



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 8, 2026 – 04:46 AM UTC

PDB ID : 1COL / pdb_00001col
Title : REFINED STRUCTURE OF THE PORE-FORMING DOMAIN OF COL-
ICIN A AT 2.4 ANGSTROMS RESOLUTION
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Deposited on : 1991-07-06
Resolution : 2.40 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

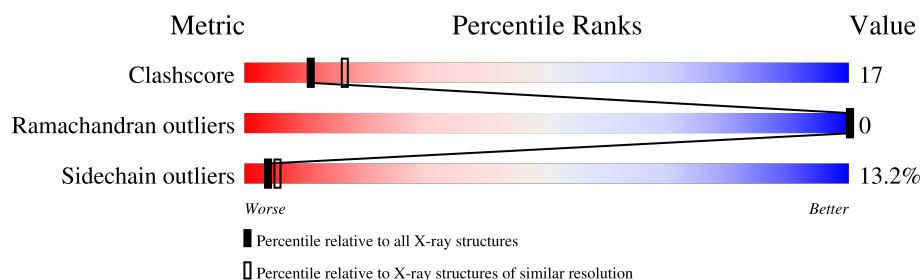
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.40 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	5391 (2.40-2.40)
Ramachandran outliers	187476	5320 (2.40-2.40)
Sidechain outliers	187428	5321 (2.40-2.40)

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	204	
1	B	204	

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 3039 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 COLICIN A.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	197	Total	C	N	O	S	0	0	0
			1478	938	251	283	6			
1	B	197	Total	C	N	O	S	0	0	0
			1478	938	251	283	6			

- Molecule 2 is water.

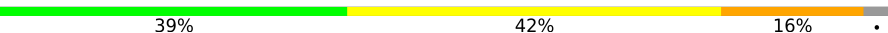
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	41	Total	O	0	0
			41	41		
2	B	42	Total	O	0	0
			42	42		

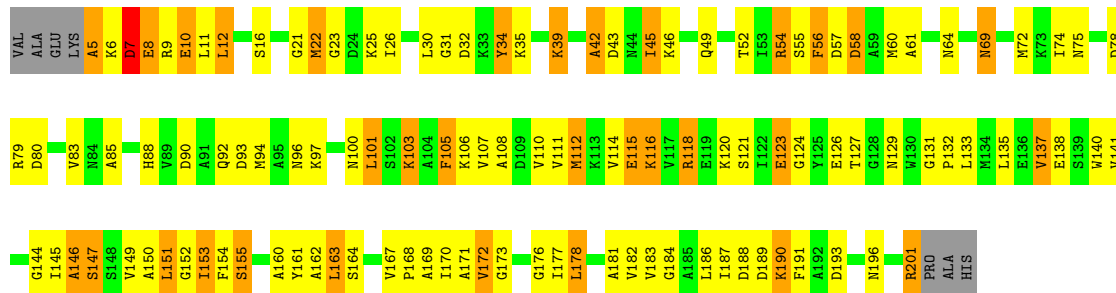
3 Residue-property plots [i](#)

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.

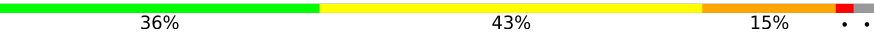
Note EDS was not executed.

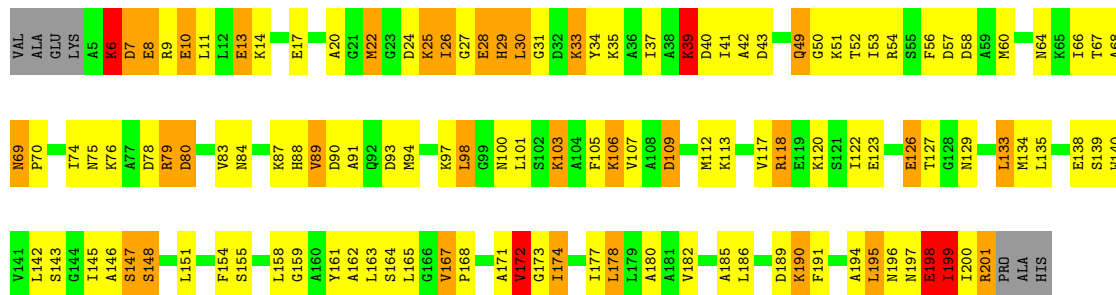
• Molecule 1: COLICIN A

Chain A: 



• Molecule 1: COLICIN A

Chain B: 



4 Data and refinement statistics

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

Property	Value	Source
Space group	P 43 21 2	Depositor
Cell constants a, b, c, α , β , γ	73.00Å 73.00Å 171.60Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	6.00 – 2.40	Depositor
% Data completeness (in resolution range)	(Not available) (6.00-2.40)	Depositor
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	PROLSQ	Depositor
R, R_{free}	0.180 , (Not available)	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	3039	wwPDB-VP
Average B, all atoms (Å ²)	35.0	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	1.16	0/1496	2.69	137/2016 (6.8%)
1	B	1.16	0/1496	2.72	147/2016 (7.3%)
All	All	1.16	0/2992	2.71	284/4032 (7.0%)

There are no bond length outliers.

All (284) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	88	HIS	CA-CB-CG	-12.06	101.74	113.80
1	A	196	ASN	CA-CB-CG	-11.13	101.47	112.60
1	A	6	LYS	N-CA-C	-10.58	101.12	114.56
1	A	151	LEU	CA-C-O	10.37	131.99	120.90
1	B	190	LYS	CA-CB-CG	10.25	134.60	114.10
1	A	171	ALA	CA-C-O	-9.85	110.55	120.70
1	A	43	ASP	CA-CB-CG	-9.42	103.18	112.60
1	A	123	GLU	CA-C-N	9.40	130.19	119.94
1	A	123	GLU	C-N-CA	9.40	130.19	119.94
1	A	137	VAL	N-CA-CB	9.35	121.49	110.55
1	A	105	PHE	N-CA-C	-9.19	101.49	112.89
1	B	28	GLU	CA-CB-CG	9.16	132.43	114.10
1	A	22	MET	N-CA-C	-9.14	101.30	111.07
1	B	162	ALA	CA-C-N	9.09	132.47	120.28
1	B	162	ALA	C-N-CA	9.09	132.47	120.28
1	A	56	PHE	CA-C-O	-8.95	111.33	120.90
1	A	137	VAL	CB-CA-C	-8.94	100.52	111.97
1	B	182	VAL	CB-CA-C	8.86	123.31	111.97
1	A	80	ASP	CA-CB-CG	8.80	121.40	112.60
1	A	32	ASP	CA-C-O	-8.72	111.31	120.55
1	B	7	ASP	CA-C-N	8.66	139.17	122.53
1	B	7	ASP	C-N-CA	8.66	139.17	122.53
1	B	158	LEU	CA-C-N	8.63	129.35	119.94
1	B	158	LEU	C-N-CA	8.63	129.35	119.94
1	B	7	ASP	CA-C-O	8.56	130.05	119.95

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	161	TYR	CA-C-N	8.55	131.74	120.28
1	A	161	TYR	C-N-CA	8.55	131.74	120.28
1	B	117	VAL	CA-C-O	8.45	129.74	120.95
1	A	115	GLU	CA-CB-CG	8.35	130.79	114.10
1	B	26	ILE	O-C-N	8.35	131.23	121.80
1	B	199	ILE	CA-C-O	-8.21	110.52	120.78
1	B	154	PHE	CA-C-O	-8.17	112.48	120.90
1	B	118	ARG	NE-CZ-NH1	-8.17	113.33	121.50
1	A	30	LEU	CB-CA-C	8.13	124.09	109.29
1	B	89	VAL	N-CA-CB	8.12	122.29	111.25
1	B	69	ASN	CA-CB-CG	-8.09	104.51	112.60
1	B	84	ASN	OD1-CG-ND2	8.04	130.65	122.60
1	A	178	LEU	CA-C-O	-8.03	111.91	120.42
1	A	127	THR	CA-CB-OG1	-7.96	97.66	109.60
1	A	172	VAL	CA-C-N	7.89	128.54	119.94
1	A	172	VAL	C-N-CA	7.89	128.54	119.94
1	B	33	LYS	CA-CB-CG	7.88	129.85	114.10
1	A	78	ASP	CA-CB-CG	-7.87	104.73	112.60
1	B	154	PHE	CA-CB-CG	7.85	121.65	113.80
1	A	69	ASN	OD1-CG-ND2	7.71	130.31	122.60
1	A	56	PHE	N-CA-CB	7.66	121.35	109.94
1	A	5	ALA	CA-C-N	7.65	133.79	122.08
1	A	5	ALA	C-N-CA	7.65	133.79	122.08
1	A	83	VAL	CA-C-N	7.63	130.50	120.28
1	A	83	VAL	C-N-CA	7.63	130.50	120.28
1	A	193	ASP	CA-CB-CG	-7.60	105.00	112.60
1	B	196	ASN	OD1-CG-ND2	-7.50	115.10	122.60
1	A	196	ASN	OD1-CG-ND2	7.49	130.09	122.60
1	A	30	LEU	N-CA-CB	-7.48	99.53	110.53
1	B	143	SER	CA-CB-OG	-7.47	96.16	111.10
1	B	8	GLU	N-CA-C	-7.46	103.80	113.12
1	A	96	ASN	CA-C-O	-7.37	113.08	120.82
1	B	90	ASP	CA-CB-CG	-7.37	105.23	112.60
1	B	148	SER	CB-CA-C	-7.36	99.04	110.81
1	A	118	ARG	NE-CZ-NH2	7.34	125.81	119.20
1	A	154	PHE	CA-C-N	7.28	129.91	120.44
1	A	154	PHE	C-N-CA	7.28	129.91	120.44
1	A	85	ALA	N-CA-C	-7.26	103.31	111.07
1	A	96	ASN	OD1-CG-ND2	-7.24	115.36	122.60
1	A	56	PHE	N-CA-C	-7.23	102.43	111.11
1	B	13	GLU	CA-C-N	7.23	129.97	120.28
1	B	13	GLU	C-N-CA	7.23	129.97	120.28

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	201	ARG	CA-C-O	-7.21	108.55	120.80
1	A	56	PHE	O-C-N	7.17	129.55	122.09
1	A	9	ARG	N-CA-C	-7.17	103.20	112.23
1	B	123	GLU	CA-C-O	-7.15	112.97	120.55
1	B	84	ASN	CA-CB-CG	-7.13	105.47	112.60
1	A	83	VAL	O-C-N	-7.11	114.95	121.91
1	A	123	GLU	CB-CG-CD	7.08	124.64	112.60
1	B	98	LEU	CA-C-N	7.07	127.95	120.03
1	B	98	LEU	C-N-CA	7.07	127.95	120.03
1	A	124	GLY	O-C-N	7.05	128.96	122.19
1	B	174	ILE	CA-C-O	-7.03	113.71	121.17
1	B	145	ILE	CA-C-O	-7.01	113.73	121.23
1	B	6	LYS	N-CA-CB	6.99	122.87	111.27
1	A	64	ASN	CA-CB-CG	-6.97	105.63	112.60
1	B	22	MET	N-CA-C	-6.92	103.73	111.28
1	A	42	ALA	CA-C-O	-6.92	112.28	120.10
1	A	21	GLY	CA-C-N	6.86	129.36	120.44
1	A	21	GLY	C-N-CA	6.86	129.36	120.44
1	A	32	ASP	O-C-N	6.85	129.38	122.12
1	A	121	SER	N-CA-C	-6.82	103.08	111.40
1	B	40	ASP	CA-CB-CG	6.82	119.42	112.60
1	B	118	ARG	NH1-CZ-NH2	6.77	128.10	119.30
1	B	53	ILE	CA-C-O	-6.75	113.31	121.54
1	A	201	ARG	CD-NE-CZ	6.73	133.82	124.40
1	B	161	TYR	CA-C-N	6.73	129.60	120.38
1	B	161	TYR	C-N-CA	6.73	129.60	120.38
1	B	126	GLU	CA-CB-CG	6.67	127.43	114.10
1	B	118	ARG	CD-NE-CZ	-6.65	115.09	124.40
1	A	83	VAL	CA-C-O	6.61	128.17	121.17
1	A	116	LYS	CA-CB-CG	-6.60	100.89	114.10
1	B	91	ALA	CA-C-O	-6.60	113.55	120.55
1	A	92	GLN	O-C-N	6.59	128.86	122.07
1	A	150	ALA	N-CA-C	-6.59	103.78	110.97
1	B	14	LYS	O-C-N	6.59	129.11	122.12
1	A	191	PHE	CA-C-O	-6.59	113.52	120.63
1	A	147	SER	N-CA-C	-6.56	103.24	111.11
1	A	141	VAL	CA-C-O	-6.56	113.69	120.71
1	B	22	MET	CA-C-N	6.55	127.26	119.98
1	B	22	MET	C-N-CA	6.55	127.26	119.98
1	B	83	VAL	N-CA-C	-6.50	104.31	110.42
1	B	146	ALA	CA-C-N	6.50	129.32	120.54
1	B	146	ALA	C-N-CA	6.50	129.32	120.54

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	85	ALA	O-C-N	-6.48	115.40	122.07
1	B	120	LYS	CB-CA-C	6.47	123.09	110.67
1	B	78	ASP	CA-C-N	6.46	128.83	120.44
1	B	78	ASP	C-N-CA	6.46	128.83	120.44
1	A	129	ASN	CA-CB-CG	6.44	119.04	112.60
1	B	165	LEU	O-C-N	6.43	130.84	122.93
1	B	80	ASP	CA-CB-CG	-6.39	106.21	112.60
1	B	93	ASP	O-C-N	6.38	128.64	122.07
1	B	148	SER	CA-CB-OG	-6.36	98.38	111.10
1	B	69	ASN	N-CA-C	-6.34	100.18	109.50
1	A	49	GLN	CB-CA-C	6.33	119.34	109.84
1	B	177	ILE	CA-C-N	6.33	128.67	120.44
1	B	177	ILE	C-N-CA	6.33	128.67	120.44
1	B	58	ASP	CA-CB-CG	6.33	118.93	112.60
1	B	29	HIS	CA-CB-CG	-6.30	107.50	113.80
1	A	94	MET	CA-CB-CG	-6.29	101.52	114.10
1	A	58	ASP	O-C-N	6.29	129.32	122.15
1	B	28	GLU	CG-CD-OE2	6.22	132.72	118.40
1	A	181	ALA	CA-C-N	6.22	128.39	120.56
1	A	181	ALA	C-N-CA	6.22	128.39	120.56
1	A	183	VAL	CB-CA-C	6.20	119.56	111.81
1	B	33	LYS	N-CA-CB	6.20	118.99	110.01
1	A	171	ALA	N-CA-CB	6.18	119.04	110.07
1	A	155	SER	CA-C-O	-6.17	114.34	120.82
1	A	187	ILE	N-CA-C	6.17	122.18	109.34
1	B	198	GLU	CB-CA-C	-6.16	97.90	109.72
1	B	94	MET	CB-CA-C	6.15	121.00	110.79
1	B	39	LYS	N-CA-C	-6.11	104.53	112.23
1	B	173	GLY	N-CA-C	-6.11	105.42	112.50
1	A	85	ALA	CB-CA-C	6.09	120.44	110.88
1	B	78	ASP	CA-CB-CG	-6.07	106.53	112.60
1	A	153	ILE	N-CA-C	6.07	116.24	110.42
1	B	20	ALA	N-CA-C	-6.06	104.79	111.82
1	B	107	VAL	CA-C-O	-6.06	113.21	120.78
1	A	169	ALA	CA-C-O	-6.05	114.13	120.55
1	A	201	ARG	NE-CZ-NH1	6.05	127.56	121.50
1	B	133	LEU	O-C-N	6.05	128.33	122.03
1	A	160	ALA	CA-C-O	6.03	126.90	119.97
1	A	151	LEU	O-C-N	-6.02	115.83	122.09
1	B	27	GLY	N-CA-C	-6.02	106.28	113.99
1	B	191	PHE	CA-C-O	-6.02	114.17	120.55
1	A	6	LYS	CA-C-O	6.02	125.41	118.55

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	155	SER	N-CA-C	5.93	117.75	111.28
1	B	123	GLU	CA-C-N	5.92	126.68	119.99
1	B	123	GLU	C-N-CA	5.92	126.68	119.99
1	B	67	THR	OG1-CB-CG2	5.91	121.12	109.30
1	B	123	GLU	CG-CD-OE2	-5.91	104.81	118.40
1	B	41	ILE	N-CA-C	-5.91	104.75	110.42
1	A	12	LEU	CA-C-N	5.89	128.45	120.44
1	A	12	LEU	C-N-CA	5.89	128.45	120.44
1	A	32	ASP	N-CA-CB	5.85	118.71	110.12
1	A	31	GLY	CA-C-N	5.84	128.11	120.28
1	A	31	GLY	C-N-CA	5.84	128.11	120.28
1	A	103	LYS	CA-CB-CG	5.83	125.77	114.10
1	B	113	LYS	CA-CB-CG	-5.83	102.44	114.10
1	B	27	GLY	O-C-N	5.83	128.95	122.54
1	A	103	LYS	CA-C-N	5.80	129.88	120.60
1	A	103	LYS	C-N-CA	5.80	129.88	120.60
1	B	147	SER	CA-C-N	5.80	128.37	120.54
1	B	147	SER	C-N-CA	5.80	128.37	120.54
1	B	196	ASN	N-CA-CB	5.80	118.38	109.91
1	A	108	ALA	CA-C-O	5.80	127.37	120.70
1	B	129	ASN	N-CA-CB	-5.79	101.00	110.21
1	A	160	ALA	CA-C-N	5.78	127.95	120.44
1	A	160	ALA	C-N-CA	5.78	127.95	120.44
1	B	126	GLU	CB-CA-C	-5.76	101.06	110.85
1	B	190	LYS	CA-C-N	5.75	127.99	120.28
1	B	190	LYS	C-N-CA	5.75	127.99	120.28
1	A	39	LYS	CA-CB-CG	-5.74	102.62	114.10
1	A	49	GLN	CA-C-O	5.72	127.19	120.96
1	B	54	ARG	NE-CZ-NH1	-5.72	115.78	121.50
1	B	147	SER	CA-CB-OG	-5.72	99.66	111.10
1	B	165	LEU	CA-C-O	-5.71	114.25	120.81
1	A	7	ASP	CA-C-N	5.70	132.00	121.52
1	A	7	ASP	C-N-CA	5.70	132.00	121.52
1	A	8	GLU	N-CA-C	-5.68	105.46	112.90
1	A	146	ALA	CA-C-N	5.66	128.18	120.54
1	A	146	ALA	C-N-CA	5.66	128.18	120.54
1	A	164	SER	CA-CB-OG	-5.64	99.83	111.10
1	B	17	GLU	CA-C-O	-5.63	114.58	120.55
1	B	105	PHE	N-CA-C	-5.63	106.36	113.18
1	B	75	ASN	CB-CA-C	5.63	121.15	110.51
1	B	83	VAL	CB-CA-C	5.62	119.12	111.87
1	B	98	LEU	CA-C-O	5.62	126.50	120.55

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	127	THR	CA-C-O	-5.62	112.55	119.18
1	B	24	ASP	CA-CB-CG	5.61	118.21	112.60
1	A	22	MET	CA-C-N	5.61	126.20	119.98
1	A	22	MET	C-N-CA	5.61	126.20	119.98
1	A	146	ALA	N-CA-CB	-5.61	101.36	109.83
1	B	197	ASN	CB-CA-C	5.61	119.68	110.88
1	A	101	LEU	N-CA-C	-5.60	105.26	111.36
1	B	8	GLU	N-CA-CB	5.59	118.98	110.42
1	B	43	ASP	N-CA-C	-5.59	105.10	111.14
1	A	69	ASN	O-C-N	5.55	126.46	121.35
1	A	93	ASP	O-C-N	5.55	127.86	122.09
1	A	182	VAL	CB-CA-C	5.55	119.07	111.97
1	B	185	ALA	CA-C-N	5.54	132.39	121.58
1	B	185	ALA	C-N-CA	5.54	132.39	121.58
1	B	167	VAL	CA-CB-CG2	5.51	119.77	110.40
1	A	12	LEU	CA-C-O	5.51	126.39	120.55
1	A	160	ALA	O-C-N	-5.51	115.50	122.27
1	A	45	ILE	CA-CB-CG2	5.48	119.81	110.50
1	B	50	GLY	CA-C-O	-5.47	113.58	119.27
1	A	144	GLY	N-CA-C	5.46	122.86	115.00
1	A	45	ILE	CB-CG1-CD1	-5.45	102.35	113.80
1	A	57	ASP	CA-CB-CG	5.44	118.04	112.60
1	A	101	LEU	CA-CB-CG	5.42	135.28	116.30
1	A	88	HIS	N-CA-CB	5.42	119.20	110.42
1	A	105	PHE	N-CA-CB	5.41	119.22	110.40
1	B	52	THR	CA-CB-CG2	5.40	119.68	110.50
1	B	54	ARG	NE-CZ-NH2	5.39	124.05	119.20
1	B	6	LYS	N-CA-C	-5.38	105.00	113.02
1	B	147	SER	O-C-N	5.37	127.67	122.09
1	B	40	ASP	CB-CA-C	5.36	119.97	110.85
1	A	79	ARG	CB-CA-C	5.35	119.68	110.79
1	A	58	ASP	CA-C-N	5.34	127.38	120.44
1	A	58	ASP	C-N-CA	5.34	127.38	120.44
1	A	46	LYS	O-C-N	5.33	128.24	122.11
1	B	164	SER	CA-C-O	-5.32	112.30	119.11
1	A	184	GLY	CA-C-N	5.32	127.40	120.28
1	A	184	GLY	C-N-CA	5.32	127.40	120.28
1	B	42	ALA	CA-C-O	-5.30	114.11	120.10
1	A	92	GLN	N-CA-CB	5.29	117.68	110.01
1	B	171	ALA	N-CA-CB	5.29	118.47	110.28
1	B	178	LEU	CA-C-O	-5.28	115.27	120.82
1	B	26	ILE	CA-C-O	-5.27	114.78	120.47

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	34	TYR	O-C-N	5.26	128.15	122.15
1	A	5	ALA	CA-C-O	5.26	129.75	120.80
1	A	23	GLY	CA-C-N	5.26	127.78	120.63
1	A	23	GLY	C-N-CA	5.26	127.78	120.63
1	B	31	GLY	N-CA-C	5.26	120.60	112.45
1	B	7	ASP	N-CA-C	-5.26	106.17	112.59
1	B	177	ILE	CA-C-O	5.26	126.33	120.71
1	A	100	ASN	CA-CB-CG	-5.25	107.35	112.60
1	B	51	LYS	CA-C-N	5.25	130.81	122.94
1	B	51	LYS	C-N-CA	5.25	130.81	122.94
1	B	138	GLU	CA-C-O	-5.24	114.99	120.55
1	B	155	SER	CA-C-N	5.24	127.73	120.29
1	B	155	SER	C-N-CA	5.24	127.73	120.29
1	A	97	LYS	CA-CB-CG	-5.24	103.62	114.10
1	B	129	ASN	CA-C-N	5.23	131.18	122.54
1	B	129	ASN	C-N-CA	5.23	131.18	122.54
1	A	114	VAL	O-C-N	5.22	127.60	121.96
1	A	90	ASP	N-CA-CB	5.22	119.00	110.39
1	B	172	VAL	CA-C-N	5.22	125.73	119.94
1	B	172	VAL	C-N-CA	5.22	125.73	119.94
1	B	171	ALA	CA-C-O	-5.21	113.98	119.97
1	B	180	ALA	CA-C-N	5.20	127.52	120.44
1	B	180	ALA	C-N-CA	5.20	127.52	120.44
1	A	189	ASP	CA-C-N	5.19	127.19	120.44
1	A	189	ASP	C-N-CA	5.19	127.19	120.44
1	A	6	LYS	CA-CB-CG	5.17	124.44	114.10
1	B	126	GLU	CA-C-O	-5.17	114.94	120.42
1	A	75	ASN	CB-CA-C	5.15	118.85	109.83
1	B	54	ARG	CA-C-N	5.15	129.57	120.87
1	B	54	ARG	C-N-CA	5.15	129.57	120.87
1	A	42	ALA	CA-C-N	5.14	127.59	120.29
1	A	42	ALA	C-N-CA	5.14	127.59	120.29
1	A	126	GLU	CA-C-O	-5.14	115.10	120.55
1	A	72	MET	N-CA-C	5.14	119.19	113.02
1	B	112	MET	CA-CB-CG	-5.14	103.82	114.10
1	B	10	GLU	CB-CA-C	-5.11	102.83	110.90
1	A	54	ARG	NH1-CZ-NH2	-5.09	112.68	119.30
1	B	109	ASP	CA-C-N	5.09	128.51	120.47
1	B	109	ASP	C-N-CA	5.09	128.51	120.47
1	B	159	GLY	N-CA-C	-5.07	106.36	112.49
1	B	155	SER	CA-CB-OG	-5.05	100.99	111.10
1	B	182	VAL	CA-CB-CG2	5.04	118.98	110.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	8	GLU	CB-CA-C	-5.03	101.26	109.56
1	B	196	ASN	O-C-N	5.02	127.25	122.03
1	B	189	ASP	CA-C-N	5.02	127.00	120.28
1	B	189	ASP	C-N-CA	5.02	127.00	120.28
1	A	39	LYS	CB-CA-C	5.01	120.60	110.38
1	A	8	GLU	CA-C-O	5.01	125.46	119.60
1	B	140	TRP	N-CA-CB	5.01	117.58	110.16

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	1478	0	1521	44	0
1	B	1478	0	1521	55	1
2	A	41	0	0	1	1
2	B	42	0	0	3	0
All	All	3039	0	3042	99	1

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 17.

All (99) 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:76:LYS:HG2	1:B:79:ARG:NH1	1.93	0.83
1:A:5:ALA:HB3	1:A:8:GLU:HG3	1.62	0.82
1:B:6:LYS:HD2	1:B:9:ARG:NH1	1.98	0.77
1:B:76:LYS:HG2	1:B:79:ARG:HH11	1.50	0.77
1:B:9:ARG:NH1	1:B:49:GLN:NE2	2.33	0.76
1:B:6:LYS:HG3	1:B:9:ARG:HD2	1.68	0.75
1:B:6:LYS:CD	1:B:9:ARG:HH11	2.06	0.68
1:B:9:ARG:NH1	1:B:49:GLN:HE22	1.92	0.68
1:B:194:ALA:O	1:B:198:GLU:HG3	1.94	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:107:VAL:HG22	1:A:110:VAL:HB	1.77	0.67
1:A:167:VAL:HB	1:A:168:PRO:HD2	1.77	0.67
1:B:6:LYS:HG3	1:B:9:ARG:HG3	1.76	0.67
1:A:146:ALA:HB3	1:A:149:VAL:HG23	1.78	0.65
1:A:167:VAL:HB	1:A:168:PRO:CD	2.28	0.63
1:A:35:LYS:O	1:A:39:LYS:HG3	1.99	0.62
1:A:140:TRP:HB3	1:A:145:ILE:HD13	1.81	0.62
1:A:103:LYS:HA	1:A:106:LYS:HE2	1.81	0.61
1:A:173:GLY:O	1:A:177:ILE:HG13	2.00	0.61
1:B:6:LYS:HG3	1:B:9:ARG:CD	2.30	0.60
1:A:149:VAL:O	1:A:153:ILE:HD12	2.02	0.59
1:B:6:LYS:CD	1:B:9:ARG:NH1	2.63	0.59
1:B:6:LYS:HG3	1:B:9:ARG:HH11	1.67	0.59
1:A:54:ARG:HG3	1:A:186:LEU:O	2.03	0.59
1:B:6:LYS:CG	1:B:9:ARG:HD2	2.32	0.58
1:A:22:MET:HE3	1:A:34:TYR:OH	2.04	0.58
1:A:103:LYS:O	1:A:106:LYS:HB2	2.04	0.57
1:B:66:ILE:HD12	1:B:200:ILE:HD11	1.85	0.57
1:B:6:LYS:HG3	1:B:9:ARG:CG	2.35	0.56
1:A:10:GLU:HA	1:A:10:GLU:OE1	2.06	0.56
1:B:98:LEU:O	1:B:101:LEU:HB2	2.05	0.56
1:A:39:LYS:HB3	2:A:234:HOH:O	2.06	0.56
1:B:56:PHE:O	1:B:60:MET:HG2	2.06	0.56
1:B:26:ILE:CG2	1:B:30:LEU:HD22	2.36	0.55
1:B:109:ASP:HA	2:B:235:HOH:O	2.06	0.55
1:B:198:GLU:C	1:B:199:ILE:HG12	2.30	0.55
1:A:107:VAL:HG11	1:A:153:ILE:HD11	1.89	0.55
1:B:29:HIS:HD2	1:B:172:VAL:HG11	1.71	0.55
1:B:37:ILE:HG21	1:B:195:LEU:HD13	1.89	0.55
1:B:6:LYS:CG	1:B:9:ARG:HH11	2.20	0.54
1:A:149:VAL:HG12	1:A:153:ILE:CD1	2.38	0.53
1:B:29:HIS:CD2	1:B:172:VAL:HG11	2.44	0.53
1:A:55:SER:O	1:A:56:PHE:C	2.51	0.53
1:A:69:ASN:OD1	1:A:69:ASN:C	2.52	0.53
1:A:58:ASP:O	1:A:61:ALA:HB3	2.09	0.52
1:A:74:ILE:HD11	1:A:178:LEU:HD11	1.91	0.52
1:A:60:MET:HE2	1:A:131:GLY:HA2	1.92	0.51
1:B:26:ILE:HG13	1:B:172:VAL:HG22	1.92	0.51
1:B:194:ALA:O	1:B:198:GLU:CG	2.58	0.51
1:B:35:LYS:O	1:B:39:LYS:HD3	2.12	0.50
1:B:76:LYS:CG	1:B:79:ARG:NH1	2.72	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:26:ILE:HG21	1:A:176:GLY:HA3	1.93	0.50
1:B:25:LYS:O	1:B:28:GLU:HG3	2.13	0.49
1:A:123:GLU:OE2	1:A:132:PRO:HG2	2.12	0.49
1:B:22:MET:HE3	1:B:34:TYR:OH	2.13	0.49
1:B:7:ASP:OD2	2:B:225:HOH:O	2.19	0.49
1:A:149:VAL:HG12	1:A:153:ILE:HD12	1.94	0.49
1:B:37:ILE:HD11	1:B:198:GLU:HG3	1.94	0.48
1:A:118:ARG:HH11	1:A:118:ARG:HG2	1.79	0.48
1:B:167:VAL:HB	1:B:168:PRO:CD	2.44	0.47
1:B:8:GLU:OE1	1:B:49:GLN:HG3	2.14	0.47
1:A:16:SER:HB2	1:A:42:ALA:O	2.14	0.47
1:A:140:TRP:HB3	1:A:145:ILE:CD1	2.43	0.47
1:B:122:ILE:O	1:B:126:GLU:HG2	2.14	0.47
1:B:69:ASN:OD1	1:B:70:PRO:HD2	2.14	0.46
1:B:198:GLU:HB2	1:B:199:ILE:HG12	1.98	0.46
1:A:8:GLU:O	1:A:12:LEU:HG	2.16	0.46
1:A:151:LEU:O	1:A:155:SER:HB2	2.16	0.46
1:B:167:VAL:HB	1:B:168:PRO:HD2	1.97	0.46
1:B:9:ARG:HG2	1:B:49:GLN:HE21	1.80	0.45
1:B:87:LYS:HA	1:B:118:ARG:HH21	1.81	0.45
1:A:151:LEU:O	1:A:152:GLY:C	2.60	0.45
1:B:57:ASP:O	2:B:214:HOH:O	2.21	0.45
1:B:64:ASN:O	1:B:68:ALA:HB3	2.16	0.45
1:B:10:GLU:O	1:B:13:GLU:HB3	2.17	0.45
1:A:25:LYS:HE2	1:A:162:ALA:O	2.17	0.45
1:B:66:ILE:HD12	1:B:200:ILE:CD1	2.48	0.44
1:A:112:MET:O	1:A:116:LYS:HG3	2.17	0.44
1:A:45:ILE:HG21	1:A:45:ILE:HD13	1.66	0.43
1:A:146:ALA:HB3	1:A:149:VAL:CG2	2.46	0.43
1:B:134:MET:HE3	1:B:186:LEU:HD21	2.00	0.43
1:B:97:LYS:O	1:B:100:ASN:HB2	2.18	0.43
1:B:103:LYS:HA	1:B:106:LYS:CD	2.48	0.43
1:A:111:VAL:O	1:A:115:GLU:HB2	2.19	0.43
1:A:151:LEU:HA	1:A:151:LEU:HD12	1.84	0.42
1:B:103:LYS:HA	1:B:106:LYS:HD2	2.01	0.42
1:B:6:LYS:HA	1:B:9:ARG:HG3	2.02	0.42
1:A:11:LEU:HD11	1:A:105:PHE:CD1	2.54	0.42
1:A:5:ALA:HB1	1:A:7:ASP:H	1.84	0.42
1:B:9:ARG:CG	1:B:49:GLN:HE21	2.33	0.41
1:B:74:ILE:HG12	1:B:174:ILE:HG21	2.03	0.41
1:A:111:VAL:O	1:A:111:VAL:HG12	2.19	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:76:LYS:HE2	1:B:79:ARG:HH12	1.84	0.41
1:B:79:ARG:HG2	1:B:80:ASP:N	2.35	0.41
1:A:116:LYS:O	1:A:120:LYS:HG3	2.21	0.41
1:A:54:ARG:O	1:A:138:GLU:OE2	2.39	0.41
1:A:163:LEU:HD12	1:A:163:LEU:HA	1.81	0.40
1:B:69:ASN:OD1	1:B:70:PRO:CD	2.69	0.40
1:B:118:ARG:HH11	1:B:118:ARG:HD3	1.54	0.40
1:A:188:ASP:OD1	1:A:190:LYS:HB2	2.21	0.40

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:57:ASP:OD2	2:A:216:HOH:O[4_455]	2.12	0.08

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	195/204 (96%)	184 (94%)	11 (6%)	0	100	100
1	B	195/204 (96%)	186 (95%)	9 (5%)	0	100	100
All	All	390/408 (96%)	370 (95%)	20 (5%)	0	100	100

There are no Ramachandran outliers to report.

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	152/157 (97%)	138 (91%)	14 (9%)	8	14
1	B	152/157 (97%)	126 (83%)	26 (17%)	2	2
All	All	304/314 (97%)	264 (87%)	40 (13%)	4	5

All (40) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	7	ASP
1	A	10	GLU
1	A	52	THR
1	A	101	LEU
1	A	112	MET
1	A	133	LEU
1	A	135	LEU
1	A	137	VAL
1	A	147	SER
1	A	163	LEU
1	A	170	ILE
1	A	172	VAL
1	A	190	LYS
1	A	201	ARG
1	B	6	LYS
1	B	11	LEU
1	B	25	LYS
1	B	30	LEU
1	B	33	LYS
1	B	39	LYS
1	B	49	GLN
1	B	79	ARG
1	B	89	VAL
1	B	103	LYS
1	B	106	LYS
1	B	133	LEU
1	B	135	LEU
1	B	139	SER
1	B	142	LEU
1	B	147	SER
1	B	148	SER
1	B	151	LEU
1	B	163	LEU

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Mol	Chain	Res	Type
1	B	172	VAL
1	B	178	LEU
1	B	190	LYS
1	B	195	LEU
1	B	198	GLU
1	B	199	ILE
1	B	201	ARG

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	29	HIS
1	A	129	ASN
1	A	197	ASN
1	B	29	HIS
1	B	44	ASN
1	B	49	GLN
1	B	96	ASN

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.