



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 8, 2026 – 02:21 AM UTC

PDB ID : 4RNT / pdb_00004rnt
Title : HIS 92 ALA MUTATION IN RIBONUCLEASE T1 INDUCES SEGMENTAL FLEXIBILITY. AN X-RAY STUDY
Authors : Saenger, W.; Koellner, G.
Deposited on : 1990-02-13
Resolution : 2.20 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
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

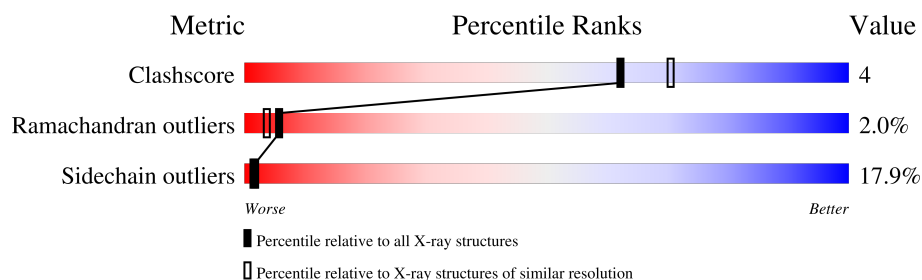
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.20 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	6851 (2.20-2.20)
Ramachandran outliers	187476	6768 (2.20-2.20)
Sidechain outliers	187428	6769 (2.20-2.20)

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	

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 846 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.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	104	Total	C	N	O	S	0	0	0
			776	477	125	170	4			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	25	LYS	GLN	conflict	UNP P00651
A	92	ALA	HIS	conflict	UNP P00651

- Molecule 2 is water.

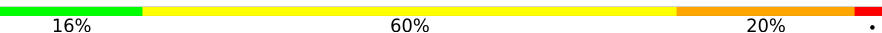
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	70	Total	O	0	0
			70	70		

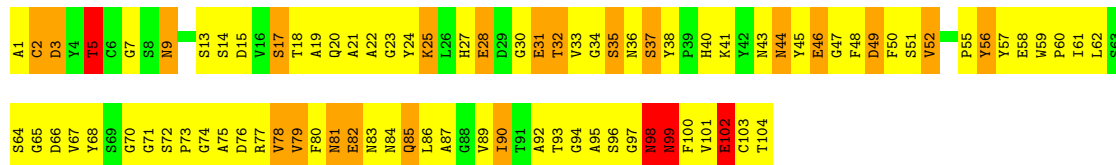
3 Residue-property plots

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

Chain A: 



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	31.04Å 62.31Å 43.70Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	10.00 – 2.20	Depositor
% Data completeness (in resolution range)	(Not available) (10.00-2.20)	Depositor
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	PROFFT	Depositor
R, R_{free}	0.162 , (Not available)	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	846	wwPDB-VP
Average B, all atoms (Å ²)	14.0	wwPDB-VP

5 Model quality

5.1 Standard geometry

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	1.99	14/796 (1.8%)	4.07	187/1084 (17.3%)

All (14) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	36	ASN	C-O	-7.72	1.13	1.24
1	A	59	TRP	NE1-CE2	6.37	1.44	1.37
1	A	27	HIS	CE1-NE2	-6.18	1.26	1.32
1	A	24	TYR	C-O	5.96	1.31	1.24
1	A	96	SER	N-CA	5.79	1.54	1.46
1	A	99	ASN	CA-C	5.75	1.60	1.53
1	A	5	THR	C-N	-5.56	1.26	1.33
1	A	77	ARG	CD-NE	5.52	1.53	1.46
1	A	3	ASP	CA-CB	-5.40	1.45	1.53
1	A	72	SER	N-CA	5.38	1.53	1.46
1	A	5	THR	CB-OG1	5.21	1.52	1.43
1	A	21	ALA	C-O	5.21	1.30	1.24
1	A	34	GLY	N-CA	5.20	1.50	1.45
1	A	62	LEU	CA-C	-5.01	1.46	1.52

All (187) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	98	ASN	CA-CB-CG	26.02	138.62	112.60
1	A	99	ASN	OD1-CG-ND2	-19.23	103.37	122.60
1	A	46	GLU	CB-CG-CD	18.93	144.78	112.60
1	A	84	ASN	OD1-CG-ND2	18.52	141.12	122.60
1	A	99	ASN	CA-CB-CG	18.11	130.71	112.60
1	A	9	ASN	CA-C-N	16.21	146.12	123.11
1	A	9	ASN	C-N-CA	16.21	146.12	123.11
1	A	99	ASN	O-C-N	-14.78	105.45	122.75
1	A	99	ASN	CB-CA-C	14.52	139.71	109.65
1	A	22	ALA	CA-C-O	14.10	135.50	120.55

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	43	ASN	OD1-CG-ND2	-13.83	108.77	122.60
1	A	98	ASN	OD1-CG-ND2	-13.68	108.92	122.60
1	A	71	GLY	O-C-N	13.28	133.91	122.88
1	A	94	GLY	CA-C-O	-13.12	103.18	119.19
1	A	99	ASN	CA-C-O	12.84	135.99	121.87
1	A	95	ALA	CA-C-O	-12.76	105.45	121.78
1	A	102	GLU	CA-CB-CG	12.73	139.56	114.10
1	A	84	ASN	CB-CG-ND2	-11.88	98.58	116.40
1	A	100	PHE	N-CA-C	-11.62	91.49	109.85
1	A	100	PHE	N-CA-CB	10.88	128.82	111.20
1	A	9	ASN	O-C-N	-10.76	109.76	122.89
1	A	93	THR	CA-C-O	10.57	133.20	120.62
1	A	9	ASN	CA-C-O	9.83	132.17	121.16
1	A	98	ASN	N-CA-CB	9.77	125.38	110.44
1	A	61	ILE	O-C-N	9.71	133.75	123.26
1	A	50	PHE	CA-CB-CG	9.62	123.42	113.80
1	A	43	ASN	CA-C-O	-9.57	108.33	120.00
1	A	27	HIS	CA-C-O	-9.46	110.77	120.90
1	A	61	ILE	N-CA-CB	9.34	124.30	111.41
1	A	74	GLY	CA-C-O	-9.29	114.02	122.57
1	A	82	GLU	CA-CB-CG	-9.22	95.65	114.10
1	A	66	ASP	CA-CB-CG	9.12	121.72	112.60
1	A	49	ASP	CB-CG-OD1	9.02	139.15	118.40
1	A	77	ARG	CA-CB-CG	8.97	132.03	114.10
1	A	20	GLN	CA-C-O	-8.95	111.48	120.70
1	A	93	THR	N-CA-CB	8.94	124.26	109.60
1	A	25	LYS	CG-CD-CE	8.91	131.80	111.30
1	A	65	GLY	N-CA-C	-8.75	102.93	115.27
1	A	43	ASN	CB-CG-ND2	8.71	129.47	116.40
1	A	22	ALA	CA-C-N	8.57	138.22	121.41
1	A	22	ALA	C-N-CA	8.57	138.22	121.41
1	A	48	PHE	CA-C-O	-8.29	112.07	121.19
1	A	32	THR	N-CA-CB	-8.25	97.88	111.66
1	A	90	ILE	O-C-N	-8.08	114.33	122.97
1	A	41	LYS	N-CA-C	8.07	121.92	110.23
1	A	92	ALA	CA-C-N	8.06	134.23	121.66
1	A	92	ALA	C-N-CA	8.06	134.23	121.66
1	A	100	PHE	CA-CB-CG	8.03	121.83	113.80
1	A	30	GLY	CA-C-O	8.03	129.51	119.80
1	A	96	SER	N-CA-C	8.02	123.06	107.98
1	A	62	LEU	N-CA-C	7.98	122.43	109.59
1	A	61	ILE	CA-C-N	-7.98	111.36	122.93

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	61	ILE	C-N-CA	-7.98	111.36	122.93
1	A	28	GLU	CA-CB-CG	7.92	129.94	114.10
1	A	95	ALA	N-CA-CB	-7.92	98.90	110.70
1	A	32	THR	OG1-CB-CG2	7.91	125.12	109.30
1	A	76	ASP	CA-CB-CG	7.90	120.50	112.60
1	A	101	VAL	N-CA-CB	7.86	126.46	111.93
1	A	36	ASN	CB-CG-ND2	-7.83	104.66	116.40
1	A	33	VAL	O-C-N	7.80	131.71	123.05
1	A	25	LYS	CA-CB-CG	7.78	129.66	114.10
1	A	68	TYR	O-C-N	7.76	132.57	122.95
1	A	79	VAL	N-CA-CB	7.72	122.32	111.82
1	A	20	GLN	OE1-CD-NE2	-7.70	114.90	122.60
1	A	48	PHE	CA-C-N	-7.68	110.55	122.08
1	A	48	PHE	C-N-CA	-7.68	110.55	122.08
1	A	55	PRO	O-C-N	7.66	135.66	121.10
1	A	33	VAL	CA-C-O	-7.61	112.39	120.76
1	A	96	SER	O-C-N	-7.52	112.66	122.43
1	A	22	ALA	N-CA-C	7.50	119.46	111.28
1	A	32	THR	N-CA-C	7.48	120.44	109.07
1	A	98	ASN	CB-CG-ND2	7.42	127.53	116.40
1	A	77	ARG	NE-CZ-NH1	7.35	128.85	121.50
1	A	73	PRO	CA-C-N	-7.33	111.42	122.06
1	A	73	PRO	C-N-CA	-7.33	111.42	122.06
1	A	97	GLY	CA-C-N	7.29	135.58	122.38
1	A	97	GLY	C-N-CA	7.29	135.58	122.38
1	A	56	TYR	CB-CG-CD1	7.28	131.72	120.80
1	A	78	VAL	CA-C-O	-7.28	112.15	121.40
1	A	51	SER	O-C-N	7.24	132.36	122.37
1	A	70	GLY	N-CA-C	-7.20	104.70	112.04
1	A	86	LEU	CA-C-O	-7.19	112.43	120.70
1	A	76	ASP	CA-C-N	-7.18	110.87	122.36
1	A	76	ASP	C-N-CA	-7.18	110.87	122.36
1	A	49	ASP	CB-CA-C	7.15	121.96	111.88
1	A	35	SER	CB-CA-C	-7.11	96.67	110.46
1	A	99	ASN	N-CA-C	-7.04	101.22	110.43
1	A	1	ALA	CB-CA-C	7.02	121.03	110.50
1	A	78	VAL	CB-CA-C	7.01	122.25	110.95
1	A	99	ASN	N-CA-CB	-6.98	100.27	110.26
1	A	89	VAL	CB-CA-C	6.95	121.11	110.96
1	A	81	ASN	OD1-CG-ND2	-6.94	115.66	122.60
1	A	58	GLU	O-C-N	6.91	132.17	123.19
1	A	2	CYS	CB-CA-C	-6.87	97.26	109.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	14	SER	CA-C-O	6.78	127.60	120.42
1	A	80	PHE	CA-C-O	-6.77	113.75	121.40
1	A	90	ILE	CA-C-N	6.73	133.40	122.29
1	A	90	ILE	C-N-CA	6.73	133.40	122.29
1	A	46	GLU	N-CA-C	-6.71	103.77	112.23
1	A	44	ASN	N-CA-CB	6.67	121.77	110.49
1	A	32	THR	CA-C-O	-6.66	114.14	121.33
1	A	51	SER	CA-C-O	-6.64	111.25	119.28
1	A	85	GLN	OE1-CD-NE2	6.60	129.20	122.60
1	A	68	TYR	CA-C-O	-6.56	113.44	120.92
1	A	104	THR	CA-CB-CG2	6.56	121.65	110.50
1	A	61	ILE	N-CA-C	-6.54	98.96	108.11
1	A	101	VAL	N-CA-C	-6.46	98.33	108.86
1	A	32	THR	O-C-N	6.44	130.60	123.25
1	A	35	SER	N-CA-C	6.43	119.98	111.75
1	A	62	LEU	N-CA-CB	-6.43	100.34	110.69
1	A	34	GLY	N-CA-C	6.41	122.87	112.61
1	A	17	SER	CA-C-O	-6.40	113.14	120.24
1	A	19	ALA	O-C-N	-6.38	114.87	122.15
1	A	99	ASN	CB-CG-ND2	6.36	125.94	116.40
1	A	25	LYS	CA-C-O	-6.33	113.84	120.55
1	A	77	ARG	O-C-N	6.24	130.83	122.96
1	A	21	ALA	CA-C-N	6.24	128.64	120.28
1	A	21	ALA	C-N-CA	6.24	128.64	120.28
1	A	5	THR	CA-CB-CG2	6.24	121.11	110.50
1	A	1	ALA	CA-C-O	-6.24	110.20	120.80
1	A	58	GLU	CA-C-O	-6.24	114.06	121.11
1	A	99	ASN	CA-C-N	6.23	133.27	122.81
1	A	99	ASN	C-N-CA	6.23	133.27	122.81
1	A	83	ASN	CA-CB-CG	6.22	118.82	112.60
1	A	32	THR	CA-CB-OG1	-6.18	100.33	109.60
1	A	7	GLY	O-C-N	6.17	130.72	122.70
1	A	43	ASN	CB-CA-C	6.10	121.64	110.11
1	A	20	GLN	O-C-N	6.08	128.65	122.09
1	A	57	TYR	CA-C-O	-6.07	114.01	121.11
1	A	49	ASP	CA-C-N	6.05	129.95	121.24
1	A	49	ASP	C-N-CA	6.05	129.95	121.24
1	A	40	HIS	O-C-N	5.94	129.93	123.10
1	A	58	GLU	OE1-CD-OE2	5.91	137.09	122.90
1	A	1	ALA	CA-C-N	5.87	131.78	122.74
1	A	1	ALA	C-N-CA	5.87	131.78	122.74
1	A	67	VAL	CA-CB-CG1	5.86	120.37	110.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	56	TYR	CB-CG-CD2	-5.83	112.05	120.80
1	A	49	ASP	O-C-N	-5.82	114.66	122.68
1	A	52	VAL	CB-CA-C	5.81	120.33	111.68
1	A	75	ALA	CA-C-N	5.76	131.23	122.65
1	A	75	ALA	C-N-CA	5.76	131.23	122.65
1	A	64	SER	N-CA-C	-5.73	105.79	112.89
1	A	77	ARG	NE-CZ-NH2	-5.71	114.06	119.20
1	A	76	ASP	N-CA-CB	-5.70	101.12	110.52
1	A	95	ALA	N-CA-C	5.70	118.52	110.14
1	A	18	THR	N-CA-C	-5.69	104.98	111.07
1	A	21	ALA	CB-CA-C	-5.62	102.05	110.88
1	A	23	GLY	N-CA-C	-5.60	99.91	113.18
1	A	25	LYS	CD-CE-NZ	5.58	129.77	111.90
1	A	5	THR	CA-CB-OG1	5.56	117.94	109.60
1	A	95	ALA	CB-CA-C	-5.52	100.53	110.36
1	A	15	ASP	CA-C-N	5.50	128.00	120.46
1	A	15	ASP	C-N-CA	5.50	128.00	120.46
1	A	83	ASN	N-CA-C	-5.50	106.34	113.16
1	A	48	PHE	CG-CD1-CE1	5.47	130.00	120.70
1	A	45	TYR	N-CA-C	-5.46	106.62	113.28
1	A	61	ILE	CA-C-O	-5.45	114.67	120.39
1	A	13	SER	O-C-N	-5.39	115.32	122.33
1	A	17	SER	CB-CA-C	5.38	120.54	110.70
1	A	15	ASP	CA-CB-CG	5.35	117.95	112.60
1	A	103	CYS	CA-CB-SG	-5.32	102.16	114.40
1	A	31	GLU	N-CA-CB	-5.31	103.09	111.05
1	A	47	GLY	CA-C-N	5.29	128.22	120.71
1	A	47	GLY	C-N-CA	5.29	128.22	120.71
1	A	59	TRP	CB-CA-C	5.27	117.17	110.16
1	A	84	ASN	CA-C-N	-5.26	114.81	122.65
1	A	84	ASN	C-N-CA	-5.26	114.81	122.65
1	A	28	GLU	CB-CA-C	-5.25	99.34	110.31
1	A	40	HIS	CG-CD2-NE2	-5.25	101.95	107.20
1	A	33	VAL	N-CA-CB	-5.24	102.85	111.45
1	A	92	ALA	CA-C-O	5.23	125.79	119.31
1	A	37	SER	CA-C-O	5.23	127.98	120.51
1	A	87	ALA	CA-C-O	5.22	126.03	120.24
1	A	2	CYS	O-C-N	-5.20	117.22	123.31
1	A	85	GLN	CA-C-O	-5.20	115.03	120.80
1	A	96	SER	N-CA-CB	-5.20	102.80	110.49
1	A	18	THR	CA-CB-OG1	-5.16	101.86	109.60
1	A	31	GLU	O-C-N	5.15	130.31	122.94

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	2	CYS	N-CA-C	5.14	117.45	108.76
1	A	60	PRO	N-CD-CG	-5.12	95.51	103.20
1	A	9	ASN	CB-CG-ND2	5.06	123.99	116.40
1	A	38	TYR	CB-CA-C	5.05	116.34	108.61
1	A	5	THR	N-CA-CB	5.04	118.51	110.65
1	A	59	TRP	CA-C-O	-5.04	115.14	119.72
1	A	52	VAL	CA-CB-CG1	5.03	118.95	110.40
1	A	98	ASN	N-CA-C	-5.02	106.94	113.16
1	A	102	GLU	CB-CG-CD	5.01	121.11	112.60

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	776	0	676	6	0
2	A	70	0	0	0	0
All	All	846	0	676	6	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 (6) 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	1.57	0.50
1:A:5:THR:HA	1:A:9:ASN:O	2.19	0.43
1:A:56:TYR:HB3	1:A:79:VAL:CG1	2.50	0.41
1:A:90:ILE:HG22	1:A:102:GLU:HA	2.02	0.41
1:A:98:ASN:O	1:A:99:ASN:C	2.63	0.41
1:A:2:CYS:O	1:A:3:ASP:C	2.63	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%)	97 (95%)	3 (3%)	2 (2%)	6 4

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	37	SER
1	A	44	ASN

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	84/84 (100%)	69 (82%)	15 (18%)	2 1

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

Mol	Chain	Res	Type
1	A	5	THR
1	A	17	SER
1	A	25	LYS
1	A	28	GLU
1	A	31	GLU
1	A	32	THR
1	A	35	SER
1	A	46	GLU
1	A	49	ASP

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Mol	Chain	Res	Type
1	A	52	VAL
1	A	78	VAL
1	A	82	GLU
1	A	98	ASN
1	A	99	ASN
1	A	102	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (3) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	20	GLN
1	A	27	HIS
1	A	85	GLN

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 ⓘ

There are no ligands in this entry.

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

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.