involved in 2 short contacts:

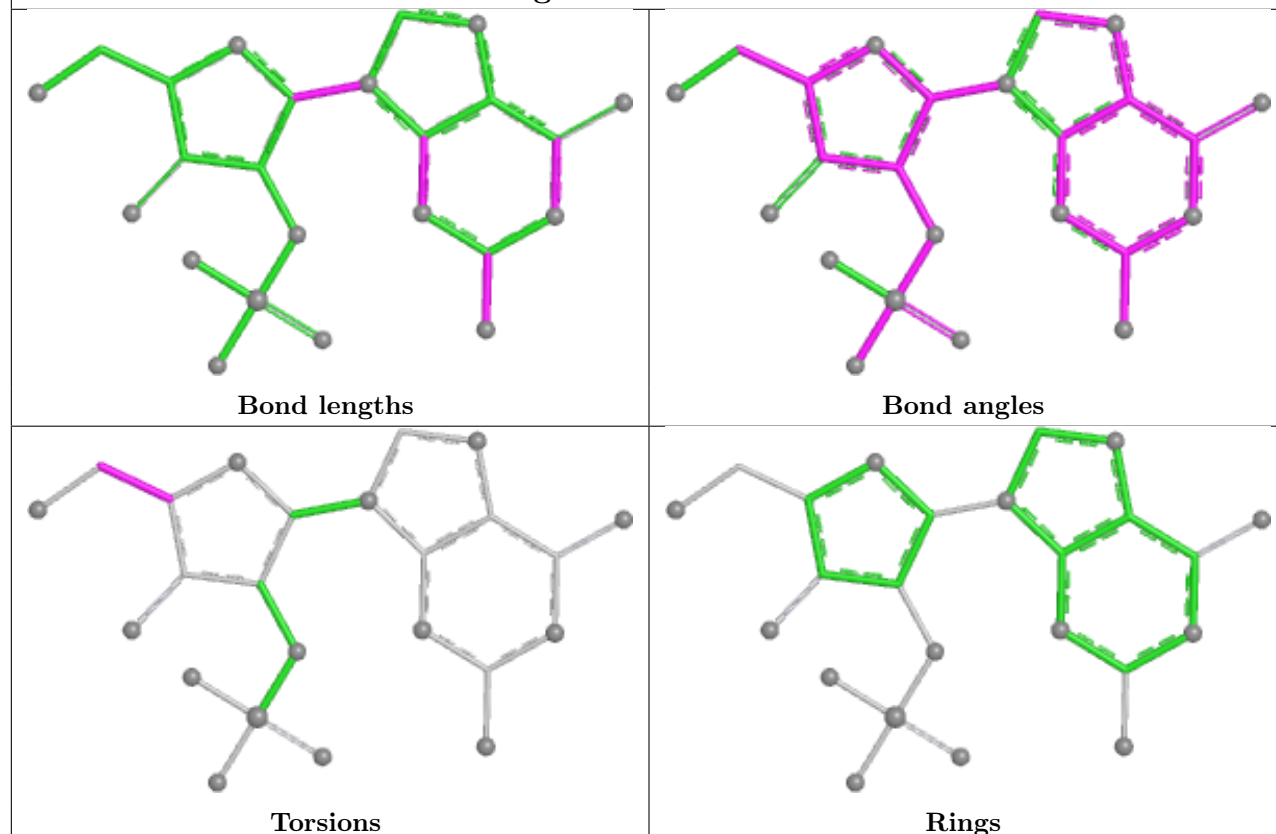
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	B	105	2GP	1	0
3	A	105	2GP	1	0

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.

Ligand 2GP B 105



Ligand 2GP A 105



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.