



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 07:47 AM UTC

PDB ID : 1BNJ / pdb_00001bnj
Title : BARNASE WILDTYPE STRUCTURE AT PH 9.0
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

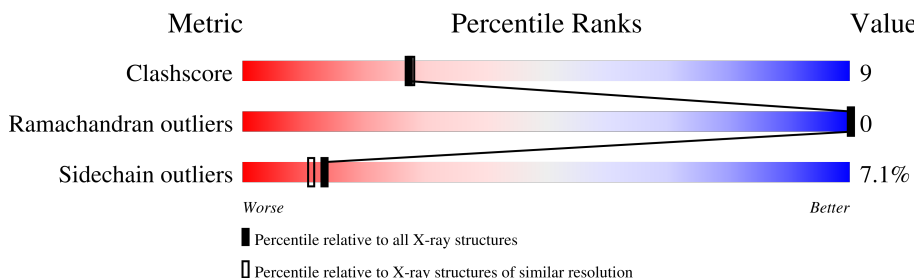
1 Overall quality at a glance

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	42% 41% 15% ..
1	B	110	36% 49% 10% ..
1	C	110	43% 46% 8% .

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 2800 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	109	Total	C	N	O	8	1	1
			863	548	151	164			
1	B	108	Total	C	N	O	2	1	0
			858	545	147	166			
1	C	107	Total	C	N	O	5	1	0
			860	545	150	165			

- Molecule 2 is water.

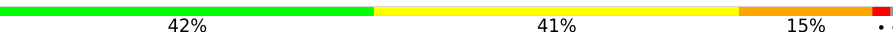
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	61	Total	O	0	0
			61	61		
2	B	78	Total	O	0	0
			78	78		
2	C	80	Total	O	0	0
			80	80		

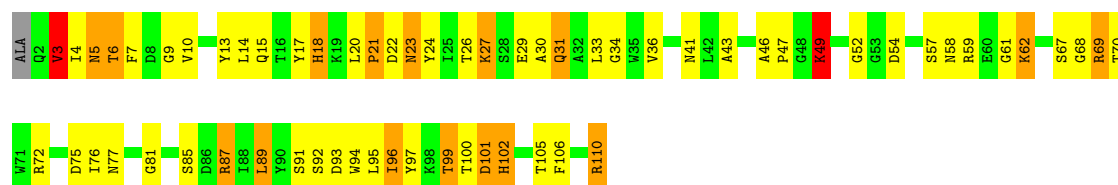
3 Residue-property plots

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.

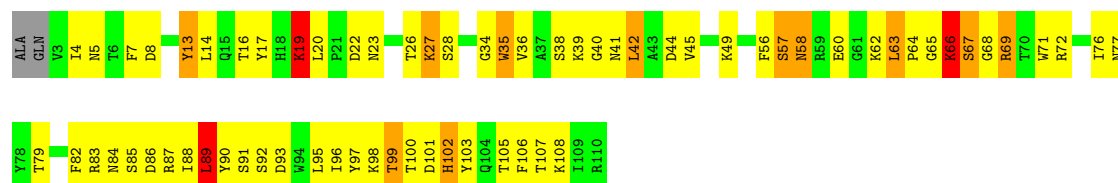
• Molecule 1: BARNASE

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	59.53Å 59.53Å 81.67Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	10.00 – 2.10	Depositor
% Data completeness (in resolution range)	83.7 (10.00-2.10)	Depositor
R_{merge}	0.05	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	PROLSQ	Depositor
R, R_{free}	0.159 , (Not available)	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	2800	wwPDB-VP
Average B, all atoms (Å ²)	13.0	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	1.48	1/890 (0.1%)	2.89	101/1204 (8.4%)
1	B	1.47	2/884 (0.2%)	2.74	90/1196 (7.5%)
1	C	1.48	2/886 (0.2%)	2.83	95/1198 (7.9%)
All	All	1.48	5/2660 (0.2%)	2.82	286/3598 (7.9%)

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	66	LYS	CE-NZ	-12.16	1.12	1.49
1	C	59	ARG	CG-CD	-8.62	1.26	1.52
1	C	11	ALA	N-CA	6.20	1.53	1.46
1	B	40	GLY	C-O	5.70	1.31	1.24
1	A	59	ARG	CB-CG	-5.46	1.36	1.52

All (286) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	3	VAL	N-CA-CB	13.95	126.38	111.46
1	C	41	ASN	OD1-CG-ND2	-12.80	109.80	122.60
1	C	56	PHE	CA-C-O	12.66	134.24	120.32
1	A	72	ARG	NE-CZ-NH2	-12.57	107.89	119.20
1	C	59	ARG	CB-CG-CD	12.35	139.71	111.30
1	A	7	PHE	CA-C-O	-11.31	108.79	120.90
1	A	23	ASN	OD1-CG-ND2	11.30	133.90	122.60
1	A	41	ASN	OD1-CG-ND2	-11.26	111.34	122.60
1	C	102	HIS	CB-CG-CD2	-10.57	117.45	131.20
1	C	18	HIS	CA-CB-CG	-10.50	103.30	113.80
1	A	20	LEU	O-C-N	10.29	132.50	121.60
1	A	67	SER	CA-C-O	10.03	132.35	120.92
1	B	5	ASN	OD1-CG-ND2	-9.94	112.66	122.60
1	B	5	ASN	CB-CG-ND2	9.89	131.24	116.40
1	A	102	HIS	CA-CB-CG	-9.89	103.91	113.80
1	B	8	ASP	CA-C-N	-9.86	109.03	119.98

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	8	ASP	C-N-CA	-9.86	109.03	119.98
1	C	104	GLN	OE1-CD-NE2	-9.80	112.80	122.60
1	C	34	GLY	CA-C-O	-9.80	108.37	118.86
1	C	59	ARG	CA-C-O	-9.58	110.39	120.55
1	C	80	SER	CA-C-O	-9.56	111.05	121.28
1	C	94	TRP	N-CA-C	9.39	124.42	111.74
1	A	20	LEU	CA-C-O	-9.33	110.61	120.87
1	A	61	GLY	CA-C-O	-9.31	108.54	119.80
1	C	41	ASN	CA-C-O	-9.22	108.81	119.78
1	A	7	PHE	O-C-N	9.20	131.66	122.09
1	B	19	LYS	CD-CE-NZ	9.15	141.17	111.90
1	A	72	ARG	NH1-CZ-NH2	9.12	131.16	119.30
1	B	22	ASP	CA-C-O	-9.12	108.46	119.49
1	A	101	ASP	CA-C-N	-8.97	109.25	122.35
1	A	101	ASP	C-N-CA	-8.97	109.25	122.35
1	B	83	ARG	CD-NE-CZ	-8.94	111.88	124.40
1	C	6	THR	O-C-N	8.91	133.10	123.03
1	A	102	HIS	CB-CG-CD2	-8.85	119.70	131.20
1	C	28	SER	CA-C-O	-8.81	110.14	120.10
1	A	105	THR	CA-C-O	8.72	131.17	121.06
1	B	63	LEU	CA-C-O	-8.55	111.82	120.63
1	B	17	TYR	CA-CB-CG	-8.46	98.67	113.90
1	B	57	SER	CA-C-O	-8.45	111.95	120.82
1	B	72	ARG	O-C-N	8.43	133.04	123.27
1	B	64	PRO	CA-C-O	8.37	130.72	120.92
1	B	76	ILE	O-C-N	8.27	131.71	123.03
1	A	110	ARG	NE-CZ-NH2	8.26	126.64	119.20
1	A	5	ASN	CB-CG-ND2	8.17	128.65	116.40
1	A	101	ASP	CA-C-O	-8.11	112.76	121.20
1	B	88	ILE	O-C-N	-8.11	114.03	123.03
1	B	71	TRP	O-C-N	8.10	133.36	123.16
1	B	108	LYS	CA-C-O	-8.03	111.58	120.81
1	C	6	THR	CA-C-O	-7.94	111.97	121.66
1	A	3	VAL	CB-CA-C	-7.90	102.74	111.35
1	B	27	LYS	CA-C-N	7.88	131.05	120.65
1	B	27	LYS	C-N-CA	7.88	131.05	120.65
1	B	66	LYS	CD-CE-NZ	7.85	137.01	111.90
1	B	93	ASP	CA-C-O	-7.78	110.45	119.56
1	C	39	LYS	CA-C-O	-7.75	110.44	119.59
1	A	3	VAL	O-C-N	7.69	131.26	122.64
1	A	47	PRO	CA-C-O	-7.67	112.96	121.32
1	B	77	ASN	OD1-CG-ND2	7.63	130.23	122.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	7	PHE	CA-CB-CG	7.59	121.39	113.80
1	A	18	HIS	CA-CB-CG	-7.58	106.22	113.80
1	C	31	GLN	OE1-CD-NE2	-7.45	115.15	122.60
1	A	57	SER	CB-CA-C	7.44	123.15	110.79
1	A	57	SER	N-CA-CB	-7.44	99.18	110.12
1	B	89	LEU	CA-C-O	-7.43	112.15	120.32
1	C	25	ILE	CA-C-O	-7.37	112.73	121.28
1	B	72	ARG	NE-CZ-NH1	-7.26	114.24	121.50
1	A	29	GLU	CA-C-N	7.25	130.30	120.44
1	A	29	GLU	C-N-CA	7.25	130.30	120.44
1	A	102	HIS	CB-CG-ND1	7.22	133.53	122.70
1	C	76	ILE	O-C-N	7.18	130.57	123.03
1	B	34	GLY	O-C-N	7.14	129.94	122.51
1	A	17	TYR	CA-CB-CG	-7.14	101.05	113.90
1	C	77	ASN	CA-C-N	-7.14	111.53	122.09
1	C	77	ASN	C-N-CA	-7.14	111.53	122.09
1	A	100	THR	N-CA-C	-7.11	102.91	112.94
1	A	102	HIS	N-CA-C	7.08	121.41	111.92
1	A	13	TYR	N-CA-CB	-7.04	99.74	110.16
1	B	8	ASP	O-C-N	6.99	130.11	122.15
1	B	66	LYS	CA-C-O	6.98	128.70	121.23
1	A	4	ILE	CA-C-O	-6.98	112.67	120.97
1	B	99	THR	CA-CB-OG1	-6.95	99.17	109.60
1	C	71	TRP	CA-C-O	-6.95	113.34	120.71
1	A	17	TYR	CA-C-O	-6.94	111.24	119.15
1	A	72	ARG	CD-NE-CZ	-6.93	114.70	124.40
1	B	28	SER	CA-CB-OG	-6.92	97.26	111.10
1	C	8	ASP	CA-CB-CG	-6.91	105.69	112.60
1	C	29	GLU	CG-CD-OE1	6.91	134.29	118.40
1	A	77	ASN	CA-C-O	-6.90	112.25	120.81
1	B	88	ILE	CA-C-N	6.90	132.71	123.05
1	B	88	ILE	C-N-CA	6.90	132.71	123.05
1	C	95	LEU	N-CA-C	-6.85	100.34	110.48
1	A	6	THR	N-CA-CB	6.85	121.80	110.63
1	B	41	ASN	N-CA-CB	-6.84	100.51	110.70
1	C	57	SER	CA-C-O	-6.84	113.82	121.00
1	A	100	THR	CA-C-N	-6.83	110.10	122.54
1	A	100	THR	C-N-CA	-6.83	110.10	122.54
1	A	17	TYR	O-C-N	6.83	131.37	122.42
1	A	30	ALA	N-CA-C	-6.78	103.82	111.14
1	C	16	THR	CA-C-O	6.77	127.79	120.55
1	B	95	LEU	N-CA-C	-6.69	99.12	109.76

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	6	THR	O-C-N	6.65	130.74	123.10
1	B	41	ASN	N-CA-C	6.62	120.27	112.72
1	C	110	ARG	NE-CZ-NH1	-6.62	114.88	121.50
1	B	72	ARG	CA-C-O	-6.62	113.39	121.06
1	B	4	ILE	CA-C-O	-6.61	113.10	120.97
1	B	101	ASP	CA-C-O	-6.61	113.66	121.32
1	C	67	SER	N-CA-CB	6.60	119.69	109.85
1	A	9	GLY	O-C-N	6.58	128.50	122.18
1	C	34	GLY	O-C-N	6.58	132.19	121.53
1	C	22	ASP	CA-CB-CG	-6.57	106.03	112.60
1	A	36	VAL	CA-C-O	-6.55	113.27	120.48
1	B	16	THR	N-CA-CB	6.54	120.32	110.19
1	A	93	ASP	CA-C-N	6.53	131.40	122.19
1	A	93	ASP	C-N-CA	6.53	131.40	122.19
1	C	36	VAL	O-C-N	6.51	130.60	122.66
1	A	33	LEU	CB-CA-C	-6.50	99.57	110.56
1	A	36	VAL	O-C-N	6.49	129.93	122.99
1	C	74	ALA	CA-C-O	-6.48	113.74	120.99
1	C	107	THR	CA-CB-OG1	-6.46	99.92	109.60
1	B	85	SER	CA-C-O	-6.45	112.02	119.56
1	B	93	ASP	CA-CB-CG	6.45	119.05	112.60
1	A	81	GLY	CA-C-O	6.42	132.24	122.28
1	B	79	THR	N-CA-C	-6.42	104.64	113.18
1	A	96	ILE	CA-CB-CG1	6.39	121.26	110.40
1	A	41	ASN	CB-CG-ND2	6.38	125.98	116.40
1	B	82	PHE	CA-C-O	-6.38	114.61	121.56
1	C	31	GLN	N-CA-CB	6.38	119.44	109.94
1	C	41	ASN	CA-CB-CG	6.35	118.95	112.60
1	A	22	ASP	O-C-N	6.32	131.75	122.39
1	B	13	TYR	CB-CG-CD2	-6.30	111.35	120.80
1	B	64	PRO	CA-C-N	6.29	127.67	121.57
1	B	64	PRO	C-N-CA	6.29	127.67	121.57
1	A	110	ARG	NE-CZ-NH1	-6.27	115.23	121.50
1	B	16	THR	CB-CA-C	-6.26	99.10	110.56
1	B	58	ASN	N-CA-C	-6.26	104.94	112.58
1	C	97	TYR	CA-C-N	-6.26	112.76	122.59
1	C	97	TYR	C-N-CA	-6.26	112.76	122.59
1	A	30	ALA	CA-C-O	-6.25	114.26	120.70
1	A	4	ILE	O-C-N	6.25	131.27	122.59
1	C	88	ILE	CA-C-N	6.24	131.78	122.99
1	C	88	ILE	C-N-CA	6.24	131.78	122.99
1	C	65	GLY	CA-C-O	6.23	127.96	121.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	41	ASN	N-CA-C	6.19	119.78	112.72
1	C	48	GLY	O-C-N	-6.18	114.53	122.39
1	C	76	ILE	CA-C-O	-6.14	113.21	121.32
1	C	79	THR	CA-CB-CG2	6.14	120.95	110.50
1	A	95	LEU	N-CA-C	-6.14	99.99	109.76
1	B	42	LEU	CA-C-N	6.14	129.12	120.28
1	B	42	LEU	C-N-CA	6.14	129.12	120.28
1	C	18	HIS	CB-CG-CD2	-6.13	123.23	131.20
1	A	101	ASP	O-C-N	6.12	129.58	121.99
1	C	72	ARG	NE-CZ-NH2	-6.11	113.70	119.20
1	B	34	GLY	N-CA-C	-6.07	106.05	116.01
1	C	80	SER	CA-CB-OG	-6.07	98.95	111.10
1	C	91	SER	O-C-N	6.05	129.86	122.84
1	A	22	ASP	CA-CB-CG	6.04	118.64	112.60
1	C	39	LYS	O-C-N	6.04	129.44	122.25
1	C	35	TRP	CG-CD2-CE3	-6.03	127.87	133.90
1	C	61	GLY	CA-C-N	6.02	129.46	120.31
1	C	61	GLY	C-N-CA	6.02	129.46	120.31
1	B	101	ASP	CA-CB-CG	6.00	118.60	112.60
1	A	22	ASP	N-CA-C	6.00	120.46	113.20
1	B	108	LYS	O-C-N	-6.00	115.55	122.93
1	B	35	TRP	CA-C-O	-6.00	113.91	120.81
1	C	6	THR	CA-CB-OG1	-5.99	100.62	109.60
1	A	100	THR	N-CA-CB	5.98	120.84	110.98
1	B	95	LEU	N-CA-CB	5.97	119.20	109.95
1	B	4	ILE	N-CA-CB	5.96	118.76	111.60
1	C	60	GLU	N-CA-C	5.92	120.12	113.02
1	C	104	GLN	CG-CD-NE2	5.92	125.28	116.40
1	C	110	ARG	N-CA-CB	5.92	120.56	110.50
1	C	72	ARG	CA-C-O	-5.90	114.74	121.58
1	C	107	THR	CA-CB-CG2	5.88	120.50	110.50
1	A	76	ILE	O-C-N	5.88	129.20	123.03
1	B	89	LEU	CB-CA-C	5.85	119.79	110.19
1	C	102	HIS	CA-CB-CG	-5.85	107.95	113.80
1	C	82	PHE	N-CA-C	-5.85	102.81	110.53
1	C	88	ILE	N-CA-C	-5.84	100.06	108.53
1	A	43	ALA	CA-C-O	-5.83	112.21	119.38
1	A	15	GLN	OE1-CD-NE2	5.81	128.41	122.60
1	C	100	THR	N-CA-C	-5.80	104.77	112.94
1	B	14	LEU	N-CA-C	5.79	118.06	111.11
1	A	22	ASP	CB-CA-C	-5.77	99.14	110.11
1	C	102	HIS	CB-CG-ND1	5.76	131.35	122.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	81	GLY	CA-C-N	5.76	131.46	120.97
1	C	81	GLY	C-N-CA	5.76	131.46	120.97
1	B	44	ASP	CA-C-O	-5.76	114.31	120.42
1	B	38	SER	N-CA-CB	5.76	120.47	110.39
1	A	87	ARG	NE-CZ-NH2	5.72	124.35	119.20
1	C	95	LEU	CA-C-O	-5.72	114.89	121.47
1	A	97	TYR	CA-C-O	5.68	128.11	121.46
1	C	19	LYS	CA-C-O	-5.68	114.85	121.10
1	B	62	LYS	CG-CD-CE	5.67	124.35	111.30
1	B	19	LYS	CB-CA-C	5.67	119.95	110.43
1	B	8	ASP	CB-CG-OD1	5.66	131.43	118.40
1	C	89	LEU	CD1-CG-CD2	5.66	123.26	110.80
1	A	9	GLY	CA-C-N	-5.66	112.38	120.42
1	A	9	GLY	C-N-CA	-5.66	112.38	120.42
1	B	34	GLY	CA-C-O	-5.63	113.48	118.77
1	C	110	ARG	CA-CB-CG	5.62	125.33	114.10
1	B	69	ARG	N-CA-CB	5.60	119.55	110.42
1	A	34	GLY	CA-C-O	-5.60	112.91	118.96
1	A	69	ARG	CA-C-O	5.59	126.47	120.32
1	C	93	ASP	CB-CA-C	5.58	120.00	111.02
1	A	52	GLY	CA-C-N	-5.57	113.83	122.69
1	A	52	GLY	C-N-CA	-5.57	113.83	122.69
1	A	23	ASN	N-CA-C	-5.56	106.47	113.20
1	C	36	VAL	N-CA-CB	5.56	118.87	112.15
1	A	72	ARG	CG-CD-NE	-5.55	99.78	112.00
1	A	14	LEU	N-CA-C	5.54	117.00	111.07
1	A	6	THR	CA-C-N	5.54	128.02	120.54
1	A	6	THR	C-N-CA	5.54	128.02	120.54
1	A	68	GLY	CA-C-O	5.53	125.42	119.06
1	B	97	TYR	CA-C-N	-5.53	113.91	122.59
1	B	97	TYR	C-N-CA	-5.53	113.91	122.59
1	A	5	ASN	CA-C-O	5.52	126.18	119.78
1	C	7	PHE	O-C-N	-5.48	116.31	122.12
1	C	42	LEU	CA-C-O	-5.48	115.03	120.90
1	B	67	SER	O-C-N	5.47	129.87	122.59
1	C	60	GLU	CA-CB-CG	-5.46	103.19	114.10
1	B	26	THR	CA-CB-OG1	-5.46	101.42	109.60
1	B	108	LYS	CA-CB-CG	-5.44	103.22	114.10
1	C	17	TYR	CA-CB-CG	-5.42	104.15	113.90
1	C	71	TRP	CH2-CZ2-CE2	-5.42	110.46	117.50
1	B	45	VAL	CG1-CB-CG2	-5.42	98.89	110.80
1	B	76	ILE	CA-C-O	-5.40	114.19	121.32

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	14	LEU	CA-C-O	5.40	126.49	120.82
1	B	13	TYR	CB-CG-CD1	5.40	128.90	120.80
1	B	5	ASN	CA-CB-CG	5.40	118.00	112.60
1	B	17	TYR	N-CA-CB	5.40	118.57	110.53
1	C	87	ARG	CD-NE-CZ	-5.39	116.85	124.40
1	A	81	GLY	O-C-N	-5.39	117.78	122.90
1	A	21	PRO	O-C-N	-5.38	116.19	122.86
1	A	31	GLN	CA-CB-CG	-5.38	103.35	114.10
1	B	105	THR	CA-CB-CG2	5.38	119.64	110.50
1	B	102	HIS	CB-CA-C	-5.37	104.66	111.86
1	B	35	TRP	O-C-N	5.37	129.53	122.93
1	A	49	LYS	CB-CA-C	-5.34	100.49	109.83
1	A	59	ARG	NE-CZ-NH2	5.34	124.00	119.20
1	B	56	PHE	CB-CA-C	5.33	118.94	110.19
1	B	107	THR	CA-CB-CG2	5.33	119.56	110.50
1	B	72	ARG	NH1-CZ-NH2	5.33	126.22	119.30
1	A	17	TYR	CB-CG-CD1	-5.32	112.82	120.80
1	A	85	SER	CA-CB-OG	-5.31	100.48	111.10
1	A	76	ILE	CA-CB-CG2	5.31	119.52	110.50
1	B	66	LYS	N-CA-C	5.29	116.89	108.79
1	C	56	PHE	CA-C-N	5.29	127.63	120.65
1	C	56	PHE	C-N-CA	5.29	127.63	120.65
1	B	20	LEU	CA-C-O	-5.27	115.21	120.64
1	C	102	HIS	CG-CD2-NE2	-5.25	101.95	107.20
1	A	93	ASP	CB-CG-OD1	5.24	130.45	118.40
1	C	85	SER	O-C-N	5.24	129.03	122.22
1	A	58	ASN	OD1-CG-ND2	5.23	127.83	122.60
1	B	101	ASP	O-C-N	5.23	128.89	121.83
1	B	90	TYR	CG-CD2-CE2	-5.22	113.36	121.20
1	A	15	GLN	O-C-N	5.22	129.42	122.43
1	B	60	GLU	CG-CD-OE1	5.22	130.41	118.40
1	B	26	THR	CA-CB-CG2	5.20	119.34	110.50
1	A	6	THR	CA-C-O	-5.20	115.14	121.28
1	A	13	TYR	CA-C-O	5.20	125.93	120.42
1	A	72	ARG	CA-C-O	-5.19	115.56	121.58
1	C	30	ALA	CA-C-N	5.18	127.53	120.54
1	C	30	ALA	C-N-CA	5.18	127.53	120.54
1	B	84	ASN	OD1-CG-ND2	-5.15	117.45	122.60
1	C	102	HIS	ND1-CG-CD2	5.10	111.20	106.10
1	A	99	THR	CA-CB-OG1	-5.09	101.96	109.60
1	B	36	VAL	CB-CA-C	5.09	117.61	110.99
1	C	65	GLY	O-C-N	-5.08	117.11	123.21

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	100	THR	CA-C-N	-5.08	113.53	123.13
1	C	100	THR	C-N-CA	-5.08	113.53	123.13
1	A	67	SER	O-C-N	-5.07	116.66	122.95
1	A	57	SER	CA-C-O	-5.06	115.18	120.55
1	C	69	ARG	CA-C-N	-5.06	114.86	122.81
1	C	69	ARG	C-N-CA	-5.06	114.86	122.81
1	B	68	GLY	O-C-N	5.06	127.36	122.41
1	C	57	SER	CA-CB-OG	-5.05	101.00	111.10
1	C	13	TYR	CB-CG-CD2	-5.05	113.22	120.80
1	B	65	GLY	CA-C-O	5.05	125.62	121.18
1	C	59	ARG	NE-CZ-NH2	5.04	123.74	119.20
1	A	13	TYR	O-C-N	-5.03	116.41	122.15
1	B	36	VAL	CA-CB-CG1	5.03	118.94	110.40
1	C	6	THR	CA-C-N	-5.02	113.55	120.28
1	C	6	THR	C-N-CA	-5.02	113.55	120.28
1	A	75	ASP	CA-C-O	-5.02	115.33	121.05
1	C	93	ASP	CA-CB-CG	5.01	117.61	112.60
1	A	23	ASN	CB-CG-ND2	-5.00	108.90	116.40

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	863	0	835	18	0
1	B	858	0	825	20	0
1	C	860	0	833	8	0
2	A	61	0	0	2	0
2	B	78	0	0	1	0
2	C	80	0	0	3	0
All	All	2800	0	2493	46	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 9.

All (46) 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:98[A]:LYS:NZ	1:B:100:THR:HG23	1.79	0.96
1:A:89:LEU:HD13	1:A:106:PHE:CE1	2.09	0.88
1:A:89:LEU:HD13	1:A:106:PHE:HE1	1.40	0.87
1:B:98[A]:LYS:HZ3	1:B:100:THR:HG23	1.47	0.78
1:A:18:HIS:HB3	1:A:94:TRP:CZ2	2.26	0.71
1:B:27:LYS:NZ	2:B:142:HOH:O	2.23	0.70
1:B:63:LEU:HD11	1:B:89:LEU:HD22	1.80	0.64
1:A:96:ILE:HB	1:A:110:ARG:HB2	1.84	0.60
1:B:89:LEU:HD13	1:B:106:PHE:HE1	1.67	0.59
1:A:87:ARG:HB2	1:A:99:THR:CG2	2.33	0.58
1:B:86:ASP:C	1:B:87:ARG:HG2	2.31	0.55
1:B:98[A]:LYS:HZ1	1:B:100:THR:HG23	1.66	0.55
1:A:89:LEU:CD1	1:A:106:PHE:HE1	2.16	0.54
1:A:46:ALA:HB1	1:A:49:LYS:HG3	1.88	0.54
1:A:69:ARG:HG3	1:A:91:SER:HB2	1.90	0.54
1:A:3:VAL:HG12	1:A:23:ASN:CB	2.40	0.52
1:B:7:PHE:CE1	1:B:98[B]:LYS:HB2	2.45	0.52
1:B:98[A]:LYS:NZ	1:B:100:THR:CG2	2.65	0.52
1:B:87:ARG:HB2	1:B:99:THR:HG22	1.92	0.51
1:C:57:SER:HB2	2:C:129:HOH:O	2.12	0.50
1:C:27:LYS:O	1:C:31:GLN:HG3	2.13	0.49
1:C:89:LEU:HD13	1:C:106:PHE:CE1	2.48	0.48
1:A:62:LYS:HZ2	1:A:62:LYS:HG2	1.56	0.48
1:B:7:PHE:CE1	1:B:98[A]:LYS:HB2	2.49	0.48
1:B:35:TRP:CD1	1:B:42:LEU:HB2	2.50	0.47
1:B:87:ARG:HB2	1:B:99:THR:CG2	2.45	0.47
1:C:27:LYS:HE2	2:C:143:HOH:O	2.15	0.46
1:C:70:THR:O	1:C:91:SER:HA	2.15	0.46
1:B:23:ASN:O	1:B:49:LYS:HA	2.15	0.46
1:C:95:LEU:C	1:C:96:ILE:HG12	2.39	0.46
1:A:62:LYS:CD	2:A:129:HOH:O	2.65	0.45
1:A:26:THR:HB	1:A:54:ASP:OD1	2.17	0.45
1:B:13:TYR:HD1	1:B:19:LYS:O	2.01	0.44
1:A:6:THR:O	1:A:10:VAL:HG23	2.16	0.44
1:B:69:ARG:HG3	1:B:91:SER:HB2	2.00	0.44
1:B:98[A]:LYS:HZ1	1:B:100:THR:CG2	2.31	0.43
1:B:66:LYS:HG2	1:B:67:SER:H	1.82	0.43
1:B:89:LEU:HD13	1:B:106:PHE:CE1	2.51	0.43
1:A:101:ASP:O	1:A:102:HIS:HB2	2.18	0.43
1:A:5:ASN:HB2	2:A:122:HOH:O	2.18	0.42
1:C:109:ILE:O	1:C:110:ARG:HD3	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:57:SER:O	1:B:58:ASN:HB3	2.20	0.42
1:A:31:GLN:HE21	1:A:31:GLN:HB2	1.66	0.41
1:C:43:ALA:HA	2:C:154:HOH:O	2.20	0.41
1:A:21:PRO:HD2	1:A:24:TYR:CD2	2.56	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	108/110 (98%)	105 (97%)	3 (3%)	0	100	100
1	B	107/110 (97%)	105 (98%)	2 (2%)	0	100	100
1	C	106/110 (96%)	103 (97%)	3 (3%)	0	100	100
All	All	321/330 (97%)	313 (98%)	8 (2%)	0	100	100

There are no Ramachandran outliers to report.

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	91/92 (99%)	83 (91%)	8 (9%)	9	7
1	B	90/92 (98%)	82 (91%)	8 (9%)	9	6
1	C	91/92 (99%)	87 (96%)	4 (4%)	25	26

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
All	All	272/276 (99%)	252 (93%)	20 (7%)	13	10

All (20) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	3	VAL
1	A	27[A]	LYS
1	A	27[B]	LYS
1	A	49	LYS
1	A	62	LYS
1	A	70	THR
1	A	89	LEU
1	A	92	SER
1	B	19	LYS
1	B	39	LYS
1	B	66	LYS
1	B	89	LEU
1	B	92	SER
1	B	96	ILE
1	B	102	HIS
1	B	103	TYR
1	C	4	ILE
1	C	67	SER
1	C	96	ILE
1	C	102	HIS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (7) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	15	GLN
1	A	31	GLN
1	B	15	GLN
1	B	31	GLN
1	B	77	ASN
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 [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.