



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 6, 2026 – 11:30 AM UTC

PDB ID : 1BAO / pdb_00001bao
Title : THE CONTRIBUTION OF BURIED HYDROGEN BONDS TO PROTEIN STABILITY: THE CRYSTAL STRUCTURES OF TWO BARNASE MUTANTS
Authors : Chen, Y.W.; Fersht, A.R.; Henrick, K.
Deposited on : 1993-05-19
Resolution : 2.20 Å(reported)

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

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

MolProbity	:	4-5-2 with Phenix2.0
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

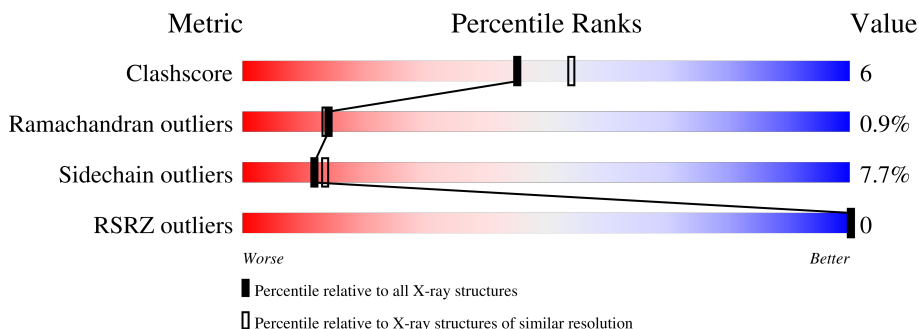
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.20 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
Clashscore	190562	6851 (2.20-2.20)
Ramachandran outliers	187476	6768 (2.20-2.20)
Sidechain outliers	187428	6769 (2.20-2.20)
RSRZ outliers	180081	6166 (2.20-2.20)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	110	
1	B	110	
1	C	110	

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 2752 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	0	0	0
			853	541	148	164			
1	B	108	Total	C	N	O	0	0	1
			842	535	144	163			
1	C	107	Total	C	N	O	0	0	0
			843	535	145	163			

There are 3 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	78	PHE	TYR	conflict	UNP P00648
B	78	PHE	TYR	conflict	UNP P00648
C	78	PHE	TYR	conflict	UNP P00648

- Molecule 2 is ZINC ION (CCD ID: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	C	1	Total	Zn	0	0
			1	1		

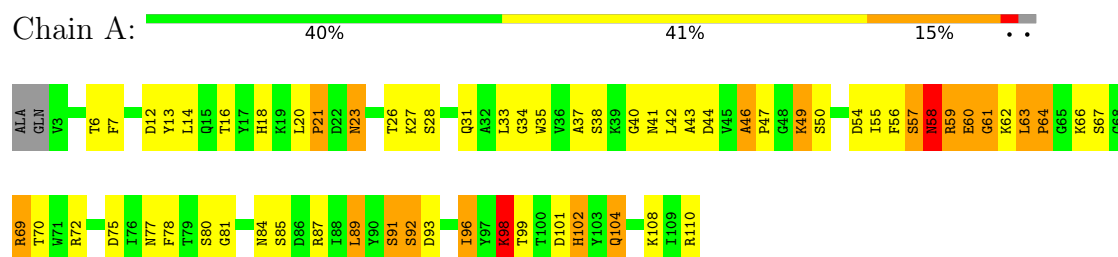
- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	72	Total	O	0	0
			72	72		
3	B	76	Total	O	0	0
			76	76		
3	C	65	Total	O	0	0
			65	65		

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 and electron density. 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. A red dot above a residue indicates a poor fit to the electron density ($RSRZ > 2$). 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.

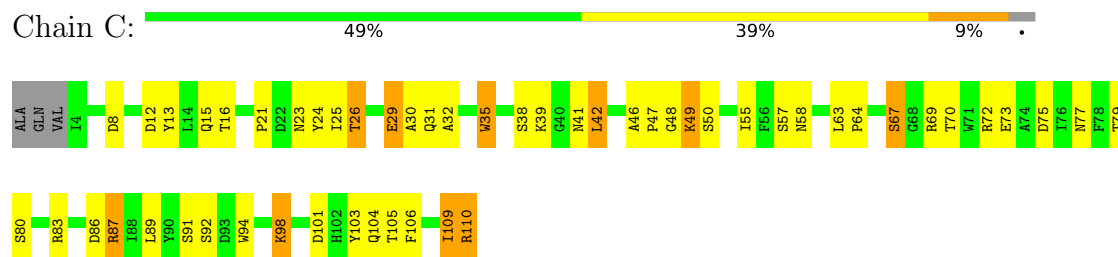
• Molecule 1: BARNASE



• Molecule 1: BARNASE



• Molecule 1: BARNASE



4 Data and refinement statistics

Property	Value	Source
Space group	P 32	Depositor
Cell constants a, b, c, α , β , γ	58.81Å 58.81Å 81.90Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	6.00 – 2.20 6.00 – 2.20	Depositor EDS
% Data completeness (in resolution range)	(Not available) (6.00-2.20) 88.3 (6.00-2.20)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.35 (at 2.20Å)	Xtriage
Refinement program	PROLSQ, X-PLOR	Depositor
R, R_{free}	0.152 , (Not available) 0.149 , (Not available)	Depositor DCC
R_{free} test set	No test flags present.	wwPDB-VP
Wilson B-factor (Å ²)	16.9	Xtriage
Anisotropy	0.197	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.38 , 92.2	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	0.006 for -h,-k,l 0.057 for h,-h-k,-l 0.028 for -k,-h,-l	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	2752	wwPDB-VP
Average B, all atoms (Å ²)	15.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 11.03% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality ⓘ

5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: ZN

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	1.39	0/874	2.83	98/1182 (8.3%)
1	B	1.40	2/863 (0.2%)	2.67	87/1168 (7.4%)
1	C	1.38	1/864 (0.1%)	2.70	78/1170 (6.7%)
All	All	1.39	3/2601 (0.1%)	2.74	263/3520 (7.5%)

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	109	ILE	CA-CB	6.59	1.61	1.54
1	B	94	TRP	CA-CB	5.10	1.60	1.53
1	B	4	ILE	CA-CB	5.03	1.59	1.54

All (263) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	110	ARG	NE-CZ-NH2	17.37	134.83	119.20
1	A	87	ARG	NE-CZ-NH2	12.07	130.06	119.20
1	A	61	GLY	CA-C-N	11.97	137.86	120.38
1	A	61	GLY	C-N-CA	11.97	137.86	120.38
1	C	87	ARG	NE-CZ-NH2	11.13	129.22	119.20
1	C	98	LYS	CA-C-O	-10.55	109.09	121.44
1	C	94	TRP	N-CA-C	10.42	126.11	111.52
1	A	104	GLN	OE1-CD-NE2	10.12	132.72	122.60
1	C	73	GLU	CA-C-O	-10.04	110.27	121.51
1	A	110	ARG	CD-NE-CZ	9.93	138.30	124.40
1	B	28	SER	CA-C-O	9.75	130.75	120.42
1	B	70	THR	CB-CA-C	9.62	126.98	109.37
1	C	8	ASP	CA-CB-CG	-9.53	103.07	112.60
1	B	58	ASN	OD1-CG-ND2	-9.15	113.45	122.60
1	B	41	ASN	N-CA-C	9.12	123.71	112.59

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	6	THR	CA-C-O	-9.07	110.91	121.16
1	A	60	GLU	CB-CG-CD	9.04	127.98	112.60
1	C	29	GLU	CB-CG-CD	9.01	127.92	112.60
1	A	93	ASP	CA-CB-CG	9.00	121.60	112.60
1	B	4	ILE	CA-C-O	-8.92	110.22	120.65
1	B	41	ASN	OD1-CG-ND2	-8.86	113.74	122.60
1	A	34	GLY	CA-C-O	-8.79	110.16	118.95
1	A	26	THR	CA-C-O	-8.73	111.67	121.89
1	B	81	GLY	O-C-N	8.56	131.16	122.86
1	A	50	SER	CA-C-O	-8.40	111.28	121.11
1	A	72	ARG	NE-CZ-NH1	8.37	129.87	121.50
1	A	57	SER	CA-C-O	-8.30	112.10	120.82
1	A	13	TYR	O-C-N	-8.21	113.42	122.12
1	A	60	GLU	CG-CD-OE2	8.16	137.17	118.40
1	A	12	ASP	CA-CB-CG	-8.05	104.55	112.60
1	C	110	ARG	NH1-CZ-NH2	-8.03	108.86	119.30
1	A	96	ILE	CB-CG1-CD1	8.01	130.62	113.80
1	C	89	LEU	CA-C-O	-7.91	111.82	120.36
1	C	83	ARG	NH1-CZ-NH2	-7.90	109.03	119.30
1	B	39	LYS	CA-C-O	-7.82	110.45	119.05
1	C	41	ASN	N-CA-C	7.75	122.04	112.59
1	B	37	ALA	N-CA-CB	7.67	121.37	109.94
1	B	37	ALA	O-C-N	7.64	130.04	122.09
1	C	58	ASN	OD1-CG-ND2	-7.64	114.96	122.60
1	A	16	THR	CA-CB-OG1	-7.62	98.17	109.60
1	A	64	PRO	CA-C-N	7.60	129.51	121.45
1	A	64	PRO	C-N-CA	7.60	129.51	121.45
1	C	105	THR	CA-C-N	7.60	134.53	122.59
1	C	105	THR	C-N-CA	7.60	134.53	122.59
1	C	32	ALA	CA-C-O	-7.54	112.55	120.55
1	C	39	LYS	CG-CD-CE	7.53	128.62	111.30
1	A	80	SER	CA-CB-OG	-7.51	96.08	111.10
1	A	59	ARG	CD-NE-CZ	7.50	134.90	124.40
1	B	52	GLY	CA-C-N	7.48	134.51	122.25
1	B	52	GLY	C-N-CA	7.48	134.51	122.25
1	C	50	SER	CA-C-O	-7.46	112.38	121.11
1	C	80	SER	CA-C-O	-7.43	113.31	121.33
1	A	102	HIS	O-C-N	-7.34	114.18	122.91
1	C	104	GLN	CA-C-N	7.31	134.35	122.29
1	C	104	GLN	C-N-CA	7.31	134.35	122.29
1	B	101	ASP	CA-CB-CG	7.27	119.87	112.60
1	C	12	ASP	CA-CB-CG	-7.26	105.34	112.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	38	SER	CA-C-O	-7.26	110.71	119.49
1	A	81	GLY	O-C-N	-7.24	113.28	122.70
1	C	12	ASP	CA-C-N	7.24	129.85	120.44
1	C	12	ASP	C-N-CA	7.24	129.85	120.44
1	B	31	GLN	OE1-CD-NE2	-7.20	115.40	122.60
1	B	6	THR	O-C-N	7.20	132.23	123.16
1	B	83	ARG	NE-CZ-NH2	7.16	125.64	119.20
1	B	94	TRP	N-CA-C	7.15	121.50	111.92
1	C	57	SER	CA-C-O	-7.14	110.45	119.31
1	A	41	ASN	OD1-CG-ND2	-7.12	115.48	122.60
1	B	57	SER	CA-C-O	-7.09	110.66	119.38
1	C	21	PRO	CA-C-O	7.07	130.79	121.95
1	A	60	GLU	CA-CB-CG	7.06	128.22	114.10
1	B	100	THR	CA-CB-OG1	-7.02	99.08	109.60
1	B	33	LEU	CA-C-O	-7.01	110.84	119.18
1	C	42	LEU	O-C-N	7.01	129.38	122.09
1	A	21	PRO	O-C-N	-7.00	114.44	122.91
1	C	42	LEU	CA-C-O	-6.95	113.47	120.90
1	C	31	GLN	CA-C-O	-6.88	113.54	120.90
1	A	23	ASN	CA-C-O	-6.88	111.11	119.43
1	B	98	LYS	CA-C-O	-6.84	113.67	121.40
1	B	104	GLN	OE1-CD-NE2	-6.84	115.76	122.60
1	A	54	ASP	CA-CB-CG	6.83	119.43	112.60
1	B	42	LEU	O-C-N	6.82	129.35	122.12
1	A	99	THR	O-C-N	-6.81	115.09	123.33
1	A	59	ARG	CA-C-O	-6.78	113.70	120.82
1	B	36	VAL	CA-C-N	6.74	129.64	120.54
1	B	36	VAL	C-N-CA	6.74	129.64	120.54
1	B	69	ARG	N-CA-CB	6.72	121.11	110.55
1	C	25	ILE	CA-C-O	-6.69	113.40	120.76
1	C	101	ASP	CA-CB-CG	6.68	119.28	112.60
1	C	16	THR	CA-CB-OG1	-6.67	99.60	109.60
1	B	26	THR	CA-CB-OG1	-6.64	99.63	109.60
1	B	8	ASP	CA-C-O	-6.61	113.41	120.42
1	C	72	ARG	NE-CZ-NH2	-6.61	113.25	119.20
1	A	16	THR	CA-C-O	-6.60	112.57	120.56
1	A	64	PRO	CA-C-O	6.59	128.54	121.03
1	A	102	HIS	CA-C-N	6.54	133.32	123.05
1	A	102	HIS	C-N-CA	6.54	133.32	123.05
1	A	38	SER	CA-CB-OG	-6.53	98.04	111.10
1	A	34	GLY	O-C-N	6.50	129.92	122.38
1	C	13	TYR	O-C-N	6.49	128.75	122.07

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	84	ASN	OD1-CG-ND2	-6.45	116.15	122.60
1	C	32	ALA	N-CA-CB	6.44	119.58	110.12
1	C	72	ARG	NE-CZ-NH1	6.42	127.92	121.50
1	B	16	THR	O-C-N	6.41	130.96	122.30
1	A	20	LEU	CB-CA-C	6.41	118.72	109.11
1	B	78	PHE	O-C-N	6.39	130.57	123.16
1	A	26	THR	CA-CB-OG1	-6.38	100.03	109.60
1	A	56	PHE	CA-C-O	-6.37	113.31	120.32
1	A	81	GLY	CA-C-O	6.37	131.66	120.57
1	B	16	THR	CA-C-O	-6.37	112.35	120.31
1	A	99	THR	CA-C-O	6.32	128.18	120.60
1	B	100	THR	CA-CB-CG2	6.31	121.23	110.50
1	C	31	GLN	N-CA-CB	6.29	119.32	109.94
1	A	40	GLY	CA-C-N	6.28	132.69	122.65
1	A	40	GLY	C-N-CA	6.28	132.69	122.65
1	A	81	GLY	CA-C-N	6.18	131.65	121.39
1	A	81	GLY	C-N-CA	6.18	131.65	121.39
1	B	74	ALA	CB-CA-C	6.18	120.98	109.86
1	B	105	THR	CA-CB-OG1	-6.16	100.37	109.60
1	A	44	ASP	CA-C-N	-6.15	112.91	121.77
1	A	44	ASP	C-N-CA	-6.15	112.91	121.77
1	C	83	ARG	NE-CZ-NH2	6.15	124.73	119.20
1	B	73	GLU	CB-CG-CD	6.14	123.03	112.60
1	A	37	ALA	CA-C-N	6.13	133.32	121.18
1	A	37	ALA	C-N-CA	6.13	133.32	121.18
1	B	8	ASP	O-C-N	6.12	129.13	122.15
1	C	24	TYR	CA-C-O	-6.11	114.07	121.28
1	A	56	PHE	CB-CA-C	6.11	120.21	110.19
1	A	66	LYS	N-CA-CB	6.09	122.05	111.39
1	B	11	ALA	CA-C-N	6.08	128.34	120.44
1	B	11	ALA	C-N-CA	6.08	128.34	120.44
1	C	67	SER	CA-CB-OG	6.07	123.24	111.10
1	A	102	HIS	CA-C-O	6.04	129.58	122.03
1	C	35	TRP	CA-C-O	-6.03	113.88	120.81
1	A	28	SER	N-CA-C	6.02	117.51	111.07
1	B	56	PHE	N-CA-C	-6.00	98.73	108.52
1	B	93	ASP	N-CA-CB	6.00	119.32	110.56
1	B	66	LYS	N-CA-CB	5.97	120.59	110.49
1	C	38	SER	CA-CB-OG	-5.97	99.16	111.10
1	C	26	THR	O-C-N	-5.96	115.38	122.65
1	C	30	ALA	CA-C-N	5.94	128.56	120.54
1	C	30	ALA	C-N-CA	5.94	128.56	120.54

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	16	THR	CB-CA-C	-5.93	99.71	110.56
1	A	98	LYS	CA-C-N	5.90	132.52	122.37
1	A	98	LYS	C-N-CA	5.90	132.52	122.37
1	B	66	LYS	CB-CG-CD	5.89	124.85	111.30
1	C	69	ARG	CA-C-O	-5.89	113.89	120.54
1	A	72	ARG	NE-CZ-NH2	-5.88	113.90	119.20
1	B	31	GLN	CG-CD-NE2	5.87	125.20	116.40
1	A	104	GLN	CA-CB-CG	-5.85	102.41	114.10
1	A	108	LYS	CA-C-O	-5.84	114.09	120.81
1	B	22	ASP	CA-CB-CG	-5.83	106.77	112.60
1	B	9	GLY	O-C-N	5.83	127.78	122.19
1	B	104	GLN	CB-CG-CD	-5.81	102.72	112.60
1	C	75	ASP	O-C-N	5.81	129.86	123.01
1	B	15	GLN	CA-C-O	-5.77	113.58	120.10
1	A	87	ARG	NE-CZ-NH1	-5.77	115.73	121.50
1	B	17	TYR	CA-CB-CG	-5.76	103.53	113.90
1	A	12	ASP	CA-C-O	-5.75	114.32	120.42
1	B	14	LEU	CA-C-N	5.74	128.55	120.28
1	B	14	LEU	C-N-CA	5.74	128.55	120.28
1	C	72	ARG	CA-C-O	-5.73	114.93	121.58
1	A	26	THR	O-C-N	5.72	129.37	122.68
1	A	27	LYS	N-CA-CB	5.70	118.50	110.12
1	A	33	LEU	CA-C-N	-5.70	114.19	122.29
1	A	33	LEU	C-N-CA	-5.70	114.19	122.29
1	A	31	GLN	CA-CB-CG	-5.67	102.77	114.10
1	B	50	SER	CA-C-O	-5.66	114.82	121.44
1	A	85	SER	N-CA-CB	-5.65	102.32	110.56
1	B	68	GLY	CA-C-N	-5.65	115.14	123.05
1	B	68	GLY	C-N-CA	-5.65	115.14	123.05
1	C	110	ARG	N-CA-CB	5.63	120.06	110.50
1	C	49	LYS	CA-C-O	5.62	128.10	121.36
1	B	54	ASP	CA-CB-CG	5.61	118.21	112.60
1	B	83	ARG	NH1-CZ-NH2	-5.60	112.01	119.30
1	B	108	LYS	CA-C-O	-5.60	114.37	120.81
1	C	91	SER	O-C-N	5.57	129.20	122.68
1	B	107	THR	CA-CB-CG2	5.56	119.96	110.50
1	A	75	ASP	CA-CB-CG	5.55	118.15	112.60
1	B	33	LEU	CA-C-N	-5.55	114.41	122.29
1	B	33	LEU	C-N-CA	-5.55	114.41	122.29
1	B	84	ASN	OD1-CG-ND2	-5.55	117.05	122.60
1	A	49	LYS	CG-CD-CE	-5.54	98.56	111.30
1	C	23	ASN	CA-C-O	-5.54	111.87	119.12

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	4	ILE	CB-CA-C	5.53	117.65	110.96
1	A	20	LEU	N-CA-CB	-5.53	102.57	110.04
1	B	70	THR	O-C-N	-5.49	116.24	123.16
1	A	58	ASN	CA-C-O	5.49	128.35	120.51
1	C	49	LYS	CA-CB-CG	5.45	125.00	114.10
1	B	53	GLY	CA-C-O	-5.43	112.98	119.01
1	C	104	GLN	CA-C-O	-5.43	114.74	120.55
1	C	77	ASN	N-CA-C	5.42	119.47	112.86
1	A	54	ASP	CA-C-N	5.41	129.82	121.71
1	A	54	ASP	C-N-CA	5.41	129.82	121.71
1	B	69	ARG	O-C-N	5.41	129.65	123.27
1	A	23	ASN	OD1-CG-ND2	5.40	128.00	122.60
1	B	57	SER	N-CA-C	5.39	119.12	112.54
1	B	110	ARG	N-CA-CB	5.38	119.65	110.50
1	C	15	GLN	CB-CG-CD	5.38	121.75	112.60
1	C	63	LEU	O-C-N	5.36	126.77	121.57
1	A	35	TRP	CA-C-N	5.36	130.38	123.10
1	A	35	TRP	C-N-CA	5.36	130.38	123.10
1	A	13	TYR	CA-C-N	5.33	127.43	120.28
1	A	13	TYR	C-N-CA	5.33	127.43	120.28
1	B	27	LYS	O-C-N	-5.33	116.47	122.12
1	A	62	LYS	CA-C-O	-5.32	114.24	120.20
1	B	81	GLY	CA-C-O	-5.32	115.13	121.83
1	C	48	GLY	CA-C-N	5.30	131.13	122.07
1	C	48	GLY	C-N-CA	5.30	131.13	122.07
1	B	37	ALA	CA-C-O	-5.30	115.23	120.90
1	A	91	SER	CA-C-N	5.29	129.56	120.72
1	A	91	SER	C-N-CA	5.29	129.56	120.72
1	A	102	HIS	CE1-NE2-CD2	5.28	114.28	109.00
1	C	31	GLN	N-CA-C	-5.28	104.78	111.11
1	A	46	ALA	O-C-N	5.27	125.04	121.19
1	B	44	ASP	O-C-N	5.26	128.54	122.17
1	A	63	LEU	CB-CA-C	5.26	116.44	108.86
1	A	54	ASP	CA-C-O	5.25	128.01	121.81
1	A	56	PHE	N-CA-C	-5.25	99.96	108.52
1	C	73	GLU	O-C-N	5.25	129.58	122.96
1	C	79	THR	CA-C-O	-5.23	113.03	120.51
1	C	109	ILE	N-CA-CB	5.22	117.95	112.21
1	A	55	ILE	CA-C-N	-5.21	115.75	123.05
1	A	55	ILE	C-N-CA	-5.21	115.75	123.05
1	C	13	TYR	CA-C-O	-5.21	115.35	120.82
1	C	86	ASP	CA-C-O	-5.21	114.66	120.54

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	6	THR	CA-CB-OG1	-5.20	101.79	109.60
1	A	70	THR	CA-C-N	-5.20	114.90	122.65
1	A	70	THR	C-N-CA	-5.20	114.90	122.65
1	A	87	ARG	CD-NE-CZ	5.20	131.68	124.40
1	B	85	SER	CA-C-N	5.20	129.32	122.30
1	B	85	SER	C-N-CA	5.20	129.32	122.30
1	C	72	ARG	CA-CB-CG	5.20	124.50	114.10
1	B	97	TYR	N-CA-C	-5.20	101.86	109.81
1	C	86	ASP	O-C-N	5.20	129.14	123.22
1	C	110	ARG	NE-CZ-NH1	-5.19	116.31	121.50
1	C	24	TYR	CB-CG-CD2	-5.19	113.02	120.80
1	C	98	LYS	N-CA-CB	-5.18	102.53	111.55
1	C	24	TYR	N-CA-C	5.17	118.49	110.17
1	B	14	LEU	N-CA-C	5.16	116.59	111.07
1	A	108	LYS	O-C-N	5.16	129.27	122.93
1	B	79	THR	O-C-N	-5.15	116.17	122.25
1	B	17	TYR	CA-C-O	-5.15	113.28	119.15
1	B	35	TRP	CG-CD2-CE3	-5.14	128.76	133.90
1	C	64	PRO	N-CA-C	5.14	119.28	110.95
1	B	9	GLY	CA-C-O	-5.14	115.46	120.75
1	C	92	SER	CA-C-O	5.14	125.70	119.49
1	B	6	THR	CA-C-N	-5.09	113.67	120.54
1	B	6	THR	C-N-CA	-5.09	113.67	120.54
1	A	69	ARG	CD-NE-CZ	-5.09	117.28	124.40
1	A	41	ASN	CB-CG-OD1	5.08	130.97	120.80
1	A	77	ASN	N-CA-CB	-5.08	104.45	112.63
1	B	36	VAL	CA-CB-CG2	5.08	119.03	110.40
1	B	106	PHE	N-CA-C	5.07	117.71	109.24
1	C	21	PRO	CA-C-N	5.06	127.57	120.28
1	C	21	PRO	C-N-CA	5.06	127.57	120.28
1	B	44	ASP	N-CA-CB	5.05	117.61	110.13
1	B	87	ARG	NE-CZ-NH1	5.05	126.56	121.50
1	C	106	PHE	CA-C-O	5.05	127.35	121.44
1	B	82	PHE	CA-CB-CG	5.05	118.85	113.80
1	A	28	SER	O-C-N	5.05	127.27	122.07
1	A	80	SER	CA-C-O	-5.03	116.05	121.38
1	C	38	SER	O-C-N	5.03	128.93	122.39
1	C	105	THR	CA-C-O	5.03	126.89	121.06

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	853	0	809	15	0
1	B	842	0	792	9	0
1	C	843	0	800	6	0
2	C	1	0	0	0	0
3	A	72	0	0	1	0
3	B	76	0	0	0	0
3	C	65	0	0	0	0
All	All	2752	0	2401	29	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 6.

All (29) 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:63:LEU:HD11	1:A:89:LEU:HG	1.75	0.68
1:B:76:ILE:O	1:B:77:ASN:HB2	2.05	0.57
1:B:46:ALA:O	1:B:49:LYS:HB2	2.09	0.52
1:C:26:THR:OG1	1:C:29:GLU:HG3	2.11	0.51
1:A:7:PHE:CE1	1:A:98:LYS:HB2	2.47	0.50
1:A:42:LEU:HD23	1:A:78:PHE:CE2	2.47	0.50
1:B:101:ASP:O	1:B:102:HIS:HB2	2.10	0.49
1:B:73:GLU:HB3	1:B:89:LEU:HD13	1.94	0.49
1:A:46:ALA:N	1:A:47:PRO:HD3	2.30	0.46
1:A:57:SER:O	1:A:58:ASN:CB	2.65	0.45
1:C:87:ARG:HG3	1:C:103:TYR:CE1	2.51	0.44
1:A:46:ALA:N	1:A:47:PRO:CD	2.80	0.44
1:B:25:ILE:HG12	1:B:49:LYS:HG3	1.99	0.44
1:C:46:ALA:N	1:C:47:PRO:HD3	2.33	0.44
1:B:13:TYR:HE1	1:B:19:LYS:HD2	1.82	0.43
1:B:81:GLY:HA2	1:C:47:PRO:HB2	1.99	0.43
1:B:98:LYS:HG2	1:B:109:ILE:CG2	2.48	0.43
1:A:63:LEU:HA	1:A:64:PRO:HD3	1.84	0.43
1:A:43:ALA:HA	3:A:142:HOH:O	2.19	0.43
1:A:101:ASP:CG	1:A:104:GLN:HB2	2.45	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:69:ARG:HG3	1:A:91:SER:HB2	2.02	0.42
1:C:109:ILE:O	1:C:110:ARG:HD3	2.20	0.42
1:A:57:SER:O	1:A:58:ASN:HB3	2.20	0.41
1:A:21:PRO:HB2	1:A:23:ASN:OD1	2.21	0.41
1:B:98:LYS:HG2	1:B:109:ILE:HG21	2.02	0.41
1:A:101:ASP:O	1:A:104:GLN:HG3	2.20	0.41
1:C:35:TRP:CD1	1:C:42:LEU:HB2	2.56	0.41
1:A:69:ARG:HA	1:A:92:SER:OG	2.21	0.40
1:A:14:LEU:O	1:A:18:HIS:HA	2.21	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	106/110 (96%)	98 (92%)	6 (6%)	2 (2%)	6	4
1	B	106/110 (96%)	98 (92%)	7 (7%)	1 (1%)	14	14
1	C	105/110 (96%)	101 (96%)	4 (4%)	0	100	100
All	All	317/330 (96%)	297 (94%)	17 (5%)	3 (1%)	14	14

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	58	ASN
1	B	60	GLU
1	A	61	GLY

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%)	78 (90%)	9 (10%)	7	7
1	B	85/92 (92%)	79 (93%)	6 (7%)	13	16
1	C	87/92 (95%)	82 (94%)	5 (6%)	18	23
All	All	259/276 (94%)	239 (92%)	20 (8%)	12	13

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

Mol	Chain	Res	Type
1	A	49	LYS
1	A	59	ARG
1	A	60	GLU
1	A	67	SER
1	A	89	LEU
1	A	92	SER
1	A	96	ILE
1	A	98	LYS
1	A	102	HIS
1	B	19	LYS
1	B	27	LYS
1	B	45	VAL
1	B	49	LYS
1	B	66	LYS
1	B	98	LYS
1	C	49	LYS
1	C	55	ILE
1	C	67	SER
1	C	70	THR
1	C	98	LYS

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

Mol	Chain	Res	Type
1	B	5	ASN

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Mol	Chain	Res	Type
1	B	31	GLN
1	C	15	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](#)

Of 1 ligands modelled in this entry, 1 is monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

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](#)

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	108/110 (98%)	-1.01	0 100 100	2, 14, 28, 41	0
1	B	108/110 (98%)	-1.11	0 100 100	3, 13, 27, 35	0
1	C	107/110 (97%)	-1.02	0 100 100	5, 13, 23, 30	0
All	All	323/330 (97%)	-1.04	0 100 100	2, 13, 27, 41	0

There are no RSRZ outliers to report.

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

There are no non-standard protein/DNA/RNA residues in this entry.

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled ‘Q< 0.9’ lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
2	ZN	C	111	1/1	0.99	0.01	18,18,18,18	0

6.5 Other polymers [i](#)

There are no such residues in this entry.