



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 01:31 PM UTC

PDB ID : 2RSP / pdb_00002rsp
Title : STRUCTURE OF THE ASPARTIC PROTEASE FROM ROUS SARCOMA RETROVIRUS REFINED AT 2 ANGSTROMS RESOLUTION
Authors : Wlodawer, A.; Miller, M.; Jaskolski, M.
Deposited on : 1989-10-17
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)	:	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

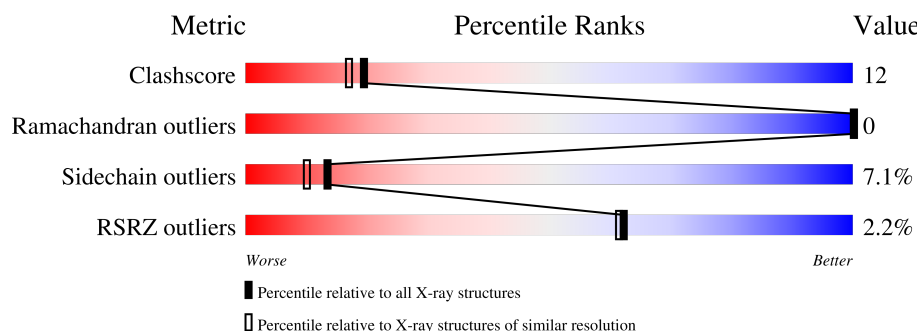
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.00 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)
RSRZ outliers	180081	10067 (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 $\leq 5\%$. 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	124	2% 33% 42% 14% • 7%
1	B	124	2% 37% 47% 6% • 9%

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 2024 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 RSV PROTEASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	115	Total	C	N	O	S	0	1	0
			891	560	159	164	8			
1	B	113	Total	C	N	O	S	0	1	0
			881	554	157	162	8			

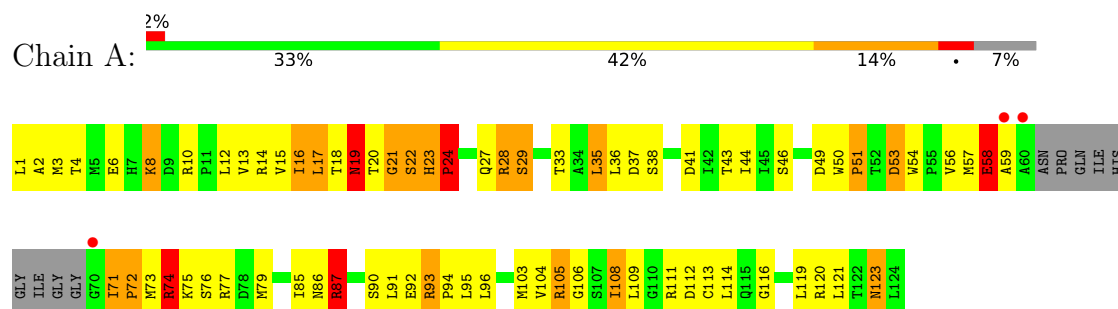
- Molecule 2 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	114	Total	O	0	0
			114	114		
2	B	138	Total	O	0	0
			138	138		

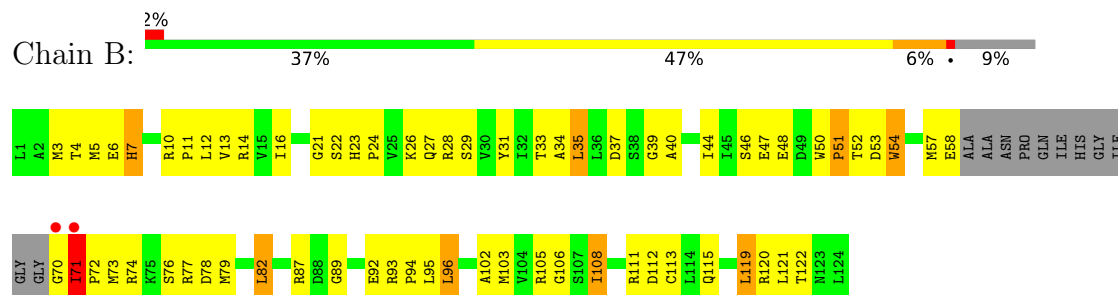
3 Residue-property plots [i](#)

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 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: RSV PROTEASE



• Molecule 1: RSV PROTEASE



4 Data and refinement statistics

Property	Value	Source
Space group	P 31 2 1	Depositor
Cell constants a, b, c, α , β , γ	88.95Å 88.95Å 78.90Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	10.00 – 2.00 10.00 – 2.06	Depositor EDS
% Data completeness (in resolution range)	(Not available) (10.00-2.00) 77.1 (10.00-2.06)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$	-	Xtriage
Refinement program	PROFFT	Depositor
R, R_{free}	0.144 , (Not available) 0.134 , (Not available)	Depositor DCC
R_{free} test set	No test flags present.	wwPDB-VP
Wilson B-factor (Å ²)	17.5	Xtriage
Anisotropy	0.184	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.30 , 82.3	EDS
L-test for twinning ¹	$\langle L \rangle = 0.44$, $\langle L^2 \rangle = 0.26$	Xtriage
Estimated twinning fraction	0.053 for -h,-k,l	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	2024	wwPDB-VP
Average B, all atoms (Å ²)	22.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.30% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Theoretical 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

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	1.61	7/909 (0.8%)	3.08	115/1229 (9.4%)
1	B	1.62	6/899 (0.7%)	2.85	98/1215 (8.1%)
All	All	1.62	13/1808 (0.7%)	2.97	213/2444 (8.7%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	1

All (13) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	119	LEU	N-CA	5.85	1.53	1.45
1	B	40	ALA	N-CA	5.58	1.52	1.46
1	B	35	LEU	C-O	5.39	1.30	1.23
1	A	14	ARG	C-N	-5.27	1.25	1.33
1	B	27	GLN	N-CA	5.26	1.52	1.46
1	A	19	ASN	CA-C	5.25	1.59	1.52
1	A	16	ILE	CA-CB	5.17	1.61	1.54
1	A	13	VAL	C-O	5.14	1.29	1.23
1	B	120	ARG	N-CA	5.10	1.52	1.45
1	B	22	SER	C-O	5.10	1.30	1.24
1	A	56	VAL	C-N	-5.08	1.27	1.33
1	A	90	SER	N-CA	5.01	1.52	1.45
1	B	111	ARG	CZ-NH1	5.01	1.39	1.32

All (213) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	87	ARG	CD-NE-CZ	25.38	159.93	124.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	74	ARG	CD-NE-CZ	23.46	157.24	124.40
1	A	28	ARG	CG-CD-NE	17.91	151.41	112.00
1	A	111	ARG	CD-NE-CZ	11.57	140.60	124.40
1	A	23	HIS	CA-CB-CG	-11.36	102.44	113.80
1	A	93	ARG	NE-CZ-NH2	-11.32	109.01	119.20
1	B	70	GLY	CA-C-N	-10.80	113.45	122.85
1	B	70	GLY	C-N-CA	-10.80	113.45	122.85
1	A	105	ARG	CD-NE-CZ	10.68	139.36	124.40
1	A	51	PRO	CB-CA-C	9.74	124.01	111.64
1	B	53	ASP	CA-C-O	-9.69	108.25	119.78
1	B	121	LEU	CA-C-O	-9.54	110.16	120.36
1	B	111	ARG	NE-CZ-NH2	9.40	127.66	119.20
1	A	6	GLU	CA-CB-CG	-9.32	95.45	114.10
1	A	49	ASP	CA-C-N	9.27	136.18	121.17
1	A	49	ASP	C-N-CA	9.27	136.18	121.17
1	A	21	GLY	O-C-N	9.26	134.74	122.70
1	B	115	GLN	CG-CD-NE2	-9.13	102.70	116.40
1	B	24	PRO	O-C-N	-9.09	111.74	123.01
1	B	112	ASP	O-C-N	-8.85	112.96	122.07
1	A	86	ASN	CB-CG-ND2	8.77	129.55	116.40
1	A	56	VAL	CA-C-O	-8.72	112.77	121.67
1	A	44	ILE	CA-C-O	-8.67	111.17	120.36
1	B	93	ARG	CD-NE-CZ	8.63	136.48	124.40
1	A	35	LEU	N-CA-CB	-8.55	96.38	110.23
1	B	112	ASP	N-CA-C	-8.34	102.14	111.07
1	B	14	ARG	CD-NE-CZ	-8.24	112.86	124.40
1	A	109	LEU	CA-C-N	8.19	133.39	121.67
1	A	109	LEU	C-N-CA	8.19	133.39	121.67
1	A	8	LYS	CB-CG-CD	8.12	129.98	111.30
1	A	58	GLU	CB-CA-C	8.11	126.31	109.68
1	A	87	ARG	CD-NE-CZ	-8.05	113.14	124.40
1	B	50	TRP	CA-C-O	-8.04	113.27	119.46
1	A	79	MET	CA-C-N	-8.03	110.64	122.68
1	A	79	MET	C-N-CA	-8.03	110.64	122.68
1	A	58	GLU	CB-CG-CD	8.01	126.22	112.60
1	B	54	TRP	N-CA-C	-7.95	98.20	109.24
1	A	27	GLN	OE1-CD-NE2	7.89	130.49	122.60
1	B	108	ILE	CB-CG1-CD1	-7.89	97.24	113.80
1	A	37	ASP	CA-CB-CG	-7.85	104.75	112.60
1	A	116	GLY	CA-C-O	-7.82	111.95	120.40
1	A	20	THR	CA-C-N	7.74	136.58	121.41
1	A	20	THR	C-N-CA	7.74	136.58	121.41

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	105	ARG	NE-CZ-NH2	-7.66	112.31	119.20
1	A	12	LEU	O-C-N	7.51	131.98	123.19
1	A	123	ASN	CA-CB-CG	7.44	120.04	112.60
1	A	113[A]	CYS	CA-C-O	-7.42	111.04	119.79
1	A	113[B]	CYS	CA-C-O	-7.42	111.04	119.79
1	B	115	GLN	CA-C-O	-7.33	112.65	120.42
1	A	51	PRO	CA-C-O	7.32	129.29	121.32
1	B	28	ARG	NE-CZ-NH2	7.30	125.77	119.20
1	A	13	VAL	CA-C-O	-7.29	114.02	121.67
1	A	105	ARG	O-C-N	-7.28	113.00	122.61
1	A	113[A]	CYS	N-CA-CB	-7.25	99.14	110.30
1	A	113[B]	CYS	N-CA-CB	-7.25	99.14	110.30
1	B	77	ARG	CD-NE-CZ	-7.19	114.34	124.40
1	B	33	THR	CA-CB-OG1	-7.18	98.82	109.60
1	B	7	HIS	O-C-N	-7.10	114.59	122.12
1	B	47	GLU	CA-CB-CG	-7.04	100.01	114.10
1	B	95	LEU	CA-C-O	-7.03	113.24	121.46
1	A	93	ARG	NE-CZ-NH1	7.01	128.51	121.50
1	A	1	LEU	CD1-CG-CD2	-7.00	95.40	110.80
1	A	108	ILE	N-CA-CB	-6.96	100.03	111.44
1	B	74	ARG	CD-NE-CZ	-6.94	114.68	124.40
1	B	74	ARG	CA-CB-CG	-6.91	100.28	114.10
1	B	10	ARG	CA-C-O	-6.90	112.80	120.25
1	B	10	ARG	CG-CD-NE	-6.86	96.91	112.00
1	B	7	HIS	CA-C-O	6.85	127.81	120.55
1	A	46	SER	CA-C-O	-6.81	114.14	121.56
1	B	106	GLY	CA-C-O	-6.78	113.54	121.61
1	A	123	ASN	N-CA-C	-6.77	103.61	112.41
1	A	43	THR	CA-CB-OG1	-6.76	99.46	109.60
1	A	24	PRO	CA-C-N	6.75	131.96	122.23
1	A	24	PRO	C-N-CA	6.75	131.96	122.23
1	A	56	VAL	O-C-N	6.71	130.38	123.00
1	A	8	LYS	N-CA-C	6.63	120.59	112.23
1	B	74	ARG	NH1-CZ-NH2	6.58	127.86	119.30
1	A	13	VAL	O-C-N	6.53	130.29	123.04
1	B	6	GLU	OE1-CD-OE2	6.53	138.57	122.90
1	B	35	LEU	N-CA-CB	-6.53	99.65	110.23
1	B	47	GLU	CA-C-O	6.51	127.49	120.20
1	A	86	ASN	OD1-CG-ND2	-6.50	116.10	122.60
1	B	26	LYS	O-C-N	6.50	129.55	122.15
1	A	36	LEU	CA-C-O	-6.48	113.28	120.60
1	B	87	ARG	CA-CB-CG	-6.45	101.19	114.10

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	71	ILE	CA-C-O	6.41	123.28	119.94
1	A	74	ARG	NE-CZ-NH1	6.41	127.91	121.50
1	B	34	ALA	CA-C-O	-6.41	113.81	120.99
1	A	76	SER	CA-CB-OG	-6.38	98.33	111.10
1	B	23	HIS	CA-CB-CG	-6.34	107.46	113.80
1	B	44	ILE	CA-C-O	-6.34	113.87	120.27
1	A	28	ARG	CA-C-N	6.33	132.44	122.94
1	A	28	ARG	C-N-CA	6.33	132.44	122.94
1	B	7	HIS	CA-CB-CG	-6.29	107.51	113.80
1	B	14	ARG	N-CA-C	-6.29	100.33	110.32
1	A	59	ALA	CA-C-O	-6.26	114.11	121.44
1	B	74	ARG	CB-CA-C	6.25	120.95	109.71
1	A	106	GLY	CA-C-O	-6.24	117.01	121.88
1	A	111	ARG	NE-CZ-NH1	6.22	127.72	121.50
1	A	49	ASP	O-C-N	-6.21	113.89	122.46
1	B	26	LYS	CA-C-N	-6.18	113.24	122.39
1	B	26	LYS	C-N-CA	-6.18	113.24	122.39
1	B	87	ARG	NE-CZ-NH2	6.18	124.76	119.20
1	B	31	TYR	O-C-N	-6.14	116.33	123.27
1	A	120	ARG	NE-CZ-NH2	-6.13	113.68	119.20
1	B	6	GLU	CA-CB-CG	-6.13	101.85	114.10
1	A	121	LEU	CB-CA-C	6.10	120.07	110.19
1	A	116	GLY	N-CA-C	-6.09	105.26	113.24
1	B	71	ILE	O-C-N	6.08	126.55	120.59
1	B	52	THR	CA-C-O	-6.07	113.24	120.10
1	A	114	LEU	CA-C-N	6.07	128.91	120.29
1	A	114	LEU	C-N-CA	6.07	128.91	120.29
1	B	121	LEU	O-C-N	6.07	130.14	123.22
1	A	79	MET	CA-C-O	-6.07	114.13	121.05
1	A	72	PRO	CB-CA-C	-6.06	104.00	111.64
1	A	37	ASP	N-CA-CB	-6.05	100.71	110.69
1	A	43	THR	CA-C-N	-6.03	114.61	122.99
1	A	43	THR	C-N-CA	-6.03	114.61	122.99
1	B	16	ILE	CB-CA-C	6.03	119.24	110.98
1	B	120	ARG	CA-C-O	-6.00	114.62	121.40
1	B	94	PRO	O-C-N	-6.00	115.57	123.01
1	B	13	VAL	CA-C-O	-6.00	115.77	121.64
1	A	14	ARG	CD-NE-CZ	-5.98	116.02	124.40
1	A	72	PRO	CA-C-O	-5.97	114.84	121.23
1	B	82	LEU	O-C-N	5.97	130.20	123.27
1	B	105	ARG	CD-NE-CZ	5.97	132.75	124.40
1	A	15	VAL	CA-C-N	-5.93	115.45	123.10

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	15	VAL	C-N-CA	-5.93	115.45	123.10
1	B	96	LEU	CA-C-O	-5.92	114.31	120.70
1	A	29	SER	CA-CB-OG	-5.91	99.28	111.10
1	B	50	TRP	CE3-CZ3-CH2	5.91	128.78	121.10
1	B	47	GLU	O-C-N	-5.91	115.47	122.20
1	B	29	SER	O-C-N	5.87	130.43	123.33
1	A	35	LEU	CA-C-O	-5.86	114.18	120.92
1	B	26	LYS	CA-C-O	-5.82	114.25	120.42
1	A	4	THR	CA-CB-OG1	-5.79	100.91	109.60
1	A	53	ASP	CA-C-O	-5.79	112.43	119.43
1	B	28	ARG	NH1-CZ-NH2	-5.79	111.78	119.30
1	A	74	ARG	N-CA-C	-5.76	101.66	109.95
1	A	76	SER	CB-CA-C	-5.75	100.18	109.72
1	B	50	TRP	CZ3-CH2-CZ2	-5.74	114.04	121.50
1	B	48	GLU	CG-CD-OE2	-5.72	105.23	118.40
1	A	96	LEU	CD1-CG-CD2	-5.72	98.21	110.80
1	B	93	ARG	NE-CZ-NH1	5.72	127.22	121.50
1	B	39	GLY	N-CA-C	-5.72	107.83	115.32
1	B	16	ILE	N-CA-CB	5.71	117.89	111.21
1	B	12	LEU	CA-C-N	-5.70	115.28	123.03
1	B	12	LEU	C-N-CA	-5.70	115.28	123.03
1	B	21	GLY	CA-C-O	5.70	130.54	122.51
1	A	33	THR	N-CA-C	-5.70	99.73	109.24
1	B	29	SER	CA-C-O	-5.68	113.79	120.60
1	A	14	ARG	N-CA-CB	5.67	119.65	110.41
1	B	120	ARG	CD-NE-CZ	-5.66	116.47	124.40
1	A	58	GLU	N-CA-C	-5.64	103.08	110.53
1	B	74	ARG	CG-CD-NE	-5.64	99.58	112.00
1	B	121	LEU	N-CA-CB	5.62	119.58	110.42
1	A	93	ARG	CA-CB-CG	-5.60	102.90	114.10
1	B	119	LEU	CA-C-O	5.60	128.41	121.81
1	A	77	ARG	CA-CB-CG	5.58	125.25	114.10
1	B	4	THR	O-C-N	-5.58	116.66	122.96
1	B	76	SER	O-C-N	-5.58	116.09	122.89
1	A	92	GLU	CA-C-N	5.57	128.14	120.39
1	A	92	GLU	C-N-CA	5.57	128.14	120.39
1	A	38	SER	N-CA-C	-5.57	105.75	112.54
1	A	71	ILE	N-CA-CB	-5.54	103.45	111.21
1	B	10	ARG	O-C-N	5.49	127.58	121.43
1	B	82	LEU	N-CA-CB	-5.48	102.10	110.65
1	B	46	SER	N-CA-CB	5.48	118.61	110.29
1	A	87	ARG	CA-C-O	-5.46	114.74	120.63

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	95	LEU	CA-C-N	5.41	130.61	122.99
1	A	95	LEU	C-N-CA	5.41	130.61	122.99
1	A	114	LEU	N-CA-C	-5.41	105.39	111.28
1	B	122	THR	N-CA-CB	-5.38	103.22	111.56
1	A	120	ARG	N-CA-CB	5.38	121.16	111.37
1	A	104	VAL	CA-C-O	5.35	127.13	121.67
1	A	121	LEU	O-C-N	-5.35	117.12	123.22
1	B	95	LEU	N-CA-CB	-5.33	102.57	111.20
1	A	35	LEU	CB-CA-C	5.33	118.32	109.53
1	B	74	ARG	NE-CZ-NH2	-5.31	114.42	119.20
1	B	103	MET	CA-C-O	-5.29	115.65	121.58
1	A	17	LEU	CA-C-O	-5.28	115.12	120.71
1	A	54	TRP	N-CA-C	-5.27	101.62	109.42
1	B	87	ARG	CB-CA-C	5.25	119.61	110.68
1	A	111	ARG	NE-CZ-NH2	-5.25	114.47	119.20
1	B	77	ARG	CA-CB-CG	-5.25	103.60	114.10
1	A	24	PRO	CB-CA-C	5.25	118.14	110.63
1	B	51	PRO	CA-C-N	5.24	127.82	120.28
1	B	51	PRO	C-N-CA	5.24	127.82	120.28
1	B	57	MET	CB-CA-C	-5.24	101.04	110.36
1	A	92	GLU	O-C-N	-5.23	116.89	122.85
1	B	37	ASP	N-CA-CB	-5.22	102.08	110.69
1	A	123	ASN	OD1-CG-ND2	5.21	127.81	122.60
1	A	92	GLU	N-CA-C	-5.18	103.56	110.55
1	A	43	THR	CA-C-O	-5.17	114.79	120.69
1	A	123	ASN	CA-C-O	-5.15	113.71	119.95
1	B	78	ASP	O-C-N	5.15	128.83	123.06
1	B	111	ARG	NH1-CZ-NH2	-5.14	112.61	119.30
1	A	18	THR	CA-C-O	-5.14	114.61	120.32
1	A	51	PRO	O-C-N	-5.13	116.58	122.85
1	A	2	ALA	N-CA-C	-5.11	99.64	108.69
1	B	92	GLU	N-CA-C	-5.11	103.18	110.59
1	A	53	ASP	CA-C-N	-5.10	114.06	121.20
1	A	53	ASP	C-N-CA	-5.10	114.06	121.20
1	B	115	GLN	CG-CD-OE1	5.10	131.00	120.80
1	B	120	ARG	N-CA-CB	-5.09	102.84	111.69
1	B	105	ARG	CA-CB-CG	5.07	124.24	114.10
1	B	89	GLY	CA-C-O	-5.06	113.39	119.06
1	A	71	ILE	CB-CG1-CD1	-5.05	103.20	113.80
1	B	34	ALA	N-CA-CB	-5.04	102.15	111.52
1	A	112	ASP	N-CA-C	-5.03	105.71	111.14
1	A	14	ARG	CA-C-O	-5.02	115.33	121.36

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	87	ARG	CA-C-O	-5.02	115.21	120.63
1	A	105	ARG	CB-CG-CD	5.00	122.81	111.30

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	87	ARG	Sidechain

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	891	0	926	26	0
1	B	881	0	916	18	0
2	A	114	0	0	5	0
2	B	138	0	0	1	0
All	All	2024	0	1842	42	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 12.

All (42) 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:79:MET:HE3	1:B:96:LEU:HD22	1.66	0.78
1:B:3:MET:HE1	1:B:11:PRO:HA	1.65	0.76
1:B:3:MET:HE1	1:B:11:PRO:CA	2.19	0.72
1:B:113[A]:CYS:SG	2:B:377:HOH:O	2.50	0.70
1:A:23:HIS:HB2	1:A:24:PRO:HD2	1.74	0.69
1:B:71:ILE:HB	1:B:73:MET:HE3	1.74	0.69
1:A:71:ILE:HG13	1:A:72:PRO:HD2	1.78	0.65
1:A:58:GLU:H	1:A:58:GLU:CD	2.05	0.65
1:A:10:ARG:NH1	2:A:289:HOH:O	2.32	0.63
1:A:19:ASN:HD22	1:A:19:ASN:C	2.09	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:91:LEU:HD12	2:A:305:HOH:O	2.03	0.59
1:B:3:MET:HE1	1:B:11:PRO:CB	2.33	0.58
1:A:35:LEU:HD23	1:A:108:ILE:CD1	2.34	0.57
1:B:73:MET:HE2	1:B:102:ALA:HB2	1.85	0.57
1:A:71:ILE:HD11	1:A:103:MET:O	2.06	0.56
1:A:41:ASP:O	1:B:7:HIS:HD2	1.89	0.56
1:B:71:ILE:HB	1:B:73:MET:CE	2.39	0.53
1:A:23:HIS:HB2	1:A:24:PRO:CD	2.39	0.51
1:A:53:ASP:OD2	1:A:53:ASP:N	2.45	0.49
1:B:11:PRO:HD2	1:B:35:LEU:HD11	1.93	0.49
1:A:19:ASN:ND2	1:A:21:GLY:H	2.11	0.48
1:A:73:MET:HE2	1:A:73:MET:HB3	1.77	0.47
1:A:19:ASN:HD22	1:A:21:GLY:H	1.62	0.47
1:A:85:ILE:HG12	1:A:91:LEU:HD13	1.96	0.46
1:B:3:MET:HB3	1:B:3:MET:HE3	1.55	0.46
1:B:51:PRO:HB2	1:B:54:TRP:CD1	2.52	0.45
1:A:91:LEU:HB3	2:A:305:HOH:O	2.15	0.45
1:B:71:ILE:HA	1:B:72:PRO:HD3	1.59	0.44
1:A:19:ASN:HD21	1:A:21:GLY:HA3	1.82	0.44
1:A:57:MET:HG3	1:A:58:GLU:O	2.19	0.43
1:A:93:ARG:HG3	1:A:94:PRO:HD2	2.00	0.43
1:A:74:ARG:NH1	2:A:363:HOH:O	2.51	0.43
1:B:82:LEU:C	1:B:82:LEU:HD23	2.44	0.42
1:A:87:ARG:HH11	1:A:87:ARG:HD2	1.56	0.42
1:B:3:MET:CE	1:B:11:PRO:CB	2.98	0.41
1:A:17:LEU:O	1:A:29:SER:HA	2.21	0.41
1:A:19:ASN:C	1:A:19:ASN:ND2	2.77	0.41
1:B:73:MET:HE2	1:B:73:MET:HB3	1.46	0.41
1:A:22:SER:N	2:A:364:HOH:O	2.54	0.41
1:A:123:ASN:HB3	1:B:119:LEU:HD23	2.03	0.41
1:A:50:TRP:HA	1:A:51:PRO:HD3	1.96	0.40
1:B:5:MET:HA	1:B:5:MET:HE2	2.03	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	112/124 (90%)	110 (98%)	2 (2%)	0	100	100
1	B	110/124 (89%)	107 (97%)	3 (3%)	0	100	100
All	All	222/248 (90%)	217 (98%)	5 (2%)	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	100/105 (95%)	89 (89%)	11 (11%)	6	3
1	B	100/105 (95%)	97 (97%)	3 (3%)	36	38
All	All	200/210 (95%)	186 (93%)	14 (7%)	13	10

All (14) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	3	MET
1	A	8	LYS
1	A	16	ILE
1	A	19	ASN
1	A	22	SER
1	A	24	PRO
1	A	28	ARG
1	A	58	GLU
1	A	74	ARG
1	A	75	LYS
1	A	105	ARG
1	B	58	GLU
1	B	71	ILE
1	B	108	ILE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (5) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	19	ASN
1	A	86	ASN
1	B	7	HIS
1	B	27	GLN
1	B	86	ASN

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 [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	115/124 (92%)	-0.86	3 (2%)	57 56	5, 16, 50, 66	1 (0%)
1	B	113/124 (91%)	-1.09	2 (1%)	67 67	7, 14, 44, 65	1 (0%)
All	All	228/248 (91%)	-0.97	5 (2%)	62 61	5, 15, 48, 66	2 (0%)

All (5) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	59	ALA	4.1
1	A	70	GLY	2.8
1	B	70	GLY	2.7
1	B	71	ILE	2.4
1	A	60	ALA	2.1

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](#)

There are no ligands in this entry.

6.5 Other polymers [i](#)

There are no such residues in this entry.