



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 11:22 AM UTC

PDB ID : 1BSD / pdb_00001bsd
Title : CRYSTAL STRUCTURAL ANALYSIS OF MUTATIONS IN THE HYDROPHOBIC CORES OF BARNASE
Authors : Buckle, A.M.; Henrick, K.; Fersht, A.R.
Deposited on : 1993-07-19
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

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

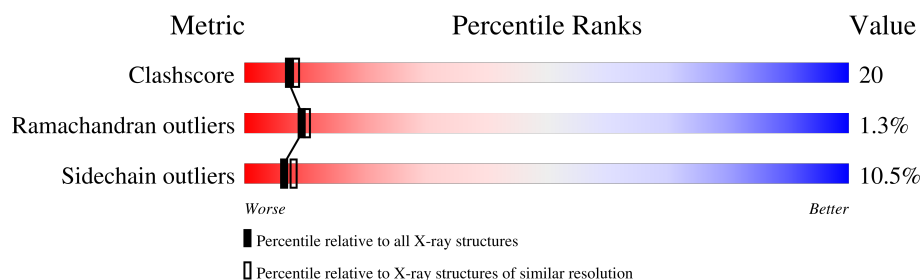
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.30 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 ≥ 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	
1	B	110	
1	C	110	

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 2780 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	107	Total	C	N	O	0	0	0
			845	536	145	164			
1	B	107	Total	C	N	O	0	0	0
			836	531	143	162			
1	C	107	Total	C	N	O	0	0	0
			834	531	144	159			

There are 3 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	96	VAL	ILE	conflict	UNP P00648
B	96	VAL	ILE	conflict	UNP P00648
C	96	VAL	ILE	conflict	UNP P00648

- Molecule 2 is water.

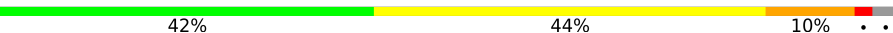
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	115	Total	O	0	0
			115	115		
2	B	72	Total	O	0	0
			72	72		
2	C	78	Total	O	0	0
			78	78		

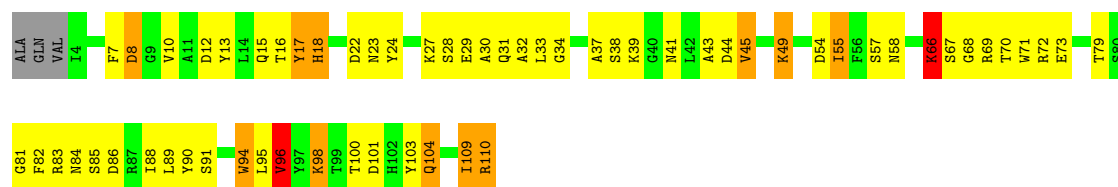
3 Residue-property plots [i](#)

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.

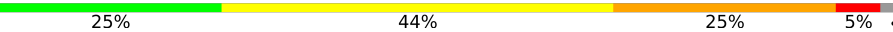
Note EDS was not executed.

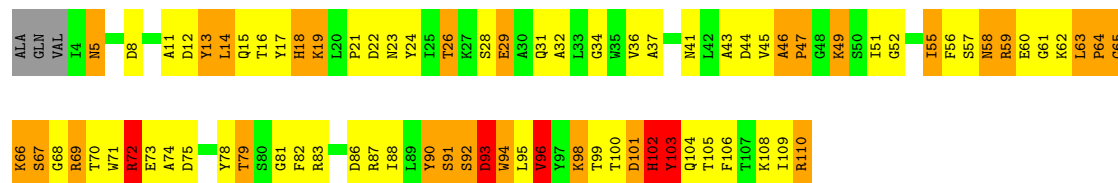
• Molecule 1: BARNASE

Chain A: 



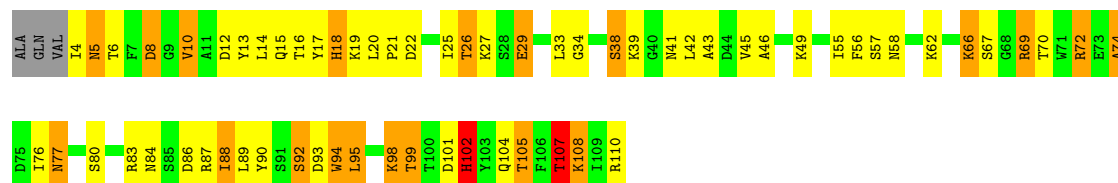
• Molecule 1: BARNASE

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	59.37Å 59.37Å 82.61Å 90.00° 90.00° 120.00°	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	PROLSQ	Depositor
R, R_{free}	0.154 , (Not available)	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	2780	wwPDB-VP
Average B, all atoms (Å ²)	16.0	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	1.36	3/866 (0.3%)	2.73	77/1173 (6.6%)
1	B	1.32	2/857 (0.2%)	2.80	92/1164 (7.9%)
1	C	1.28	1/855 (0.1%)	2.70	82/1160 (7.1%)
All	All	1.32	6/2578 (0.2%)	2.75	251/3497 (7.2%)

All (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	94	TRP	CA-CB	6.16	1.63	1.53
1	B	24	TYR	CA-CB	5.57	1.62	1.53
1	B	95	LEU	CA-C	5.36	1.59	1.52
1	A	24	TYR	CA-CB	5.24	1.61	1.53
1	C	39	LYS	C-N	-5.17	1.28	1.33
1	A	44	ASP	C-N	-5.02	1.27	1.33

All (251) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	72	ARG	CD-NE-CZ	25.45	160.03	124.40
1	B	93	ASP	CA-CB-CG	23.97	136.57	112.60
1	B	110	ARG	NE-CZ-NH2	13.26	131.13	119.20
1	A	72	ARG	NE-CZ-NH2	-12.13	108.29	119.20
1	B	22	ASP	CA-C-O	-11.86	106.70	120.10
1	A	15	GLN	CB-CG-CD	11.37	131.93	112.60
1	C	45	VAL	CA-C-N	-10.88	112.25	122.37
1	C	45	VAL	C-N-CA	-10.88	112.25	122.37
1	C	21	PRO	CA-C-N	10.62	135.88	120.38
1	C	21	PRO	C-N-CA	10.62	135.88	120.38
1	A	10	VAL	O-C-N	10.60	132.92	121.90
1	A	57	SER	N-CA-C	10.52	122.33	111.07
1	C	12	ASP	CA-CB-CG	-10.25	102.35	112.60
1	C	49	LYS	CA-C-O	10.03	133.90	121.66
1	C	107	THR	O-C-N	9.42	134.76	123.27

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	65	GLY	CA-C-O	9.02	129.94	121.64
1	C	41	ASN	CA-C-O	-9.00	109.03	119.56
1	B	96	VAL	CB-CA-C	8.95	123.40	110.33
1	B	11	ALA	O-C-N	8.83	131.16	122.07
1	A	12	ASP	CA-CB-CG	-8.81	103.79	112.60
1	A	10	VAL	CA-C-O	-8.71	111.38	121.05
1	C	5	ASN	CB-CG-ND2	8.62	129.34	116.40
1	B	64	PRO	CA-C-N	8.50	130.32	120.71
1	B	64	PRO	C-N-CA	8.50	130.32	120.71
1	A	58	ASN	CA-C-N	8.38	131.34	120.44
1	A	58	ASN	C-N-CA	8.38	131.34	120.44
1	B	16	THR	N-CA-CB	8.33	122.61	110.20
1	A	95	LEU	N-CA-C	-8.29	99.36	110.55
1	A	83	ARG	NE-CZ-NH2	8.27	126.64	119.20
1	A	94	TRP	N-CA-C	8.27	122.67	112.58
1	B	90	TYR	CA-C-O	8.26	130.16	120.66
1	B	109	ILE	CA-C-O	8.11	126.28	118.98
1	C	110	ARG	CA-CB-CG	8.06	130.22	114.10
1	A	69	ARG	NE-CZ-NH2	-8.03	111.98	119.20
1	C	38	SER	N-CA-C	8.02	122.17	112.38
1	B	94	TRP	CA-C-N	7.95	132.87	121.50
1	B	94	TRP	C-N-CA	7.95	132.87	121.50
1	B	69	ARG	N-CA-CB	7.89	122.93	110.55
1	C	42	LEU	N-CA-C	7.84	120.81	111.33
1	B	28	SER	CB-CA-C	7.83	124.16	110.85
1	A	23	ASN	OD1-CG-ND2	7.78	130.38	122.60
1	C	70	THR	CA-C-N	7.77	134.22	122.65
1	C	70	THR	C-N-CA	7.77	134.22	122.65
1	C	34	GLY	CA-C-O	-7.77	111.18	118.95
1	B	67	SER	O-C-N	7.74	132.04	123.13
1	C	10	VAL	CB-CA-C	7.68	122.09	112.02
1	B	21	PRO	N-CA-CB	7.68	110.61	103.39
1	A	83	ARG	NE-CZ-NH1	-7.66	113.84	121.50
1	C	72	ARG	NE-CZ-NH2	-7.66	112.31	119.20
1	A	38	SER	N-CA-C	7.63	120.48	111.71
1	A	83	ARG	CD-NE-CZ	-7.57	113.80	124.40
1	C	57	SER	CA-C-O	-7.57	112.40	120.42
1	A	45	VAL	CA-C-N	-7.55	115.34	122.37
1	A	45	VAL	C-N-CA	-7.55	115.34	122.37
1	A	23	ASN	CA-CB-CG	7.47	120.07	112.60
1	A	15	GLN	OE1-CD-NE2	-7.45	115.15	122.60
1	B	110	ARG	NH1-CZ-NH2	-7.43	109.64	119.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	45	VAL	O-C-N	7.40	130.91	122.18
1	B	8	ASP	CA-C-N	-7.37	111.89	120.00
1	B	8	ASP	C-N-CA	-7.37	111.89	120.00
1	C	102	HIS	CA-CB-CG	-7.37	106.43	113.80
1	B	8	ASP	CA-C-O	-7.32	111.16	119.79
1	C	39	LYS	CA-C-N	7.22	131.01	120.11
1	C	39	LYS	C-N-CA	7.22	131.01	120.11
1	A	85	SER	O-C-N	7.19	130.94	122.24
1	A	57	SER	CA-C-O	-7.16	113.30	120.82
1	C	98	LYS	O-C-N	7.09	131.49	123.27
1	B	14	LEU	N-CA-C	7.07	119.88	111.33
1	C	108	LYS	CA-C-O	-7.07	112.99	121.05
1	C	99	THR	CA-C-O	7.06	129.37	121.11
1	B	51	ILE	CA-C-N	7.05	131.39	121.09
1	B	51	ILE	C-N-CA	7.05	131.39	121.09
1	B	78	TYR	O-C-N	7.03	131.32	123.16
1	B	95	LEU	N-CA-C	-7.01	98.61	109.76
1	C	93	ASP	CA-C-O	7.00	128.12	119.78
1	A	38	SER	CA-CB-OG	-6.97	97.16	111.10
1	C	4	ILE	N-CA-CB	6.97	123.35	111.50
1	B	102	HIS	CA-CB-CG	-6.95	106.85	113.80
1	B	37	ALA	CA-C-O	-6.91	113.51	120.90
1	B	82	PHE	N-CA-C	-6.89	100.78	110.50
1	C	95	LEU	CA-C-O	-6.88	113.10	121.36
1	C	16	THR	N-CA-CB	6.87	120.03	110.07
1	B	36	VAL	CA-C-N	6.87	129.81	120.54
1	B	36	VAL	C-N-CA	6.87	129.81	120.54
1	A	96	VAL	N-CA-CB	6.86	122.69	111.58
1	A	18	HIS	CA-CB-CG	-6.84	106.95	113.80
1	A	41	ASN	N-CA-C	6.81	121.30	112.92
1	C	77	ASN	CA-C-O	-6.80	112.30	120.12
1	A	57	SER	CA-CB-OG	-6.70	97.70	111.10
1	A	72	ARG	NE-CZ-NH1	6.68	128.18	121.50
1	C	8	ASP	CA-CB-CG	-6.67	105.92	112.60
1	C	107	THR	N-CA-CB	6.67	123.08	111.00
1	B	18	HIS	CA-CB-CG	-6.66	107.14	113.80
1	C	56	PHE	O-C-N	6.60	131.06	123.27
1	C	58	ASN	CA-CB-CG	-6.59	106.01	112.60
1	B	75	ASP	CA-CB-CG	6.58	119.18	112.60
1	C	107	THR	CA-C-O	-6.57	113.11	120.66
1	A	69	ARG	CD-NE-CZ	6.54	133.56	124.40
1	A	8	ASP	CA-C-O	6.52	127.33	120.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	17	TYR	N-CA-C	6.52	121.44	112.90
1	C	86	ASP	CA-C-O	6.51	127.53	120.43
1	B	63	LEU	O-C-N	6.51	127.40	121.80
1	A	17	TYR	CA-CB-CG	-6.49	102.22	113.90
1	C	80	SER	CA-C-O	-6.49	114.50	121.38
1	C	66	LYS	CA-CB-CG	6.45	126.99	114.10
1	C	107	THR	CB-CA-C	-6.43	96.62	109.35
1	A	49	LYS	CA-C-N	6.38	132.58	122.62
1	A	49	LYS	C-N-CA	6.38	132.58	122.62
1	C	83	ARG	O-C-N	6.38	130.67	122.89
1	B	81	GLY	O-C-N	6.37	130.99	122.70
1	C	29	GLU	CB-CG-CD	6.34	123.39	112.60
1	C	18	HIS	CA-CB-CG	-6.33	107.47	113.80
1	B	86	ASP	CA-CB-CG	6.32	118.92	112.60
1	C	108	LYS	O-C-N	6.31	130.46	123.01
1	B	83	ARG	CD-NE-CZ	-6.29	115.60	124.40
1	A	31	GLN	N-CA-CB	6.24	119.30	109.82
1	B	15	GLN	OE1-CD-NE2	6.23	128.83	122.60
1	A	90	TYR	CA-C-O	6.21	127.81	120.66
1	B	37	ALA	O-C-N	6.19	128.52	122.09
1	B	29	GLU	CG-CD-OE1	6.18	132.62	118.40
1	B	52	GLY	N-CA-C	6.18	120.12	110.91
1	B	29	GLU	CB-CG-CD	6.16	123.06	112.60
1	B	68	GLY	O-C-N	6.11	129.01	122.41
1	B	72	ARG	CD-NE-CZ	6.11	132.95	124.40
1	C	105	THR	CA-C-O	6.11	127.83	120.99
1	C	46	ALA	O-C-N	6.09	125.63	121.19
1	B	41	ASN	N-CA-CB	-6.06	101.71	110.56
1	B	92	SER	CA-CB-OG	6.05	123.21	111.10
1	A	39	LYS	CA-C-O	-6.05	112.27	119.35
1	C	66	LYS	CA-C-O	-6.05	113.97	120.75
1	B	73	GLU	CA-C-N	6.04	131.91	121.64
1	B	73	GLU	C-N-CA	6.04	131.91	121.64
1	A	30	ALA	O-C-N	6.02	128.51	122.12
1	C	22	ASP	CA-C-O	-6.00	113.48	120.20
1	C	15	GLN	CB-CA-C	5.99	121.71	109.67
1	C	38	SER	CA-CB-OG	-5.97	99.16	111.10
1	B	44	ASP	CA-C-O	-5.96	113.63	120.24
1	B	106	PHE	N-CA-C	5.96	119.19	109.24
1	B	8	ASP	O-C-N	5.95	130.31	122.33
1	B	91	SER	CA-C-O	5.93	128.89	121.66
1	B	56	PHE	CA-C-O	5.92	126.84	120.32

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	81	GLY	CA-C-N	5.92	130.24	120.94
1	B	81	GLY	C-N-CA	5.92	130.24	120.94
1	B	59	ARG	N-CA-C	-5.91	103.81	111.02
1	A	22	ASP	CA-CB-CG	-5.90	106.70	112.60
1	B	34	GLY	N-CA-C	-5.90	106.84	115.63
1	C	69	ARG	O-C-N	5.90	130.25	123.29
1	A	104	GLN	CB-CG-CD	-5.88	102.61	112.60
1	A	16	THR	CA-CB-OG1	-5.86	100.81	109.60
1	B	41	ASN	CA-C-N	5.85	128.39	120.38
1	B	41	ASN	C-N-CA	5.85	128.39	120.38
1	B	23	ASN	OD1-CG-ND2	5.84	128.44	122.60
1	B	49	LYS	CA-C-O	5.81	128.13	121.28
1	A	41	ASN	OD1-CG-ND2	-5.80	116.80	122.60
1	A	110	ARG	CA-C-O	-5.79	110.95	120.80
1	B	87	ARG	NE-CZ-NH1	5.77	127.27	121.50
1	A	79	THR	CB-CA-C	5.77	121.90	110.42
1	C	8	ASP	O-C-N	5.75	128.00	122.07
1	B	68	GLY	N-CA-C	-5.75	104.93	114.48
1	C	70	THR	CB-CA-C	5.74	120.63	109.33
1	B	12	ASP	CA-C-O	-5.71	115.01	121.00
1	C	72	ARG	NE-CZ-NH1	5.71	127.21	121.50
1	B	94	TRP	CA-C-O	5.69	127.40	120.57
1	C	41	ASN	N-CA-C	5.69	119.91	112.92
1	A	38	SER	CA-C-O	5.68	126.52	120.10
1	C	17	TYR	N-CA-C	5.67	120.35	113.38
1	C	107	THR	CA-CB-CG2	-5.66	100.89	110.50
1	B	101	ASP	N-CA-CB	-5.62	103.19	111.51
1	A	81	GLY	O-C-N	-5.59	118.09	122.90
1	B	13	TYR	O-C-N	-5.58	115.44	122.20
1	A	69	ARG	NE-CZ-NH1	5.58	127.08	121.50
1	A	82	PHE	CA-C-O	-5.57	115.41	121.87
1	A	28	SER	O-C-N	5.55	129.44	122.23
1	B	94	TRP	N-CA-C	5.54	119.34	112.58
1	C	16	THR	CB-CA-C	-5.54	102.15	110.90
1	A	88	ILE	CB-CA-C	5.53	119.22	110.81
1	C	87	ARG	CA-C-O	5.53	127.18	120.99
1	B	69	ARG	NE-CZ-NH2	5.51	124.16	119.20
1	C	26	THR	CA-C-O	5.51	128.31	121.81
1	A	66	LYS	CA-C-O	-5.50	115.05	121.10
1	B	46	ALA	O-C-N	5.50	126.28	121.17
1	A	68	GLY	N-CA-C	-5.48	108.17	115.40
1	A	110	ARG	N-CA-CB	5.48	119.81	110.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	18	HIS	CA-C-N	5.48	132.00	121.54
1	B	18	HIS	C-N-CA	5.48	132.00	121.54
1	A	45	VAL	O-C-N	5.47	128.64	122.18
1	C	5	ASN	CB-CG-OD1	-5.46	109.88	120.80
1	B	13	TYR	CA-C-N	5.44	127.83	120.38
1	B	13	TYR	C-N-CA	5.44	127.83	120.38
1	A	12	ASP	N-CA-C	5.40	117.16	111.28
1	A	98	LYS	CA-CB-CG	5.38	124.87	114.10
1	C	57	SER	N-CA-C	5.38	117.23	111.36
1	A	85	SER	CA-C-O	-5.38	112.92	119.32
1	C	49	LYS	N-CA-CB	5.38	118.95	110.56
1	C	84	ASN	OD1-CG-ND2	-5.38	117.22	122.60
1	B	16	THR	CA-C-N	-5.38	114.09	122.37
1	B	16	THR	C-N-CA	-5.38	114.09	122.37
1	B	44	ASP	CB-CG-OD1	-5.37	106.06	118.40
1	A	109	ILE	CA-C-O	-5.36	114.15	118.98
1	C	69	ARG	CA-C-O	-5.36	114.54	120.38
1	A	41	ASN	N-CA-CB	-5.34	102.76	110.56
1	C	69	ARG	CA-C-N	-5.34	114.43	122.81
1	C	69	ARG	C-N-CA	-5.34	114.43	122.81
1	A	73	GLU	CA-C-N	5.32	131.53	121.69
1	A	73	GLU	C-N-CA	5.32	131.53	121.69
1	B	29	GLU	N-CA-CB	5.32	117.72	110.01
1	A	110	ARG	NE-CZ-NH2	-5.30	114.43	119.20
1	C	33	LEU	CA-C-O	5.29	125.48	119.18
1	B	69	ARG	NE-CZ-NH1	-5.29	116.21	121.50
1	C	20	LEU	O-C-N	5.27	128.33	121.64
1	C	95	LEU	CA-C-N	-5.25	115.69	122.99
1	C	95	LEU	C-N-CA	-5.25	115.69	122.99
1	B	16	THR	O-C-N	5.25	129.05	122.23
1	B	98	LYS	CA-CB-CG	5.24	124.58	114.10
1	B	31	GLN	OE1-CD-NE2	-5.24	117.36	122.60
1	B	70	THR	CA-C-N	5.23	129.94	122.72
1	B	70	THR	C-N-CA	5.23	129.94	122.72
1	A	84	ASN	OD1-CG-ND2	5.23	127.83	122.60
1	C	20	LEU	N-CA-C	-5.22	102.62	110.24
1	A	28	SER	N-CA-C	-5.19	105.31	111.69
1	C	105	THR	CB-CA-C	5.19	120.99	109.94
1	A	71	TRP	O-C-N	5.18	129.79	123.21
1	A	90	TYR	CB-CG-CD2	-5.17	113.05	120.80
1	C	94	TRP	N-CA-C	5.16	118.70	111.74
1	C	107	THR	OG1-CB-CG2	5.15	119.60	109.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	58	ASN	OD1-CG-ND2	5.15	127.75	122.60
1	B	96	VAL	CA-CB-CG1	5.14	119.14	110.40
1	C	72	ARG	CA-C-O	-5.14	115.09	121.11
1	A	39	LYS	O-C-N	5.13	128.76	122.34
1	C	88	ILE	N-CA-C	-5.13	101.09	108.89
1	B	5	ASN	CB-CG-ND2	5.13	124.09	116.40
1	B	73	GLU	CB-CG-CD	5.12	121.31	112.60
1	C	89	LEU	O-C-N	5.11	129.25	123.27
1	C	15	GLN	N-CA-C	-5.11	106.21	112.90
1	A	54	ASP	CA-C-N	5.11	127.92	120.98
1	A	54	ASP	C-N-CA	5.11	127.92	120.98
1	A	103	TYR	CA-C-O	-5.09	114.49	120.81
1	A	100	THR	N-CA-C	-5.07	105.41	112.30
1	A	37	ALA	CA-C-N	5.07	127.58	120.28
1	A	37	ALA	C-N-CA	5.07	127.58	120.28
1	A	90	TYR	CB-CG-CD1	5.07	128.40	120.80
1	B	11	ALA	CA-C-O	-5.07	115.50	120.82
1	C	39	LYS	CA-C-O	-5.06	113.30	119.32
1	C	45	VAL	CA-C-O	-5.05	113.76	119.42
1	B	78	TYR	CA-C-O	-5.04	115.12	120.92
1	C	74	ALA	CA-C-O	-5.04	114.49	120.43
1	A	33	LEU	CA-C-N	5.02	129.56	122.63
1	A	33	LEU	C-N-CA	5.02	129.56	122.63
1	B	29	GLU	O-C-N	5.02	127.25	122.07
1	B	26	THR	CA-C-N	5.00	126.98	120.28
1	B	26	THR	C-N-CA	5.00	126.98	120.28

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	845	0	799	29	0
1	B	836	0	785	41	0
1	C	834	0	784	32	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	A	115	0	0	8	0
2	B	72	0	0	5	0
2	C	78	0	0	7	0
All	All	2780	0	2368	100	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 20.

All (100) 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:96:VAL:HG13	1:B:110:ARG:HB2	1.33	1.05
1:B:64:PRO:O	1:B:69:ARG:NH1	1.92	1.02
1:C:102:HIS:HB2	2:C:153:HOH:O	1.61	0.99
1:A:96:VAL:HG13	1:A:110:ARG:HB2	1.51	0.91
1:C:107:THR:HG21	2:C:123:HOH:O	1.72	0.90
1:C:107:THR:CG2	2:C:123:HOH:O	2.23	0.87
1:B:26:THR:OG1	1:B:29:GLU:HG3	1.82	0.80
1:B:100:THR:O	2:B:176:HOH:O	2.02	0.77
1:A:32:ALA:HB3	2:A:146:HOH:O	1.85	0.75
1:C:18:HIS:HB3	1:C:94:TRP:CZ2	2.26	0.71
1:B:18:HIS:HB3	1:B:94:TRP:CZ2	2.26	0.70
1:A:43:ALA:HA	2:A:198:HOH:O	1.92	0.68
1:C:101:ASP:O	1:C:104:GLN:HG3	1.93	0.68
1:A:101:ASP:O	1:A:104:GLN:HG2	1.94	0.66
1:B:64:PRO:C	1:B:69:ARG:NH1	2.54	0.66
1:C:14:LEU:O	1:C:18:HIS:HA	1.97	0.64
1:B:64:PRO:C	1:B:69:ARG:HH11	2.04	0.62
1:C:13:TYR:HD2	1:C:19:LYS:O	1.83	0.61
1:B:96:VAL:CG1	1:B:110:ARG:HB2	2.22	0.60
1:C:5:ASN:HB2	2:C:111:HOH:O	2.01	0.60
1:C:107:THR:HG22	1:C:108:LYS:N	2.17	0.59
1:B:101:ASP:OD2	1:B:105:THR:OG1	2.19	0.59
1:A:96:VAL:HG13	1:A:110:ARG:CB	2.29	0.58
1:B:17:TYR:O	1:B:18:HIS:C	2.46	0.57
1:B:72:ARG:HB3	1:B:90:TYR:CZ	2.39	0.56
1:B:65:GLY:O	1:B:66:LYS:HG2	2.05	0.56
1:B:14:LEU:O	1:B:18:HIS:N	2.39	0.56
1:B:46:ALA:N	1:B:47:PRO:HD3	2.21	0.55
1:C:101:ASP:OD2	1:C:105:THR:OG1	2.21	0.55
1:A:13:TYR:CE2	1:A:17:TYR:CE2	2.94	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:45:VAL:C	1:B:47:PRO:HD3	2.32	0.55
1:C:107:THR:HG22	2:C:123:HOH:O	1.99	0.55
1:B:14:LEU:O	1:B:18:HIS:HA	2.06	0.55
1:C:13:TYR:HE2	1:C:19:LYS:HZ2	1.54	0.54
1:A:13:TYR:CE2	1:A:17:TYR:CD2	2.95	0.54
1:B:13:TYR:HD1	1:B:19:LYS:O	1.90	0.53
1:B:69:ARG:NE	1:B:93:ASP:OD1	2.30	0.52
1:B:32:ALA:HB3	2:B:161:HOH:O	2.10	0.52
1:C:62:LYS:HE3	2:C:168:HOH:O	2.08	0.52
1:A:13:TYR:O	1:A:17:TYR:HB2	2.10	0.51
1:B:63:LEU:HD13	1:B:71:TRP:CD2	2.45	0.51
1:C:26:THR:OG1	1:C:29:GLU:HG3	2.10	0.51
1:B:13:TYR:CD1	1:B:19:LYS:O	2.64	0.51
1:A:43:ALA:HB3	2:A:115:HOH:O	2.10	0.50
1:B:101:ASP:O	1:B:104:GLN:HG3	2.11	0.50
1:C:55:ILE:HG12	1:C:72:ARG:NH1	2.27	0.50
1:A:96:VAL:CG1	1:A:110:ARG:HB2	2.33	0.50
1:B:55:ILE:HD13	1:B:72:ARG:HG3	1.93	0.50
1:C:90:TYR:HA	1:C:95:LEU:O	2.11	0.50
1:B:64:PRO:O	1:B:69:ARG:HD2	2.13	0.49
1:C:69:ARG:HA	1:C:92:SER:OG	2.13	0.49
1:A:27:LYS:NZ	2:A:225:HOH:O	2.46	0.48
1:B:74:ALA:HB3	1:B:88:ILE:CG2	2.43	0.48
1:B:99:THR:HG21	1:B:103:TYR:HA	1.94	0.48
1:A:7:PHE:CZ	1:A:86:ASP:HB3	2.48	0.48
1:B:14:LEU:O	1:B:18:HIS:CA	2.61	0.48
1:B:102:HIS:O	1:B:104:GLN:HG3	2.13	0.47
1:B:5:ASN:HB2	2:B:130:HOH:O	2.13	0.47
1:B:55:ILE:HD13	1:B:55:ILE:HA	1.72	0.47
1:B:60:GLU:O	1:B:62:LYS:N	2.47	0.47
1:B:79:THR:OG1	2:B:160:HOH:O	2.00	0.46
1:A:18:HIS:HD2	1:A:94:TRP:CD2	2.35	0.45
1:C:6:THR:O	1:C:10:VAL:HG23	2.17	0.45
1:A:70:THR:O	1:A:91:SER:HA	2.17	0.45
1:B:58:ASN:O	1:B:59:ARG:C	2.60	0.45
1:A:45:VAL:HA	1:B:108:LYS:HD3	1.98	0.45
1:B:43:ALA:HA	2:B:166:HOH:O	2.16	0.44
1:C:13:TYR:CD2	1:C:19:LYS:O	2.68	0.44
1:C:107:THR:HG22	1:C:108:LYS:H	1.82	0.44
1:A:34:GLY:HA2	1:B:64:PRO:CG	2.47	0.44
1:A:66:LYS:HZ2	1:A:66:LYS:HG2	1.66	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:70:THR:HG23	2:A:222:HOH:O	2.17	0.44
1:C:76:ILE:O	1:C:77:ASN:HB2	2.16	0.44
1:C:99:THR:OG1	1:C:101:ASP:OD1	2.35	0.44
1:A:18:HIS:CD2	1:A:94:TRP:CE2	3.06	0.43
1:C:101:ASP:O	1:C:102:HIS:CB	2.63	0.43
1:A:29:GLU:OE1	2:A:162:HOH:O	2.21	0.43
1:C:43:ALA:HB3	2:C:115:HOH:O	2.18	0.43
1:B:101:ASP:CG	1:B:105:THR:OG1	2.62	0.43
1:A:13:TYR:CD2	1:A:17:TYR:CD2	3.06	0.43
1:A:32:ALA:CB	2:A:146:HOH:O	2.54	0.43
1:A:49:LYS:CE	2:A:176:HOH:O	2.67	0.42
1:A:96:VAL:HG22	1:A:109:ILE:HG13	2.01	0.42
1:C:74:ALA:HB3	1:C:88:ILE:HG22	2.01	0.42
1:C:14:LEU:O	1:C:18:HIS:N	2.53	0.42
1:C:25:ILE:HD13	1:C:25:ILE:HG21	1.83	0.42
1:A:96:VAL:HG22	1:A:109:ILE:CG1	2.50	0.41
1:B:46:ALA:N	1:B:47:PRO:CD	2.83	0.41
1:C:26:THR:O	1:C:27:LYS:C	2.63	0.41
1:C:13:TYR:CE2	1:C:19:LYS:NZ	2.89	0.41
1:A:18:HIS:CD2	1:A:94:TRP:CD2	3.09	0.41
1:A:96:VAL:HG13	1:A:110:ARG:CG	2.51	0.41
1:A:109:ILE:O	1:A:110:ARG:HD3	2.21	0.41
1:B:65:GLY:O	1:B:66:LYS:CG	2.69	0.41
1:B:71:TRP:CZ3	1:B:91:SER:HB3	2.56	0.41
1:A:55:ILE:HD13	1:A:55:ILE:HA	1.90	0.40
1:B:49:LYS:HA	1:B:49:LYS:HD2	1.85	0.40
1:C:13:TYR:HE2	1:C:19:LYS:NZ	2.18	0.40
1:C:66:LYS:HD3	1:C:69:ARG:NH2	2.36	0.40
1:C:13:TYR:OH	1:C:19:LYS:NZ	2.54	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	105/110 (96%)	98 (93%)	7 (7%)	0	100	100
1	B	105/110 (96%)	92 (88%)	9 (9%)	4 (4%)	2	1
1	C	105/110 (96%)	102 (97%)	3 (3%)	0	100	100
All	All	315/330 (96%)	292 (93%)	19 (6%)	4 (1%)	9	10

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	61	GLY
1	B	19	LYS
1	B	103	TYR
1	B	58	ASN

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%)	80 (92%)	7 (8%)	11	15
1	B	85/92 (92%)	72 (85%)	13 (15%)	3	3
1	C	84/92 (91%)	77 (92%)	7 (8%)	10	14
All	All	256/276 (93%)	229 (90%)	27 (10%)	6	8

All (27) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	8	ASP
1	A	55	ILE
1	A	66	LYS
1	A	67	SER
1	A	89	LEU
1	A	96	VAL
1	A	98	LYS
1	B	47	PRO
1	B	55	ILE

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Mol	Chain	Res	Type
1	B	57	SER
1	B	66	LYS
1	B	67	SER
1	B	72	ARG
1	B	79	THR
1	B	92	SER
1	B	93	ASP
1	B	96	VAL
1	B	98	LYS
1	B	102	HIS
1	B	103	TYR
1	C	8	ASP
1	C	38	SER
1	C	67	SER
1	C	92	SER
1	C	98	LYS
1	C	102	HIS
1	C	107	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (1) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	18	HIS

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 ⓘ

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.