



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 8, 2026 – 10:51 AM UTC

PDB ID : 1BNI / pdb_00001bni
Title : BARNASE WILDTYPE STRUCTURE AT PH 6.0
Authors : Cameron, A.; Henrick, K.; Fersht, A.R.; Dodson, G.; Buckle, A.M.
Deposited on : 1995-05-17
Resolution : 2.10 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

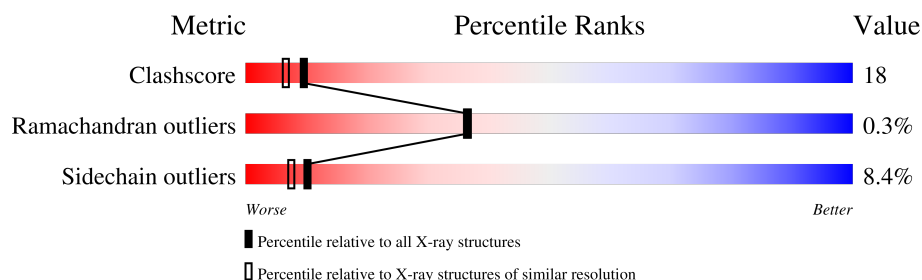
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.10 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	7164 (2.10-2.10)
Ramachandran outliers	187476	7099 (2.10-2.10)
Sidechain outliers	187428	7100 (2.10-2.10)

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	110	 39% 35% 24% ..
1	B	110	 31% 39% 25% . .
1	C	110	 37% 46% 14% ..

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 2763 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 BARNASE.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
1	A	108	Total	C	N	O	6	0	0
			851	541	147	163			
1	B	108	Total	C	N	O	1	0	0
			844	537	144	163			
1	C	108	Total	C	N	O	0	0	0
			852	541	145	166			

- Molecule 2 is water.

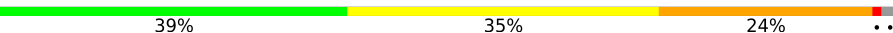
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	63	Total	O	0	0
			63	63		
2	B	72	Total	O	0	0
			72	72		
2	C	81	Total	O	0	0
			81	81		

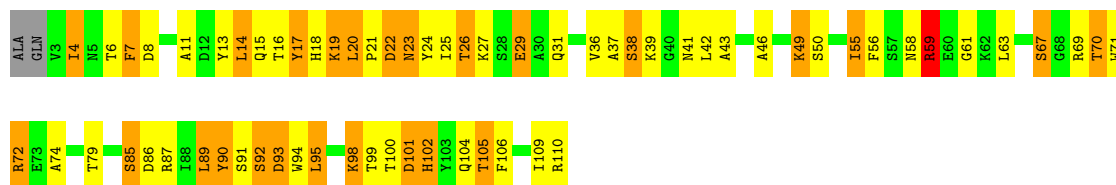
3 Residue-property plots

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.

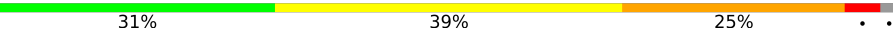
Note EDS was not executed.

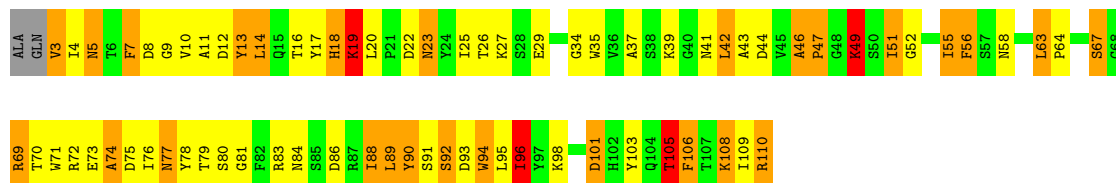
• Molecule 1: BARNASE

Chain A: 



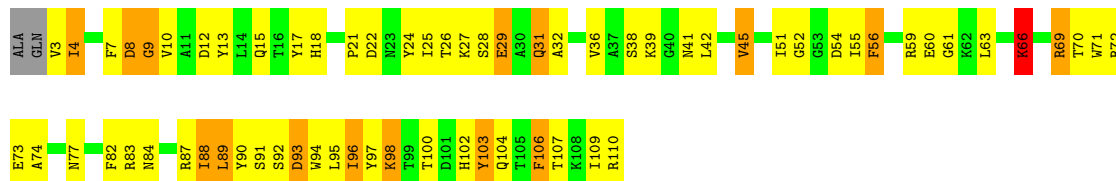
• Molecule 1: BARNASE

Chain B: 



• Molecule 1: BARNASE

Chain C: 



4 Data and refinement statistics

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

Property	Value	Source
Space group	P 32	Depositor
Cell constants a, b, c, α , β , γ	59.39Å 59.39Å 82.59Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	10.00 – 2.10	Depositor
% Data completeness (in resolution range)	80.0 (10.00-2.10)	Depositor
R_{merge}	0.09	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	PROLSQ	Depositor
R, R_{free}	0.179 , (Not available)	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	2763	wwPDB-VP
Average B, all atoms (Å ²)	15.0	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	1.50	2/872 (0.2%)	2.90	85/1183 (7.2%)
1	B	1.59	6/865 (0.7%)	3.01	108/1175 (9.2%)
1	C	1.49	3/873 (0.3%)	2.91	97/1183 (8.2%)
All	All	1.53	11/2610 (0.4%)	2.94	290/3541 (8.2%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	1

All (11) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	59	ARG	CB-CG	-20.95	0.89	1.52
1	B	67	SER	CB-OG	-19.04	1.04	1.42
1	B	84	ASN	C-O	8.19	1.33	1.23
1	B	89	LEU	N-CA	6.26	1.53	1.46
1	B	110	ARG	CZ-NH2	-5.59	1.26	1.33
1	B	25	ILE	C-O	5.38	1.29	1.23
1	C	7	PHE	N-CA	5.29	1.52	1.46
1	A	26	THR	CA-CB	5.26	1.61	1.53
1	C	107	THR	CA-CB	5.24	1.61	1.53
1	C	96	ILE	CA-CB	5.24	1.61	1.54
1	B	51	ILE	N-CA	5.23	1.52	1.46

All (290) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	59	ARG	CA-CB-CG	15.04	144.18	114.10
1	B	67	SER	CA-CB-OG	14.54	140.19	111.10

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	22	ASP	CA-CB-CG	13.36	125.96	112.60
1	B	46	ALA	O-C-N	13.21	131.93	121.23
1	A	29	GLU	CA-C-N	12.06	136.12	120.44
1	A	29	GLU	C-N-CA	12.06	136.12	120.44
1	A	46	ALA	O-C-N	11.88	129.86	121.19
1	C	18	HIS	CA-CB-CG	-11.64	102.16	113.80
1	B	8	ASP	O-C-N	11.59	138.81	122.36
1	B	109	ILE	CA-C-O	11.52	129.35	118.98
1	A	61	GLY	CA-C-N	11.36	135.50	120.28
1	A	61	GLY	C-N-CA	11.36	135.50	120.28
1	C	102	HIS	CB-CG-CD2	-10.95	116.97	131.20
1	B	27	LYS	CA-C-O	10.91	132.41	120.63
1	B	8	ASP	CA-C-O	-10.42	107.41	119.60
1	C	25	ILE	CA-C-O	-10.42	110.24	121.28
1	A	74	ALA	CA-C-N	10.33	135.41	120.95
1	A	74	ALA	C-N-CA	10.33	135.41	120.95
1	A	59	ARG	CD-NE-CZ	10.32	138.85	124.40
1	A	20	LEU	O-C-N	9.90	132.52	121.43
1	C	59	ARG	CA-C-O	-9.85	109.97	120.42
1	B	105	THR	CA-CB-CG2	9.81	127.18	110.50
1	A	67	SER	CA-C-O	9.80	131.94	120.58
1	C	10	VAL	CA-C-O	-9.74	110.85	121.17
1	A	72	ARG	NE-CZ-NH2	-9.50	110.65	119.20
1	C	77	ASN	CA-C-O	-9.39	109.73	119.78
1	B	110	ARG	NE-CZ-NH2	9.20	127.48	119.20
1	C	36	VAL	CA-C-O	-9.12	110.44	120.48
1	B	27	LYS	CA-C-N	9.12	132.29	120.44
1	B	27	LYS	C-N-CA	9.12	132.29	120.44
1	C	39	LYS	CA-C-O	-9.11	108.69	119.35
1	C	72	ARG	NE-CZ-NH2	-9.10	111.01	119.20
1	B	56	PHE	CA-C-N	9.07	133.40	120.79
1	B	56	PHE	C-N-CA	9.07	133.40	120.79
1	C	66	LYS	CG-CD-CE	9.06	132.14	111.30
1	A	104	GLN	CA-C-N	9.02	137.34	122.73
1	A	104	GLN	C-N-CA	9.02	137.34	122.73
1	C	8	ASP	CA-CB-CG	-8.78	103.82	112.60
1	B	92	SER	O-C-N	8.74	132.45	122.22
1	A	23	ASN	OD1-CG-ND2	8.71	131.31	122.60
1	B	11	ALA	O-C-N	8.71	131.50	122.09
1	A	101	ASP	CA-C-N	-8.67	109.69	122.35
1	A	101	ASP	C-N-CA	-8.67	109.69	122.35
1	B	81	GLY	O-C-N	8.66	130.07	122.88

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	70	THR	N-CA-CB	-8.63	96.80	110.69
1	A	70	THR	CB-CA-C	8.62	124.89	109.38
1	A	58	ASN	CA-CB-CG	-8.59	104.02	112.60
1	C	54	ASP	CA-C-N	8.48	132.52	120.98
1	C	54	ASP	C-N-CA	8.48	132.52	120.98
1	A	29	GLU	CB-CG-CD	8.47	127.00	112.60
1	C	7	PHE	CA-C-O	8.46	129.71	120.82
1	A	4	ILE	O-C-N	8.41	134.39	122.62
1	B	88	ILE	CA-C-O	-8.35	111.63	120.57
1	B	37	ALA	O-C-N	8.30	130.72	122.09
1	A	49	LYS	CA-C-N	8.25	136.10	122.73
1	A	49	LYS	C-N-CA	8.25	136.10	122.73
1	A	23	ASN	CA-CB-CG	8.17	120.77	112.60
1	A	27	LYS	O-C-N	7.99	130.58	122.12
1	C	15	GLN	CB-CG-CD	7.95	126.11	112.60
1	A	92	SER	CA-C-O	-7.88	109.69	119.38
1	B	5	ASN	OD1-CG-ND2	-7.85	114.75	122.60
1	B	63	LEU	CA-C-O	-7.79	112.61	120.63
1	B	101	ASP	CA-CB-CG	7.78	120.38	112.60
1	B	55	ILE	O-C-N	7.78	130.87	122.63
1	C	7	PHE	O-C-N	-7.77	114.07	122.07
1	B	22	ASP	CA-C-O	-7.75	109.84	119.38
1	A	93	ASP	CA-C-O	7.74	129.09	119.95
1	B	11	ALA	CA-C-O	-7.74	112.73	120.70
1	B	17	TYR	CA-C-O	-7.65	110.16	119.18
1	C	41	ASN	O-C-N	7.61	131.30	122.25
1	C	17	TYR	O-C-N	7.53	132.28	122.42
1	A	27	LYS	CA-C-O	-7.50	112.60	120.55
1	B	70	THR	CA-CB-OG1	-7.49	98.37	109.60
1	B	89	LEU	CB-CA-C	7.47	122.57	110.16
1	B	67	SER	N-CA-CB	7.45	120.95	109.85
1	C	55	ILE	CA-C-N	7.45	132.68	122.77
1	C	55	ILE	C-N-CA	7.45	132.68	122.77
1	A	42	LEU	CA-C-N	7.43	130.24	120.28
1	A	42	LEU	C-N-CA	7.43	130.24	120.28
1	B	96	ILE	CA-C-O	-7.41	112.68	120.39
1	C	60	GLU	CA-C-N	7.40	131.28	120.11
1	C	60	GLU	C-N-CA	7.40	131.28	120.11
1	C	97	TYR	CA-C-N	-7.35	111.05	122.59
1	C	97	TYR	C-N-CA	-7.35	111.05	122.59
1	C	9	GLY	O-C-N	7.35	132.25	122.70
1	A	69	ARG	N-CA-CB	7.31	122.43	110.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	80	SER	O-C-N	7.31	130.60	123.29
1	C	102	HIS	CA-C-O	-7.30	113.10	121.65
1	A	31	GLN	OE1-CD-NE2	-7.29	115.31	122.60
1	C	104	GLN	CA-C-O	7.24	128.07	119.60
1	B	41	ASN	N-CA-C	7.23	120.96	112.72
1	C	15	GLN	CA-CB-CG	-7.22	99.66	114.10
1	C	42	LEU	CA-C-O	-7.18	113.22	120.90
1	C	83	ARG	NE-CZ-NH2	7.18	125.66	119.20
1	B	34	GLY	O-C-N	7.13	129.92	122.51
1	C	17	TYR	CA-C-O	-7.11	111.04	119.15
1	C	41	ASN	CA-C-O	-7.10	111.21	119.59
1	A	72	ARG	NH1-CZ-NH2	7.10	128.53	119.30
1	B	19	LYS	CA-C-O	7.07	130.62	120.51
1	B	76	ILE	O-C-N	7.02	130.30	123.14
1	C	17	TYR	N-CA-C	7.01	122.00	113.38
1	C	10	VAL	O-C-N	7.00	128.77	121.91
1	B	109	ILE	O-C-N	-6.97	113.10	122.03
1	C	56	PHE	CA-CB-CG	-6.94	106.86	113.80
1	A	49	LYS	N-CA-CB	6.89	121.88	110.85
1	C	17	TYR	CB-CG-CD2	-6.86	110.51	120.80
1	C	31	GLN	OE1-CD-NE2	-6.86	115.74	122.60
1	A	93	ASP	CB-CG-OD2	-6.85	102.65	118.40
1	C	24	TYR	CA-CB-CG	-6.82	101.62	113.90
1	B	18	HIS	CA-C-N	6.76	134.45	121.54
1	B	18	HIS	C-N-CA	6.76	134.45	121.54
1	B	25	ILE	CA-C-O	-6.75	114.12	121.28
1	A	8	ASP	O-C-N	6.70	129.79	122.15
1	C	82	PHE	CA-CB-CG	-6.67	107.13	113.80
1	B	72	ARG	O-C-N	6.66	131.81	123.15
1	B	27	LYS	O-C-N	-6.65	115.08	122.12
1	A	4	ILE	CA-C-O	-6.61	112.08	120.86
1	A	19	LYS	CA-CB-CG	6.58	127.27	114.10
1	C	95	LEU	N-CA-C	-6.58	99.86	110.32
1	B	34	GLY	CA-C-O	-6.58	112.59	118.77
1	C	36	VAL	O-C-N	6.54	129.99	122.99
1	B	16	THR	N-CA-C	-6.53	103.38	112.45
1	B	13	TYR	O-C-N	-6.52	115.31	122.09
1	B	18	HIS	CA-C-O	6.51	129.82	120.51
1	A	41	ASN	CA-C-O	-6.47	111.60	119.43
1	A	72	ARG	CD-NE-CZ	-6.47	115.34	124.40
1	C	102	HIS	CB-CG-ND1	6.46	132.39	122.70
1	C	73	GLU	CA-C-O	-6.42	113.92	121.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	7	PHE	CA-CB-CG	6.42	120.22	113.80
1	B	108	LYS	CA-C-O	-6.39	113.46	120.81
1	C	12	ASP	N-CA-C	6.38	118.23	111.28
1	C	17	TYR	CB-CA-C	-6.31	98.66	109.65
1	A	42	LEU	N-CA-C	6.31	118.97	111.33
1	C	29	GLU	N-CA-CB	6.30	119.49	110.16
1	B	79	THR	CA-CB-OG1	-6.28	100.18	109.60
1	B	110	ARG	NE-CZ-NH1	-6.25	115.25	121.50
1	C	70	THR	CA-C-N	6.24	132.29	122.94
1	C	70	THR	C-N-CA	6.24	132.29	122.94
1	C	104	GLN	O-C-N	-6.23	113.51	122.36
1	A	29	GLU	CA-CB-CG	6.22	126.53	114.10
1	A	29	GLU	CG-CD-OE2	6.21	132.69	118.40
1	A	59	ARG	CB-CG-CD	6.21	125.58	111.30
1	A	11	ALA	N-CA-C	-6.20	104.44	111.07
1	C	88	ILE	CA-C-O	-6.20	113.65	120.72
1	B	16	THR	CA-C-N	-6.19	112.63	122.29
1	B	16	THR	C-N-CA	-6.19	112.63	122.29
1	B	93	ASP	CA-CB-CG	6.18	118.78	112.60
1	A	15	GLN	CA-C-O	-6.17	113.39	120.24
1	B	26	THR	CA-CB-OG1	-6.17	100.34	109.60
1	B	4	ILE	CA-CB-CG1	-6.14	99.95	110.40
1	A	110	ARG	NE-CZ-NH1	6.14	127.64	121.50
1	C	22	ASP	CA-CB-CG	-6.14	106.46	112.60
1	B	110	ARG	CD-NE-CZ	-6.14	115.80	124.40
1	A	72	ARG	CB-CG-CD	-6.12	97.22	111.30
1	B	42	LEU	CA-C-O	-6.11	114.08	120.55
1	C	31	GLN	CB-CG-CD	-6.11	102.22	112.60
1	A	59	ARG	CG-CD-NE	6.10	125.43	112.00
1	B	55	ILE	CA-C-O	-6.10	114.65	121.36
1	A	29	GLU	CA-C-O	6.09	126.87	120.42
1	B	4	ILE	CA-C-O	-6.06	113.31	120.76
1	B	20	LEU	O-C-N	6.05	128.19	121.53
1	A	7	PHE	O-C-N	6.05	128.38	122.09
1	B	13	TYR	CA-C-N	6.04	129.19	120.38
1	B	13	TYR	C-N-CA	6.04	129.19	120.38
1	A	109	ILE	N-CA-CB	6.03	121.19	111.23
1	B	83	ARG	NE-CZ-NH2	6.02	124.62	119.20
1	B	23	ASN	O-C-N	-6.01	113.49	122.39
1	C	45	VAL	CA-CB-CG1	-6.01	100.18	110.40
1	C	7	PHE	CA-C-N	5.99	128.59	120.44
1	C	7	PHE	C-N-CA	5.99	128.59	120.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	102	HIS	CB-CG-CD2	-5.97	123.44	131.20
1	C	17	TYR	CA-CB-CG	-5.93	103.23	113.90
1	C	42	LEU	O-C-N	5.93	128.25	122.09
1	C	72	ARG	NH1-CZ-NH2	5.92	127.00	119.30
1	C	94	TRP	N-CA-C	5.92	119.73	111.74
1	B	5	ASN	CA-C-O	-5.91	113.36	119.51
1	C	71	TRP	O-C-N	5.91	130.92	123.23
1	B	39	LYS	N-CA-CB	5.91	119.10	110.47
1	C	95	LEU	CA-C-O	-5.90	114.28	121.36
1	C	84	ASN	CB-CG-ND2	-5.90	107.56	116.40
1	C	4	ILE	N-CA-CB	-5.86	101.84	111.45
1	A	86	ASP	CA-C-O	5.86	126.81	120.43
1	C	8	ASP	O-C-N	5.85	128.41	122.09
1	A	72	ARG	O-C-N	5.85	130.25	123.17
1	A	16	THR	N-CA-CB	5.85	118.46	109.98
1	C	17	TYR	CB-CG-CD1	5.83	129.54	120.80
1	B	94	TRP	CA-C-N	5.81	129.81	121.50
1	B	94	TRP	C-N-CA	5.81	129.81	121.50
1	B	67	SER	O-C-N	5.81	130.07	122.93
1	B	12	ASP	CA-C-N	-5.80	112.71	120.54
1	B	12	ASP	C-N-CA	-5.80	112.71	120.54
1	C	61	GLY	O-C-N	5.78	127.19	122.51
1	B	8	ASP	N-CA-CB	5.77	118.99	110.33
1	B	19	LYS	CA-CB-CG	-5.76	102.59	114.10
1	C	93	ASP	CB-CA-C	5.75	120.39	111.13
1	A	19	LYS	O-C-N	5.75	129.57	123.42
1	B	3	VAL	N-CA-CB	5.74	121.26	111.50
1	A	14	LEU	CA-C-O	5.71	126.60	120.55
1	B	29	GLU	CG-CD-OE1	5.70	131.50	118.40
1	B	90	TYR	CA-C-O	5.68	126.62	120.32
1	B	106	PHE	CA-CB-CG	-5.64	108.16	113.80
1	B	41	ASN	OD1-CG-ND2	-5.62	116.97	122.60
1	A	105	THR	CA-C-O	5.62	127.12	120.66
1	C	38	SER	CA-CB-OG	-5.61	99.88	111.10
1	B	8	ASP	CA-C-N	-5.59	113.73	119.94
1	B	8	ASP	C-N-CA	-5.59	113.73	119.94
1	C	21	PRO	CA-C-N	5.58	128.32	120.28
1	C	21	PRO	C-N-CA	5.58	128.32	120.28
1	A	100	THR	CA-C-N	-5.58	112.34	122.50
1	A	100	THR	C-N-CA	-5.58	112.34	122.50
1	B	10	VAL	N-CA-C	5.57	116.34	110.72
1	C	39	LYS	O-C-N	5.56	129.29	122.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	79	THR	CA-C-N	-5.55	111.76	122.09
1	B	79	THR	C-N-CA	-5.55	111.76	122.09
1	C	12	ASP	CA-C-O	5.55	126.43	120.55
1	A	69	ARG	CA-C-O	5.54	126.31	120.54
1	C	32	ALA	O-C-N	-5.54	116.25	122.12
1	A	95	LEU	O-C-N	5.53	129.52	123.22
1	B	74	ALA	CA-C-N	5.52	128.68	120.95
1	B	74	ALA	C-N-CA	5.52	128.68	120.95
1	B	7	PHE	N-CA-CB	5.52	118.23	110.12
1	C	106	PHE	CA-C-N	5.51	130.54	122.77
1	C	106	PHE	C-N-CA	5.51	130.54	122.77
1	B	13	TYR	N-CA-C	5.51	117.72	111.11
1	B	22	ASP	CA-CB-CG	5.51	118.11	112.60
1	C	51	ILE	N-CA-CB	5.51	116.53	110.53
1	B	77	ASN	CB-CG-ND2	-5.50	108.15	116.40
1	C	110	ARG	NE-CZ-NH2	5.48	124.13	119.20
1	A	17	TYR	N-CA-C	5.47	120.22	113.50
1	A	15	GLN	O-C-N	5.46	129.33	122.23
1	B	23	ASN	CA-CB-CG	-5.46	107.14	112.60
1	C	90	TYR	CB-CG-CD2	-5.44	112.64	120.80
1	A	102	HIS	CA-C-O	-5.43	114.24	120.98
1	B	58	ASN	N-CA-C	-5.43	103.79	111.56
1	C	69	ARG	CA-C-O	5.41	126.86	120.69
1	C	72	ARG	CD-NE-CZ	5.39	131.95	124.40
1	A	38	SER	N-CA-C	5.39	118.96	112.38
1	B	79	THR	CA-C-O	-5.38	112.26	119.47
1	C	55	ILE	N-CA-CB	5.36	116.90	110.31
1	C	60	GLU	O-C-N	5.31	129.17	122.37
1	C	38	SER	N-CA-C	5.30	118.85	112.38
1	A	85	SER	CA-C-O	-5.28	113.36	119.59
1	A	72	ARG	CA-C-O	-5.27	115.44	121.40
1	B	14	LEU	N-CA-C	5.27	118.49	111.75
1	B	78	TYR	O-C-N	5.26	129.26	123.16
1	C	100	THR	CA-CB-CG2	5.26	119.44	110.50
1	B	4	ILE	CB-CA-C	5.25	116.90	111.23
1	A	105	THR	CB-CA-C	-5.25	98.96	109.35
1	B	89	LEU	O-C-N	-5.24	117.19	123.27
1	A	93	ASP	CA-C-N	5.22	129.55	122.19
1	A	93	ASP	C-N-CA	5.22	129.55	122.19
1	C	90	TYR	CB-CG-CD1	5.22	128.63	120.80
1	A	49	LYS	O-C-N	5.22	129.73	123.16
1	B	14	LEU	CA-C-O	5.21	126.04	120.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	23	ASN	CA-C-O	5.20	125.93	119.12
1	B	47	PRO	CB-CA-C	5.19	118.23	111.64
1	A	55	ILE	O-C-N	5.18	128.32	122.67
1	B	56	PHE	CB-CA-C	5.18	118.58	110.19
1	C	55	ILE	CA-CB-CG1	5.17	119.20	110.40
1	C	7	PHE	N-CA-C	5.17	116.61	111.07
1	A	79	THR	CA-C-O	-5.17	113.12	120.51
1	B	105	THR	CA-CB-OG1	-5.17	101.85	109.60
1	A	100	THR	OG1-CB-CG2	5.16	119.62	109.30
1	B	8	ASP	CB-CG-OD1	5.16	130.26	118.40
1	B	13	TYR	CB-CG-CD2	-5.16	113.07	120.80
1	C	104	GLN	OE1-CD-NE2	-5.16	117.44	122.60
1	A	6	THR	O-C-N	5.15	129.02	123.10
1	B	58	ASN	CB-CA-C	5.15	118.41	111.82
1	C	15	GLN	CA-C-N	5.14	127.62	120.63
1	C	15	GLN	C-N-CA	5.14	127.62	120.63
1	B	26	THR	N-CA-CB	-5.14	103.09	110.44
1	C	13	TYR	N-CA-CB	-5.14	102.57	110.12
1	B	69	ARG	CA-C-O	5.13	126.34	120.54
1	C	94	TRP	CA-CB-CG	-5.13	103.85	113.60
1	B	79	THR	N-CA-C	-5.13	106.36	113.18
1	B	44	ASP	CA-CB-CG	5.12	117.72	112.60
1	A	86	ASP	CB-CG-OD1	5.11	130.16	118.40
1	B	110	ARG	N-CA-CB	5.11	119.19	110.50
1	B	49	LYS	O-C-N	5.10	128.79	123.03
1	A	90	TYR	O-C-N	5.10	129.49	123.27
1	C	29	GLU	CA-C-O	-5.09	115.02	120.42
1	C	4	ILE	CA-C-O	-5.09	115.16	120.76
1	B	13	TYR	CB-CG-CD1	5.08	128.42	120.80
1	C	103	TYR	CA-CB-CG	5.07	123.03	113.90
1	A	37	ALA	CB-CA-C	5.05	119.27	110.68
1	A	93	ASP	CB-CG-OD1	5.04	129.99	118.40
1	A	8	ASP	CA-CB-CG	-5.03	107.57	112.60
1	A	72	ARG	CA-CB-CG	-5.01	104.09	114.10
1	C	91	SER	CA-C-N	5.00	127.49	120.28
1	C	91	SER	C-N-CA	5.00	127.49	120.28

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	59	ARG	Sidechain

5.2 Too-close contacts ⓘ

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	851	0	809	35	0
1	B	844	0	796	34	0
1	C	852	0	809	20	0
2	A	63	0	0	2	0
2	B	72	0	0	2	0
2	C	81	0	0	0	0
All	All	2763	0	2414	88	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 18.

All (88) 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:B:14:LEU:O	1:B:18:HIS:HA	1.75	0.86
1:A:101:ASP:O	1:A:102:HIS:HB2	1.81	0.79
1:B:101:ASP:OD2	1:B:105:THR:OG1	2.01	0.78
1:B:18:HIS:HB3	1:B:94:TRP:CZ2	2.21	0.74
1:A:14:LEU:O	1:A:18:HIS:HA	1.87	0.74
1:B:14:LEU:O	1:B:18:HIS:CA	2.37	0.73
1:A:14:LEU:HD22	1:A:94:TRP:HZ3	1.57	0.70
1:A:36:VAL:HB	1:A:39:LYS:HG3	1.73	0.70
1:A:13:TYR:CE2	1:A:17:TYR:CE2	2.80	0.69
1:C:66:LYS:NZ	1:C:93:ASP:OD2	2.26	0.68
1:C:74:ALA:HB3	1:C:88:ILE:HG22	1.77	0.66
1:A:26:THR:OG1	1:A:29:GLU:HG3	1.96	0.66
1:C:63:LEU:HD11	1:C:89:LEU:HD22	1.78	0.65
1:B:56:PHE:CE2	1:B:63:LEU:HD12	2.31	0.65
1:B:69:ARG:HG3	1:B:91:SER:HB2	1.79	0.65
1:B:89:LEU:HD13	1:B:106:PHE:HE1	1.61	0.64
1:B:56:PHE:HE2	1:B:63:LEU:HD12	1.63	0.62
1:B:77:ASN:ND2	1:B:86:ASP:OD2	2.27	0.61
1:C:3:VAL:C	1:C:4:ILE:HD12	2.25	0.60
1:C:26:THR:OG1	1:C:29:GLU:HG3	2.02	0.59
1:B:5:ASN:HB2	2:B:123:HOH:O	2.02	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:7:PHE:CE1	1:B:98:LYS:HB2	2.38	0.59
1:B:64:PRO:O	1:B:69:ARG:NH1	2.36	0.59
1:B:14:LEU:O	1:B:18:HIS:N	2.36	0.58
1:B:96:ILE:HG13	1:B:110:ARG:HB2	1.85	0.57
1:C:28:SER:HA	1:C:31:GLN:HE21	1.68	0.57
1:A:13:TYR:CD2	1:A:17:TYR:CE2	2.93	0.57
1:C:56:PHE:CD2	1:C:89:LEU:CD2	2.88	0.57
1:B:13:TYR:HD1	1:B:19:LYS:O	1.88	0.56
1:A:90:TYR:HA	1:A:95:LEU:O	2.06	0.56
1:C:98:LYS:HG2	1:C:109:ILE:HG21	1.88	0.55
1:A:56:PHE:CE2	1:A:63:LEU:HD12	2.42	0.55
1:B:108:LYS:HD3	1:C:45:VAL:HA	1.87	0.54
1:A:101:ASP:O	1:A:102:HIS:CB	2.50	0.54
1:A:71:TRP:CH2	1:A:91:SER:HB3	2.42	0.54
1:B:3:VAL:HG12	1:B:23:ASN:HB3	1.89	0.53
1:C:4:ILE:HG21	1:C:9:GLY:C	2.32	0.53
1:A:25:ILE:HG23	1:A:49:LYS:HD2	1.89	0.53
1:B:63:LEU:HD11	1:B:89:LEU:HD22	1.90	0.53
1:C:56:PHE:CG	1:C:89:LEU:HD21	2.44	0.53
1:A:13:TYR:HD1	1:A:19:LYS:O	1.91	0.52
1:B:13:TYR:CD1	1:B:19:LYS:O	2.62	0.52
1:A:55:ILE:HD13	1:A:72:ARG:HG3	1.90	0.52
1:A:43:ALA:HB3	2:A:139:HOH:O	2.07	0.52
1:B:74:ALA:HB3	1:B:88:ILE:CG2	2.40	0.51
1:A:14:LEU:O	1:A:18:HIS:CA	2.57	0.51
1:A:71:TRP:CZ3	1:A:91:SER:HB3	2.44	0.51
1:C:98:LYS:HG2	1:C:109:ILE:CG2	2.40	0.51
1:B:46:ALA:HB1	1:B:49:LYS:HG3	1.93	0.50
1:A:71:TRP:O	1:A:72:ARG:HG3	2.12	0.49
1:A:13:TYR:CD1	1:A:19:LYS:O	2.65	0.49
1:B:18:HIS:HB3	1:B:94:TRP:CE2	2.47	0.49
1:A:23:ASN:O	1:A:49:LYS:HD3	2.12	0.49
1:B:35:TRP:CD1	1:B:42:LEU:HB2	2.47	0.49
1:A:4:ILE:HD12	1:A:21:PRO:HB3	1.95	0.48
1:A:87:ARG:HB2	1:A:99:THR:HG22	1.96	0.48
1:B:56:PHE:HB2	1:B:73:GLU:HG2	1.95	0.48
1:B:101:ASP:CG	1:B:105:THR:OG1	2.57	0.48
1:C:87:ARG:HG3	1:C:103:TYR:CE1	2.49	0.48
1:C:106:PHE:CD1	1:C:106:PHE:N	2.82	0.48
1:B:52:GLY:HA2	1:B:74:ALA:HA	1.95	0.47
1:A:13:TYR:CD2	1:A:17:TYR:HE2	2.32	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:74:ALA:HB3	1:B:88:ILE:HG22	1.97	0.47
1:A:89:LEU:HD13	1:A:106:PHE:HE2	1.81	0.46
1:A:24:TYR:HA	1:A:50:SER:O	2.16	0.46
1:B:64:PRO:HG2	1:B:71:TRP:HZ2	1.81	0.46
1:B:89:LEU:HD13	1:B:106:PHE:CE1	2.48	0.46
1:A:89:LEU:HD13	1:A:106:PHE:CE2	2.51	0.45
1:B:43:ALA:O	1:B:47:PRO:HG3	2.16	0.45
1:C:98:LYS:H	1:C:98:LYS:HG3	1.64	0.45
1:A:56:PHE:HE2	1:A:63:LEU:HD12	1.81	0.45
1:C:74:ALA:HB3	1:C:88:ILE:CG2	2.44	0.44
1:A:56:PHE:CG	1:A:89:LEU:HD21	2.53	0.44
1:C:27:LYS:O	1:C:31:GLN:HG3	2.18	0.44
1:A:20:LEU:HA	1:A:21:PRO:HD3	1.86	0.43
1:A:14:LEU:O	1:A:18:HIS:N	2.52	0.43
1:A:98:LYS:O	1:A:98:LYS:HG3	2.16	0.42
1:B:9:GLY:HA3	2:B:146:HOH:O	2.20	0.42
1:B:90:TYR:HA	1:B:95:LEU:O	2.20	0.42
1:B:51:ILE:O	1:B:75:ASP:HB2	2.19	0.41
1:A:13:TYR:CZ	1:A:17:TYR:CD2	3.08	0.41
1:C:63:LEU:CD1	1:C:89:LEU:HD22	2.47	0.41
1:C:52:GLY:HA2	1:C:74:ALA:HA	2.03	0.41
1:A:29:GLU:HA	2:A:158:HOH:O	2.20	0.41
1:A:7:PHE:CE1	1:A:98:LYS:HB2	2.55	0.41
1:A:85:SER:HB3	1:A:102:HIS:CE1	2.56	0.41
1:C:69:ARG:HA	1:C:92:SER:OG	2.22	0.40
1:B:101:ASP:CG	1:B:105:THR:H	2.29	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	106/110 (96%)	101 (95%)	5 (5%)	0	100	100
1	B	106/110 (96%)	100 (94%)	5 (5%)	1 (1%)	14	10
1	C	106/110 (96%)	106 (100%)	0	0	100	100
All	All	318/330 (96%)	307 (96%)	10 (3%)	1 (0%)	36	36

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	19	LYS

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	87/92 (95%)	77 (88%)	10 (12%)	5	3
1	B	86/92 (94%)	79 (92%)	7 (8%)	11	8
1	C	88/92 (96%)	83 (94%)	5 (6%)	18	17
All	All	261/276 (95%)	239 (92%)	22 (8%)	10	7

All (22) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	22	ASP
1	A	38	SER
1	A	59	ARG
1	A	67	SER
1	A	70	THR
1	A	89	LEU
1	A	92	SER
1	A	93	ASP
1	A	98	LYS
1	A	105	THR
1	B	49	LYS
1	B	55	ILE

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Mol	Chain	Res	Type
1	B	67	SER
1	B	92	SER
1	B	96	ILE
1	B	103	TYR
1	B	105	THR
1	C	8	ASP
1	C	66	LYS
1	C	89	LEU
1	C	96	ILE
1	C	98	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (4) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	15	GLN
1	B	31	GLN
1	C	18	HIS
1	C	31	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.