



# Full wwPDB X-ray Structure Validation Report ⓘ

Mar 10, 2026 – 04:23 AM UTC

PDB ID : 1RTC / pdb\_00001rtc  
Title : THE STRUCTURE OF RECOMBINANT RICIN A CHAIN AT 2.3  
ANGSTROMS  
Authors : Mlsna, D.; Monzingo, A.F.; Katzin, B.J.; Ernst, S.; Robertus, J.D.  
Deposited on : 1992-10-29  
Resolution : 2.30 Å(reported)

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

We welcome your comments at [validation@mail.wwpdb.org](mailto: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>.

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The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity : 4-5-2 with Phenix2.0  
Xtrriage (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

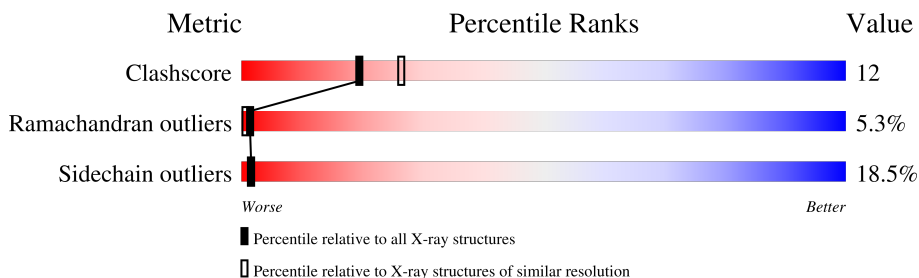
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.30 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
Clashscore	190562	6919 (2.30-2.30)
Ramachandran outliers	187476	6854 (2.30-2.30)
Sidechain outliers	187428	6854 (2.30-2.30)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 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	268	

## 2 Entry composition [i](#)

There are 2 unique types of molecules in this entry. The entry contains 2180 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 RICIN.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	268	2132	1354	374	398	6	0	2	0

- Molecule 2 is water.

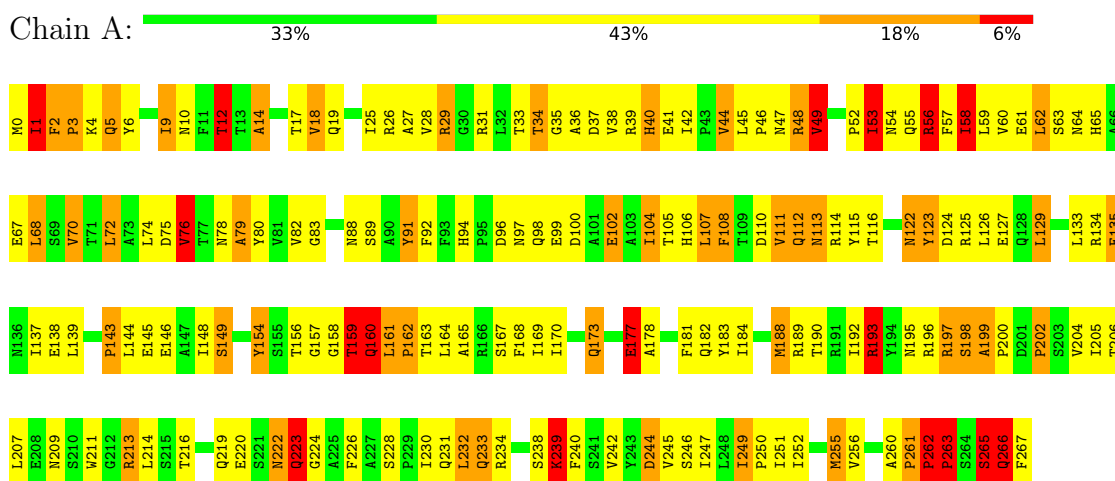
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	48	Total	O	0	0
			48	48		

### 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: RICIN



## 4 Data and refinement statistics

Xtrriage (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, $\alpha$ , $\beta$ , $\gamma$	42.60Å 68.10Å 50.20Å 90.00° 112.90° 90.00°	Depositor
Resolution (Å)	(Not available) – 2.30	Depositor
% Data completeness (in resolution range)	(Not available) ((Not available)-2.30)	Depositor
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
Refinement program	X-PLOR	Depositor
R, $R_{free}$	0.230 , (Not available)	Depositor
Estimated twinning fraction	No twinning to report.	Xtrriage
Total number of atoms	2180	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	17.0	wwPDB-VP

## 5 Model quality i

### 5.1 Standard geometry i

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	43/2188 (2.0%)	2.71	206/2974 (6.9%)

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	5

All (43) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	206	THR	C-N	-8.79	1.22	1.33
1	A	170	ILE	CA-CB	8.45	1.64	1.54
1	A	234	ARG	NE-CZ	7.87	1.41	1.33
1	A	94	HIS	CD2-NE2	-7.62	1.29	1.37
1	A	94	HIS	CG-ND1	-7.35	1.30	1.38
1	A	65	HIS	CD2-NE2	-7.10	1.30	1.37
1	A	110	ASP	CA-CB	-6.90	1.43	1.53
1	A	40	HIS	CD2-NE2	-6.88	1.30	1.37
1	A	159	THR	CA-CB	6.79	1.65	1.53
1	A	207	LEU	CA-C	-6.67	1.44	1.52
1	A	102	GLU	CA-CB	6.59	1.63	1.53
1	A	58	ILE	N-CA	-6.55	1.38	1.46
1	A	192	ILE	CA-CB	6.40	1.62	1.54
1	A	177	GLU	CA-CB	-6.40	1.43	1.53
1	A	61	GLU	CA-CB	-6.34	1.44	1.53
1	A	46	PRO	CA-C	-6.26	1.44	1.52
1	A	198	SER	CA-C	-6.19	1.45	1.52
1	A	45	LEU	C-O	6.14	1.30	1.24
1	A	261	PRO	N-CD	-6.13	1.39	1.47
1	A	249	ILE	CA-CB	6.01	1.57	1.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	260	ALA	C-N	5.97	1.40	1.33
1	A	19	GLN	CA-CB	-5.96	1.46	1.53
1	A	205	ILE	CA-CB	-5.94	1.47	1.54
1	A	82	VAL	CA-CB	5.92	1.62	1.54
1	A	256	VAL	CA-CB	5.73	1.61	1.54
1	A	19	GLN	CA-C	-5.67	1.47	1.53
1	A	158	GLY	N-CA	5.63	1.53	1.45
1	A	65	HIS	C-N	5.61	1.41	1.33
1	A	156	THR	N-CA	5.54	1.54	1.46
1	A	167	SER	C-O	-5.51	1.17	1.24
1	A	182	GLN	C-O	-5.49	1.17	1.24
1	A	165	ALA	CA-CB	-5.49	1.44	1.53
1	A	58	ILE	CA-C	5.41	1.59	1.52
1	A	107	LEU	N-CA	-5.38	1.39	1.46
1	A	133	LEU	C-O	-5.34	1.17	1.23
1	A	18	VAL	C-N	5.34	1.40	1.33
1	A	146	GLU	CA-C	-5.30	1.45	1.52
1	A	106	HIS	CD2-NE2	-5.29	1.32	1.37
1	A	29	ARG	N-CA	5.24	1.52	1.46
1	A	200	PRO	N-CA	-5.16	1.41	1.47
1	A	200	PRO	CA-CB	-5.10	1.46	1.53
1	A	193	ARG	NE-CZ	5.07	1.38	1.33
1	A	70	VAL	N-CA	5.04	1.51	1.46

All (206) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	36	ALA	N-CA-C	16.53	132.58	109.11
1	A	49	VAL	N-CA-C	12.65	123.50	110.72
1	A	112	GLN	O-C-N	-11.92	109.09	123.04
1	A	261	PRO	N-CA-C	10.68	123.73	110.70
1	A	37	ASP	N-CA-C	-10.54	89.58	108.02
1	A	98	GLN	OE1-CD-NE2	-10.44	112.16	122.60
1	A	112	GLN	OE1-CD-NE2	-9.78	112.82	122.60
1	A	205	ILE	CA-C-O	-9.71	110.88	121.17
1	A	53	ILE	CB-CA-C	-9.46	95.77	111.29
1	A	78	ASN	OD1-CG-ND2	-9.19	113.41	122.60
1	A	231	GLN	OE1-CD-NE2	-9.00	113.60	122.60
1	A	202	PRO	N-CA-C	9.00	125.10	114.03
1	A	160	GLN	OE1-CD-NE2	-8.89	113.71	122.60
1	A	14	ALA	CA-C-O	-8.81	107.91	120.51
1	A	158	GLY	CA-C-N	8.80	138.35	121.54

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	158	GLY	C-N-CA	8.80	138.35	121.54
1	A	112	GLN	CB-CG-CD	8.66	127.33	112.60
1	A	88	ASN	CA-C-O	-8.61	109.30	119.03
1	A	45	LEU	N-CA-CB	-8.47	94.17	110.10
1	A	233	GLN	OE1-CD-NE2	-8.30	114.30	122.60
1	A	182	GLN	OE1-CD-NE2	-8.18	114.42	122.60
1	A	2	PHE	CA-C-N	8.17	130.05	119.84
1	A	2	PHE	C-N-CA	8.17	130.05	119.84
1	A	2	PHE	N-CA-C	8.10	127.71	109.81
1	A	216	THR	N-CA-C	-8.07	102.07	111.03
1	A	159	THR	OG1-CB-CG2	-8.07	93.16	109.30
1	A	164	LEU	O-C-N	-8.05	113.59	122.12
1	A	112	GLN	N-CA-C	-8.03	97.00	109.76
1	A	12	THR	CA-CB-CG2	7.95	124.01	110.50
1	A	211	TRP	CG-CD2-CE3	7.94	141.84	133.90
1	A	12	THR	CA-CB-OG1	-7.94	97.69	109.60
1	A	149	SER	CA-CB-OG	-7.90	95.30	111.10
1	A	266	GLN	OE1-CD-NE2	-7.90	114.70	122.60
1	A	56	ARG	CG-CD-NE	-7.88	94.66	112.00
1	A	143	PRO	CA-N-CD	-7.85	101.01	112.00
1	A	45	LEU	CB-CA-C	7.83	120.90	108.91
1	A	196	ARG	O-C-N	-7.81	114.20	123.03
1	A	167	SER	O-C-N	-7.76	112.72	122.27
1	A	246	SER	O-C-N	7.71	130.11	122.09
1	A	88	ASN	CA-CB-CG	7.60	120.20	112.60
1	A	159	THR	CA-CB-CG2	7.60	123.42	110.50
1	A	262	PRO	CA-N-CD	-7.57	101.40	112.00
1	A	154	TYR	N-CA-C	-7.50	103.10	111.28
1	A	63	SER	CA-C-O	7.47	129.85	121.11
1	A	94	HIS	CB-CG-CD2	-7.43	121.54	131.20
1	A	219	GLN	CA-CB-CG	-7.43	99.24	114.10
1	A	45	LEU	N-CA-C	-7.42	99.22	110.50
1	A	97	ASN	CB-CG-ND2	7.42	127.53	116.40
1	A	222	ASN	OD1-CG-ND2	-7.35	115.25	122.60
1	A	74	LEU	O-C-N	-7.34	113.89	123.21
1	A	137	ILE	N-CA-CB	-7.22	102.77	111.00
1	A	168	PHE	N-CA-C	-7.21	103.50	111.36
1	A	3	PRO	CA-N-CD	-7.13	102.01	112.00
1	A	5	GLN	OE1-CD-NE2	-7.12	115.48	122.60
1	A	168	PHE	CA-C-O	-7.08	112.92	120.42
1	A	97	ASN	OD1-CG-ND2	-6.97	115.63	122.60
1	A	0	MET	N-CA-C	-6.89	91.69	111.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	28	VAL	CB-CA-C	6.82	120.70	111.97
1	A	26	ARG	CA-CB-CG	-6.78	100.54	114.10
1	A	3	PRO	N-CA-C	6.76	126.40	112.47
1	A	54	ASN	OD1-CG-ND2	-6.75	115.85	122.60
1	A	256	VAL	O-C-N	-6.75	114.29	122.59
1	A	104	ILE	CA-CB-CG2	6.74	121.96	110.50
1	A	9	ILE	N-CA-C	-6.68	98.86	108.48
1	A	219	GLN	OE1-CD-NE2	-6.68	115.92	122.60
1	A	249	ILE	N-CA-CB	-6.67	106.30	110.50
1	A	265	SER	O-C-N	-6.66	113.73	122.59
1	A	197	ARG	N-CA-C	-6.65	97.53	108.76
1	A	56	ARG	NE-CZ-NH2	-6.61	113.25	119.20
1	A	70	VAL	CB-CA-C	6.57	120.54	110.55
1	A	70	VAL	N-CA-CB	-6.53	101.47	112.44
1	A	27	ALA	CA-C-N	6.50	128.75	120.56
1	A	27	ALA	C-N-CA	6.50	128.75	120.56
1	A	28	VAL	O-C-N	-6.49	115.55	121.91
1	A	240	PHE	O-C-N	-6.49	115.25	123.24
1	A	40	HIS	CB-CG-CD2	-6.48	122.77	131.20
1	A	249	ILE	CA-C-O	-6.45	113.36	118.85
1	A	104	ILE	CA-CB-CG1	-6.42	99.49	110.40
1	A	125	ARG	CB-CG-CD	6.41	126.04	111.30
1	A	79	ALA	N-CA-C	6.39	124.40	110.80
1	A	251	ILE	CA-C-O	-6.37	114.00	120.69
1	A	220	GLU	CA-CB-CG	6.36	126.82	114.10
1	A	52	PRO	CA-C-O	-6.36	114.16	121.98
1	A	91	TYR	CA-C-O	-6.30	113.89	120.70
1	A	161	LEU	CB-CA-C	-6.30	98.70	112.38
1	A	133	LEU	CA-C-N	6.26	129.52	120.38
1	A	133	LEU	C-N-CA	6.26	129.52	120.38
1	A	27	ALA	O-C-N	-6.25	115.49	122.12
1	A	113	ASN	CB-CA-C	-6.21	98.07	110.42
1	A	113	ASN	CA-CB-CG	6.17	118.77	112.60
1	A	148	ILE	O-C-N	-6.17	115.87	121.91
1	A	250	PRO	CA-C-N	6.16	129.96	122.63
1	A	250	PRO	C-N-CA	6.16	129.96	122.63
1	A	188	MET	CG-SD-CE	-6.11	87.47	100.90
1	A	223	GLN	CA-C-O	6.10	129.24	120.51
1	A	38	VAL	O-C-N	6.09	129.51	123.18
1	A	213	ARG	O-C-N	-6.08	115.21	122.15
1	A	145	GLU	CB-CA-C	-6.08	98.32	110.42
1	A	214	LEU	N-CA-C	-6.06	104.59	111.07

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	34	THR	N-CA-CB	-6.03	100.30	110.49
1	A	107	LEU	CA-C-N	-6.00	113.99	123.24
1	A	107	LEU	C-N-CA	-6.00	113.99	123.24
1	A	265	SER	CA-CB-OG	5.99	123.08	111.10
1	A	244	ASP	CA-C-O	-5.98	114.12	121.06
1	A	63	SER	O-C-N	-5.98	115.89	123.24
1	A	219	GLN	CB-CG-CD	5.97	122.75	112.60
1	A	107	LEU	O-C-N	-5.97	115.46	122.32
1	A	133	LEU	CA-C-O	-5.96	115.06	121.56
1	A	114	ARG	CB-CG-CD	-5.96	97.60	111.30
1	A	222	ASN	CB-CG-ND2	5.96	125.33	116.40
1	A	53	ILE	N-CA-CB	5.91	120.98	111.23
1	A	2	PHE	CA-CB-CG	5.91	119.70	113.80
1	A	192	ILE	CA-C-O	-5.89	114.51	121.05
1	A	206	THR	CA-CB-OG1	-5.88	100.78	109.60
1	A	124	ASP	O-C-N	-5.87	116.03	122.07
1	A	161	LEU	CA-CB-CG	5.87	136.83	116.30
1	A	246	SER	N-CA-C	5.84	118.12	111.11
1	A	56	ARG	N-CA-C	5.83	119.58	112.23
1	A	144	LEU	CA-C-O	-5.82	114.70	120.82
1	A	255	MET	CA-C-O	-5.82	114.54	121.11
1	A	173	GLN	OE1-CD-NE2	-5.81	116.79	122.60
1	A	70	VAL	O-C-N	-5.81	116.59	123.04
1	A	211	TRP	CE2-CD2-CG	-5.78	100.27	107.20
1	A	182	GLN	N-CA-C	-5.76	105.09	111.71
1	A	260	ALA	N-CA-C	5.76	118.84	110.14
1	A	58	ILE	CB-CA-C	5.72	120.94	110.71
1	A	46	PRO	CA-C-O	5.71	127.86	121.34
1	A	98	GLN	CG-CD-NE2	5.70	124.95	116.40
1	A	159	THR	N-CA-CB	-5.68	100.88	110.49
1	A	44	VAL	N-CA-C	-5.68	100.39	109.20
1	A	34	THR	CA-C-O	5.68	128.63	120.51
1	A	188	MET	O-C-N	-5.67	115.69	122.15
1	A	244	ASP	N-CA-CB	-5.61	101.10	111.53
1	A	58	ILE	N-CA-C	-5.60	99.73	108.81
1	A	34	THR	CA-CB-CG2	-5.60	100.98	110.50
1	A	211	TRP	O-C-N	-5.59	115.83	122.20
1	A	68	LEU	N-CA-C	-5.59	99.79	108.90
1	A	113	ASN	N-CA-CB	5.59	119.93	110.49
1	A	169	ILE	CA-C-N	5.58	127.70	120.56
1	A	169	ILE	C-N-CA	5.58	127.70	120.56
1	A	83	GLY	O-C-N	-5.56	118.25	123.81

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	112	GLN	CG-CD-NE2	5.55	124.73	116.40
1	A	92	PHE	O-C-N	-5.55	115.97	123.19
1	A	111	VAL	N-CA-C	-5.55	100.46	108.89
1	A	199	ALA	O-C-N	-5.55	115.72	121.60
1	A	58	ILE	N-CA-CB	-5.54	101.56	111.92
1	A	105	THR	N-CA-C	-5.54	106.53	113.28
1	A	25	ILE	CA-C-O	-5.54	114.98	120.85
1	A	72	LEU	CA-C-O	-5.54	114.66	120.80
1	A	204	VAL	N-CA-C	-5.54	105.22	110.42
1	A	200	PRO	CB-CA-C	5.53	118.56	111.21
1	A	228	SER	O-C-N	-5.53	116.68	121.71
1	A	233	GLN	O-C-N	-5.53	116.44	123.24
1	A	10	ASN	N-CA-C	5.52	118.73	109.95
1	A	17	THR	CA-CB-OG1	-5.49	101.37	109.60
1	A	161	LEU	CA-C-N	5.48	125.57	119.32
1	A	161	LEU	C-N-CA	5.48	125.57	119.32
1	A	159	THR	CA-C-N	5.37	131.80	121.54
1	A	159	THR	C-N-CA	5.37	131.80	121.54
1	A	48	ARG	N-CA-C	-5.37	106.23	112.89
1	A	5	GLN	CG-CD-NE2	5.37	124.45	116.40
1	A	75	ASP	O-C-N	-5.36	117.11	123.22
1	A	65	HIS	CB-CA-C	-5.35	99.78	110.42
1	A	202	PRO	N-CA-CB	-5.35	98.38	103.41
1	A	211	TRP	N-CA-C	5.35	118.60	111.75
1	A	41	GLU	CA-CB-CG	-5.33	103.44	114.10
1	A	54	ASN	CB-CG-ND2	5.31	124.37	116.40
1	A	190	THR	CA-CB-CG2	5.30	119.51	110.50
1	A	1	ILE	O-C-N	-5.30	115.95	122.57
1	A	55	GLN	OE1-CD-NE2	-5.29	117.31	122.60
1	A	116	THR	O-C-N	-5.28	117.06	123.29
1	A	244	ASP	N-CA-C	5.26	117.39	109.23
1	A	48	ARG	CD-NE-CZ	5.25	131.75	124.40
1	A	125	ARG	N-CA-C	-5.25	105.00	111.40
1	A	100	ASP	CA-CB-CG	-5.25	107.35	112.60
1	A	159	THR	CA-CB-OG1	-5.24	101.73	109.60
1	A	250	PRO	N-CA-CB	5.24	108.54	103.51
1	A	170	ILE	O-C-N	-5.24	116.45	121.90
1	A	239[A]	LYS	N-CA-C	-5.22	100.66	109.07
1	A	239[B]	LYS	N-CA-C	-5.22	100.66	109.07
1	A	148	ILE	N-CA-CB	-5.22	104.45	110.55
1	A	240	PHE	CA-C-O	-5.22	115.01	121.11
1	A	177	GLU	CB-CG-CD	5.21	121.46	112.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	76	VAL	N-CA-CB	-5.20	100.12	111.05
1	A	1	ILE	CA-C-O	-5.20	114.28	120.78
1	A	28	VAL	N-CA-C	-5.18	105.45	110.42
1	A	242	VAL	CG1-CB-CG2	-5.17	99.42	110.80
1	A	6	TYR	CA-C-N	5.16	125.45	119.93
1	A	6	TYR	C-N-CA	5.16	125.45	119.93
1	A	80	TYR	CA-C-O	5.16	127.55	121.36
1	A	108	PHE	N-CA-C	-5.14	96.92	107.67
1	A	46	PRO	N-CA-C	5.14	119.15	111.14
1	A	88	ASN	N-CA-C	-5.13	105.79	113.89
1	A	238	SER	O-C-N	5.13	128.64	122.79
1	A	199	ALA	CA-C-N	5.10	124.86	119.76
1	A	199	ALA	C-N-CA	5.10	124.86	119.76
1	A	5	GLN	N-CA-CB	-5.09	102.12	110.41
1	A	195	ASN	CA-CB-CG	-5.08	107.52	112.60
1	A	26	ARG	CA-C-O	-5.07	114.14	119.97
1	A	196	ARG	NH1-CZ-NH2	-5.06	112.72	119.30
1	A	183	TYR	O-C-N	-5.05	116.77	122.03
1	A	28	VAL	N-CA-CB	-5.05	104.64	110.55
1	A	163	THR	CA-CB-OG1	-5.05	102.03	109.60
1	A	263	PRO	N-CA-C	-5.03	102.10	112.47
1	A	94	HIS	CA-C-O	-5.01	114.53	119.49
1	A	178	ALA	O-C-N	-5.00	116.37	122.22

There are no chirality outliers.

All (5) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	1	ILE	Peptide
1	A	115	TYR	Sidechain
1	A	223	GLN	Mainchain
1	A	56	ARG	Sidechain
1	A	91	TYR	Sidechain

## 5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2132	0	2104	49	0
2	A	48	0	0	4	0
All	All	2180	0	2104	49	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 12.

All (49) 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:161:LEU:HD23	2:A:299:HOH:O	1.80	0.82
1:A:138:GLU:HB2	2:A:292:HOH:O	1.81	0.80
1:A:139:LEU:HD13	1:A:188:MET:HE1	1.61	0.80
1:A:143:PRO:HG3	2:A:292:HOH:O	1.84	0.75
1:A:123:TYR:O	1:A:127:GLU:HG3	1.89	0.73
1:A:161:LEU:HB2	1:A:162:PRO:HD3	1.76	0.66
1:A:122:ASN:HD22	1:A:122:ASN:H	1.46	0.64
1:A:135:GLU:O	1:A:199:ALA:HB1	2.04	0.57
1:A:129:LEU:HD23	1:A:161:LEU:HD13	1.87	0.56
1:A:224:GLY:O	1:A:245:VAL:HG23	2.06	0.56
1:A:159:THR:HG22	1:A:160:GLN:H	1.70	0.55
1:A:9:ILE:HD11	1:A:31:ARG:HG3	1.89	0.55
1:A:122:ASN:H	1:A:122:ASN:ND2	2.03	0.53
1:A:154:TYR:HD1	1:A:159:THR:HA	1.74	0.53
1:A:108:PHE:O	1:A:111:VAL:HG22	2.09	0.52
1:A:47:ASN:OD1	1:A:49:VAL:HG23	2.11	0.51
1:A:1:ILE:HG12	1:A:2:PHE:N	2.25	0.50
1:A:262:PRO:HD2	1:A:263:PRO:HD2	1.93	0.50
1:A:12:THR:HG23	1:A:14:ALA:HB3	1.93	0.49
1:A:154:TYR:CE1	1:A:159:THR:HG23	2.49	0.48
1:A:134:ARG:HH12	1:A:209:ASN:ND2	2.12	0.48
1:A:173:GLN:HA	1:A:177:GLU:HB2	1.96	0.48
1:A:226:PHE:CD2	1:A:230:ILE:HG12	2.49	0.47
1:A:202:PRO:HB3	1:A:233:GLN:NE2	2.30	0.46
1:A:60:VAL:HG12	1:A:62:LEU:HD13	1.97	0.46
1:A:134:ARG:HH22	1:A:209:ASN:HD21	1.63	0.46
1:A:129:LEU:CD2	1:A:161:LEU:HD22	2.46	0.46
1:A:56:ARG:O	1:A:76:VAL:HB	2.16	0.45
1:A:143:PRO:HD3	1:A:197:ARG:CZ	2.47	0.45
1:A:42:ILE:HD13	1:A:252:ILE:HG23	1.98	0.45
1:A:53:ILE:HD13	2:A:332:HOH:O	2.16	0.44
1:A:232:LEU:HD12	1:A:232:LEU:HA	1.85	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:202:PRO:HB3	1:A:233:GLN:HE22	1.82	0.44
1:A:154:TYR:HE1	1:A:159:THR:HG23	1.82	0.43
1:A:181:PHE:CD2	1:A:184:ILE:HD12	2.53	0.42
1:A:33:THR:C	1:A:35:GLY:H	2.25	0.42
1:A:57:PHE:O	1:A:58:ILE:HD12	2.20	0.42
1:A:157:GLY:C	1:A:159:THR:H	2.28	0.42
1:A:226:PHE:CE2	1:A:230:ILE:HG12	2.56	0.41
1:A:266:GLN:O	1:A:267:PHE:CD1	2.73	0.41
1:A:139:LEU:CD1	1:A:188:MET:HE1	2.41	0.41
1:A:68:LEU:C	1:A:68:LEU:HD12	2.45	0.41
1:A:18:VAL:HG21	1:A:193:ARG:HG2	2.02	0.41
1:A:42:ILE:HB	1:A:255:MET:HE2	2.02	0.41
1:A:64:ASN:ND2	1:A:149:SER:OG	2.53	0.41
1:A:161:LEU:HB2	1:A:162:PRO:CD	2.46	0.41
1:A:249:ILE:HD13	1:A:249:ILE:HG21	1.88	0.41
1:A:266:GLN:C	1:A:266:GLN:HE21	2.29	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	268/268 (100%)	233 (87%)	21 (8%)	14 (5%)	<b>1</b> <b>1</b>

All (14) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	3	PRO
1	A	67	GLU
1	A	159	THR
1	A	262	PRO
1	A	79	ALA

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Mol	Chain	Res	Type
1	A	265	SER
1	A	4	LYS
1	A	160	GLN
1	A	123	TYR
1	A	40	HIS
1	A	113	ASN
1	A	1	ILE
1	A	263	PRO
1	A	261	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
1	A	229/227 (101%)	185 (81%)	44 (19%)	<b>1</b> <b>1</b>

All (44) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	1	ILE
1	A	5	GLN
1	A	12	THR
1	A	29	ARG
1	A	34	THR
1	A	39	ARG
1	A	44	VAL
1	A	48	ARG
1	A	49	VAL
1	A	53	ILE
1	A	56	ARG
1	A	58	ILE
1	A	59	LEU
1	A	62	LEU
1	A	70	VAL
1	A	72	LEU
1	A	76	VAL

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Mol	Chain	Res	Type
1	A	89	SER
1	A	96	ASP
1	A	99[A]	GLU
1	A	99[B]	GLU
1	A	102	GLU
1	A	104	ILE
1	A	107	LEU
1	A	112	GLN
1	A	122	ASN
1	A	126	LEU
1	A	129	LEU
1	A	135	GLU
1	A	162	PRO
1	A	177	GLU
1	A	189	ARG
1	A	193	ARG
1	A	198	SER
1	A	213	ARG
1	A	222	ASN
1	A	223	GLN
1	A	232	LEU
1	A	239[A]	LYS
1	A	239[B]	LYS
1	A	244	ASP
1	A	247	ILE
1	A	265	SER
1	A	266	GLN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (12) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	54	ASN
1	A	55	GLN
1	A	113	ASN
1	A	122	ASN
1	A	160	GLN
1	A	173	GLN
1	A	182	GLN
1	A	209	ASN
1	A	219	GLN
1	A	223	GLN
1	A	233	GLN

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Mol	Chain	Res	Type
1	A	266	GLN

### 5.3.3 RNA [i](#)

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](#)

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 [i](#)

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

EDS was not executed - this section is therefore empty.

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

EDS was not executed - this section is therefore empty.

### 6.3 Carbohydrates [i](#)

EDS was not executed - this section is therefore empty.

### 6.4 Ligands [i](#)

EDS was not executed - this section is therefore empty.

### 6.5 Other polymers [i](#)

EDS was not executed - this section is therefore empty.