



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 01:14 AM UTC

PDB ID : 1BSE / pdb_00001bse
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 : 2.00 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

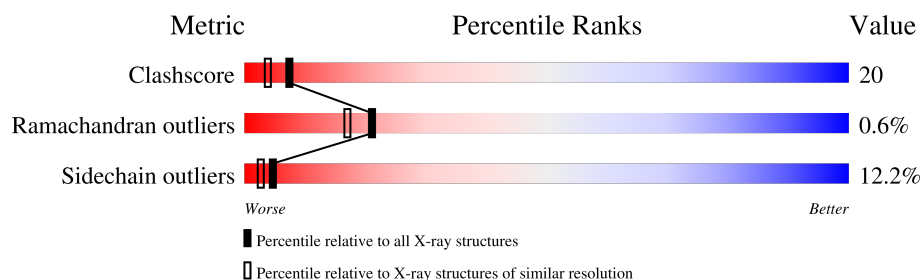
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.00 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	11152 (2.00-2.00)
Ramachandran outliers	187476	11031 (2.00-2.00)
Sidechain outliers	187428	11029 (2.00-2.00)

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 2736 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	542	147	164			
1	B	108	Total	C	N	O	0	0	0
			851	540	145	166			
1	C	108	Total	C	N	O	0	0	0
			843	534	144	165			

There are 3 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	89	VAL	LEU	conflict	UNP P00648
B	89	VAL	LEU	conflict	UNP P00648
C	89	VAL	LEU	conflict	UNP P00648

- Molecule 2 is water.

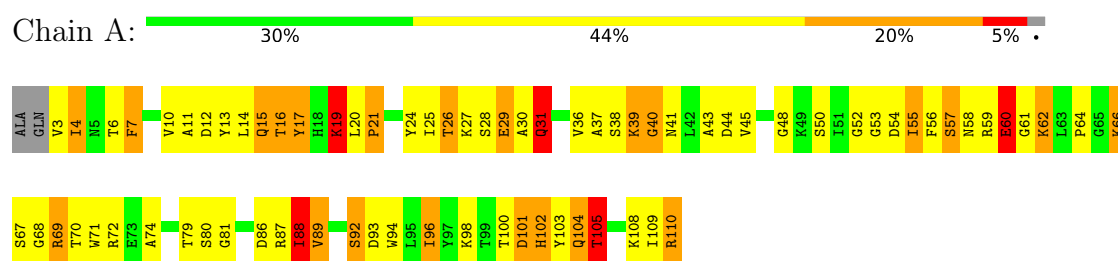
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	58	Total	O	0	0
			58	58		
2	B	64	Total	O	0	0
			64	64		
2	C	67	Total	O	0	0
			67	67		

3 Residue-property plots

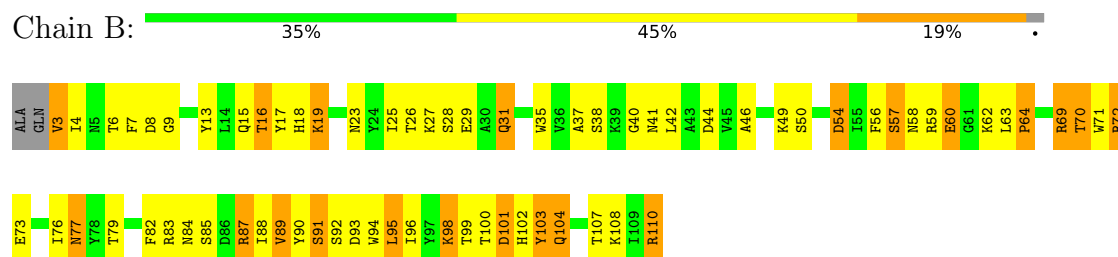
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry. Residues are color-coded 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.

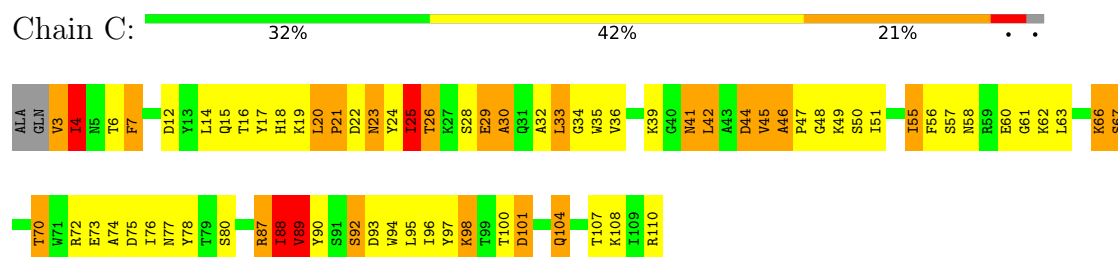
• Molecule 1: BARNASE



• Molecule 1: BARNASE



• Molecule 1: BARNASE



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	58.91Å 58.91Å 81.68Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	(Not available) – 2.00	Depositor
% Data completeness (in resolution range)	(Not available) ((Not available)-2.00)	Depositor
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	PROLSQ	Depositor
R, R_{free}	0.178 , (Not available)	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	2736	wwPDB-VP
Average B, all atoms (Å ²)	22.0	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	1.29	2/874 (0.2%)	3.04	109/1185 (9.2%)
1	B	1.37	0/872	2.77	94/1184 (7.9%)
1	C	1.36	1/864 (0.1%)	3.33	126/1174 (10.7%)
All	All	1.34	3/2610 (0.1%)	3.05	329/3543 (9.3%)

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	60	GLU	N-CA	5.62	1.53	1.46
1	A	11	ALA	N-CA	5.18	1.52	1.46
1	A	105	THR	CB-OG1	5.03	1.51	1.43

All (329) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	60	GLU	CA-CB-CG	32.02	178.15	114.10
1	C	60	GLU	CA-CB-CG	23.07	160.25	114.10
1	C	60	GLU	CG-CD-OE2	20.74	166.10	118.40
1	C	60	GLU	CB-CG-CD	19.88	146.40	112.60
1	C	61	GLY	O-C-N	-16.23	106.50	122.41
1	C	50	SER	CA-C-O	-15.85	102.68	121.06
1	C	61	GLY	CA-C-O	13.91	136.63	119.80
1	A	89	VAL	CB-CA-C	13.75	130.29	110.77
1	C	60	GLU	OE1-CD-OE2	-13.22	91.18	122.90
1	B	31	GLN	OE1-CD-NE2	11.81	134.41	122.60
1	C	18	HIS	CA-CB-CG	-11.28	102.52	113.80
1	A	57	SER	CA-C-O	-10.87	107.47	119.97
1	B	101	ASP	CA-CB-CG	10.44	123.04	112.60
1	A	69	ARG	CA-C-O	10.39	132.33	120.80
1	B	89	VAL	CB-CA-C	10.31	125.89	110.63
1	C	50	SER	O-C-N	10.05	134.93	123.27
1	C	23	ASN	CA-C-O	-9.88	106.39	120.51
1	C	87	ARG	NE-CZ-NH2	9.87	128.08	119.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	87	ARG	NH1-CZ-NH2	-9.78	106.59	119.30
1	C	101	ASP	CA-C-O	-9.56	111.26	121.20
1	A	68	GLY	N-CA-C	-9.49	103.39	114.69
1	A	102	HIS	CB-CG-CD2	-9.34	119.06	131.20
1	A	21	PRO	CB-CA-C	9.26	123.06	111.12
1	C	4	ILE	N-CA-CB	9.17	126.37	111.23
1	B	104	GLN	OE1-CD-NE2	9.09	131.69	122.60
1	B	44	ASP	CA-CB-CG	-9.07	103.53	112.60
1	A	101	ASP	CA-CB-CG	9.00	121.60	112.60
1	A	102	HIS	CA-CB-CG	-8.97	104.83	113.80
1	B	87	ARG	NE-CZ-NH2	8.84	127.16	119.20
1	C	48	GLY	CA-C-O	-8.81	110.48	119.20
1	C	42	LEU	CA-C-O	-8.73	111.21	120.63
1	C	93	ASP	CA-C-N	8.70	134.51	122.07
1	C	93	ASP	C-N-CA	8.70	134.51	122.07
1	C	29	GLU	CA-CB-CG	8.68	131.47	114.10
1	A	64	PRO	CA-C-N	8.43	131.27	120.64
1	A	64	PRO	C-N-CA	8.43	131.27	120.64
1	A	105	THR	N-CA-CB	-8.42	96.18	110.83
1	A	29	GLU	CA-C-O	8.41	129.33	120.42
1	A	104	GLN	CA-C-O	8.38	129.33	120.70
1	C	93	ASP	O-C-N	-8.38	111.38	122.19
1	C	73	GLU	CB-CG-CD	8.37	126.83	112.60
1	C	30	ALA	O-C-N	-8.22	113.54	122.09
1	C	32	ALA	CA-C-N	8.22	137.45	121.18
1	C	32	ALA	C-N-CA	8.22	137.45	121.18
1	C	46	ALA	O-C-N	8.16	127.15	121.19
1	B	17	TYR	CA-C-O	-8.11	109.53	119.18
1	A	16	THR	CA-CB-OG1	-8.09	97.46	109.60
1	A	110	ARG	CD-NE-CZ	8.07	135.70	124.40
1	B	94	TRP	CA-CB-CG	-8.05	98.31	113.60
1	C	26	THR	CA-CB-OG1	-8.04	97.55	109.60
1	C	20	LEU	CA-C-N	8.03	127.98	120.03
1	C	20	LEU	C-N-CA	8.03	127.98	120.03
1	C	12	ASP	CA-C-N	8.00	130.83	120.44
1	C	12	ASP	C-N-CA	8.00	130.83	120.44
1	A	96	ILE	CA-C-O	7.99	128.34	120.27
1	C	7	PHE	CA-CB-CG	7.98	121.78	113.80
1	C	36	VAL	CA-C-O	-7.96	112.15	120.51
1	C	60	GLU	O-C-N	-7.96	111.48	122.46
1	C	24	TYR	CA-C-O	-7.95	112.13	121.11
1	A	4	ILE	CA-C-O	-7.94	111.53	120.74

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	21	PRO	O-C-N	-7.86	113.40	122.91
1	C	36	VAL	O-C-N	7.84	130.32	122.71
1	A	94	TRP	CA-CB-CG	-7.84	98.71	113.60
1	C	44	ASP	CA-CB-CG	-7.79	104.81	112.60
1	A	21	PRO	CA-C-O	7.72	131.60	121.95
1	C	58	ASN	OD1-CG-ND2	-7.71	114.89	122.60
1	B	50	SER	O-C-N	7.71	132.21	123.27
1	C	107	THR	CA-C-O	-7.57	110.97	120.28
1	C	67	SER	N-CA-C	-7.53	98.88	110.10
1	A	53	GLY	CA-C-O	-7.52	110.45	119.03
1	B	8	ASP	CA-C-N	7.52	128.29	119.94
1	B	8	ASP	C-N-CA	7.52	128.29	119.94
1	C	60	GLU	N-CA-C	-7.49	104.02	113.01
1	A	15	GLN	O-C-N	7.49	132.79	122.46
1	A	14	LEU	N-CA-C	7.44	120.34	111.33
1	B	95	LEU	N-CA-CB	7.38	121.20	110.06
1	C	23	ASN	OD1-CG-ND2	7.38	129.98	122.60
1	C	70	THR	CA-C-O	-7.37	112.74	120.70
1	C	93	ASP	CA-C-O	7.35	129.63	120.15
1	A	50	SER	CA-C-O	-7.34	112.53	121.11
1	B	37	ALA	CA-C-O	-7.33	112.72	120.63
1	B	26	THR	CA-CB-OG1	-7.32	98.62	109.60
1	B	16	THR	O-C-N	7.32	130.74	122.32
1	C	88	ILE	CB-CA-C	7.31	121.93	110.81
1	A	88	ILE	N-CA-C	-7.30	97.95	108.17
1	A	60	GLU	CG-CD-OE2	7.29	135.16	118.40
1	B	83	ARG	CD-NE-CZ	-7.29	114.20	124.40
1	B	38	SER	CA-C-O	7.25	128.26	119.49
1	A	48	GLY	CA-C-N	7.25	134.96	122.64
1	A	48	GLY	C-N-CA	7.25	134.96	122.64
1	C	78	TYR	CA-C-O	-7.21	112.47	120.69
1	A	80	SER	CA-C-O	-7.21	113.57	121.28
1	B	4	ILE	CA-C-O	-7.20	112.38	120.74
1	C	107	THR	O-C-N	7.19	132.13	123.36
1	C	94	TRP	N-CA-C	7.16	121.27	111.54
1	B	41	ASN	N-CA-C	7.13	120.84	112.72
1	C	110	ARG	N-CA-CB	7.12	122.61	110.50
1	A	31	GLN	OE1-CD-NE2	7.07	129.67	122.60
1	A	60	GLU	CG-CD-OE1	-7.06	102.17	118.40
1	A	69	ARG	CA-C-N	7.06	133.61	122.74
1	A	69	ARG	C-N-CA	7.06	133.61	122.74
1	B	60	GLU	CA-CB-CG	7.05	128.19	114.10

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	19	LYS	CA-CB-CG	7.03	128.16	114.10
1	A	68	GLY	CA-C-N	-7.03	112.17	122.65
1	A	68	GLY	C-N-CA	-7.03	112.17	122.65
1	B	31	GLN	CG-CD-NE2	-7.03	105.86	116.40
1	B	93	ASP	O-C-N	6.99	131.41	121.97
1	C	66	LYS	CB-CA-C	-6.92	98.86	109.99
1	C	101	ASP	O-C-N	6.92	130.56	121.99
1	C	89	VAL	CA-CB-CG1	6.90	122.13	110.40
1	B	69	ARG	CD-NE-CZ	6.86	134.00	124.40
1	B	28	SER	CA-C-O	6.85	127.68	120.42
1	A	80	SER	O-C-N	6.85	130.14	123.29
1	B	77	ASN	OD1-CG-ND2	6.84	129.44	122.60
1	C	26	THR	N-CA-CB	-6.83	100.67	110.44
1	C	60	GLU	CG-CD-OE1	-6.83	102.70	118.40
1	C	89	VAL	CG1-CB-CG2	-6.82	95.79	110.80
1	A	31	GLN	CB-CG-CD	-6.76	101.10	112.60
1	C	30	ALA	CA-C-O	6.72	128.09	120.90
1	B	70	THR	CB-CA-C	6.71	122.68	109.66
1	A	28	SER	N-CA-CB	-6.71	99.89	110.22
1	B	94	TRP	N-CA-C	6.71	120.66	111.54
1	C	3	VAL	CA-C-N	6.71	134.04	121.97
1	C	3	VAL	C-N-CA	6.71	134.04	121.97
1	C	29	GLU	CB-CG-CD	6.70	123.99	112.60
1	B	54	ASP	O-C-N	6.69	130.51	122.96
1	A	16	THR	O-C-N	6.64	129.55	122.38
1	A	26	THR	CA-CB-OG1	-6.63	99.65	109.60
1	C	97	TYR	CA-C-O	-6.63	113.68	121.44
1	A	102	HIS	CB-CG-ND1	6.61	132.62	122.70
1	C	28	SER	CA-C-O	-6.58	112.02	119.79
1	A	28	SER	CB-CA-C	6.57	122.78	110.63
1	A	105	THR	CA-CB-OG1	-6.57	99.75	109.60
1	A	36	VAL	CA-C-O	-6.54	113.90	120.31
1	B	9	GLY	O-C-N	6.54	128.46	122.18
1	B	17	TYR	CA-CB-CG	-6.53	102.14	113.90
1	B	104	GLN	CA-CB-CG	-6.53	101.04	114.10
1	C	42	LEU	O-C-N	6.53	129.04	122.12
1	A	69	ARG	O-C-N	-6.53	115.55	123.19
1	B	89	VAL	CG1-CB-CG2	-6.49	96.53	110.80
1	B	41	ASN	CA-CB-CG	6.47	119.07	112.60
1	B	25	ILE	O-C-N	-6.44	115.92	123.00
1	B	107	THR	CA-CB-OG1	-6.42	99.98	109.60
1	A	89	VAL	CG1-CB-CG2	-6.41	96.70	110.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	31	GLN	CB-CG-CD	-6.41	101.70	112.60
1	B	103	TYR	CA-C-O	-6.41	112.87	120.81
1	A	87	ARG	CD-NE-CZ	6.38	133.33	124.40
1	C	60	GLU	CA-C-O	6.37	127.33	119.05
1	B	89	VAL	CA-C-O	6.34	127.05	120.39
1	C	21	PRO	CA-C-N	6.34	128.78	120.28
1	C	21	PRO	C-N-CA	6.34	128.78	120.28
1	C	41	ASN	CB-CA-C	-6.34	100.81	111.02
1	C	57	SER	CA-C-O	-6.33	112.69	119.97
1	A	3	VAL	O-C-N	6.32	133.11	123.00
1	A	21	PRO	N-CA-C	-6.31	101.56	111.34
1	A	104	GLN	CA-C-N	6.30	132.38	122.94
1	A	104	GLN	C-N-CA	6.30	132.38	122.94
1	A	38	SER	CA-CB-OG	-6.28	98.53	111.10
1	A	89	VAL	CA-CB-CG2	6.27	121.05	110.40
1	A	104	GLN	OE1-CD-NE2	6.25	128.85	122.60
1	C	22	ASP	O-C-N	6.25	128.74	122.12
1	C	18	HIS	CA-C-O	-6.24	113.08	120.81
1	C	36	VAL	CA-C-N	6.22	131.07	121.19
1	C	36	VAL	C-N-CA	6.22	131.07	121.19
1	B	50	SER	CA-C-O	-6.19	113.88	121.06
1	A	36	VAL	O-C-N	6.16	129.00	123.03
1	A	86	ASP	CB-CG-OD1	6.15	132.55	118.40
1	C	17	TYR	CB-CG-CD1	-6.14	111.59	120.80
1	C	25	ILE	CA-C-O	-6.14	114.87	121.19
1	C	41	ASN	N-CA-C	6.13	120.06	112.59
1	B	89	VAL	O-C-N	-6.11	116.66	123.26
1	A	56	PHE	CB-CA-C	6.09	120.06	110.19
1	A	6	THR	CA-CB-OG1	-6.08	100.48	109.60
1	A	60	GLU	N-CA-CB	6.07	118.93	110.56
1	B	59	ARG	CA-C-O	6.06	127.19	120.82
1	A	59	ARG	CA-C-O	-6.06	111.92	119.38
1	B	64	PRO	CA-C-N	6.05	127.37	120.53
1	B	64	PRO	C-N-CA	6.05	127.37	120.53
1	B	84	ASN	CA-C-N	-6.03	113.01	122.65
1	B	84	ASN	C-N-CA	-6.03	113.01	122.65
1	B	100	THR	CB-CA-C	6.02	120.72	110.85
1	B	46	ALA	O-C-N	6.02	126.10	121.23
1	C	29	GLU	N-CA-C	-6.01	104.65	111.14
1	C	39	LYS	N-CA-CB	-6.01	101.58	110.53
1	A	29	GLU	CG-CD-OE2	6.00	132.19	118.40
1	A	3	VAL	CA-C-N	-5.99	115.09	122.93

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	3	VAL	C-N-CA	-5.99	115.09	122.93
1	C	29	GLU	O-C-N	-5.98	115.63	122.09
1	B	29	GLU	O-C-N	5.97	128.22	122.07
1	C	100	THR	CA-CB-CG2	5.97	120.65	110.50
1	B	23	ASN	CA-CB-CG	5.97	118.57	112.60
1	C	7	PHE	N-CA-CB	5.96	118.99	110.16
1	B	4	ILE	N-CA-C	-5.96	98.64	107.51
1	B	84	ASN	CA-C-O	-5.94	114.30	120.89
1	B	82	PHE	O-C-N	5.93	130.13	122.89
1	C	14	LEU	O-C-N	5.92	128.16	122.07
1	B	28	SER	N-CA-CB	-5.91	101.41	110.16
1	A	29	GLU	OE1-CD-OE2	-5.91	108.72	122.90
1	A	79	THR	CA-C-O	-5.91	112.06	120.51
1	B	18	HIS	CA-CB-CG	-5.91	107.89	113.80
1	C	80	SER	CA-CB-OG	-5.91	99.29	111.10
1	C	6	THR	CA-CB-OG1	-5.90	100.74	109.60
1	A	89	VAL	N-CA-C	-5.90	99.13	107.75
1	A	44	ASP	CA-C-O	-5.89	113.70	120.24
1	A	12	ASP	CA-C-O	-5.88	114.65	120.70
1	A	105	THR	CA-CB-CG2	5.86	120.47	110.50
1	C	60	GLU	CB-CA-C	5.86	122.13	110.17
1	A	81	GLY	CA-C-N	5.86	130.14	120.94
1	A	81	GLY	C-N-CA	5.86	130.14	120.94
1	B	82	PHE	CA-C-O	-5.85	114.60	121.16
1	C	87	ARG	N-CA-CB	5.84	122.38	111.52
1	C	67	SER	N-CA-CB	5.82	118.60	109.69
1	C	95	LEU	O-C-N	-5.82	116.15	123.01
1	A	13	TYR	O-C-N	-5.79	116.07	122.09
1	C	93	ASP	CB-CA-C	5.79	120.03	111.06
1	A	57	SER	CA-CB-OG	-5.76	99.57	111.10
1	A	92	SER	O-C-N	5.76	128.96	122.22
1	C	15	GLN	CB-CG-CD	5.75	122.38	112.60
1	C	20	LEU	O-C-N	5.75	127.97	121.53
1	C	15	GLN	CG-CD-NE2	5.75	125.02	116.40
1	A	37	ALA	CA-C-O	-5.74	114.43	120.63
1	B	49	LYS	CA-C-O	5.74	128.50	121.72
1	A	80	SER	CA-CB-OG	-5.74	99.62	111.10
1	B	3	VAL	N-CA-CB	-5.74	101.75	111.50
1	C	29	GLU	CG-CD-OE2	5.73	131.58	118.40
1	B	72	ARG	NE-CZ-NH2	5.73	124.35	119.20
1	A	29	GLU	CA-CB-CG	5.72	125.54	114.10
1	C	33	LEU	N-CA-C	5.72	119.88	113.01

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	4	ILE	O-C-N	5.71	129.71	122.57
1	C	92	SER	N-CA-CB	5.71	118.52	110.12
1	A	72	ARG	N-CA-CB	5.70	121.75	111.37
1	A	29	GLU	N-CA-CB	5.70	118.59	110.16
1	A	88	ILE	CB-CA-C	5.69	119.31	110.83
1	A	81	GLY	O-C-N	-5.69	118.16	122.88
1	B	25	ILE	CA-C-O	5.67	127.03	121.19
1	C	66	LYS	N-CA-C	5.66	117.13	108.52
1	B	77	ASN	CA-C-O	-5.66	113.78	120.57
1	B	63	LEU	CB-CA-C	5.65	116.51	108.76
1	B	35	TRP	CA-C-O	-5.65	114.31	120.81
1	B	15	GLN	OE1-CD-NE2	-5.64	116.96	122.60
1	B	94	TRP	CA-C-N	-5.63	113.37	121.42
1	B	94	TRP	C-N-CA	-5.63	113.37	121.42
1	A	13	TYR	CA-C-O	5.63	126.92	120.90
1	C	32	ALA	CB-CA-C	5.62	120.41	110.85
1	B	29	GLU	N-CA-CB	5.62	118.16	110.01
1	B	15	GLN	O-C-N	-5.61	115.37	122.27
1	B	57	SER	CB-CA-C	-5.60	101.44	110.74
1	A	31	GLN	CG-CD-NE2	-5.59	108.01	116.40
1	C	62	LYS	N-CA-C	5.59	119.94	113.18
1	A	30	ALA	CA-C-O	-5.59	114.95	120.82
1	B	110	ARG	N-CA-CB	5.58	119.99	110.50
1	C	23	ASN	CA-CB-CG	-5.57	107.03	112.60
1	C	66	LYS	CA-C-N	-5.57	112.97	120.82
1	C	66	LYS	C-N-CA	-5.57	112.97	120.82
1	C	17	TYR	CB-CG-CD2	5.56	129.14	120.80
1	B	18	HIS	N-CA-C	5.52	119.01	111.39
1	C	50	SER	CB-CA-C	-5.52	97.31	109.56
1	B	29	GLU	CG-CD-OE2	-5.51	105.73	118.40
1	C	16	THR	CA-CB-CG2	5.51	119.86	110.50
1	C	93	ASP	N-CA-CB	-5.50	102.22	110.91
1	A	36	VAL	N-CA-CB	-5.50	105.07	112.10
1	C	74	ALA	CA-C-N	5.48	128.50	120.71
1	C	74	ALA	C-N-CA	5.48	128.50	120.71
1	A	54	ASP	O-C-N	-5.47	116.78	122.96
1	B	42	LEU	CA-C-N	5.46	129.34	120.60
1	B	42	LEU	C-N-CA	5.46	129.34	120.60
1	A	7	PHE	CA-C-O	5.44	126.72	120.90
1	A	101	ASP	O-C-N	5.42	128.72	121.99
1	C	78	TYR	O-C-N	5.41	129.37	123.04
1	A	39	LYS	CA-C-N	5.40	128.26	120.11

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	39	LYS	C-N-CA	5.40	128.26	120.11
1	B	35	TRP	O-C-N	5.40	129.57	122.93
1	B	63	LEU	CA-C-N	5.39	126.23	119.98
1	B	63	LEU	C-N-CA	5.39	126.23	119.98
1	C	18	HIS	O-C-N	5.39	131.53	122.21
1	C	89	VAL	CB-CA-C	5.36	118.56	110.63
1	B	40	GLY	O-C-N	-5.35	117.70	122.57
1	A	57	SER	CA-C-N	-5.34	115.70	123.93
1	A	57	SER	C-N-CA	-5.34	115.70	123.93
1	C	94	TRP	CA-CB-CG	-5.34	103.45	113.60
1	C	26	THR	CA-CB-CG2	5.34	119.58	110.50
1	C	48	GLY	CA-C-N	5.33	132.51	121.32
1	C	48	GLY	C-N-CA	5.33	132.51	121.32
1	B	91	SER	O-C-N	5.31	130.35	122.97
1	B	57	SER	N-CA-C	5.31	120.13	111.37
1	C	108	LYS	CA-C-O	-5.31	114.71	120.81
1	C	88	ILE	CA-C-O	5.30	126.76	120.72
1	C	104	GLN	CA-CB-CG	-5.29	103.51	114.10
1	B	16	THR	CA-CB-CG2	5.27	119.46	110.50
1	C	56	PHE	CA-CB-CG	5.27	119.07	113.80
1	A	37	ALA	O-C-N	5.27	127.70	122.12
1	C	4	ILE	CA-CB-CG1	5.26	119.35	110.40
1	C	45	VAL	CA-C-N	-5.26	117.48	122.37
1	C	45	VAL	C-N-CA	-5.26	117.48	122.37
1	B	104	GLN	N-CA-C	-5.26	104.47	112.04
1	C	96	ILE	N-CA-CB	5.25	118.39	111.25
1	A	45	VAL	N-CA-CB	-5.24	102.92	111.98
1	A	100	THR	N-CA-C	-5.23	105.61	112.41
1	B	79	THR	CB-CA-C	5.22	118.94	110.37
1	A	10	VAL	N-CA-C	-5.22	105.75	110.82
1	A	25	ILE	CA-C-O	-5.22	115.75	121.28
1	C	67	SER	CA-C-N	5.22	131.65	121.41
1	C	67	SER	C-N-CA	5.22	131.65	121.41
1	A	96	ILE	N-CA-C	5.21	115.48	107.77
1	C	90	TYR	CA-C-O	5.21	126.65	120.66
1	C	15	GLN	OE1-CD-NE2	-5.20	117.40	122.60
1	A	31	GLN	O-C-N	5.19	127.62	122.12
1	C	4	ILE	CA-C-O	5.19	127.26	120.78
1	A	12	ASP	CB-CG-OD2	-5.17	106.51	118.40
1	A	50	SER	CA-CB-OG	5.17	121.44	111.10
1	A	41	ASN	N-CA-CB	-5.16	103.01	110.70
1	B	38	SER	CA-C-N	5.16	130.84	121.92

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	38	SER	C-N-CA	5.16	130.84	121.92
1	B	6	THR	CA-C-O	-5.14	115.34	121.56
1	A	108	LYS	CA-C-O	-5.13	114.91	120.81
1	B	64	PRO	CA-CB-CG	-5.13	94.76	104.50
1	B	16	THR	CA-CB-OG1	-5.12	101.92	109.60
1	B	98	LYS	CA-C-O	-5.12	115.61	121.40
1	A	40	GLY	O-C-N	-5.12	118.36	122.51
1	B	15	GLN	CA-C-N	5.12	131.18	121.81
1	B	15	GLN	C-N-CA	5.12	131.18	121.81
1	A	69	ARG	NE-CZ-NH2	-5.11	114.60	119.20
1	B	56	PHE	O-C-N	-5.09	117.37	123.27
1	A	6	THR	OG1-CB-CG2	5.07	119.44	109.30
1	C	96	ILE	CB-CA-C	-5.06	103.29	110.83
1	C	48	GLY	O-C-N	5.06	128.57	122.25
1	B	38	SER	O-C-N	-5.02	115.86	122.39
1	A	43	ALA	N-CA-CB	5.02	117.95	110.22
1	B	18	HIS	O-C-N	-5.01	116.34	122.55

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	818	49	0
1	B	851	0	804	22	0
1	C	843	0	787	30	0
2	A	58	0	0	6	0
2	B	64	0	0	4	0
2	C	67	0	0	5	0
All	All	2736	0	2409	101	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 (101) 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:60:GLU:HG2	1:A:62:LYS:HD2	1.26	1.11
1:A:26:THR:OG1	1:A:29:GLU:HG3	1.59	1.01
1:A:101:ASP:O	1:A:104:GLN:HG3	1.61	0.98
1:A:55:ILE:HD11	1:A:70:THR:HG23	1.41	0.98
1:A:16:THR:HB	1:A:17:TYR:CD1	2.12	0.84
1:A:60:GLU:HG2	1:A:62:LYS:CD	2.07	0.84
1:A:55:ILE:CD1	1:A:70:THR:HG23	2.07	0.83
1:A:17:TYR:H	1:A:17:TYR:HD1	1.25	0.82
1:B:19:LYS:HE3	2:B:167:HOH:O	1.83	0.78
1:A:55:ILE:HD11	1:A:70:THR:CG2	2.13	0.77
1:A:26:THR:HG1	1:A:29:GLU:HG3	1.48	0.77
1:A:66:LYS:HG3	1:A:67:SER:N	2.00	0.76
1:A:17:TYR:CD1	1:A:17:TYR:N	2.52	0.76
1:A:21:PRO:O	2:A:156:HOH:O	2.06	0.74
1:C:25:ILE:HD12	1:C:30:ALA:HB2	1.69	0.72
1:B:64:PRO:O	1:B:69:ARG:NH1	2.17	0.71
1:C:3:VAL:HA	2:C:156:HOH:O	1.89	0.71
1:A:16:THR:HB	1:A:17:TYR:CE1	2.26	0.69
1:C:76:ILE:HG13	1:C:88:ILE:HB	1.73	0.69
1:C:3:VAL:O	1:C:23:ASN:OD1	2.09	0.69
1:A:62:LYS:HE3	1:A:104:GLN:O	1.93	0.68
1:B:85:SER:HB3	1:B:102:HIS:CE1	2.31	0.65
1:C:89:VAL:HG22	2:C:148:HOH:O	1.95	0.65
1:A:16:THR:HB	1:A:17:TYR:HD1	1.60	0.64
1:C:76:ILE:O	1:C:77:ASN:HB2	1.98	0.64
1:C:26:THR:OG1	1:C:29:GLU:HG3	1.97	0.64
1:B:85:SER:HB3	1:B:102:HIS:ND1	2.13	0.63
1:B:19:LYS:CE	2:B:167:HOH:O	2.44	0.62
1:A:60:GLU:CG	1:A:62:LYS:HD2	2.16	0.62
1:A:16:THR:CG2	1:A:17:TYR:CE1	2.84	0.60
1:B:108:LYS:NZ	2:B:166:HOH:O	2.26	0.60
1:C:89:VAL:HG13	2:C:148:HOH:O	2.02	0.60
1:A:17:TYR:HD1	1:A:17:TYR:N	1.95	0.60
1:A:57:SER:O	1:A:58:ASN:HB3	2.02	0.59
1:C:98:LYS:O	1:C:98:LYS:HG3	2.00	0.59
1:C:41:ASN:O	1:C:44:ASP:HB2	2.03	0.59
1:A:16:THR:CB	1:A:17:TYR:CD1	2.86	0.57
1:C:55:ILE:HG12	1:C:72:ARG:HG2	1.86	0.56
1:B:57:SER:OG	1:B:58:ASN:N	2.38	0.56
1:C:7:PHE:CE1	1:C:98:LYS:HB2	2.41	0.56
1:B:101:ASP:O	1:B:104:GLN:HG3	2.07	0.54
1:B:64:PRO:HG2	1:B:71:TRP:HZ2	1.73	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:66:LYS:HB3	1:A:69:ARG:NH1	2.22	0.54
1:C:7:PHE:HD1	1:C:88:ILE:HG13	1.72	0.54
1:C:89:VAL:CG2	2:C:148:HOH:O	2.52	0.54
1:A:16:THR:HG21	1:A:17:TYR:CE1	2.44	0.53
1:A:101:ASP:O	1:A:104:GLN:CG	2.47	0.53
1:A:74:ALA:HB3	1:A:88:ILE:HG22	1.90	0.53
1:C:66:LYS:O	1:C:67:SER:C	2.50	0.52
1:B:13:TYR:HE1	1:B:19:LYS:HE2	1.75	0.51
1:A:57:SER:O	1:A:58:ASN:CB	2.59	0.51
1:B:27:LYS:HE2	1:B:54:ASP:OD2	2.10	0.51
1:C:51:ILE:O	1:C:75:ASP:HB2	2.11	0.51
1:A:16:THR:CG2	1:A:17:TYR:CD1	2.94	0.51
1:B:64:PRO:O	1:B:64:PRO:HG2	2.10	0.50
1:A:19:LYS:HZ3	1:A:19:LYS:CB	2.24	0.50
1:C:25:ILE:HA	1:C:29:GLU:OE2	2.11	0.50
1:B:101:ASP:O	1:B:102:HIS:C	2.54	0.49
1:C:25:ILE:CD1	1:C:30:ALA:HB2	2.41	0.49
1:A:52:GLY:HA2	1:A:74:ALA:HA	1.95	0.49
1:C:23:ASN:OD1	1:C:23:ASN:N	2.40	0.48
1:A:96:ILE:HB	1:A:110:ARG:HB2	1.96	0.48
1:B:87:ARG:HB2	1:B:99:THR:HG22	1.94	0.48
1:A:27:LYS:O	1:A:31:GLN:NE2	2.48	0.47
1:C:35:TRP:CD1	1:C:42:LEU:HB2	2.49	0.47
1:A:101:ASP:OD2	1:A:105:THR:HB	2.15	0.47
1:A:15:GLN:HG3	1:A:96:ILE:HD11	1.97	0.46
1:B:96:ILE:HB	1:B:110:ARG:HB2	1.97	0.46
1:B:72:ARG:HB2	1:B:90:TYR:CZ	2.51	0.46
1:C:87:ARG:HH11	1:C:87:ARG:HD3	1.52	0.46
1:A:27:LYS:NZ	2:A:126:HOH:O	2.40	0.46
1:B:62:LYS:HB2	2:B:125:HOH:O	2.17	0.45
1:C:20:LEU:HA	1:C:21:PRO:HD3	1.75	0.45
1:A:21:PRO:HD2	1:A:24:TYR:CD1	2.51	0.44
1:C:63:LEU:HD11	1:C:89:VAL:HG11	1.99	0.44
1:B:7:PHE:CZ	1:B:98:LYS:HE2	2.53	0.44
1:A:39:LYS:HE2	2:A:147:HOH:O	2.17	0.44
1:A:60:GLU:HG2	1:A:62:LYS:CE	2.48	0.43
1:A:96:ILE:HG22	1:A:109:ILE:HG13	1.98	0.43
1:A:102:HIS:C	1:A:103:TYR:CD1	2.97	0.43
1:C:76:ILE:CG1	1:C:88:ILE:HB	2.46	0.43
1:A:62:LYS:HE2	2:A:155:HOH:O	2.18	0.43
1:A:55:ILE:HD13	1:A:71:TRP:O	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:3:VAL:CB	2:C:158:HOH:O	2.68	0.42
1:A:7:PHE:CE1	1:A:98:LYS:HB2	2.55	0.42
1:A:16:THR:HG22	1:A:17:TYR:CD1	2.55	0.42
1:C:41:ASN:HB2	1:C:44:ASP:HB2	2.02	0.42
1:A:40:GLY:HA2	2:A:131:HOH:O	2.20	0.41
1:B:73:GLU:HA	1:B:88:ILE:O	2.20	0.41
1:A:93:ASP:OD1	1:A:93:ASP:N	2.54	0.41
1:B:76:ILE:O	1:B:77:ASN:HB2	2.19	0.41
1:C:46:ALA:N	1:C:47:PRO:HD3	2.35	0.41
1:A:16:THR:CB	1:A:17:TYR:CE1	3.01	0.41
1:A:96:ILE:HD12	1:A:110:ARG:HB2	2.02	0.41
1:B:27:LYS:CE	1:B:54:ASP:OD2	2.69	0.41
1:B:69:ARG:HG3	1:B:91:SER:HB2	2.03	0.41
1:C:101:ASP:CG	1:C:104:GLN:HB2	2.46	0.41
1:C:29:GLU:O	1:C:30:ALA:C	2.63	0.40
1:A:20:LEU:HA	1:A:21:PRO:HD3	1.86	0.40
1:C:34:GLY:O	1:C:45:VAL:HG11	2.21	0.40
1:A:4:ILE:HA	2:A:158:HOH:O	2.21	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%)	100 (94%)	5 (5%)	1 (1%)	14	9
1	B	106/110 (96%)	102 (96%)	4 (4%)	0	100	100
1	C	106/110 (96%)	101 (95%)	4 (4%)	1 (1%)	14	9
All	All	318/330 (96%)	303 (95%)	13 (4%)	2 (1%)	21	17

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	4	ILE
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	89/92 (97%)	78 (88%)	11 (12%)	4	2
1	B	88/92 (96%)	78 (89%)	10 (11%)	5	3
1	C	86/92 (94%)	75 (87%)	11 (13%)	4	2
All	All	263/276 (95%)	231 (88%)	32 (12%)	5	3

All (32) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	17	TYR
1	A	19	LYS
1	A	31	GLN
1	A	55	ILE
1	A	60	GLU
1	A	62	LYS
1	A	66	LYS
1	A	88	ILE
1	A	89	VAL
1	A	92	SER
1	A	105	THR
1	B	3	VAL
1	B	16	THR
1	B	19	LYS
1	B	31	GLN
1	B	60	GLU
1	B	70	THR
1	B	89	VAL
1	B	92	SER
1	B	95	LEU
1	B	103	TYR

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Mol	Chain	Res	Type
1	C	4	ILE
1	C	19	LYS
1	C	25	ILE
1	C	33	LEU
1	C	49	LYS
1	C	55	ILE
1	C	70	THR
1	C	88	ILE
1	C	89	VAL
1	C	92	SER
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	A	18	HIS
1	A	102	HIS
1	C	104	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.