



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 10, 2026 – 06:20 AM UTC

PDB ID : 1RBB / pdb_00001rbb
Title : THE CRYSTAL STRUCTURE OF RIBONUCLEASE B AT 2.5-
ANGSTROMS RESOLUTION
Authors : Williams, R.L.; Greene, S.M.; McPherson, A.
Deposited on : 1987-09-14
Resolution : 2.50 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

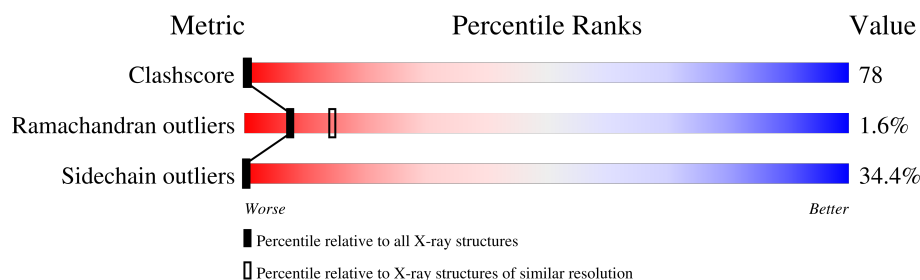
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.50 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	6492 (2.50-2.50)
Ramachandran outliers	187476	6378 (2.50-2.50)
Sidechain outliers	187428	6380 (2.50-2.50)

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	124	
1	B	124	

2 Entry composition

There is only 1 type of molecule in this entry. The entry contains 1900 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 RIBONUCLEASE B.

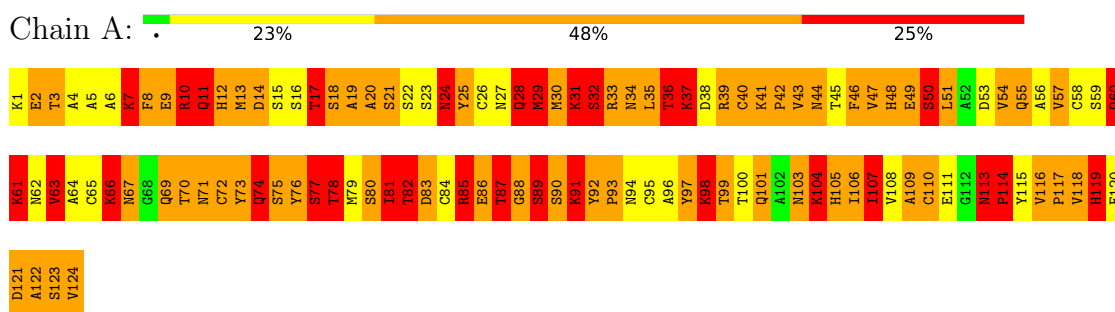
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	124	Total	C	N	O	S	0	0	0
			950	575	171	192	12			
1	B	124	Total	C	N	O	S	0	0	0
			950	575	171	192	12			

3 Residue-property plots

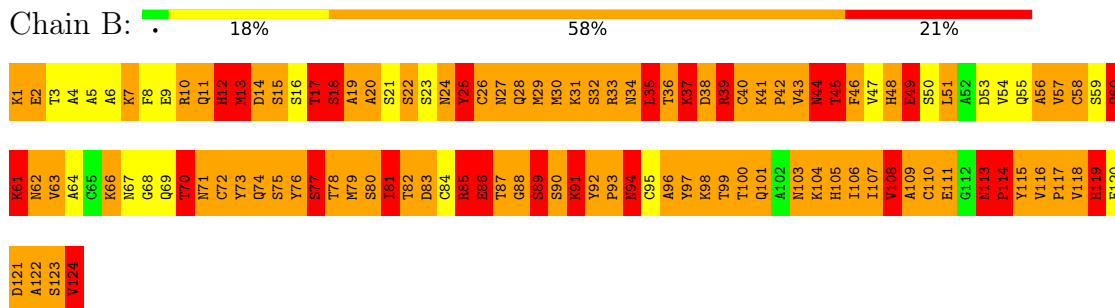
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry. Residues are color-coded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



• Molecule 1: RIBONUCLEASE B



4 Data and refinement statistics

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

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	101.81Å 33.36Å 73.60Å 90.00° 90.40° 90.00°	Depositor
Resolution (Å)	(Not available) – 2.50	Depositor
% Data completeness (in resolution range)	(Not available) ((Not available)-2.50)	Depositor
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	CORELS	Depositor
R, R_{free}	0.218 , (Not available)	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	1900	wwPDB-VP
Average B, all atoms (Å ²)	11.0	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	4.19	203/966 (21.0%)	3.72	194/1304 (14.9%)
1	B	4.07	198/966 (20.5%)	3.78	196/1304 (15.0%)
All	All	4.13	401/1932 (20.8%)	3.75	390/2608 (15.0%)

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	2
1	B	0	2
All	All	0	4

All (401) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	97	TYR	CA-C	13.77	1.69	1.52
1	A	97	TYR	CA-C	13.76	1.69	1.52
1	B	105	HIS	CD2-NE2	13.06	1.52	1.37
1	A	96	ALA	N-CA	12.98	1.62	1.46
1	A	90	SER	CA-C	12.87	1.69	1.52
1	A	27	ASN	C-O	12.78	1.38	1.24
1	A	82	THR	CA-C	12.66	1.67	1.52
1	B	118	VAL	N-CA	12.60	1.58	1.46
1	A	94	ASN	N-CA	12.55	1.64	1.46
1	B	63	VAL	CA-C	12.47	1.67	1.52
1	A	63	VAL	CA-C	12.43	1.67	1.52
1	B	90	SER	CA-C	12.42	1.69	1.52
1	B	96	ALA	N-CA	12.37	1.61	1.46
1	A	105	HIS	CD2-NE2	12.31	1.51	1.37
1	B	27	ASN	C-O	12.30	1.38	1.24
1	A	44	ASN	CA-C	12.28	1.68	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	106	ILE	N-CA	12.18	1.61	1.46
1	B	106	ILE	N-CA	12.18	1.61	1.46
1	A	118	VAL	N-CA	11.99	1.57	1.46
1	A	123	SER	N-CA	11.96	1.60	1.45
1	A	62	ASN	N-CA	11.95	1.60	1.46
1	B	94	ASN	N-CA	11.93	1.63	1.46
1	A	48	HIS	C-O	11.87	1.39	1.24
1	A	39	ARG	CA-C	11.83	1.67	1.52
1	B	39	ARG	CA-C	11.82	1.66	1.52
1	A	5	ALA	C-O	11.60	1.37	1.24
1	B	48	HIS	C-O	11.55	1.38	1.24
1	A	26	CYS	N-CA	11.44	1.60	1.46
1	A	64	ALA	N-CA	11.41	1.59	1.46
1	B	123	SER	N-CA	11.41	1.60	1.46
1	B	67	ASN	C-O	11.39	1.39	1.24
1	A	33	ARG	CA-C	11.36	1.68	1.52
1	A	4	ALA	CA-C	11.35	1.67	1.52
1	B	5	ALA	C-O	11.34	1.37	1.24
1	A	95	CYS	CA-C	11.17	1.67	1.52
1	B	62	ASN	N-CA	11.13	1.60	1.46
1	B	44	ASN	CA-C	11.12	1.67	1.52
1	B	82	THR	CA-C	11.10	1.66	1.52
1	A	67	ASN	C-O	10.78	1.39	1.24
1	B	64	ALA	N-CA	10.74	1.59	1.46
1	A	85	ARG	CZ-NH2	10.69	1.47	1.33
1	B	95	CYS	CA-C	10.66	1.66	1.52
1	B	26	CYS	N-CA	10.56	1.58	1.46
1	B	105	HIS	CA-C	10.50	1.66	1.52
1	B	85	ARG	CZ-NH2	10.48	1.47	1.33
1	B	4	ALA	CA-C	10.48	1.66	1.52
1	A	91	LYS	N-CA	10.44	1.58	1.46
1	A	117	PRO	N-CD	10.42	1.62	1.47
1	A	29	MET	CA-C	10.42	1.66	1.52
1	A	5	ALA	N-CA	10.36	1.58	1.46
1	B	91	LYS	N-CA	10.27	1.58	1.46
1	A	105	HIS	CA-C	10.24	1.66	1.52
1	B	80	SER	CA-C	10.21	1.65	1.52
1	A	40	CYS	N-CA	10.19	1.59	1.46
1	A	32	SER	CA-CB	10.18	1.69	1.53
1	B	43	VAL	N-CA	10.14	1.58	1.46
1	A	33	ARG	CZ-NH2	10.13	1.46	1.33
1	A	12	HIS	CG-CD2	10.12	1.47	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	88	GLY	N-CA	10.09	1.59	1.45
1	B	12	HIS	CG-CD2	10.02	1.46	1.35
1	B	76	TYR	N-CA	10.01	1.58	1.46
1	B	105	HIS	CB-CG	10.00	1.64	1.50
1	B	29	MET	CA-C	9.99	1.65	1.52
1	A	76	TYR	N-CA	9.87	1.58	1.46
1	A	13	MET	N-CA	9.87	1.58	1.46
1	A	31	LYS	C-O	9.87	1.35	1.24
1	A	30	MET	N-CA	9.83	1.58	1.46
1	A	105	HIS	CB-CG	9.80	1.63	1.50
1	A	120	PHE	N-CA	9.79	1.58	1.46
1	A	12	HIS	ND1-CE1	9.77	1.42	1.32
1	A	110	CYS	CA-C	9.77	1.64	1.52
1	A	85	ARG	CD-NE	9.72	1.59	1.46
1	B	31	LYS	C-O	9.71	1.35	1.24
1	B	85	ARG	CD-NE	9.69	1.59	1.46
1	A	14	ASP	CA-C	9.69	1.67	1.53
1	B	40	CYS	N-CA	9.63	1.58	1.46
1	B	32	SER	CA-CB	9.58	1.68	1.53
1	B	117	PRO	N-CD	9.58	1.61	1.47
1	A	2	GLU	N-CA	9.56	1.58	1.46
1	B	5	ALA	N-CA	9.56	1.58	1.46
1	B	110	CYS	CA-C	9.52	1.64	1.52
1	B	88	GLY	C-O	9.42	1.35	1.23
1	A	18	SER	CA-CB	9.39	1.69	1.53
1	A	50	SER	CA-C	9.38	1.65	1.52
1	A	82	THR	C-O	9.38	1.34	1.24
1	B	4	ALA	C-O	9.38	1.35	1.24
1	B	2	GLU	N-CA	9.36	1.58	1.46
1	B	33	ARG	CZ-NH2	9.32	1.45	1.33
1	A	43	VAL	N-CA	9.25	1.57	1.46
1	A	80	SER	CA-C	9.23	1.65	1.52
1	A	89	SER	N-CA	9.21	1.58	1.46
1	B	69	GLN	CA-C	9.21	1.64	1.52
1	B	120	PHE	N-CA	9.20	1.58	1.46
1	A	86	GLU	CA-CB	9.19	1.68	1.53
1	A	87	THR	C-O	9.19	1.35	1.23
1	A	25	TYR	CA-C	9.15	1.65	1.52
1	B	14	ASP	CA-C	9.15	1.67	1.53
1	B	87	THR	C-O	9.14	1.35	1.23
1	A	108	VAL	N-CA	9.13	1.56	1.46
1	B	117	PRO	CA-C	9.12	1.63	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	117	PRO	CA-C	9.07	1.62	1.52
1	B	98	LYS	N-CA	9.06	1.57	1.46
1	A	4	ALA	C-O	9.06	1.34	1.24
1	B	67	ASN	N-CA	8.99	1.57	1.46
1	A	69	GLN	CA-C	8.99	1.64	1.52
1	B	12	HIS	ND1-CE1	8.99	1.41	1.32
1	B	30	MET	N-CA	8.95	1.57	1.46
1	A	67	ASN	N-CA	8.93	1.58	1.46
1	A	115	TYR	C-O	8.91	1.34	1.24
1	B	82	THR	C-O	8.89	1.34	1.24
1	B	81	ILE	N-CA	8.89	1.55	1.46
1	A	98	LYS	N-CA	8.87	1.57	1.46
1	B	13	MET	N-CA	8.84	1.57	1.46
1	A	122	ALA	CA-C	8.77	1.63	1.52
1	B	18	SER	CA-CB	8.76	1.68	1.53
1	A	81	ILE	C-O	8.72	1.32	1.24
1	A	88	GLY	N-CA	8.72	1.58	1.45
1	A	45	THR	N-CA	8.70	1.56	1.46
1	A	37	LYS	N-CA	8.64	1.57	1.46
1	B	115	TYR	C-O	8.61	1.34	1.24
1	B	50	SER	CA-C	8.53	1.63	1.52
1	A	58	CYS	N-CA	8.51	1.57	1.46
1	B	64	ALA	C-O	8.51	1.34	1.23
1	A	64	ALA	C-O	8.49	1.34	1.23
1	A	101	GLN	C-O	8.48	1.34	1.23
1	B	37	LYS	N-CA	8.47	1.56	1.46
1	B	86	GLU	CA-CB	8.46	1.67	1.53
1	A	72	CYS	CA-C	8.45	1.64	1.52
1	A	24	ASN	N-CA	8.44	1.57	1.46
1	A	88	GLY	C-O	8.43	1.35	1.23
1	A	66	LYS	CA-C	8.40	1.64	1.52
1	A	56	ALA	CA-CB	8.39	1.67	1.53
1	B	108	VAL	N-CA	8.38	1.56	1.46
1	B	55	GLN	N-CA	8.38	1.56	1.46
1	B	45	THR	N-CA	8.37	1.56	1.46
1	A	41	LYS	CA-C	8.36	1.62	1.53
1	B	41	LYS	CA-C	8.32	1.62	1.53
1	A	8	PHE	N-CA	8.32	1.56	1.46
1	A	105	HIS	ND1-CE1	8.29	1.40	1.32
1	A	74	GLN	CA-C	8.27	1.62	1.52
1	A	43	VAL	C-O	8.26	1.32	1.24
1	B	77	SER	CB-OG	8.26	1.58	1.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	21	SER	N-CA	8.24	1.56	1.46
1	A	22	SER	CA-C	8.24	1.62	1.52
1	B	105	HIS	ND1-CE1	8.24	1.40	1.32
1	A	113	ASN	C-O	8.22	1.33	1.24
1	B	2	GLU	CD-OE2	8.22	1.41	1.25
1	B	24	ASN	N-CA	8.22	1.57	1.46
1	B	11	GLN	CA-C	8.21	1.64	1.52
1	A	11	GLN	CA-C	8.21	1.64	1.52
1	A	77	SER	CB-OG	8.21	1.58	1.42
1	B	8	PHE	N-CA	8.21	1.56	1.46
1	B	81	ILE	C-O	8.21	1.32	1.23
1	B	122	ALA	CA-C	8.19	1.62	1.52
1	B	72	CYS	CA-C	8.16	1.64	1.53
1	A	23	SER	CA-C	8.15	1.64	1.52
1	B	89	SER	N-CA	8.15	1.56	1.46
1	A	81	ILE	N-CA	8.15	1.55	1.46
1	A	33	ARG	CD-NE	8.14	1.57	1.46
1	A	42	PRO	N-CD	8.13	1.59	1.47
1	A	55	GLN	N-CA	8.13	1.56	1.46
1	A	12	HIS	CB-CG	8.12	1.61	1.50
1	B	12	HIS	C-O	8.09	1.34	1.24
1	B	43	VAL	C-O	8.09	1.32	1.24
1	A	30	MET	C-O	8.08	1.33	1.24
1	A	2	GLU	CD-OE2	8.07	1.40	1.25
1	B	23	SER	CA-C	8.07	1.64	1.52
1	A	38	ASP	N-CA	8.06	1.56	1.46
1	B	30	MET	C-O	8.04	1.33	1.24
1	B	38	ASP	N-CA	8.03	1.56	1.45
1	B	73	TYR	N-CA	8.01	1.55	1.46
1	B	46	PHE	CA-C	8.01	1.62	1.52
1	A	71	ASN	CA-C	8.00	1.63	1.52
1	B	58	CYS	N-CA	8.00	1.56	1.46
1	A	107	ILE	CA-C	7.98	1.63	1.52
1	B	74	GLN	CA-C	7.91	1.62	1.52
1	B	107	ILE	CA-C	7.90	1.63	1.52
1	A	20	ALA	CA-C	7.84	1.63	1.52
1	B	101	GLN	C-O	7.81	1.33	1.24
1	B	14	ASP	C-O	7.80	1.34	1.23
1	B	42	PRO	CA-C	7.76	1.63	1.52
1	A	73	TYR	CA-C	7.75	1.61	1.52
1	B	9	GLU	C-O	7.74	1.33	1.24
1	A	34	ASN	CG-ND2	7.74	1.49	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	21	SER	N-CA	7.74	1.56	1.46
1	B	25	TYR	CA-C	7.71	1.64	1.52
1	A	9	GLU	C-O	7.69	1.33	1.24
1	B	56	ALA	CA-CB	7.69	1.66	1.53
1	A	51	LEU	N-CA	7.68	1.55	1.46
1	B	34	ASN	CG-ND2	7.67	1.49	1.33
1	B	71	ASN	CA-C	7.66	1.63	1.52
1	B	73	TYR	CA-C	7.65	1.62	1.52
1	B	100	THR	N-CA	7.65	1.55	1.46
1	A	21	SER	C-O	7.63	1.34	1.23
1	A	117	PRO	CA-CB	7.61	1.63	1.53
1	A	34	ASN	N-CA	7.59	1.58	1.46
1	A	83	ASP	N-CA	7.58	1.55	1.46
1	B	34	ASN	N-CA	7.57	1.57	1.46
1	B	33	ARG	CD-NE	7.57	1.56	1.46
1	A	12	HIS	C-O	7.57	1.34	1.24
1	B	66	LYS	CA-C	7.55	1.63	1.52
1	A	12	HIS	N-CA	7.54	1.56	1.45
1	B	113	ASN	C-O	7.50	1.33	1.24
1	A	10	ARG	CA-CB	7.50	1.65	1.53
1	B	28	GLN	CD-OE1	7.47	1.37	1.23
1	A	73	TYR	N-CA	7.47	1.55	1.46
1	A	23	SER	C-O	7.46	1.33	1.24
1	B	42	PRO	N-CD	7.46	1.58	1.47
1	A	42	PRO	CA-C	7.46	1.62	1.52
1	B	111	GLU	N-CA	7.46	1.55	1.46
1	B	47	VAL	N-CA	7.43	1.55	1.46
1	A	63	VAL	C-O	7.41	1.31	1.23
1	B	10	ARG	CA-CB	7.40	1.65	1.53
1	A	100	THR	N-CA	7.33	1.55	1.46
1	B	20	ALA	CA-C	7.32	1.62	1.52
1	B	21	SER	C-O	7.32	1.34	1.23
1	A	24	ASN	CG-OD1	7.31	1.37	1.23
1	A	111	GLU	N-CA	7.30	1.55	1.46
1	B	22	SER	CA-C	7.27	1.61	1.52
1	B	12	HIS	CB-CG	7.26	1.60	1.50
1	A	107	ILE	N-CA	7.21	1.55	1.46
1	A	14	ASP	C-O	7.19	1.34	1.23
1	A	34	ASN	C-O	7.14	1.33	1.23
1	B	15	SER	N-CA	7.13	1.55	1.46
1	A	116	VAL	C-O	7.12	1.33	1.24
1	B	103	ASN	CA-CB	7.11	1.63	1.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	28	GLN	CA-CB	7.09	1.64	1.53
1	B	12	HIS	CE1-NE2	7.06	1.39	1.32
1	A	8	PHE	CA-C	7.05	1.61	1.52
1	B	117	PRO	CA-CB	7.00	1.62	1.53
1	B	107	ILE	N-CA	6.99	1.55	1.46
1	A	59	SER	CA-C	6.96	1.61	1.52
1	A	119	HIS	CA-C	6.94	1.61	1.52
1	A	28	GLN	CD-OE1	6.92	1.36	1.23
1	A	78	THR	CB-OG1	6.91	1.54	1.43
1	B	51	LEU	N-CA	6.91	1.54	1.46
1	B	119	HIS	CA-C	6.89	1.60	1.52
1	A	15	SER	N-CA	6.85	1.55	1.46
1	A	89	SER	CA-CB	6.85	1.65	1.53
1	B	24	ASN	CG-OD1	6.84	1.36	1.23
1	B	63	VAL	C-O	6.82	1.31	1.23
1	A	46	PHE	CA-C	6.82	1.60	1.52
1	B	83	ASP	N-CA	6.82	1.54	1.46
1	A	75	SER	N-CA	6.76	1.54	1.46
1	A	37	LYS	CA-C	6.70	1.61	1.52
1	B	54	VAL	N-CA	6.70	1.54	1.46
1	A	23	SER	N-CA	6.68	1.55	1.46
1	B	12	HIS	N-CA	6.65	1.55	1.45
1	B	34	ASN	C-O	6.64	1.33	1.23
1	B	7	LYS	CA-C	6.63	1.61	1.52
1	B	46	PHE	C-O	6.62	1.32	1.24
1	B	22	SER	CB-OG	6.61	1.55	1.42
1	A	7	LYS	CA-C	6.59	1.61	1.52
1	A	9	GLU	CD-OE2	6.57	1.37	1.25
1	B	37	LYS	CA-C	6.56	1.61	1.52
1	B	23	SER	C-O	6.55	1.32	1.24
1	B	28	GLN	CA-CB	6.54	1.63	1.53
1	A	3	THR	CB-OG1	6.54	1.54	1.43
1	A	46	PHE	C-O	6.54	1.32	1.24
1	B	89	SER	CA-CB	6.52	1.64	1.53
1	A	47	VAL	N-CA	6.51	1.54	1.46
1	B	109	ALA	CA-CB	6.50	1.62	1.53
1	A	97	TYR	CB-CG	6.47	1.65	1.51
1	A	75	SER	CA-C	6.43	1.61	1.52
1	B	74	GLN	N-CA	6.43	1.53	1.46
1	A	22	SER	CB-OG	6.41	1.54	1.42
1	B	33	ARG	NE-CZ	6.38	1.40	1.33
1	B	59	SER	CA-C	6.37	1.61	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	54	VAL	N-CA	6.37	1.55	1.46
1	A	74	GLN	N-CA	6.31	1.53	1.46
1	B	97	TYR	CB-CG	6.30	1.65	1.51
1	B	49	GLU	C-O	6.29	1.31	1.23
1	B	78	THR	CB-OG1	6.29	1.53	1.43
1	A	67	ASN	CG-ND2	6.28	1.46	1.33
1	A	12	HIS	CE1-NE2	6.27	1.38	1.32
1	A	12	HIS	CA-C	6.27	1.60	1.52
1	B	83	ASP	CG-OD2	6.27	1.37	1.25
1	B	75	SER	CA-C	6.26	1.61	1.52
1	B	116	VAL	C-O	6.26	1.32	1.24
1	B	9	GLU	CD-OE2	6.25	1.37	1.25
1	A	120	PHE	CB-CG	6.22	1.65	1.50
1	A	109	ALA	N-CA	6.21	1.53	1.46
1	A	49	GLU	CG-CD	6.18	1.67	1.52
1	A	103	ASN	CA-CB	6.17	1.63	1.53
1	A	101	GLN	CD-OE1	6.17	1.35	1.23
1	B	120	PHE	CB-CG	6.16	1.64	1.50
1	A	115	TYR	CG-CD1	6.14	1.52	1.39
1	B	49	GLU	CG-CD	6.14	1.67	1.52
1	A	83	ASP	CG-OD2	6.09	1.36	1.25
1	B	67	ASN	CG-ND2	6.09	1.46	1.33
1	A	35	LEU	CA-CB	6.08	1.64	1.53
1	B	35	LEU	CA-CB	6.08	1.64	1.53
1	A	58	CYS	C-O	6.07	1.31	1.24
1	A	10	ARG	CZ-NH1	6.03	1.41	1.32
1	B	101	GLN	CD-OE1	6.01	1.34	1.23
1	B	116	VAL	N-CA	5.99	1.53	1.46
1	A	53	ASP	CG-OD2	5.94	1.36	1.25
1	B	3	THR	CB-OG1	5.94	1.53	1.43
1	A	93	PRO	CA-C	5.92	1.64	1.52
1	B	75	SER	N-CA	5.92	1.53	1.46
1	B	8	PHE	CG-CD2	5.89	1.51	1.38
1	A	8	PHE	CG-CD2	5.87	1.51	1.38
1	B	115	TYR	CG-CD1	5.87	1.51	1.39
1	B	69	GLN	C-O	5.86	1.31	1.23
1	A	28	GLN	C-O	5.85	1.30	1.24
1	B	113	ASN	N-CA	5.85	1.54	1.45
1	B	23	SER	N-CA	5.84	1.54	1.46
1	B	61	LYS	CA-CB	5.84	1.60	1.53
1	A	49	GLU	C-O	5.83	1.31	1.23
1	B	19	ALA	CA-CB	5.82	1.63	1.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	28	GLN	C-O	5.82	1.30	1.24
1	A	77	SER	C-O	5.81	1.31	1.23
1	B	36	THR	CA-C	5.80	1.60	1.53
1	B	77	SER	C-O	5.79	1.30	1.23
1	A	109	ALA	CA-CB	5.78	1.62	1.53
1	A	69	GLN	C-O	5.78	1.30	1.23
1	A	92	TYR	CA-CB	5.78	1.62	1.53
1	B	14	ASP	N-CA	5.76	1.55	1.47
1	A	16	SER	CA-CB	5.75	1.63	1.53
1	A	26	CYS	C-O	5.75	1.30	1.24
1	A	1	LYS	CA-C	5.74	1.65	1.52
1	A	84	CYS	CA-C	5.74	1.59	1.52
1	B	87	THR	CB-OG1	5.74	1.52	1.43
1	B	54	VAL	CA-C	5.72	1.59	1.52
1	A	36	THR	CA-C	5.72	1.60	1.53
1	B	26	CYS	C-O	5.71	1.30	1.24
1	B	1	LYS	CA-C	5.69	1.65	1.52
1	A	116	VAL	N-CA	5.66	1.53	1.46
1	B	12	HIS	CA-C	5.66	1.60	1.52
1	B	53	ASP	CG-OD2	5.66	1.36	1.25
1	B	92	TYR	CA-CB	5.66	1.62	1.53
1	A	99	THR	C-O	5.66	1.30	1.24
1	B	7	LYS	C-O	5.66	1.30	1.24
1	A	53	ASP	CA-C	5.65	1.60	1.52
1	A	60	GLN	N-CA	5.62	1.53	1.46
1	B	8	PHE	CA-C	5.60	1.60	1.52
1	B	93	PRO	CA-C	5.59	1.64	1.52
1	B	58	CYS	C-O	5.59	1.31	1.24
1	B	109	ALA	N-CA	5.58	1.53	1.46
1	A	14	ASP	N-CA	5.57	1.56	1.47
1	A	50	SER	N-CA	5.56	1.52	1.46
1	B	50	SER	N-CA	5.56	1.52	1.46
1	B	8	PHE	C-O	5.55	1.30	1.24
1	B	99	THR	C-O	5.54	1.30	1.24
1	A	85	ARG	CZ-NH1	5.52	1.40	1.32
1	A	62	ASN	CB-CG	5.51	1.65	1.52
1	A	24	ASN	C-O	5.49	1.31	1.24
1	A	76	TYR	CA-C	5.47	1.59	1.52
1	A	120	PHE	CD2-CE2	5.47	1.55	1.38
1	A	124	VAL	CA-C	5.46	1.64	1.52
1	B	1	LYS	N-CA	5.42	1.56	1.46
1	B	79	MET	CA-CB	5.42	1.65	1.54

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	120	PHE	CD2-CE2	5.41	1.54	1.38
1	B	24	ASN	C-O	5.39	1.31	1.24
1	B	38	ASP	C-O	5.37	1.30	1.23
1	A	90	SER	CA-CB	-5.36	1.44	1.53
1	B	76	TYR	CA-C	5.36	1.59	1.52
1	A	13	MET	SD-CE	5.35	1.93	1.79
1	A	17	THR	CA-CB	5.34	1.61	1.53
1	A	1	LYS	N-CA	5.32	1.56	1.46
1	B	53	ASP	CA-C	5.31	1.59	1.52
1	A	114	PRO	N-CA	5.31	1.54	1.47
1	A	86	GLU	CG-CD	5.30	1.65	1.52
1	A	8	PHE	C-O	5.30	1.30	1.24
1	A	111	GLU	CD-OE2	5.30	1.35	1.25
1	A	19	ALA	CA-CB	5.30	1.63	1.53
1	B	86	GLU	CG-CD	5.30	1.65	1.52
1	B	124	VAL	CA-C	5.30	1.64	1.52
1	B	62	ASN	CB-CG	5.29	1.65	1.52
1	A	87	THR	CB-OG1	5.28	1.52	1.43
1	A	33	ARG	NE-CZ	5.26	1.38	1.33
1	B	60	GLN	N-CA	5.26	1.52	1.46
1	A	116	VAL	CB-CG2	5.24	1.69	1.52
1	A	20	ALA	C-O	5.24	1.30	1.23
1	A	36	THR	CA-CB	5.24	1.60	1.53
1	A	47	VAL	CA-C	5.24	1.58	1.52
1	A	97	TYR	CD2-CE2	5.22	1.54	1.38
1	B	61	LYS	CA-C	5.22	1.59	1.52
1	B	88	GLY	CA-C	-5.21	1.44	1.52
1	A	61	LYS	CA-C	5.21	1.59	1.52
1	B	116	VAL	CB-CG2	5.19	1.69	1.52
1	B	20	ALA	C-O	5.19	1.30	1.23
1	A	22	SER	C-O	5.18	1.29	1.23
1	A	73	TYR	CE1-CZ	5.18	1.50	1.38
1	B	111	GLU	CD-OE2	5.18	1.35	1.25
1	B	97	TYR	CD2-CE2	5.17	1.54	1.38
1	A	114	PRO	CA-CB	5.17	1.61	1.53
1	A	38	ASP	CG-OD2	5.16	1.35	1.25
1	B	53	ASP	CA-CB	5.16	1.61	1.53
1	B	84	CYS	CA-C	5.15	1.58	1.52
1	B	73	TYR	CE1-CZ	5.15	1.50	1.38
1	B	16	SER	CA-CB	5.15	1.62	1.53
1	B	85	ARG	CZ-NH1	5.09	1.39	1.32
1	A	37	LYS	CG-CD	5.09	1.67	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	54	VAL	CA-C	5.07	1.59	1.52
1	A	95	CYS	CB-SG	5.05	1.98	1.81
1	B	10	ARG	CZ-NH1	5.04	1.39	1.32
1	B	31	LYS	CD-CE	5.04	1.67	1.52
1	B	114	PRO	N-CA	5.02	1.53	1.47
1	A	12	HIS	CD2-NE2	5.01	1.43	1.37
1	A	30	MET	SD-CE	5.01	1.92	1.79

All (390) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	113	ASN	O-C-N	-35.49	87.14	121.57
1	A	113	ASN	O-C-N	-27.24	89.25	121.39
1	B	92	TYR	O-C-N	-25.66	91.81	121.32
1	A	92	TYR	O-C-N	-24.11	93.60	121.32
1	A	10	ARG	NE-CZ-NH1	17.22	138.72	121.50
1	B	10	ARG	NE-CZ-NH1	16.49	137.99	121.50
1	B	34	ASN	OD1-CG-ND2	13.85	136.44	122.60
1	A	70	THR	N-CA-CB	-13.70	90.56	110.56
1	A	34	ASN	OD1-CG-ND2	13.48	136.08	122.60
1	A	17	THR	N-CA-CB	-13.48	88.28	110.52
1	B	88	GLY	CA-C-O	-13.00	106.06	122.82
1	A	10	ARG	NE-CZ-NH2	-12.94	107.56	119.20
1	B	70	THR	N-CA-CB	-12.65	91.50	110.61
1	B	95	CYS	O-C-N	12.51	137.77	123.01
1	B	17	THR	N-CA-CB	-12.24	88.84	111.00
1	B	118	VAL	N-CA-CB	-11.91	96.04	112.12
1	B	10	ARG	NE-CZ-NH2	-11.82	108.56	119.20
1	B	66	LYS	O-C-N	11.79	135.64	122.20
1	A	95	CYS	O-C-N	11.74	136.86	123.01
1	A	73	TYR	O-C-N	11.60	137.37	123.33
1	B	118	VAL	CB-CA-C	11.52	121.94	110.65
1	A	118	VAL	N-CA-CB	-11.45	96.67	112.12
1	A	53	ASP	O-C-N	11.04	134.79	122.20
1	B	122	ALA	O-C-N	10.63	133.26	123.26
1	A	118	VAL	CB-CA-C	10.60	121.03	110.65
1	A	10	ARG	CD-NE-CZ	10.50	139.10	124.40
1	B	61	LYS	O-C-N	10.48	136.44	122.82
1	A	39	ARG	O-C-N	10.47	133.10	123.26
1	B	34	ASN	CB-CG-OD1	-10.42	99.95	120.80
1	A	70	THR	CA-CB-OG1	-10.39	94.02	109.60
1	A	34	ASN	CB-CG-OD1	-10.30	100.20	120.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	12	HIS	O-C-N	10.20	134.24	122.20
1	B	70	THR	CA-CB-OG1	-10.10	94.46	109.60
1	A	46	PHE	CA-CB-CG	-10.02	103.78	113.80
1	B	10	ARG	CD-NE-CZ	9.99	138.39	124.40
1	B	73	TYR	O-C-N	9.98	135.09	123.41
1	A	87	THR	N-CA-CB	-9.98	95.12	110.29
1	A	93	PRO	CA-C-N	-9.97	108.35	122.41
1	A	93	PRO	C-N-CA	-9.97	108.35	122.41
1	B	90	SER	O-C-N	9.92	135.13	122.93
1	A	24	ASN	CA-CB-CG	-9.85	102.75	112.60
1	A	66	LYS	O-C-N	9.61	133.47	122.22
1	B	46	PHE	CA-CB-CG	-9.61	104.19	113.80
1	B	87	THR	N-CA-CB	-9.56	95.64	110.56
1	A	105	HIS	O-C-N	9.50	134.22	123.01
1	B	12	HIS	O-C-N	9.47	131.94	122.19
1	A	83	ASP	CA-C-O	-9.46	109.85	120.54
1	B	105	HIS	CA-C-N	-9.36	108.64	122.68
1	B	105	HIS	C-N-CA	-9.36	108.64	122.68
1	A	95	CYS	CA-C-N	-9.35	107.59	122.73
1	A	95	CYS	C-N-CA	-9.35	107.59	122.73
1	A	17	THR	CA-CB-OG1	-9.34	95.59	109.60
1	B	1	LYS	O-C-N	9.28	137.84	123.00
1	A	105	HIS	CA-C-N	-9.25	108.81	122.68
1	A	105	HIS	C-N-CA	-9.25	108.81	122.68
1	A	12	HIS	CA-C-N	-9.21	110.02	122.72
1	A	12	HIS	C-N-CA	-9.21	110.02	122.72
1	A	63	VAL	O-C-N	9.18	133.23	123.04
1	A	61	LYS	O-C-N	9.14	134.48	122.96
1	B	39	ARG	O-C-N	9.09	132.80	123.26
1	B	83	ASP	CA-C-O	-8.96	110.41	120.54
1	A	90	SER	O-C-N	8.95	134.05	122.95
1	B	24	ASN	CA-CB-CG	-8.93	103.67	112.60
1	B	73	TYR	CA-C-N	-8.92	110.69	123.00
1	B	73	TYR	C-N-CA	-8.92	110.69	123.00
1	A	72	CYS	O-C-N	8.90	133.09	123.03
1	B	95	CYS	CA-C-N	-8.88	109.07	122.74
1	B	95	CYS	C-N-CA	-8.88	109.07	122.74
1	A	1	LYS	O-C-N	8.73	136.97	123.00
1	B	17	THR	CA-CB-OG1	-8.73	96.51	109.60
1	B	54	VAL	O-C-N	8.71	130.44	121.91
1	B	93	PRO	CA-C-N	-8.69	109.91	123.12
1	B	93	PRO	C-N-CA	-8.69	109.91	123.12

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	57	VAL	O-C-N	8.54	131.79	122.06
1	A	50	SER	O-C-N	8.52	133.28	122.81
1	B	63	VAL	CA-C-N	-8.48	109.30	121.42
1	B	63	VAL	C-N-CA	-8.48	109.30	121.42
1	B	117	PRO	CA-C-N	-8.43	111.59	121.71
1	B	117	PRO	C-N-CA	-8.43	111.59	121.71
1	A	20	ALA	N-CA-C	-8.38	97.61	110.10
1	A	122	ALA	O-C-N	8.34	130.92	123.41
1	B	105	HIS	O-C-N	8.30	133.01	122.89
1	B	70	THR	CA-CB-CG2	8.27	124.56	110.50
1	A	117	PRO	O-C-N	8.26	132.36	123.03
1	B	63	VAL	O-C-N	8.15	132.09	123.04
1	B	20	ALA	N-CA-C	-8.15	97.74	109.96
1	B	47	VAL	O-C-N	8.14	131.73	123.18
1	A	74	GLN	OE1-CD-NE2	8.13	130.73	122.60
1	B	12	HIS	CA-C-N	-8.08	109.06	121.02
1	B	12	HIS	C-N-CA	-8.08	109.06	121.02
1	B	108	VAL	O-C-N	8.08	131.38	122.98
1	B	76	TYR	O-C-N	8.05	130.66	122.12
1	B	74	GLN	OE1-CD-NE2	8.03	130.63	122.60
1	A	11	GLN	O-C-N	8.03	133.76	122.36
1	B	88	GLY	N-CA-C	-7.95	101.59	112.25
1	B	122	ALA	CA-C-N	-7.94	111.03	122.94
1	B	122	ALA	C-N-CA	-7.94	111.03	122.94
1	A	44	ASN	CA-C-N	-7.94	111.42	122.93
1	A	44	ASN	C-N-CA	-7.94	111.42	122.93
1	A	70	THR	CA-CB-CG2	7.92	123.97	110.50
1	B	53	ASP	O-C-N	7.91	132.51	122.23
1	B	57	VAL	O-C-N	7.89	132.39	122.05
1	A	17	THR	OG1-CB-CG2	7.87	125.03	109.30
1	B	124	VAL	N-CA-CB	-7.86	98.14	111.50
1	A	117	PRO	CA-C-N	-7.84	112.30	121.71
1	A	117	PRO	C-N-CA	-7.84	112.30	121.71
1	B	25	TYR	CA-C-N	-7.80	110.30	120.44
1	B	25	TYR	C-N-CA	-7.80	110.30	120.44
1	B	50	SER	O-C-N	7.78	132.38	122.81
1	A	108	VAL	O-C-N	7.76	131.18	123.03
1	B	61	LYS	CA-C-N	-7.76	109.88	120.82
1	B	61	LYS	C-N-CA	-7.76	109.88	120.82
1	A	73	TYR	CA-C-N	-7.73	112.33	123.00
1	A	73	TYR	C-N-CA	-7.73	112.33	123.00
1	A	124	VAL	N-CA-CB	-7.73	98.36	111.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	88	GLY	CA-C-O	-7.71	107.15	120.57
1	A	122	ALA	CA-C-N	-7.71	110.70	122.81
1	A	122	ALA	C-N-CA	-7.71	110.70	122.81
1	A	25	TYR	O-C-N	7.65	130.05	122.09
1	B	71	ASN	O-C-N	7.64	132.75	122.59
1	A	121	ASP	CA-C-O	-7.63	110.78	120.31
1	B	40	CYS	CA-C-O	-7.63	112.74	120.98
1	B	11	GLN	O-C-N	7.60	132.52	122.33
1	B	36	THR	O-C-N	7.60	131.93	122.20
1	B	90	SER	CA-C-N	-7.58	111.45	122.44
1	B	90	SER	C-N-CA	-7.58	111.45	122.44
1	A	62	ASN	CA-CB-CG	7.55	120.15	112.60
1	B	17	THR	OG1-CB-CG2	7.54	124.37	109.30
1	B	39	ARG	CA-C-N	-7.52	109.99	122.17
1	B	39	ARG	C-N-CA	-7.52	109.99	122.17
1	A	47	VAL	O-C-N	7.50	131.06	123.18
1	A	90	SER	CA-C-N	-7.49	110.44	121.76
1	A	90	SER	C-N-CA	-7.49	110.44	121.76
1	A	93	PRO	O-C-N	7.49	135.33	121.10
1	A	13	MET	CA-C-O	-7.47	112.28	120.43
1	A	76	TYR	O-C-N	7.47	130.04	122.12
1	A	1	LYS	CA-C-N	-7.45	110.31	120.82
1	A	1	LYS	C-N-CA	-7.45	110.31	120.82
1	B	1	LYS	CA-C-N	-7.44	109.96	121.56
1	B	1	LYS	C-N-CA	-7.44	109.96	121.56
1	B	25	TYR	O-C-N	7.42	130.64	122.11
1	B	18	SER	CA-CB-OG	-7.38	96.35	111.10
1	B	72	CYS	O-C-N	7.34	131.16	122.94
1	B	93	PRO	O-C-N	7.34	135.05	121.10
1	A	104	LYS	CB-CA-C	-7.32	96.83	111.17
1	B	4	ALA	O-C-N	7.28	129.84	122.12
1	B	121	ASP	CA-C-O	-7.28	111.21	120.31
1	A	61	LYS	CA-C-N	-7.27	110.77	120.95
1	A	61	LYS	C-N-CA	-7.27	110.77	120.95
1	B	29	MET	O-C-N	7.27	130.44	122.15
1	A	97	TYR	CA-C-N	-7.25	111.96	122.19
1	A	97	TYR	C-N-CA	-7.25	111.96	122.19
1	B	119	HIS	CA-C-N	-7.17	113.52	122.84
1	B	119	HIS	C-N-CA	-7.17	113.52	122.84
1	A	18	SER	CA-CB-OG	-7.15	96.81	111.10
1	A	87	THR	OG1-CB-CG2	7.11	123.52	109.30
1	B	83	ASP	CA-CB-CG	-7.11	105.50	112.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	106	ILE	O-C-N	7.09	130.35	122.98
1	B	97	TYR	CA-C-N	-7.08	111.37	121.50
1	B	97	TYR	C-N-CA	-7.08	111.37	121.50
1	B	13	MET	CA-C-O	-7.07	112.57	120.70
1	B	87	THR	OG1-CB-CG2	7.02	123.34	109.30
1	A	124	VAL	CB-CA-C	7.00	124.71	111.40
1	A	33	ARG	CA-C-N	-6.99	111.80	122.08
1	A	33	ARG	C-N-CA	-6.99	111.80	122.08
1	B	55	GLN	OE1-CD-NE2	6.95	129.55	122.60
1	A	44	ASN	O-C-N	6.88	131.46	123.41
1	A	4	ALA	O-C-N	6.82	129.35	122.12
1	A	46	PHE	CA-C-N	-6.79	114.76	123.19
1	A	46	PHE	C-N-CA	-6.79	114.76	123.19
1	A	119	HIS	CA-C-N	-6.79	113.74	122.77
1	A	119	HIS	C-N-CA	-6.79	113.74	122.77
1	B	99	THR	CB-CA-C	-6.79	99.19	110.19
1	A	33	ARG	O-C-N	6.78	131.61	122.59
1	B	99	THR	CA-CB-OG1	-6.76	99.46	109.60
1	B	53	ASP	CA-C-N	-6.75	112.05	120.56
1	B	53	ASP	C-N-CA	-6.75	112.05	120.56
1	B	62	ASN	CA-CB-CG	6.75	119.35	112.60
1	B	34	ASN	CA-C-O	-6.71	112.49	120.81
1	B	34	ASN	CA-CB-CG	-6.69	105.91	112.60
1	A	106	ILE	CA-C-N	-6.68	114.22	123.10
1	A	106	ILE	C-N-CA	-6.68	114.22	123.10
1	A	118	VAL	CG1-CB-CG2	6.67	125.48	110.80
1	A	63	VAL	CA-C-N	-6.66	111.41	120.87
1	A	63	VAL	C-N-CA	-6.66	111.41	120.87
1	B	118	VAL	CG1-CB-CG2	6.66	125.46	110.80
1	A	75	SER	N-CA-CB	6.65	120.19	109.28
1	A	94	ASN	CA-CB-CG	-6.63	105.97	112.60
1	A	36	THR	O-C-N	6.63	130.68	122.20
1	B	124	VAL	CB-CA-C	6.62	123.99	111.40
1	A	99	THR	CA-CB-OG1	-6.61	99.68	109.60
1	A	34	ASN	CA-C-O	-6.60	112.83	121.08
1	A	55	GLN	OE1-CD-NE2	6.58	129.18	122.60
1	A	47	VAL	N-CA-CB	-6.57	102.31	111.25
1	A	99	THR	CB-CA-C	-6.56	99.56	110.19
1	A	73	TYR	CA-C-O	-6.55	112.74	120.60
1	B	80	SER	O-C-N	6.54	130.68	123.22
1	A	83	ASP	CA-CB-CG	-6.54	106.06	112.60
1	A	11	GLN	CA-C-N	-6.53	112.10	122.29

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	11	GLN	C-N-CA	-6.53	112.10	122.29
1	A	61	LYS	CA-C-O	-6.51	113.03	120.58
1	B	53	ASP	CA-C-O	-6.51	113.02	120.24
1	B	50	SER	CA-C-N	-6.50	111.56	120.28
1	B	50	SER	C-N-CA	-6.50	111.56	120.28
1	B	44	ASN	CA-C-N	-6.50	113.19	122.94
1	B	44	ASN	C-N-CA	-6.50	113.19	122.94
1	A	58	CYS	N-CA-CB	6.48	121.74	110.39
1	A	34	ASN	CA-CB-CG	-6.44	106.16	112.60
1	B	16	SER	N-CA-CB	-6.44	100.35	110.46
1	B	58	CYS	N-CA-CB	6.42	122.01	110.32
1	B	66	LYS	CA-C-N	-6.41	111.54	122.56
1	B	66	LYS	C-N-CA	-6.41	111.54	122.56
1	A	12	HIS	CA-C-O	-6.39	111.64	119.18
1	A	16	SER	N-CA-CB	-6.38	100.48	110.44
1	B	113	ASN	CB-CA-C	6.36	118.44	108.84
1	B	16	SER	CB-CA-C	6.29	121.79	109.72
1	A	16	SER	CB-CA-C	6.28	122.29	109.55
1	B	74	GLN	CG-CD-OE1	-6.26	108.27	120.80
1	A	66	LYS	CA-C-N	-6.25	109.82	122.31
1	A	66	LYS	C-N-CA	-6.25	109.82	122.31
1	A	113	ASN	CB-CA-C	6.24	118.23	108.63
1	A	13	MET	O-C-N	6.23	130.31	123.27
1	A	29	MET	O-C-N	6.22	130.87	122.59
1	A	116	VAL	CA-CB-CG1	6.21	120.97	110.40
1	A	42	PRO	CA-C-N	-6.21	113.77	122.71
1	A	42	PRO	C-N-CA	-6.21	113.77	122.71
1	B	61	LYS	CA-C-O	-6.21	113.58	120.60
1	A	118	VAL	N-CA-C	-6.20	107.45	113.53
1	B	103	ASN	CA-C-O	-6.19	113.84	120.46
1	A	121	ASP	O-C-N	6.19	130.65	122.30
1	B	47	VAL	CA-C-O	-6.18	113.93	120.48
1	B	73	TYR	CA-C-O	-6.17	112.94	120.54
1	B	72	CYS	CA-C-N	-6.15	111.11	121.94
1	B	72	CYS	C-N-CA	-6.15	111.11	121.94
1	A	1	LYS	CA-C-O	-6.15	110.35	120.80
1	A	74	GLN	CG-CD-OE1	-6.15	108.51	120.80
1	B	29	MET	CA-C-N	-6.14	111.97	120.38
1	B	29	MET	C-N-CA	-6.14	111.97	120.38
1	A	61	LYS	CG-CD-CE	6.13	125.41	111.30
1	B	46	PHE	CA-C-N	-6.13	115.58	123.19
1	B	46	PHE	C-N-CA	-6.13	115.58	123.19

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	37	LYS	N-CA-C	6.13	118.04	111.36
1	B	75	SER	N-CA-CB	6.13	119.19	109.51
1	A	98	LYS	CA-C-O	-6.12	113.62	120.54
1	B	96	ALA	CA-C-O	-6.12	113.53	120.32
1	B	85	ARG	N-CA-CB	-6.11	100.98	110.57
1	B	106	ILE	CA-C-N	-6.08	115.01	123.10
1	B	106	ILE	C-N-CA	-6.08	115.01	123.10
1	B	23	SER	CA-C-O	6.06	126.73	119.10
1	B	27	ASN	OD1-CG-ND2	6.05	128.65	122.60
1	A	47	VAL	CA-C-O	-6.04	114.08	120.48
1	A	23	SER	CA-CB-OG	-6.04	99.03	111.10
1	B	94	ASN	CA-CB-CG	-6.00	106.60	112.60
1	B	1	LYS	CA-C-O	-6.00	110.60	120.80
1	B	12	HIS	CA-C-O	-5.98	111.81	118.69
1	A	97	TYR	O-C-N	5.97	130.56	123.27
1	B	44	ASN	O-C-N	5.96	130.52	122.59
1	A	99	THR	CA-C-N	-5.96	114.71	123.05
1	A	99	THR	C-N-CA	-5.96	114.71	123.05
1	B	47	VAL	N-CA-CB	-5.95	103.17	111.25
1	B	61	LYS	CG-CD-CE	5.93	124.95	111.30
1	B	56	ALA	CA-C-O	-5.92	112.10	119.38
1	A	17	THR	CB-CA-C	5.91	119.42	109.48
1	B	11	GLN	CA-C-N	-5.89	112.96	121.98
1	B	11	GLN	C-N-CA	-5.89	112.96	121.98
1	B	74	GLN	CA-C-O	5.89	126.81	120.38
1	A	85	ARG	CG-CD-NE	-5.89	99.05	112.00
1	A	56	ALA	CA-C-O	-5.89	113.20	119.97
1	A	50	SER	CA-C-N	-5.88	112.40	120.28
1	A	50	SER	C-N-CA	-5.88	112.40	120.28
1	A	27	ASN	OD1-CG-ND2	5.87	128.47	122.60
1	A	87	THR	CA-CB-OG1	-5.87	100.80	109.60
1	B	97	TYR	O-C-N	5.86	130.84	123.23
1	A	96	ALA	CA-C-O	-5.81	113.97	120.66
1	A	17	THR	CA-C-O	-5.81	114.35	120.80
1	A	111	GLU	O-C-N	5.81	129.21	123.46
1	B	81	ILE	CA-CB-CG1	-5.80	100.55	110.40
1	B	21	SER	CA-CB-OG	-5.79	99.52	111.10
1	B	116	VAL	CA-CB-CG1	5.78	120.23	110.40
1	A	103	ASN	CA-C-O	-5.77	114.10	120.33
1	A	80	SER	CA-C-N	-5.76	113.53	122.69
1	A	80	SER	C-N-CA	-5.76	113.53	122.69
1	A	119	HIS	CA-CB-CG	5.76	119.56	113.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	87	THR	CA-CB-OG1	-5.74	100.98	109.60
1	B	87	THR	CA-C-N	-5.73	113.61	121.06
1	B	87	THR	C-N-CA	-5.73	113.61	121.06
1	B	51	LEU	N-CA-C	-5.72	105.04	111.28
1	A	72	CYS	CA-C-N	-5.71	112.54	122.37
1	A	72	CYS	C-N-CA	-5.71	112.54	122.37
1	B	69	GLN	N-CA-C	-5.71	102.59	110.35
1	A	23	SER	CA-C-O	5.69	126.27	119.10
1	A	66	LYS	N-CA-CB	-5.68	101.47	110.22
1	B	118	VAL	N-CA-C	-5.67	107.97	113.53
1	A	24	ASN	OD1-CG-ND2	5.66	128.26	122.60
1	A	66	LYS	CB-CA-C	5.66	121.10	110.63
1	B	23	SER	CA-CB-OG	-5.65	99.79	111.10
1	B	53	ASP	N-CA-CB	5.63	118.59	110.20
1	A	73	TYR	CG-CD2-CE2	5.63	129.65	121.20
1	A	21	SER	CA-CB-OG	-5.62	99.85	111.10
1	B	91	LYS	CA-C-O	-5.61	113.18	120.25
1	B	104	LYS	CB-CA-C	-5.61	97.73	110.07
1	A	51	LEU	N-CA-C	-5.60	105.17	111.28
1	B	85	ARG	CG-CD-NE	-5.60	99.68	112.00
1	A	63	VAL	CB-CA-C	5.59	119.05	110.55
1	B	80	SER	CA-CB-OG	-5.59	99.92	111.10
1	A	20	ALA	CA-C-N	-5.58	113.33	122.54
1	A	20	ALA	C-N-CA	-5.58	113.33	122.54
1	A	64	ALA	N-CA-C	-5.58	102.02	110.28
1	B	27	ASN	CB-CG-ND2	-5.58	108.02	116.40
1	A	78	THR	N-CA-C	-5.58	103.02	110.55
1	B	75	SER	CA-C-N	-5.58	112.80	120.28
1	B	75	SER	C-N-CA	-5.58	112.80	120.28
1	A	85	ARG	N-CA-CB	-5.56	101.18	110.80
1	A	53	ASP	CA-C-O	-5.55	113.98	120.20
1	B	33	ARG	CA-C-N	-5.52	114.39	122.40
1	B	33	ARG	C-N-CA	-5.52	114.39	122.40
1	B	17	THR	CB-CA-C	5.51	120.27	109.35
1	B	121	ASP	O-C-N	5.50	129.73	122.30
1	B	113	ASN	CA-C-O	-5.49	113.87	120.41
1	A	78	THR	CA-CB-CG2	5.49	119.83	110.50
1	B	85	ARG	CB-CG-CD	-5.48	98.69	111.30
1	B	108	VAL	CA-C-N	-5.48	114.46	122.19
1	B	108	VAL	C-N-CA	-5.48	114.46	122.19
1	A	27	ASN	CB-CG-ND2	-5.47	108.19	116.40
1	A	86	GLU	CB-CA-C	5.46	118.42	109.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	17	THR	CA-C-O	-5.46	114.39	120.66
1	A	25	TYR	CA-C-N	-5.43	113.05	120.44
1	A	25	TYR	C-N-CA	-5.43	113.05	120.44
1	A	75	SER	CA-C-O	5.43	126.66	120.80
1	A	80	SER	CA-CB-OG	-5.43	100.24	111.10
1	A	113	ASN	CA-C-O	-5.43	113.86	120.54
1	B	16	SER	CA-C-O	5.43	125.64	119.18
1	B	4	ALA	CA-C-N	-5.42	111.65	120.71
1	B	4	ALA	C-N-CA	-5.42	111.65	120.71
1	A	74	GLN	CA-C-O	5.41	126.28	120.38
1	A	81	ILE	CA-CB-CG1	-5.39	101.23	110.40
1	B	78	THR	CA-CB-CG2	5.39	119.66	110.50
1	A	43	VAL	CA-C-O	-5.39	114.83	120.76
1	B	37	LYS	O-C-N	5.39	128.29	122.15
1	B	119	HIS	CA-CB-CG	5.38	119.18	113.80
1	A	107	ILE	O-C-N	5.38	128.90	123.20
1	B	73	TYR	CG-CD2-CE2	5.38	129.27	121.20
1	A	8	PHE	CA-C-O	5.37	126.46	120.82
1	B	62	ASN	OD1-CG-ND2	-5.36	117.25	122.60
1	A	88	GLY	N-CA-C	-5.35	100.50	113.18
1	B	42	PRO	CA-C-N	-5.35	115.01	122.71
1	B	42	PRO	C-N-CA	-5.35	115.01	122.71
1	B	111	GLU	O-C-N	5.34	129.14	123.42
1	A	62	ASN	OD1-CG-ND2	-5.33	117.27	122.60
1	B	80	SER	CA-C-N	-5.33	114.25	122.68
1	B	80	SER	C-N-CA	-5.33	114.25	122.68
1	A	106	ILE	O-C-N	5.29	128.49	122.98
1	B	8	PHE	CA-C-O	5.29	126.57	120.90
1	A	110	CYS	CA-C-N	-5.28	111.20	121.91
1	A	110	CYS	C-N-CA	-5.28	111.20	121.91
1	B	86	GLU	CB-CA-C	5.26	118.44	109.72
1	A	6	ALA	CA-C-O	-5.25	114.41	120.24
1	A	32	SER	CB-CA-C	5.25	119.50	110.79
1	A	11	GLN	OE1-CD-NE2	-5.24	117.36	122.60
1	B	98	LYS	CA-C-O	-5.24	114.72	120.69
1	B	41	LYS	N-CA-C	-5.23	101.94	109.48
1	A	30	MET	CA-C-O	5.22	125.95	120.42
1	A	16	SER	CA-C-O	5.21	125.37	119.27
1	A	59	SER	O-C-N	5.21	128.99	122.22
1	B	117	PRO	O-C-N	5.19	128.91	123.10
1	B	97	TYR	CA-C-O	5.18	126.29	120.70
1	A	109	ALA	N-CA-CB	5.17	119.06	110.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	7	LYS	CA-C-O	5.17	126.03	120.55
1	A	85	ARG	CB-CG-CD	-5.16	99.44	111.30
1	B	66	LYS	CB-CA-C	5.16	120.46	110.46
1	A	12	HIS	N-CA-C	5.15	121.33	113.61
1	A	37	LYS	O-C-N	5.15	128.40	122.17
1	B	2	GLU	CA-C-O	-5.14	115.81	120.95
1	A	117	PRO	CB-CA-C	5.13	117.11	111.11
1	B	86	GLU	CB-CG-CD	5.11	121.29	112.60
1	A	37	LYS	N-CA-C	5.10	117.63	111.40
1	B	78	THR	OG1-CB-CG2	-5.09	99.12	109.30
1	A	56	ALA	O-C-N	5.08	128.52	122.27
1	B	6	ALA	CA-C-O	-5.08	115.14	120.63
1	B	107	ILE	CA-C-N	-5.07	115.07	122.68
1	B	107	ILE	C-N-CA	-5.07	115.07	122.68
1	B	22	SER	O-C-N	5.06	128.84	123.42
1	A	78	THR	OG1-CB-CG2	-5.04	99.21	109.30
1	A	46	PHE	N-CA-CB	5.04	119.60	110.83
1	B	83	ASP	OD1-CG-OD2	5.04	134.99	122.90
1	A	53	ASP	N-CA-CB	5.02	118.08	110.14
1	A	70	THR	CB-CA-C	5.02	119.05	110.56
1	B	20	ALA	CA-C-N	-5.02	114.26	122.54
1	B	20	ALA	C-N-CA	-5.02	114.26	122.54
1	A	69	GLN	N-CA-C	-5.02	102.34	110.32

There are no chirality outliers.

All (4) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	113	ASN	Peptide,Mainchain
1	B	113	ASN	Peptide,Mainchain

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	950	0	905	135	1
1	B	950	0	905	156	2

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
All	All	1900	0	1810	289	2

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 78.

All (289) 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:10:ARG:O	1:B:33:ARG:HD2	1.26	1.29
1:B:108:VAL:CG1	1:B:117:PRO:HB3	1.67	1.24
1:B:17:THR:HG23	1:B:48:HIS:ND1	1.55	1.21
1:A:14:ASP:OD1	1:A:29:MET:HE1	1.36	1.20
1:A:25:TYR:O	1:A:29:MET:HB2	1.43	1.19
1:A:20:ALA:HB2	1:A:82:THR:OG1	1.42	1.18
1:A:109:ALA:CB	1:A:119:HIS:CD2	2.27	1.17
1:A:106:ILE:C	1:A:107:ILE:HD12	1.69	1.17
1:B:60:GLN:HG2	1:B:76:TYR:CD2	1.80	1.17
1:A:109:ALA:CB	1:A:119:HIS:HD2	1.58	1.16
1:B:91:LYS:HD3	1:B:91:LYS:C	1.71	1.16
1:B:43:VAL:CG2	1:B:85:ARG:HH12	1.59	1.13
1:A:109:ALA:HB2	1:A:119:HIS:CD2	1.83	1.10
1:B:78:THR:HG22	1:B:105:HIS:CD2	1.86	1.09
1:A:91:LYS:O	1:A:91:LYS:HG3	1.47	1.07
1:A:43:VAL:HG22	1:A:85:ARG:CD	1.84	1.07
1:A:85:ARG:NH1	1:A:85:ARG:HG2	1.62	1.07
1:A:19:ALA:HA	1:A:48:HIS:CD2	1.88	1.06
1:B:108:VAL:HG11	1:B:117:PRO:HB3	1.07	1.06
1:A:109:ALA:HB3	1:A:119:HIS:HD2	1.18	1.04
1:A:71:ASN:HD21	1:A:109:ALA:HB1	1.18	1.04
1:B:91:LYS:HD3	1:B:91:LYS:O	1.58	1.03
1:A:91:LYS:O	1:A:91:LYS:CG	2.07	1.02
1:B:14:ASP:OD2	1:B:17:THR:HG21	1.59	1.02
1:A:106:ILE:O	1:A:107:ILE:HD12	1.61	1.00
1:B:43:VAL:HG22	1:B:85:ARG:HH12	1.21	0.99
1:A:71:ASN:ND2	1:A:109:ALA:HB1	1.77	0.99
1:A:109:ALA:HB3	1:A:119:HIS:CD2	1.94	0.99
1:A:51:LEU:O	1:A:55:GLN:HG3	1.61	0.99
1:B:43:VAL:HG22	1:B:85:ARG:NH1	1.79	0.97
1:B:2:GLU:OE2	1:B:7:LYS:HA	1.64	0.97
1:A:85:ARG:HG2	1:A:85:ARG:HH11	1.25	0.95
1:A:106:ILE:C	1:A:107:ILE:CD1	2.40	0.95

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:31:LYS:HA	1:A:36:THR:HG23	1.46	0.93
1:A:87:THR:HG23	1:A:88:GLY:O	1.69	0.93
1:A:107:ILE:CD1	1:A:107:ILE:N	2.33	0.92
1:B:108:VAL:HG11	1:B:117:PRO:CB	2.00	0.92
1:A:67:ASN:ND2	1:A:69:GLN:HG3	1.86	0.91
1:B:41:LYS:HZ3	1:B:44:ASN:HB2	1.35	0.91
1:A:24:ASN:HB3	1:A:28:GLN:HE21	1.33	0.91
1:A:50:SER:O	1:A:54:VAL:HG23	1.71	0.90
1:A:60:GLN:HG2	1:A:76:TYR:CD2	2.09	0.88
1:B:43:VAL:CG2	1:B:85:ARG:NH1	2.34	0.88
1:B:109:ALA:HB3	1:B:119:HIS:HB3	1.56	0.87
1:A:85:ARG:HH11	1:A:85:ARG:CG	1.86	0.86
1:B:10:ARG:O	1:B:33:ARG:CD	2.18	0.86
1:B:91:LYS:C	1:B:91:LYS:CD	2.48	0.86
1:B:90:SER:HB3	1:B:96:ALA:H	1.37	0.86
1:B:41:LYS:NZ	1:B:44:ASN:HB2	1.91	0.85
1:A:43:VAL:HG22	1:A:85:ARG:HD3	1.59	0.82
1:A:30:MET:HE2	1:A:97:TYR:CE1	2.15	0.82
1:A:86:GLU:HG2	1:A:90:SER:CB	2.10	0.81
1:B:30:MET:HG3	1:B:97:TYR:CD2	2.15	0.81
1:B:40:CYS:SG	1:B:92:TYR:HA	2.20	0.81
1:B:44:ASN:C	1:B:44:ASN:HD22	1.88	0.81
1:A:24:ASN:HB3	1:A:28:GLN:NE2	1.95	0.81
1:A:14:ASP:CG	1:A:29:MET:HE1	2.06	0.81
1:B:33:ARG:HB2	1:B:35:LEU:HD11	1.62	0.81
1:A:78:THR:HG23	1:A:105:HIS:CE1	2.17	0.80
1:B:78:THR:HG22	1:B:105:HIS:HD2	1.41	0.80
1:B:90:SER:OG	1:B:96:ALA:HB3	1.82	0.80
1:B:24:ASN:ND2	1:B:28:GLN:HE22	1.81	0.78
1:A:87:THR:C	1:A:88:GLY:O	2.20	0.76
1:A:7:LYS:O	1:A:11:GLN:HG3	1.86	0.76
1:B:91:LYS:CD	1:B:92:TYR:O	2.34	0.75
1:A:67:ASN:CG	1:A:69:GLN:HG3	2.11	0.75
1:B:2:GLU:OE2	1:B:7:LYS:CA	2.34	0.74
1:B:82:THR:CG2	1:B:99:THR:HG23	2.17	0.74
1:A:25:TYR:CZ	1:A:29:MET:HG3	2.23	0.74
1:A:107:ILE:N	1:A:107:ILE:HD13	2.01	0.74
1:A:78:THR:HG22	1:A:104:LYS:HA	1.70	0.73
1:A:10:ARG:O	1:A:33:ARG:HD2	1.89	0.73
1:B:42:PRO:HA	1:B:86:GLU:HB2	1.69	0.73
1:A:14:ASP:OD1	1:A:29:MET:CE	2.28	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:25:TYR:OH	1:A:29:MET:HE3	1.90	0.72
1:B:91:LYS:HD3	1:B:92:TYR:O	1.89	0.71
1:B:44:ASN:C	1:B:44:ASN:ND2	2.47	0.71
1:B:74:GLN:HG2	1:B:75:SER:N	2.05	0.71
1:A:57:VAL:HG23	1:A:79:MET:HE1	1.70	0.71
1:B:60:GLN:CG	1:B:76:TYR:CD2	2.68	0.71
1:B:108:VAL:HG12	1:B:117:PRO:HB3	1.69	0.70
1:B:90:SER:CB	1:B:96:ALA:H	2.03	0.70
1:A:75:SER:HB3	1:A:79:MET:HE3	1.74	0.69
1:A:75:SER:HG	1:A:105:HIS:HA	1.56	0.69
1:B:11:GLN:O	1:B:46:PHE:CE1	2.46	0.69
1:A:30:MET:SD	1:A:44:ASN:HB3	2.33	0.68
1:B:43:VAL:HG21	1:B:85:ARG:HH12	1.57	0.68
1:A:19:ALA:HA	1:A:48:HIS:HD2	1.53	0.67
1:A:86:GLU:HG2	1:A:90:SER:HB3	1.76	0.67
1:B:49:GLU:OE1	1:B:79:MET:HB3	1.94	0.67
1:A:7:LYS:O	1:A:11:GLN:CG	2.42	0.67
1:B:12:HIS:HA	1:B:46:PHE:CD1	2.29	0.66
1:B:25:TYR:C	1:B:25:TYR:CD2	2.74	0.66
1:A:61:LYS:HB2	1:A:76:TYR:HE1	1.60	0.66
1:B:19:ALA:HB1	1:B:101:GLN:OE1	1.95	0.66
1:B:30:MET:O	1:B:35:LEU:HD12	1.96	0.66
1:A:20:ALA:CB	1:A:82:THR:OG1	2.34	0.66
1:A:17:THR:O	1:A:48:HIS:HB3	1.96	0.65
1:B:14:ASP:OD2	1:B:17:THR:CG2	2.39	0.65
1:B:83:ASP:N	1:B:100:THR:O	2.20	0.65
1:B:13:MET:O	1:B:33:ARG:NH1	2.29	0.64
1:B:107:ILE:HD11	1:B:124:VAL:HG11	1.79	0.64
1:B:24:ASN:HB3	1:B:28:GLN:OE1	1.98	0.64
1:B:87:THR:C	1:B:88:GLY:O	2.37	0.63
1:A:7:LYS:CD	1:A:10:ARG:HH11	2.12	0.63
1:B:82:THR:HG21	1:B:99:THR:HG23	1.80	0.63
1:A:57:VAL:CG2	1:A:79:MET:HE1	2.28	0.63
1:A:14:ASP:CG	1:A:29:MET:CE	2.71	0.62
1:B:17:THR:HG23	1:B:48:HIS:CE1	2.33	0.62
1:B:61:LYS:NZ	1:B:76:TYR:CD1	2.66	0.62
1:A:107:ILE:N	1:A:122:ALA:O	2.30	0.62
1:B:20:ALA:HA	1:B:25:TYR:CD1	2.34	0.61
1:A:78:THR:HG22	1:A:104:LYS:CA	2.30	0.61
1:B:78:THR:CG2	1:B:105:HIS:CD2	2.76	0.61
1:A:24:ASN:O	1:A:28:GLN:HG3	2.01	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:26:CYS:HB2	1:B:99:THR:OG1	2.01	0.61
1:B:30:MET:HA	1:B:35:LEU:HD12	1.83	0.60
1:A:42:PRO:C	1:A:43:VAL:HG23	2.25	0.60
1:A:75:SER:O	1:A:105:HIS:CD2	2.54	0.60
1:B:27:ASN:H	1:B:27:ASN:ND2	1.98	0.60
1:B:17:THR:CG2	1:B:48:HIS:ND1	2.48	0.60
1:B:17:THR:O	1:B:48:HIS:HB3	2.02	0.60
1:B:91:LYS:O	1:B:92:TYR:C	2.45	0.59
1:A:19:ALA:HB1	1:A:101:GLN:CD	2.27	0.59
1:B:24:ASN:O	1:B:28:GLN:OE1	2.18	0.59
1:B:20:ALA:HB2	1:B:82:THR:OG1	2.03	0.59
1:A:25:TYR:CD2	1:A:82:THR:HG21	2.38	0.59
1:A:41:LYS:HD3	1:A:44:ASN:HB2	1.82	0.59
1:B:41:LYS:O	1:B:97:TYR:CE1	2.56	0.59
1:A:74:GLN:O	1:A:74:GLN:HG2	2.03	0.58
1:A:109:ALA:HB2	1:A:119:HIS:NE2	2.18	0.58
1:B:40:CYS:SG	1:B:92:TYR:CA	2.91	0.58
1:B:121:ASP:O	1:B:122:ALA:HB2	2.02	0.58
1:A:25:TYR:O	1:A:29:MET:CB	2.36	0.58
1:B:11:GLN:HB2	1:B:12:HIS:CD2	2.39	0.58
1:A:32:SER:C	1:A:34:ASN:H	2.12	0.58
1:A:43:VAL:HG22	1:A:85:ARG:NE	2.19	0.57
1:A:49:GLU:HG3	1:A:79:MET:HB3	1.85	0.57
1:B:61:LYS:NZ	1:B:76:TYR:HD1	2.02	0.57
1:B:24:ASN:O	1:B:28:GLN:CD	2.48	0.56
1:A:14:ASP:OD2	1:A:17:THR:HB	2.05	0.56
1:B:12:HIS:HB3	1:B:45:THR:O	2.06	0.56
1:B:30:MET:CB	1:B:97:TYR:CE2	2.89	0.56
1:B:49:GLU:OE1	1:B:79:MET:HA	2.06	0.55
1:A:75:SER:OG	1:A:105:HIS:HA	2.05	0.55
1:B:12:HIS:CD2	1:B:12:HIS:N	2.74	0.55
1:B:14:ASP:O	1:B:17:THR:HG22	2.06	0.55
1:A:57:VAL:CG2	1:A:79:MET:CE	2.85	0.54
1:A:31:LYS:HA	1:A:36:THR:CG2	2.28	0.54
1:A:107:ILE:O	1:A:121:ASP:N	2.35	0.54
1:A:9:GLU:HA	1:A:13:MET:HG2	1.89	0.54
1:B:49:GLU:OE1	1:B:79:MET:CA	2.55	0.54
1:A:51:LEU:O	1:A:55:GLN:CG	2.48	0.54
1:A:61:LYS:HB2	1:A:76:TYR:CE1	2.42	0.54
1:A:43:VAL:CG2	1:A:85:ARG:NE	2.70	0.54
1:A:113:ASN:C	1:A:114:PRO:O	2.50	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:41:LYS:O	1:B:97:TYR:HE1	1.90	0.54
1:A:7:LYS:HD3	1:A:10:ARG:HH11	1.73	0.53
1:A:8:PHE:CD1	1:A:12:HIS:CD2	2.97	0.53
1:B:12:HIS:HA	1:B:46:PHE:HD1	1.70	0.53
1:B:113:ASN:C	1:B:114:PRO:O	2.51	0.53
1:B:24:ASN:CG	1:B:28:GLN:HE22	2.16	0.53
1:B:32:SER:C	1:B:34:ASN:H	2.15	0.53
1:A:30:MET:O	1:A:35:LEU:HB2	2.09	0.53
1:A:88:GLY:O	1:A:89:SER:CB	2.56	0.53
1:A:19:ALA:CA	1:A:48:HIS:CD2	2.79	0.53
1:A:11:GLN:O	1:A:46:PHE:CE1	2.62	0.52
1:B:60:GLN:HG2	1:B:76:TYR:CE2	2.38	0.52
1:A:10:ARG:HG3	1:B:76:TYR:CE1	2.45	0.52
1:B:91:LYS:N	1:B:94:ASN:O	2.36	0.52
1:A:29:MET:O	1:A:33:ARG:HG2	2.10	0.52
1:B:85:ARG:HB3	1:B:98:LYS:HB3	1.91	0.51
1:B:13:MET:HE2	1:B:49:GLU:O	2.11	0.51
1:B:49:GLU:OE1	1:B:79:MET:CB	2.58	0.51
1:B:91:LYS:O	1:B:91:LYS:CD	2.47	0.51
1:A:7:LYS:HD2	1:A:10:ARG:HH11	1.75	0.51
1:A:43:VAL:CG2	1:A:85:ARG:CD	2.74	0.50
1:B:57:VAL:CG2	1:B:79:MET:HE1	2.41	0.50
1:B:30:MET:HA	1:B:35:LEU:CD1	2.42	0.50
1:B:73:TYR:HD2	1:B:110:CYS:SG	2.35	0.50
1:B:88:GLY:O	1:B:89:SER:HB3	2.12	0.50
1:B:57:VAL:HG23	1:B:79:MET:HE1	1.94	0.49
1:B:73:TYR:CD2	1:B:110:CYS:SG	3.06	0.49
1:A:65:CYS:HB2	1:A:67:ASN:OD1	2.13	0.49
1:A:60:GLN:HG2	1:A:76:TYR:CG	2.47	0.49
1:A:91:LYS:O	1:A:92:TYR:C	2.55	0.48
1:B:104:LYS:HD3	1:B:123:SER:HB2	1.94	0.48
1:A:81:ILE:HD11	1:A:104:LYS:HG3	1.93	0.48
1:A:60:GLN:HG2	1:A:76:TYR:CE2	2.47	0.48
1:A:86:GLU:HG2	1:A:90:SER:OG	2.12	0.48
1:B:14:ASP:O	1:B:48:HIS:HA	2.13	0.48
1:B:19:ALA:HA	1:B:48:HIS:CE1	2.48	0.48
1:B:72:CYS:HA	1:B:108:VAL:O	2.13	0.48
1:B:13:MET:CE	1:B:49:GLU:O	2.61	0.48
1:A:66:LYS:HE3	1:A:121:ASP:OD1	2.14	0.48
1:B:91:LYS:HD3	1:B:92:TYR:N	2.24	0.48
1:A:8:PHE:CD1	1:A:12:HIS:HD2	2.32	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:7:LYS:HD2	1:A:10:ARG:NH1	2.29	0.47
1:B:7:LYS:HZ2	1:B:10:ARG:HH11	1.62	0.47
1:B:58:CYS:HB3	1:B:115:TYR:CD2	2.50	0.47
1:A:105:HIS:O	1:A:124:VAL:N	2.45	0.47
1:B:90:SER:HB3	1:B:96:ALA:N	2.17	0.47
1:B:110:CYS:HB2	1:B:115:TYR:CE2	2.49	0.47
1:B:60:GLN:CG	1:B:76:TYR:CE2	2.97	0.47
1:B:78:THR:HG22	1:B:105:HIS:NE2	2.27	0.47
1:A:72:CYS:HB3	1:A:107:ILE:CG2	2.46	0.47
1:A:123:SER:C	1:A:124:VAL:HG23	2.39	0.47
1:B:71:ASN:ND2	1:B:110:CYS:O	2.48	0.47
1:A:37:LYS:HE2	1:A:37:LYS:HA	1.95	0.46
1:A:63:VAL:O	1:A:72:CYS:HB2	2.15	0.46
1:A:85:ARG:HH11	1:A:85:ARG:CB	2.27	0.46
1:B:18:SER:O	1:B:19:ALA:HB2	2.14	0.46
1:A:78:THR:HG23	1:A:105:HIS:ND1	2.30	0.46
1:B:33:ARG:HB2	1:B:35:LEU:CD1	2.39	0.46
1:B:90:SER:OG	1:B:96:ALA:CB	2.59	0.46
1:A:43:VAL:HG22	1:A:85:ARG:HD2	1.88	0.46
1:B:91:LYS:HD3	1:B:92:TYR:C	2.41	0.46
1:B:88:GLY:O	1:B:89:SER:CB	2.64	0.46
1:B:73:TYR:CE2	1:B:115:TYR:HE2	2.34	0.46
1:B:90:SER:CB	1:B:96:ALA:N	2.76	0.46
1:A:106:ILE:C	1:A:107:ILE:HD13	2.34	0.46
1:B:36:THR:HA	1:B:39:ARG:O	2.16	0.46
1:B:45:THR:HG22	1:B:81:ILE:HB	1.97	0.46
1:A:13:MET:O	1:A:33:ARG:NH1	2.49	0.45
1:A:67:ASN:HD21	1:A:69:GLN:HG3	1.78	0.45
1:B:62:ASN:ND2	1:B:70:THR:O	2.40	0.45
1:B:70:THR:C	1:B:72:CYS:H	2.25	0.45
1:B:60:GLN:HG2	1:B:76:TYR:CG	2.44	0.45
1:A:42:PRO:C	1:A:43:VAL:CG2	2.89	0.45
1:B:105:HIS:O	1:B:123:SER:HA	2.17	0.45
1:A:105:HIS:O	1:A:123:SER:HA	2.17	0.45
1:B:30:MET:C	1:B:35:LEU:HD12	2.41	0.45
1:B:39:ARG:HD2	1:B:39:ARG:C	2.42	0.45
1:A:19:ALA:O	1:A:20:ALA:C	2.60	0.45
1:B:36:THR:HG22	1:B:97:TYR:OH	2.16	0.45
1:A:78:THR:HG23	1:A:105:HIS:HE1	1.76	0.45
1:A:98:LYS:HA	1:A:98:LYS:HD3	1.48	0.45
1:B:87:THR:HG22	1:B:88:GLY:O	2.17	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:56:ALA:O	1:B:60:GLN:NE2	2.50	0.45
1:A:17:THR:HG22	1:A:48:HIS:ND1	2.31	0.44
1:B:33:ARG:O	1:B:34:ASN:HB2	2.18	0.44
1:A:7:LYS:O	1:A:11:GLN:HG2	2.17	0.44
1:B:43:VAL:HG22	1:B:85:ARG:CZ	2.45	0.44
1:B:25:TYR:C	1:B:25:TYR:HD2	2.24	0.44
1:B:108:VAL:CG1	1:B:117:PRO:CB	2.63	0.44
1:B:109:ALA:CB	1:B:119:HIS:HB3	2.38	0.44
1:A:31:LYS:CA	1:A:36:THR:HG23	2.33	0.44
1:A:61:LYS:HG2	1:A:63:VAL:CG1	2.48	0.44
1:A:103:ASN:C	1:A:104:LYS:HG2	2.40	0.44
1:B:1:LYS:O	1:B:2:GLU:C	2.61	0.44
1:B:110:CYS:HA	1:B:116:VAL:O	2.17	0.44
1:B:30:MET:HB3	1:B:97:TYR:CE2	2.53	0.44
1:B:39:ARG:HA	1:B:92:TYR:CD1	2.52	0.44
1:A:71:ASN:HD22	1:A:110:CYS:H	1.66	0.43
1:B:34:ASN:CG	1:B:37:LYS:HE3	2.43	0.43
1:A:10:ARG:HG3	1:B:76:TYR:CD1	2.53	0.43
1:A:30:MET:HE2	1:A:97:TYR:CZ	2.52	0.43
1:A:34:ASN:N	1:A:34:ASN:OD1	2.50	0.43
1:B:24:ASN:OD1	1:B:27:ASN:ND2	2.52	0.43
1:B:49:GLU:CD	1:B:79:MET:HB3	2.43	0.43
1:A:2:GLU:OE1	1:A:7:LYS:HD3	2.18	0.43
1:A:61:LYS:O	1:A:63:VAL:HG13	2.19	0.43
1:B:44:ASN:ND2	1:B:45:THR:N	2.67	0.43
1:B:57:VAL:CG2	1:B:79:MET:CE	2.97	0.43
1:A:25:TYR:CE1	1:A:29:MET:HG3	2.52	0.43
1:B:61:LYS:HG2	1:B:63:VAL:HG13	2.01	0.43
1:A:72:CYS:C	1:A:73:TYR:CD2	2.97	0.42
1:B:11:GLN:HE21	1:B:35:LEU:HD23	1.84	0.42
1:A:20:ALA:HB1	1:A:99:THR:HG21	2.01	0.42
1:B:58:CYS:HB3	1:B:115:TYR:HD2	1.85	0.42
1:A:8:PHE:CD2	1:A:117:PRO:HB2	2.55	0.42
1:B:85:ARG:O	1:B:97:TYR:HA	2.19	0.42
1:B:26:CYS:HB3	1:B:97:TYR:HB2	2.01	0.42
1:A:78:THR:CG2	1:A:104:LYS:HA	2.46	0.42
1:A:47:VAL:HG22	1:A:81:ILE:HG22	2.02	0.41
1:B:82:THR:CG2	1:B:99:THR:CG2	2.93	0.41
1:B:91:LYS:HE2	1:B:92:TYR:N	2.35	0.41
1:B:105:HIS:O	1:B:124:VAL:N	2.43	0.41
1:B:2:GLU:OE2	1:B:7:LYS:N	2.54	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:73:TYR:O	1:B:107:ILE:HA	2.21	0.41
1:B:11:GLN:NE2	1:B:35:LEU:HD23	2.35	0.41
1:A:24:ASN:O	1:A:28:GLN:CD	2.63	0.41
1:B:78:THR:CG2	1:B:105:HIS:HD2	2.23	0.41
1:A:75:SER:OG	1:A:105:HIS:CA	2.70	0.41
1:B:75:SER:OG	1:B:77:SER:O	2.34	0.40
1:B:29:MET:HB3	1:B:46:PHE:CE2	2.57	0.40
1:B:24:ASN:C	1:B:28:GLN:OE1	2.64	0.40
1:B:48:HIS:NE2	1:B:82:THR:OG1	2.48	0.40
1:A:91:LYS:O	1:A:91:LYS:HG2	2.10	0.40

All (2) 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:A:77:SER:OG	1:B:68:GLY:O[4_656]	1.82	0.38
1:B:92:TYR:CD2	1:B:92:TYR:CD2[2_657]	2.05	0.15

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	122/124 (98%)	109 (89%)	10 (8%)	3 (2%)	4	7
1	B	122/124 (98%)	110 (90%)	11 (9%)	1 (1%)	16	31
All	All	244/248 (98%)	219 (90%)	21 (9%)	4 (2%)	7	14

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	114	PRO
1	B	114	PRO

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Mol	Chain	Res	Type
1	A	89	SER
1	A	40	CYS

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	109/109 (100%)	70 (64%)	39 (36%)	0	0
1	B	109/109 (100%)	73 (67%)	36 (33%)	0	0
All	All	218/218 (100%)	143 (66%)	75 (34%)	0	0

All (75) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	3	THR
1	A	7	LYS
1	A	10	ARG
1	A	11	GLN
1	A	17	THR
1	A	18	SER
1	A	21	SER
1	A	24	ASN
1	A	28	GLN
1	A	29	MET
1	A	31	LYS
1	A	32	SER
1	A	36	THR
1	A	37	LYS
1	A	39	ARG
1	A	50	SER
1	A	60	GLN
1	A	61	LYS
1	A	63	VAL
1	A	66	LYS
1	A	70	THR

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Mol	Chain	Res	Type
1	A	74	GLN
1	A	77	SER
1	A	78	THR
1	A	80	SER
1	A	81	ILE
1	A	82	THR
1	A	83	ASP
1	A	85	ARG
1	A	87	THR
1	A	89	SER
1	A	91	LYS
1	A	93	PRO
1	A	98	LYS
1	A	104	LYS
1	A	107	ILE
1	A	116	VAL
1	A	118	VAL
1	A	119	HIS
1	B	12	HIS
1	B	13	MET
1	B	15	SER
1	B	17	THR
1	B	18	SER
1	B	22	SER
1	B	25	TYR
1	B	31	LYS
1	B	35	LEU
1	B	37	LYS
1	B	38	ASP
1	B	39	ARG
1	B	44	ASN
1	B	45	THR
1	B	49	GLU
1	B	51	LEU
1	B	60	GLN
1	B	61	LYS
1	B	66	LYS
1	B	70	THR
1	B	77	SER
1	B	80	SER
1	B	81	ILE
1	B	85	ARG

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Mol	Chain	Res	Type
1	B	86	GLU
1	B	89	SER
1	B	91	LYS
1	B	93	PRO
1	B	94	ASN
1	B	103	ASN
1	B	106	ILE
1	B	108	VAL
1	B	111	GLU
1	B	118	VAL
1	B	119	HIS
1	B	124	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (14) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	12	HIS
1	A	28	GLN
1	A	44	ASN
1	A	69	GLN
1	A	71	ASN
1	A	113	ASN
1	A	119	HIS
1	B	11	GLN
1	B	12	HIS
1	B	24	ASN
1	B	27	ASN
1	B	69	GLN
1	B	71	ASN
1	B	113	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 [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

There are no ligands in this entry.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

EDS was not executed - this section is therefore empty.

6.2 Non-standard residues in protein, DNA, RNA chains

EDS was not executed - this section is therefore empty.

6.3 Carbohydrates

EDS was not executed - this section is therefore empty.

6.4 Ligands

EDS was not executed - this section is therefore empty.

6.5 Other polymers

EDS was not executed - this section is therefore empty.