



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 07:12 AM UTC

PDB ID : 1ATT / pdb_00001att
Title : CRYSTAL STRUCTURE OF CLEAVED BOVINE ANTITHROMBIN III AT
3.2 ANGSTROMS RESOLUTION
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Deposited on : 1993-03-29
Resolution : 3.20 Å(reported)

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

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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

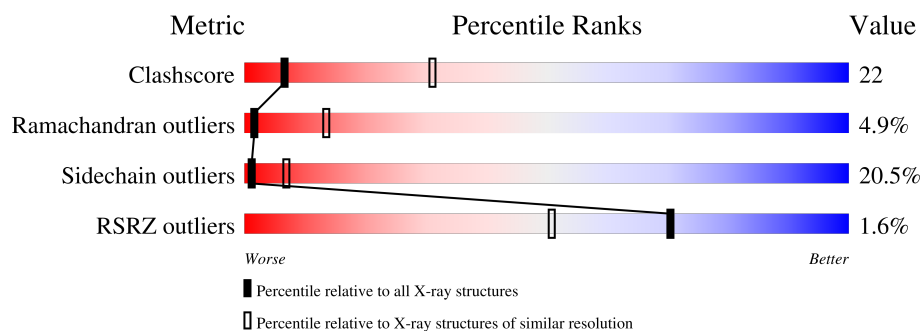
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.20 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
Clashscore	190562	1573 (3.20-3.20)
Ramachandran outliers	187476	1548 (3.20-3.20)
Sidechain outliers	187428	1547 (3.20-3.20)
RSRZ outliers	180081	1466 (3.20-3.20)

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

Mol	Chain	Length	Quality of chain
1	A	429	
1	B	429	

2 Entry composition

There is only 1 type of molecule in this entry. The entry contains 6640 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.

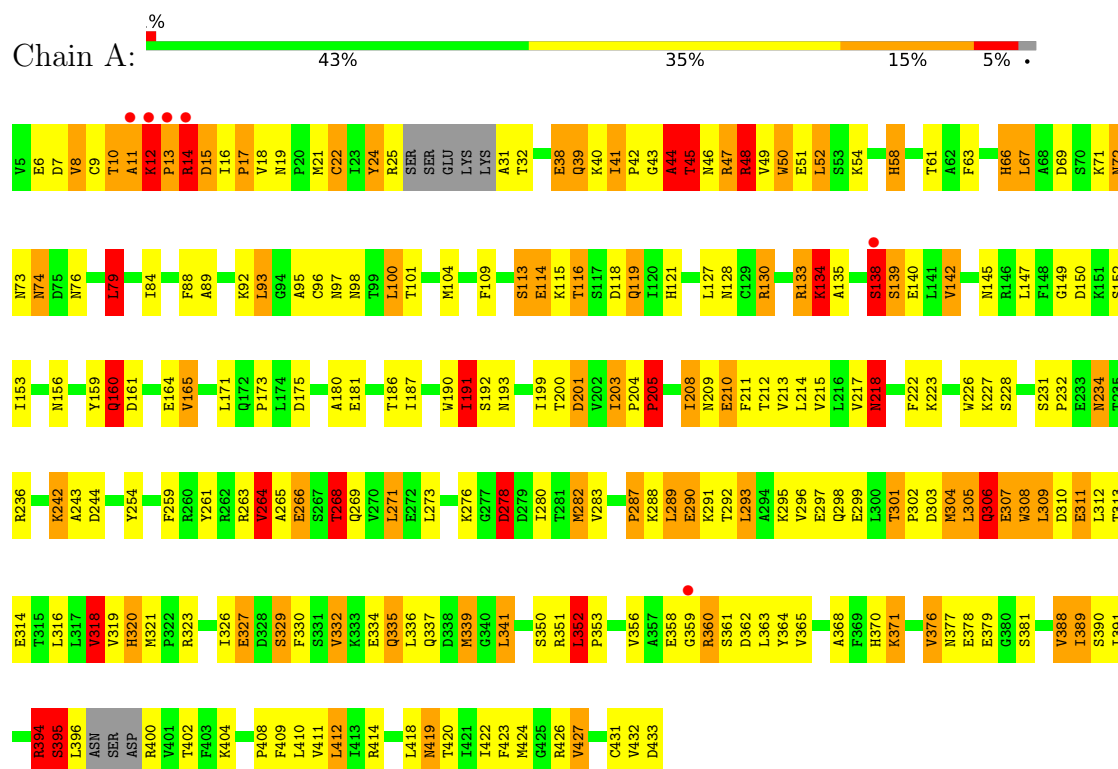
- Molecule 1 is a protein called ANTITHROMBIN III.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	421	Total	C	N	O	S	0	0	1
			3354	2131	568	639	16			
1	B	411	Total	C	N	O	S	0	0	1
			3286	2090	558	623	15			

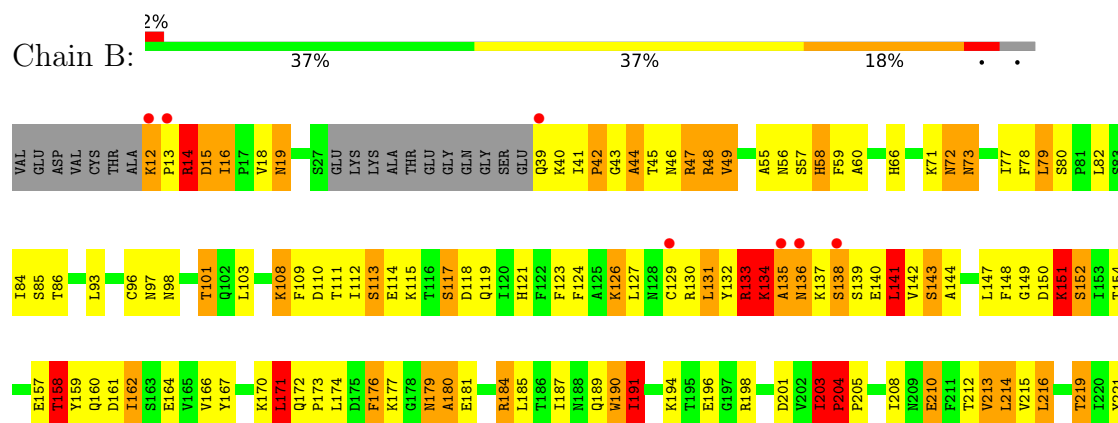
3 Residue-property plots

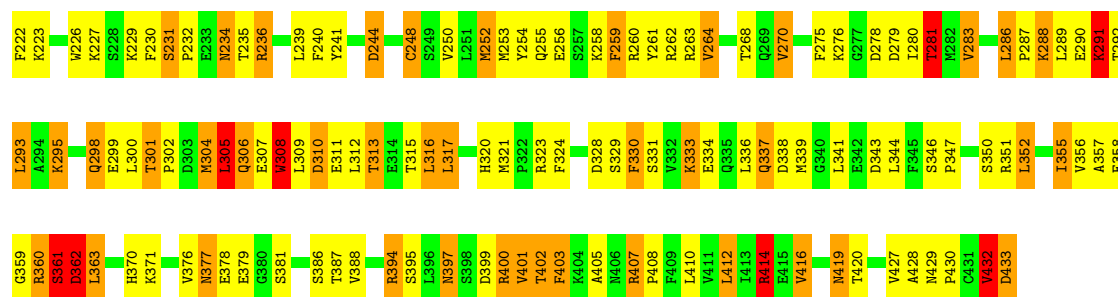
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ($RSRZ > 2$). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

• Molecule 1: ANTITHROMBIN III



• Molecule 1: ANTITHROMBIN III





4 Data and refinement statistics

Property	Value	Source
Space group	P 43 21 2	Depositor
Cell constants a, b, c, α , β , γ	91.30Å 91.30Å 383.10Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	8.00 – 3.20 8.00 – 3.20	Depositor EDS
% Data completeness (in resolution range)	(Not available) (8.00-3.20) 74.1 (8.00-3.20)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	4.51 (at 3.19Å)	Xtriage
Refinement program	X-PLOR	Depositor
R, R_{free}	0.212 , (Not available) 0.214 , (Not available)	Depositor DCC
R_{free} test set	No test flags present.	wwPDB-VP
Wilson B-factor (Å ²)	59.5	Xtriage
Anisotropy	0.305	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.22 , 68.0	EDS
L-test for twinning ²	$\langle L \rangle = 0.47$, $\langle L^2 \rangle = 0.30$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.90	EDS
Total number of atoms	6640	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 2.93% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

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

5 Model quality

5.1 Standard geometry

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	15/3417 (0.4%)	2.07	126/4616 (2.7%)
1	B	1.12	18/3349 (0.5%)	2.09	134/4523 (3.0%)
All	All	1.14	33/6766 (0.5%)	2.08	260/9139 (2.8%)

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
1	B	0	3
All	All	0	4

All (33) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	134	LYS	C-N	10.62	1.46	1.33
1	A	17	PRO	C-N	9.75	1.44	1.33
1	B	203	ILE	CA-CB	8.66	1.65	1.54
1	B	126	LYS	C-N	-8.64	1.22	1.33
1	A	395	SER	C-N	-7.72	1.22	1.33
1	A	223	LYS	C-N	-7.70	1.22	1.33
1	A	204	PRO	CA-CB	-7.58	1.47	1.54
1	A	121	HIS	CD2-NE2	-7.51	1.29	1.37
1	A	66	HIS	CD2-NE2	-7.04	1.30	1.37
1	A	320	HIS	CD2-NE2	-6.92	1.30	1.37
1	B	118	ASP	C-N	-6.87	1.25	1.33
1	B	213	VAL	CA-CB	6.68	1.62	1.54
1	A	14	ARG	N-CA	6.68	1.56	1.46
1	B	305	LEU	C-N	6.61	1.43	1.33
1	A	370	HIS	CD2-NE2	-6.60	1.30	1.37
1	B	395	SER	C-N	-6.60	1.24	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	66	HIS	CD2-NE2	-6.56	1.30	1.37
1	B	58	HIS	CD2-NE2	-6.29	1.30	1.37
1	B	48	ARG	CA-CB	-6.17	1.45	1.54
1	B	370	HIS	CD2-NE2	-5.89	1.31	1.37
1	B	317	LEU	C-N	-5.81	1.25	1.33
1	B	162	ILE	CA-CB	5.71	1.61	1.54
1	B	41	ILE	CA-CB	5.67	1.59	1.53
1	A	45	THR	CA-CB	5.66	1.63	1.53
1	B	370	HIS	CG-ND1	-5.64	1.32	1.38
1	A	226	TRP	NE1-CE2	-5.64	1.31	1.37
1	A	231	SER	CA-CB	-5.61	1.44	1.53
1	A	58	HIS	CD2-NE2	-5.55	1.31	1.37
1	A	389	ILE	CA-CB	5.41	1.61	1.54
1	B	416	VAL	CA-CB	5.37	1.60	1.54
1	B	171	LEU	C-N	-5.17	1.29	1.33
1	A	50	TRP	CG-CD2	-5.13	1.34	1.43
1	B	308	TRP	NE1-CE2	-5.02	1.31	1.37

All (260) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	305	LEU	N-CA-C	-17.05	95.19	114.62
1	B	234	ASN	CA-CB-CG	15.65	128.25	112.60
1	A	38	GLU	N-CA-C	14.11	128.53	110.33
1	B	401	VAL	N-CA-C	12.20	128.00	111.17
1	A	44	ALA	O-C-N	-11.79	110.27	123.48
1	B	56	ASN	CA-CB-CG	11.50	124.10	112.60
1	A	310	ASP	CA-CB-CG	11.05	123.66	112.60
1	A	13	PRO	O-C-N	-10.49	110.22	122.91
1	B	304	MET	CA-C-O	10.06	132.85	121.58
1	B	278	ASP	N-CA-C	10.03	125.14	111.90
1	A	304	MET	N-CA-C	-9.84	98.92	112.30
1	B	140	GLU	CA-C-O	-9.79	108.71	119.97
1	B	397	ASN	OD1-CG-ND2	-9.76	112.84	122.60
1	A	48	ARG	N-CA-C	-9.48	100.07	112.68
1	A	145	ASN	OD1-CG-ND2	-9.22	113.38	122.60
1	A	200	THR	CA-CB-OG1	-9.21	95.78	109.60
1	A	278	ASP	N-CA-C	8.65	129.23	110.80
1	B	126	LYS	CA-C-N	8.57	132.46	120.29
1	B	126	LYS	C-N-CA	8.57	132.46	120.29
1	A	218	ASN	OD1-CG-ND2	-8.44	114.16	122.60
1	A	14	ARG	N-CA-C	8.28	118.89	108.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	12	LYS	O-C-N	-8.10	112.00	121.32
1	B	359	GLY	O-C-N	8.01	129.23	123.14
1	B	362	ASP	CA-CB-CG	8.00	120.60	112.60
1	A	389	ILE	CB-CA-C	7.95	122.39	110.63
1	B	403	PHE	CA-CB-CG	-7.91	105.89	113.80
1	A	121	HIS	CB-CG-CD2	-7.81	121.05	131.20
1	B	201	ASP	CA-CB-CG	7.79	120.39	112.60
1	A	389	ILE	N-CA-C	-7.76	97.25	108.11
1	B	58	HIS	CB-CG-CD2	-7.75	121.13	131.20
1	B	78	PHE	CA-CB-CG	-7.66	106.14	113.80
1	B	72	ASN	CA-CB-CG	7.66	120.26	112.60
1	A	13	PRO	N-CA-C	-7.66	99.47	111.34
1	A	211	PHE	CA-CB-CG	7.61	121.41	113.80
1	B	164	GLU	N-CA-C	7.53	119.12	111.07
1	B	234	ASN	OD1-CG-ND2	-7.39	115.21	122.60
1	B	161	ASP	CA-CB-CG	7.35	119.95	112.60
1	B	402	THR	N-CA-C	7.34	126.43	110.80
1	A	74	ASN	OD1-CG-ND2	-7.29	115.31	122.60
1	B	343	ASP	N-CA-C	7.28	118.90	110.97
1	A	388	VAL	N-CA-C	-7.22	97.62	108.17
1	A	209	ASN	OD1-CG-ND2	-7.21	115.39	122.60
1	B	47	ARG	CB-CG-CD	7.12	127.68	111.30
1	A	47	ARG	O-C-N	7.11	132.15	122.83
1	B	316	LEU	N-CA-C	-7.11	98.46	109.76
1	A	390	SER	O-C-N	-7.05	115.31	123.27
1	B	71	LYS	N-CA-C	-7.04	97.92	109.40
1	B	59	PHE	N-CA-C	-7.04	103.03	111.69
1	A	352	LEU	O-C-N	-7.01	115.55	121.23
1	A	210	GLU	CA-CB-CG	6.99	128.07	114.10
1	B	361	SER	N-CA-C	6.98	120.14	108.20
1	A	320	HIS	CB-CG-CD2	-6.96	122.15	131.20
1	B	317	LEU	CA-C-N	6.94	131.79	122.90
1	B	317	LEU	C-N-CA	6.94	131.79	122.90
1	B	429	ASN	CB-CG-ND2	6.94	126.81	116.40
1	B	138	SER	N-CA-C	6.94	120.19	111.24
1	A	128	ASN	CA-CB-CG	6.88	119.48	112.60
1	A	204	PRO	CA-C-N	6.88	128.44	119.84
1	A	204	PRO	C-N-CA	6.88	128.44	119.84
1	A	323	ARG	CB-CG-CD	-6.84	95.57	111.30
1	A	134	LYS	CG-CD-CE	6.81	126.96	111.30
1	B	136	ASN	O-C-N	6.79	131.26	122.43
1	A	46	ASN	CB-CG-ND2	6.79	126.58	116.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	126	LYS	O-C-N	-6.77	115.10	122.07
1	B	231	SER	CA-C-N	6.77	126.01	118.97
1	B	231	SER	C-N-CA	6.77	126.01	118.97
1	A	263	ARG	N-CA-C	-6.73	97.54	108.52
1	A	269	GLN	OE1-CD-NE2	-6.73	115.87	122.60
1	A	156	ASN	OD1-CG-ND2	-6.72	115.88	122.60
1	A	52	LEU	N-CA-C	-6.71	103.58	111.03
1	B	179	ASN	CA-C-O	6.71	130.10	120.51
1	B	79	LEU	O-C-N	-6.69	115.99	123.48
1	A	47	ARG	CA-C-O	6.64	131.40	122.51
1	A	13	PRO	CB-CA-C	6.56	119.58	111.12
1	B	234	ASN	CB-CG-ND2	6.54	126.22	116.40
1	A	192	SER	CA-CB-OG	6.54	124.18	111.10
1	A	114	GLU	N-CA-C	-6.54	99.37	109.24
1	B	46	ASN	O-C-N	-6.53	113.91	122.59
1	A	218	ASN	CB-CG-ND2	6.51	126.17	116.40
1	A	259	PHE	CA-CB-CG	6.51	120.31	113.80
1	A	330	PHE	CA-CB-CG	6.51	120.31	113.80
1	A	433	ASP	CA-CB-CG	6.50	119.10	112.60
1	B	136	ASN	CA-CB-CG	6.49	119.09	112.60
1	A	205	PRO	N-CA-C	6.47	125.79	112.47
1	B	377	ASN	N-CA-CB	-6.47	101.50	111.46
1	B	268	THR	N-CA-CB	-6.46	100.86	110.17
1	A	8	VAL	O-C-N	6.46	128.48	121.83
1	B	399	ASP	N-CA-C	-6.36	104.39	111.71
1	B	416	VAL	CB-CA-C	-6.33	103.90	111.81
1	B	118	ASP	CA-C-N	6.33	128.76	120.28
1	B	118	ASP	C-N-CA	6.33	128.76	120.28
1	A	244	ASP	CA-CB-CG	6.30	118.91	112.60
1	B	86	THR	N-CA-C	6.29	117.80	111.07
1	A	201	ASP	CA-CB-CG	6.25	118.86	112.60
1	B	399	ASP	CA-CB-CG	6.25	118.85	112.60
1	A	306	GLN	N-CA-C	-6.23	104.18	110.97
1	B	227	LYS	N-CA-C	-6.22	104.13	111.03
1	A	426	ARG	N-CA-C	-6.21	97.05	107.80
1	A	46	ASN	CA-C-N	-6.20	113.44	122.06
1	A	46	ASN	C-N-CA	-6.20	113.44	122.06
1	A	142	VAL	O-C-N	-6.19	116.37	123.00
1	A	327	GLU	CA-C-O	-6.19	113.55	120.66
1	B	135	ALA	N-CA-C	6.17	118.84	107.73
1	A	134	LYS	N-CA-C	6.16	123.92	110.80
1	B	191	ILE	CA-CB-CG2	-6.14	100.06	110.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	175	ASP	CA-CB-CG	6.13	118.73	112.60
1	A	361	SER	CA-CB-OG	6.13	123.37	111.10
1	A	156	ASN	CB-CG-ND2	6.11	125.57	116.40
1	A	308	TRP	CG-CD2-CE3	6.11	140.01	133.90
1	A	318	VAL	N-CA-C	-6.11	97.00	106.72
1	A	17	PRO	CA-C-N	-6.11	114.73	122.43
1	A	17	PRO	C-N-CA	-6.11	114.73	122.43
1	B	86	THR	CA-CB-OG1	-6.10	100.45	109.60
1	B	133	ARG	CD-NE-CZ	6.10	132.94	124.40
1	A	335	GLN	OE1-CD-NE2	-6.10	116.50	122.60
1	A	50	TRP	CE2-CD2-CE3	6.09	124.89	118.80
1	A	180	ALA	N-CA-C	6.06	118.67	111.33
1	A	203	ILE	CA-C-N	6.00	123.98	119.66
1	A	203	ILE	C-N-CA	6.00	123.98	119.66
1	B	191	ILE	N-CA-C	-6.00	104.66	110.42
1	B	414	ARG	N-CA-C	5.98	117.33	108.60
1	A	190	TRP	CG-CD2-CE3	5.98	139.88	133.90
1	B	235	THR	N-CA-C	-5.97	99.45	109.07
1	B	216	LEU	O-C-N	-5.94	116.56	123.27
1	A	327	GLU	O-C-N	-5.93	116.03	123.27
1	A	186	THR	CA-CB-OG1	-5.92	100.72	109.60
1	A	268	THR	N-CA-CB	-5.92	100.65	110.47
1	A	390	SER	CA-C-O	-5.90	114.00	120.43
1	A	376	VAL	N-CA-C	-5.89	99.98	108.53
1	A	93	LEU	N-CA-C	-5.89	104.94	111.36
1	A	427	VAL	N-CA-C	-5.88	98.55	107.73
1	A	121	HIS	CA-CB-CG	-5.87	107.93	113.80
1	A	24	TYR	N-CA-C	-5.85	100.75	110.17
1	B	159	TYR	N-CA-C	-5.85	104.98	111.36
1	B	387	THR	N-CA-C	-5.85	100.26	109.50
1	B	263	ARG	N-CA-C	-5.84	99.21	108.73
1	B	338	ASP	CA-CB-CG	5.83	118.44	112.60
1	A	409	PHE	CA-CB-CG	5.83	119.63	113.80
1	B	240	PHE	N-CA-C	5.82	117.50	111.03
1	A	79	LEU	CD1-CG-CD2	-5.82	98.01	110.80
1	A	142	VAL	N-CA-CB	-5.81	101.19	111.93
1	B	361	SER	O-C-N	-5.81	116.14	123.05
1	B	170	LYS	O-C-N	-5.79	116.73	123.27
1	A	190	TRP	N-CA-C	-5.78	104.88	111.07
1	B	328	ASP	CA-CB-CG	5.78	118.38	112.60
1	A	119	GLN	N-CA-C	5.76	117.56	111.28
1	B	283	VAL	CA-CB-CG2	-5.76	100.61	110.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	77	ILE	CB-CA-C	-5.75	103.52	110.99
1	B	379	GLU	CB-CG-CD	5.74	122.36	112.60
1	B	363	LEU	N-CA-C	5.72	118.63	110.10
1	A	377	ASN	OD1-CG-ND2	-5.72	116.88	122.60
1	B	293	LEU	N-CA-C	-5.70	105.14	111.36
1	B	244	ASP	CA-CB-CG	5.70	118.30	112.60
1	A	46	ASN	OD1-CG-ND2	-5.68	116.92	122.60
1	B	151	LYS	N-CA-C	5.67	122.88	110.80
1	A	69	ASP	N-CA-C	-5.66	105.03	111.14
1	B	141	LEU	N-CA-C	5.65	122.83	110.80
1	A	282	MET	N-CA-C	-5.64	99.70	108.90
1	B	432	VAL	N-CA-CB	-5.64	101.93	111.23
1	B	181	GLU	CB-CG-CD	5.63	122.17	112.60
1	B	110	ASP	CA-CB-CG	5.62	118.22	112.60
1	B	117	SER	N-CA-C	5.62	119.65	112.34
1	A	370	HIS	CB-CG-CD2	-5.62	123.90	131.20
1	B	360	ARG	CB-CG-CD	5.60	124.18	111.30
1	B	429	ASN	OD1-CG-ND2	-5.59	117.01	122.60
1	A	191	ILE	CB-CA-C	-5.58	104.60	112.14
1	A	319	VAL	N-CA-C	5.58	116.62	108.58
1	A	76	ASN	CA-CB-CG	5.57	118.17	112.60
1	B	189	GLN	OE1-CD-NE2	-5.57	117.03	122.60
1	B	180	ALA	N-CA-C	5.57	118.19	111.40
1	A	121	HIS	CB-CG-ND1	5.56	131.03	122.70
1	B	142	VAL	N-CA-CB	-5.56	102.06	111.23
1	A	145	ASN	CB-CG-ND2	5.55	124.73	116.40
1	B	109	PHE	CA-CB-CG	5.55	119.35	113.80
1	B	268	THR	CB-CA-C	5.55	119.75	109.54
1	A	234	ASN	N-CA-C	-5.55	101.89	109.71
1	A	138	SER	N-CA-C	5.54	122.61	110.80
1	B	259	PHE	CB-CA-C	-5.54	100.31	110.62
1	A	308	TRP	CB-CG-CD1	-5.53	118.60	126.90
1	A	358	GLU	N-CA-C	5.53	119.64	113.01
1	B	47	ARG	O-C-N	5.52	129.50	122.65
1	B	324	PHE	N-CA-C	5.52	118.26	110.14
1	B	158	THR	CA-CB-OG1	-5.51	101.34	109.60
1	A	46	ASN	CA-C-O	-5.50	115.77	122.64
1	B	43	GLY	N-CA-C	-5.50	100.16	113.18
1	B	240	PHE	CA-C-O	-5.49	115.25	120.90
1	B	346	SER	CA-C-N	5.47	125.30	119.28
1	B	346	SER	C-N-CA	5.47	125.30	119.28
1	A	84	ILE	CA-C-O	-5.47	115.37	121.17

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	113	SER	CA-C-O	5.47	127.70	121.58
1	B	48	ARG	N-CA-C	-5.46	106.99	113.97
1	B	400	ARG	N-CA-C	-5.45	102.42	110.48
1	A	268	THR	CB-CA-C	5.43	119.65	110.79
1	B	140	GLU	N-CA-C	5.43	118.12	111.82
1	A	161	ASP	CA-C-O	-5.42	114.75	120.55
1	A	362	ASP	CA-CB-CG	5.41	118.01	112.60
1	A	160	GLN	OE1-CD-NE2	-5.40	117.20	122.60
1	A	303	ASP	N-CA-C	-5.40	103.84	110.65
1	A	72	ASN	OD1-CG-ND2	-5.40	117.20	122.60
1	A	199	ILE	N-CA-C	-5.40	98.72	106.55
1	B	357	ALA	N-CA-C	-5.40	96.42	107.70
1	B	298	GLN	CA-CB-CG	5.39	124.88	114.10
1	A	200	THR	CA-CB-CG2	5.38	119.64	110.50
1	B	361	SER	N-CA-CB	-5.38	101.50	110.37
1	B	355	ILE	N-CA-C	-5.36	105.17	113.16
1	B	298	GLN	OE1-CD-NE2	-5.36	117.24	122.60
1	A	411	VAL	CA-C-O	-5.36	114.76	120.39
1	B	290	GLU	N-CA-C	-5.36	103.24	110.68
1	B	143	SER	CA-CB-OG	5.35	121.81	111.10
1	B	407	ARG	CA-C-N	5.35	125.65	119.93
1	B	407	ARG	C-N-CA	5.35	125.65	119.93
1	A	223	LYS	N-CA-C	-5.35	99.73	108.76
1	B	360	ARG	CA-CB-CG	5.34	124.79	114.10
1	A	289	LEU	N-CA-CB	-5.34	101.46	110.49
1	B	310	ASP	O-C-N	5.33	129.15	122.22
1	B	46	ASN	OD1-CG-ND2	-5.32	117.28	122.60
1	B	80	SER	CA-C-N	5.31	124.82	119.19
1	B	80	SER	C-N-CA	5.31	124.82	119.19
1	B	261	TYR	O-C-N	-5.30	117.43	123.48
1	B	19	ASN	OD1-CG-ND2	-5.29	117.31	122.60
1	B	176	PHE	CA-CB-CG	5.27	119.07	113.80
1	B	14	ARG	NE-CZ-NH2	5.27	123.94	119.20
1	A	371	LYS	N-CA-C	-5.26	101.36	109.52
1	B	394	ARG	O-C-N	5.26	128.74	122.27
1	B	419	ASN	CA-CB-CG	-5.26	107.34	112.60
1	B	158	THR	CA-CB-CG2	5.25	119.43	110.50
1	A	341	LEU	N-CA-C	-5.25	99.20	108.23
1	A	47	ARG	CB-CG-CD	5.23	123.32	111.30
1	A	88	PHE	CA-C-O	-5.22	114.44	120.24
1	A	227	LYS	N-CA-C	-5.22	105.23	111.03
1	B	291	LYS	CA-CB-CG	5.22	124.54	114.10

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	39	GLN	CA-C-N	5.21	131.49	121.54
1	B	39	GLN	C-N-CA	5.21	131.49	121.54
1	B	204	PRO	CA-C-N	5.21	125.15	119.78
1	B	204	PRO	C-N-CA	5.21	125.15	119.78
1	B	416	VAL	N-CA-CB	5.21	116.30	110.62
1	B	283	VAL	CA-CB-CG1	5.21	119.25	110.40
1	A	13	PRO	CA-N-CD	5.20	119.27	112.00
1	B	136	ASN	CA-C-O	5.18	127.39	121.58
1	A	201	ASP	N-CA-C	5.18	121.83	110.80
1	A	320	HIS	CB-CG-ND1	5.18	130.47	122.70
1	A	323	ARG	N-CA-C	-5.16	100.83	109.24
1	B	281	THR	N-CA-CB	-5.14	102.88	111.20
1	A	66	HIS	CB-CG-CD2	-5.13	124.53	131.20
1	A	377	ASN	CB-CG-ND2	5.12	124.09	116.40
1	A	47	ARG	CA-CB-CG	-5.10	103.90	114.10
1	A	306	GLN	OE1-CD-NE2	-5.08	117.52	122.60
1	B	412	LEU	CA-C-O	-5.08	113.25	120.51
1	A	66	HIS	CA-C-O	-5.08	115.67	121.00
1	B	191	ILE	CA-CB-CG1	5.07	119.02	110.40
1	B	190	TRP	CE2-CD2-CG	-5.06	101.13	107.20
1	B	352	LEU	O-C-N	-5.06	115.50	121.32
1	A	88	PHE	CA-CB-CG	-5.06	108.74	113.80
1	B	226	TRP	CB-CG-CD1	-5.05	119.32	126.90
1	B	305	LEU	O-C-N	-5.05	115.10	121.67
1	B	330	PHE	CA-CB-CG	5.05	118.86	113.80
1	A	133	ARG	NE-CZ-NH1	5.04	126.55	121.50
1	B	313	THR	N-CA-C	-5.04	99.08	107.80
1	A	424	MET	O-C-N	-5.01	117.77	123.48
1	B	48	ARG	CG-CD-NE	-5.01	100.99	112.00

There are no chirality outliers.

All (4) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	44	ALA	Mainchain
1	B	134	LYS	Mainchain
1	B	167	TYR	Sidechain
1	B	18	VAL	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	3354	0	3345	149	0
1	B	3286	0	3282	137	0
All	All	6640	0	6627	286	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 22.

All (286) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:41:ILE:N	1:A:42:PRO:HD3	1.53	1.16
1:A:11:ALA:HB1	1:A:12:LYS:HE2	1.37	1.05
1:A:41:ILE:N	1:A:42:PRO:CD	2.28	0.97
1:A:153:ILE:HD13	1:A:213:VAL:HG13	1.51	0.93
1:B:317:LEU:HD13	1:B:401:VAL:HG23	1.50	0.91
1:A:63:PHE:HD1	1:A:339:MET:HE1	1.42	0.84
1:A:10:THR:HA	1:A:14:ARG:NH1	1.92	0.84
1:A:305:LEU:HA	1:A:308:TRP:CE3	2.14	0.82
1:A:40:LYS:C	1:A:42:PRO:HD3	2.04	0.82
1:A:305:LEU:HA	1:A:308:TRP:HE3	1.46	0.81
1:B:12:LYS:HG2	1:B:12:LYS:O	1.82	0.80
1:A:41:ILE:H	1:A:42:PRO:HD3	1.51	0.76
1:A:11:ALA:HB1	1:A:12:LYS:CE	2.16	0.74
1:A:21:MET:SD	1:A:353:PRO:HB2	2.28	0.74
1:B:236:ARG:HH21	1:B:254:TYR:HD1	1.36	0.73
1:A:134:LYS:NZ	1:A:134:LYS:HA	2.05	0.72
1:B:236:ARG:NH1	1:B:252:MET:HB3	2.03	0.72
1:B:236:ARG:HH11	1:B:252:MET:HB3	1.56	0.71
1:A:271:LEU:HD22	1:A:273:LEU:HG	1.72	0.71
1:B:49:VAL:HG23	1:B:127:LEU:HB2	1.71	0.71
1:B:184:ARG:HE	1:B:205:PRO:HA	1.56	0.70
1:A:97:ASN:OD1	1:A:351:ARG:NH1	2.25	0.70
1:A:10:THR:HA	1:A:14:ARG:HH11	1.55	0.69
1:B:283:VAL:HG21	1:B:308:TRP:NE1	2.08	0.69
1:B:203:ILE:HD11	1:B:208:ILE:HG12	1.75	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:191:ILE:HD12	1:A:217:VAL:HG11	1.75	0.68
1:B:13:PRO:HD2	1:B:126:LYS:HE3	1.76	0.67
1:A:41:ILE:HG23	1:A:41:ILE:O	1.95	0.67
1:A:264:VAL:HG11	1:A:307:GLU:HG3	1.76	0.67
1:A:16:ILE:HG23	1:A:17:PRO:HD2	1.77	0.67
1:A:63:PHE:CD1	1:A:339:MET:HE1	2.29	0.67
1:A:287:PRO:HG3	1:A:293:LEU:HD23	1.77	0.67
1:A:95:ALA:HA	1:A:352:LEU:HD12	1.77	0.66
1:A:8:VAL:HG21	1:A:16:ILE:HG13	1.76	0.66
1:B:291:LYS:HZ2	1:B:292:THR:H	1.42	0.66
1:B:160:GLN:HE22	1:B:171:LEU:HB2	1.59	0.66
1:B:252:MET:SD	1:B:320:HIS:HB3	2.35	0.66
1:A:40:LYS:N	1:A:42:PRO:HD3	2.11	0.65
1:A:288:LYS:HB3	1:A:291:LYS:HD2	1.77	0.65
1:B:408:PRO:HB3	1:B:428:ALA:HA	1.78	0.64
1:B:264:VAL:HG11	1:B:307:GLU:HG2	1.78	0.64
1:A:74:ASN:OD1	1:A:243:ALA:HB3	1.97	0.64
1:A:48:ARG:NH2	1:A:113:SER:HB2	2.13	0.64
1:B:134:LYS:N	1:B:134:LYS:HD3	2.13	0.63
1:A:254:TYR:HE1	1:A:318:VAL:HG23	1.63	0.63
1:A:288:LYS:HD3	1:A:291:LYS:NZ	2.14	0.62
1:A:222:PHE:CE2	1:A:280:ILE:HG21	2.33	0.62
1:B:158:THR:O	1:B:162:ILE:HG22	2.00	0.62
1:A:134:LYS:HA	1:A:134:LYS:HZ2	1.64	0.62
1:A:39:GLN:HA	1:A:50:TRP:CD1	2.35	0.61
1:B:321:MET:HE1	1:B:376:VAL:HG11	1.82	0.61
1:A:58:HIS:HA	1:A:302:PRO:HG3	1.82	0.61
1:A:337:GLN:HA	1:A:341:LEU:O	2.01	0.60
1:A:133:ARG:HD2	1:A:134:LYS:N	2.16	0.60
1:B:351:ARG:HE	1:B:361:SER:HB3	1.67	0.60
1:B:48:ARG:HH12	1:B:113:SER:HB2	1.67	0.59
1:A:22:CYS:CB	1:A:96:CYS:SG	2.90	0.59
1:B:97:ASN:ND2	1:B:351:ARG:HH11	2.00	0.59
1:B:47:ARG:HH12	1:B:130:ARG:NH2	2.00	0.59
1:B:329:SER:HB3	1:B:371:LYS:HG3	1.84	0.59
1:B:187:ILE:HD13	1:B:215:VAL:HG11	1.85	0.59
1:A:96:CYS:SG	1:A:97:ASN:N	2.75	0.59
1:A:187:ILE:HD13	1:A:215:VAL:HG11	1.84	0.59
1:B:236:ARG:H	1:B:236:ARG:HD2	1.68	0.58
1:B:214:LEU:HD12	1:B:355:ILE:HD12	1.86	0.58
1:A:264:VAL:HG12	1:A:265:ALA:H	1.69	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:236:ARG:NH2	1:B:254:TYR:HD1	2.02	0.58
1:A:394:ARG:HH21	1:A:395:SER:HA	1.70	0.57
1:A:16:ILE:CG2	1:A:18:VAL:HG23	2.33	0.57
1:B:147:LEU:HD22	1:B:216:LEU:HG	1.86	0.57
1:A:138:SER:HA	1:A:276:LYS:O	2.05	0.57
1:A:326:ILE:HG21	1:A:427:VAL:HG23	1.85	0.57
1:A:25:ARG:HB2	1:A:115:LYS:O	2.05	0.56
1:A:66:HIS:CD2	1:A:339:MET:SD	2.99	0.56
1:A:21:MET:HB3	1:A:22:CYS:SG	2.46	0.56
1:B:47:ARG:HH12	1:B:130:ARG:CZ	2.19	0.56
1:A:336:LEU:HD23	1:A:339:MET:HE2	1.88	0.56
1:B:260:ARG:HA	1:B:313:THR:O	2.06	0.56
1:B:270:VAL:HG21	1:B:307:GLU:HB3	1.87	0.56
1:B:230:PHE:HD2	1:B:253:MET:SD	2.29	0.55
1:B:236:ARG:HH22	1:B:320:HIS:CG	2.24	0.55
1:B:281:THR:HG21	1:B:308:TRP:CZ2	2.41	0.55
1:B:150:ASP:HA	1:B:174:LEU:O	2.05	0.55
1:A:67:LEU:HD12	1:A:79:LEU:HD23	1.88	0.55
1:A:8:VAL:CG2	1:A:16:ILE:HG13	2.35	0.55
1:A:16:ILE:HG23	1:A:165:VAL:HG11	1.89	0.55
1:A:16:ILE:HG22	1:A:18:VAL:HG23	1.87	0.55
1:A:16:ILE:HD12	1:A:16:ILE:N	2.22	0.55
1:B:308:TRP:CZ2	1:B:414:ARG:HD2	2.42	0.54
1:A:130:ARG:HB3	1:A:418:LEU:HD21	1.88	0.54
1:B:362:ASP:HA	1:B:394:ARG:HE	1.72	0.54
1:B:255:GLN:HE21	1:B:259:PHE:HZ	1.54	0.54
1:B:15:ASP:O	1:B:16:ILE:C	2.49	0.54
1:A:22:CYS:HG	1:A:96:CYS:HG	0.62	0.54
1:A:48:ARG:HD2	1:A:48:ARG:N	2.21	0.54
1:A:39:GLN:HA	1:A:50:TRP:HD1	1.71	0.54
1:B:180:ALA:HB1	1:B:208:ILE:HG22	1.91	0.53
1:B:121:HIS:HB3	1:B:166:VAL:HG11	1.90	0.53
1:A:150:ASP:HB3	1:A:153:ILE:HD12	1.89	0.53
1:B:230:PHE:CD2	1:B:253:MET:SD	3.02	0.53
1:A:12:LYS:O	1:A:14:ARG:NH2	2.41	0.53
1:A:203:ILE:HG21	1:A:208:ILE:HD12	1.91	0.53
1:A:334:GLU:HB2	1:A:335:GLN:OE1	2.09	0.53
1:A:306:GLN:HA	1:A:309:LEU:HD22	1.89	0.53
1:A:288:LYS:HD3	1:A:291:LYS:HZ1	1.74	0.52
1:B:114:GLU:HG3	1:B:123:PHE:HZ	1.74	0.52
1:A:10:THR:HG22	1:A:14:ARG:HH12	1.75	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:282:MET:HE1	1:A:376:VAL:CG2	2.40	0.52
1:B:288:LYS:HD3	1:B:289:LEU:H	1.74	0.52
1:A:271:LEU:CD2	1:A:273:LEU:HG	2.37	0.52
1:A:191:ILE:CD1	1:A:217:VAL:HG11	2.39	0.52
1:B:203:ILE:HD12	1:B:204:PRO:HD2	1.91	0.52
1:A:93:LEU:HB3	1:A:159:TYR:HE1	1.76	0.51
1:B:331:SER:OG	1:B:333:LYS:HB2	2.10	0.51
1:B:48:ARG:NH1	1:B:113:SER:HB2	2.25	0.51
1:B:133:ARG:HG2	1:B:133:ARG:HH11	1.76	0.51
1:A:208:ILE:HD11	1:A:215:VAL:HG21	1.93	0.51
1:B:141:LEU:HD12	1:B:222:PHE:HB2	1.92	0.51
1:B:279:ASP:O	1:B:416:VAL:HG23	2.11	0.51
1:A:213:VAL:HG21	1:A:363:LEU:HD12	1.92	0.51
1:B:97:ASN:ND2	1:B:351:ARG:HD3	2.26	0.51
1:B:397:ASN:O	1:B:400:ARG:HG2	2.10	0.51
1:A:10:THR:O	1:A:11:ALA:C	2.54	0.50
1:A:11:ALA:C	1:A:12:LYS:HG3	2.36	0.50
1:A:283:VAL:HB	1:A:412:LEU:HB2	1.92	0.50
1:B:98:ASN:HA	1:B:101:THR:OG1	2.11	0.50
1:B:288:LYS:HD3	1:B:289:LEU:N	2.26	0.50
1:A:16:ILE:CG2	1:A:17:PRO:HD2	2.42	0.50
1:A:268:THR:HA	1:A:287:PRO:HA	1.92	0.50
1:B:40:LYS:O	1:B:42:PRO:HD3	2.12	0.50
1:A:363:LEU:HD22	1:A:363:LEU:H	1.76	0.50
1:B:184:ARG:HH11	1:B:184:ARG:HG2	1.76	0.50
1:B:262:ARG:CZ	1:B:310:ASP:HB2	2.42	0.50
1:B:347:PRO:HB2	1:B:394:ARG:HD3	1.94	0.50
1:A:25:ARG:NH2	1:A:31:ALA:HB3	2.26	0.50
1:B:134:LYS:N	1:B:134:LYS:CD	2.75	0.50
1:B:321:MET:CE	1:B:376:VAL:HG11	2.41	0.50
1:B:286:LEU:HD13	1:B:405:ALA:HA	1.94	0.49
1:B:347:PRO:HB2	1:B:394:ARG:HB3	1.93	0.49
1:B:148:PHE:CE2	1:B:187:ILE:HG23	2.47	0.49
1:B:44:ALA:HB3	1:B:47:ARG:CG	2.43	0.49
1:A:293:LEU:HD13	1:A:297:GLU:HG3	1.94	0.49
1:B:253:MET:HE2	1:B:323:ARG:HA	1.95	0.49
1:A:12:LYS:O	1:A:13:PRO:C	2.51	0.49
1:A:135:ALA:HB1	1:A:138:SER:OG	2.13	0.49
1:B:262:ARG:HB2	1:B:270:VAL:HG23	1.95	0.49
1:A:293:LEU:HD22	1:A:296:VAL:CG1	2.43	0.49
1:B:160:GLN:NE2	1:B:171:LEU:HB2	2.28	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:254:TYR:CE1	1:A:318:VAL:HG23	2.45	0.48
1:A:22:CYS:CB	1:A:96:CYS:HG	2.18	0.48
1:B:337:GLN:HA	1:B:341:LEU:O	2.12	0.48
1:A:49:VAL:HG13	1:A:127:LEU:HB2	1.95	0.48
1:B:184:ARG:NE	1:B:205:PRO:HA	2.27	0.48
1:B:121:HIS:H	1:B:121:HIS:CD2	2.32	0.48
1:B:253:MET:O	1:B:320:HIS:HA	2.14	0.47
1:A:208:ILE:HG12	1:A:212:THR:HG21	1.95	0.47
1:A:365:VAL:HG22	1:A:391:ILE:HG22	1.95	0.47
1:B:256:GLU:HA	1:B:317:LEU:O	2.13	0.47
1:A:116:THR:HB	1:A:118:ASP:OD1	2.15	0.47
1:A:41:ILE:O	1:A:41:ILE:CG2	2.61	0.47
1:A:360:ARG:N	1:A:396:LEU:N	2.61	0.47
1:B:301:THR:H	1:B:304:MET:HE2	1.78	0.47
1:A:12:LYS:CB	1:A:13:PRO:HD2	2.44	0.47
1:B:138:SER:C	1:B:276:LYS:HE2	2.39	0.47
1:A:89:ALA:HB2	1:A:109:PHE:CZ	2.50	0.47
1:A:353:PRO:HB3	1:A:360:ARG:CZ	2.44	0.47
1:B:230:PHE:HB2	1:B:378:GLU:HA	1.95	0.47
1:A:422:ILE:HG22	1:A:423:PHE:CD1	2.50	0.46
1:B:58:HIS:CE1	1:B:108:LYS:HE2	2.50	0.46
1:A:114:GLU:CD	1:A:119:GLN:HG3	2.40	0.46
1:A:187:ILE:HG22	1:A:191:ILE:HD11	1.96	0.46
1:A:261:TYR:C	1:A:311:GLU:HB2	2.41	0.46
1:B:138:SER:O	1:B:276:LYS:HE2	2.14	0.46
1:A:320:HIS:HB2	1:A:404:LYS:HA	1.98	0.46
1:A:15:ASP:C	1:A:16:ILE:HD12	2.40	0.46
1:B:57:SER:O	1:B:60:ALA:HB3	2.15	0.46
1:B:305:LEU:O	1:B:308:TRP:N	2.49	0.46
1:A:293:LEU:HD21	1:A:410:LEU:HD23	1.96	0.46
1:B:108:LYS:O	1:B:111:THR:HG23	2.15	0.46
1:B:132:TYR:CE2	1:B:143:SER:HB2	2.50	0.46
1:B:135:ALA:HB1	1:B:138:SER:OG	2.15	0.46
1:B:250:VAL:HG21	1:B:430:PRO:HB2	1.98	0.46
1:A:293:LEU:HA	1:A:296:VAL:HG12	1.98	0.45
1:B:97:ASN:HD21	1:B:351:ARG:HH11	1.62	0.45
1:A:318:VAL:HG13	1:A:402:THR:HA	1.98	0.45
1:B:121:HIS:CD2	1:B:121:HIS:N	2.84	0.45
1:B:239:LEU:HA	1:B:248:CYS:O	2.17	0.45
1:A:21:MET:C	1:A:22:CYS:SG	2.97	0.45
1:A:394:ARG:O	1:A:395:SER:HB2	2.16	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:96:CYS:SG	1:B:97:ASN:N	2.89	0.45
1:B:194:LYS:HB3	1:B:219:THR:HG21	1.98	0.45
1:B:275:PHE:HE2	1:B:381:SER:H	1.65	0.45
1:B:305:LEU:O	1:B:306:GLN:C	2.60	0.45
1:A:22:CYS:SG	1:A:96:CYS:CB	3.05	0.45
1:A:24:TYR:CD2	1:A:104:MET:HG3	2.52	0.45
1:B:432:VAL:HG22	1:B:433:ASP:H	1.81	0.44
1:A:11:ALA:CB	1:A:12:LYS:HE2	2.26	0.44
1:A:12:LYS:C	1:A:13:PRO:O	2.59	0.44
1:B:134:LYS:H	1:B:134:LYS:HE2	1.82	0.44
1:B:147:LEU:HB3	1:B:214:LEU:HD21	1.98	0.44
1:A:243:ALA:HB2	1:A:408:PRO:HG2	1.98	0.44
1:B:317:LEU:HD11	1:B:403:PHE:HB2	1.99	0.44
1:B:305:LEU:HG	1:B:309:LEU:HD23	1.99	0.44
1:B:280:ILE:HA	1:B:414:ARG:O	2.17	0.44
1:A:100:LEU:O	1:A:101:THR:C	2.61	0.44
1:B:149:GLY:O	1:B:173:PRO:HA	2.18	0.44
1:A:92:LYS:HD2	1:A:104:MET:SD	2.57	0.44
1:A:134:LYS:HA	1:A:134:LYS:CE	2.48	0.44
1:A:288:LYS:HG2	1:A:290:GLU:HG2	2.00	0.44
1:A:308:TRP:CD1	1:A:414:ARG:HD2	2.52	0.44
1:B:58:HIS:CD2	1:B:302:PRO:HG3	2.53	0.44
1:B:283:VAL:HG21	1:B:308:TRP:CE2	2.52	0.44
1:B:288:LYS:O	1:B:291:LYS:HB3	2.17	0.44
1:A:89:ALA:HB2	1:A:109:PHE:HZ	1.82	0.43
1:B:44:ALA:HB3	1:B:47:ARG:HG3	2.00	0.43
1:B:287:PRO:HG3	1:B:293:LEU:HA	1.99	0.43
1:B:291:LYS:HZ2	1:B:292:THR:N	2.15	0.43
1:A:301:THR:O	1:A:304:MET:HB2	2.18	0.43
1:A:40:LYS:H	1:A:42:PRO:HG3	1.83	0.43
1:A:193:ASN:N	1:A:193:ASN:HD22	2.16	0.43
1:B:336:LEU:HA	1:B:339:MET:HB2	1.99	0.43
1:B:231:SER:HA	1:B:232:PRO:HD3	1.87	0.43
1:B:97:ASN:HD22	1:B:351:ARG:HD3	1.83	0.43
1:B:300:LEU:HD11	1:B:410:LEU:HD21	2.01	0.42
1:B:174:LEU:HB2	1:B:176:PHE:CE1	2.55	0.42
1:A:288:LYS:HD3	1:A:291:LYS:HZ3	1.83	0.42
1:A:376:VAL:HA	1:A:381:SER:HB3	2.01	0.42
1:A:350:SER:OG	1:A:364:TYR:HA	2.20	0.42
1:A:356:VAL:HG12	1:A:359:GLY:H	1.83	0.42
1:A:394:ARG:NH2	1:A:395:SER:HA	2.32	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:341:LEU:HD13	1:B:344:LEU:HD22	2.01	0.42
1:B:355:ILE:HG13	1:B:356:VAL:HG13	2.00	0.42
1:B:362:ASP:OD1	1:B:394:ARG:HG2	2.18	0.42
1:A:288:LYS:HB3	1:A:291:LYS:CD	2.47	0.42
1:B:103:LEU:HD23	1:B:341:LEU:HD21	2.00	0.42
1:A:150:ASP:OD2	1:A:152:SER:HB2	2.19	0.42
1:A:12:LYS:CB	1:A:13:PRO:CD	2.97	0.42
1:A:38:GLU:HA	1:A:39:GLN:OE1	2.20	0.42
1:A:213:VAL:HG21	1:A:363:LEU:CD1	2.49	0.42
1:B:55:ALA:O	1:B:58:HIS:HB3	2.20	0.42
1:B:230:PHE:HD1	1:B:255:GLN:HB2	1.84	0.42
1:B:232:PRO:HA	1:B:378:GLU:HG2	2.02	0.42
1:A:217:VAL:HG12	1:A:218:ASN:N	2.35	0.42
1:A:422:ILE:HG22	1:A:423:PHE:CE1	2.55	0.42
1:B:184:ARG:HH12	1:B:185:LEU:HD23	1.84	0.42
1:B:187:ILE:O	1:B:190:TRP:HB3	2.19	0.42
1:B:308:TRP:CH2	1:B:414:ARG:HD2	2.55	0.42
1:A:160:GLN:HE21	1:A:160:GLN:HB2	1.68	0.41
1:B:260:ARG:HB3	1:B:311:GLU:HG2	2.02	0.41
1:A:149:GLY:HA2	1:A:214:LEU:HA	2.03	0.41
1:A:16:ILE:HG21	1:A:18:VAL:HG23	2.02	0.41
1:A:273:LEU:HD11	1:A:321:MET:HE1	2.03	0.41
1:A:332:VAL:HG12	1:A:368:ALA:HB3	2.01	0.41
1:A:332:VAL:HG12	1:A:368:ALA:O	2.21	0.41
1:B:204:PRO:HB2	1:B:205:PRO:HD2	2.03	0.41
1:A:48:ARG:O	1:A:51:GLU:N	2.54	0.41
1:A:54:LYS:HB2	1:A:54:LYS:HE2	1.83	0.41
1:A:332:VAL:HG12	1:A:368:ALA:CB	2.51	0.41
1:A:42:PRO:O	1:A:44:ALA:N	2.54	0.41
1:A:133:ARG:HD2	1:A:134:LYS:CA	2.51	0.41
1:B:177:LYS:HA	1:B:177:LYS:HD2	1.90	0.41
1:B:292:THR:HG23	1:B:295:LYS:H	1.86	0.41
1:A:363:LEU:HD22	1:A:363:LEU:N	2.36	0.41
1:B:126:LYS:HD2	1:B:126:LYS:HA	1.96	0.40
1:B:131:LEU:HD11	1:B:420:THR:HG21	2.04	0.40
1:B:331:SER:HG	1:B:333:LYS:HB2	1.87	0.40
1:A:234:ASN:HB3	1:A:254:TYR:HD2	1.86	0.40
1:B:93:LEU:HG	1:B:121:HIS:CE1	2.56	0.40
1:B:119:GLN:OE1	1:B:119:GLN:HA	2.20	0.40
1:B:196:GLU:HB2	1:B:221:TYR:CE2	2.55	0.40
1:B:214:LEU:HD13	1:B:216:LEU:HD11	2.04	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:230:PHE:CD1	1:B:255:GLN:HB2	2.56	0.40
1:B:258:LYS:HA	1:B:315:THR:O	2.22	0.40
1:B:408:PRO:CB	1:B:428:ALA:HA	2.48	0.40
1:A:67:LEU:HD22	1:A:71:LYS:HD2	2.02	0.40
1:A:266:GLU:O	1:A:291:LYS:HE2	2.22	0.40
1:A:295:LYS:HA	1:A:298:GLN:OE1	2.21	0.40
1:A:329:SER:HA	1:A:371:LYS:HA	2.03	0.40
1:A:419:ASN:O	1:A:419:ASN:CG	2.64	0.40
1:B:151:LYS:HG3	1:B:152:SER:N	2.37	0.40
1:B:293:LEU:HD11	1:B:410:LEU:HD13	2.03	0.40
1:B:295:LYS:HB3	1:B:295:LYS:HE2	1.91	0.40
1:A:242:LYS:HE3	1:A:242:LYS:HB2	1.79	0.40
1:A:376:VAL:HG22	1:A:381:SER:HB3	2.04	0.40
1:B:144:ALA:HB3	1:B:219:THR:HB	2.04	0.40
1:B:191:ILE:HG21	1:B:386:SER:OG	2.20	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	415/429 (97%)	348 (84%)	52 (12%)	15 (4%)	2	19
1	B	405/429 (94%)	334 (82%)	46 (11%)	25 (6%)	1	9
All	All	820/858 (96%)	682 (83%)	98 (12%)	40 (5%)	1	13

All (40) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	11	ALA
1	A	12	LYS
1	A	278	ASP

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Mol	Chain	Res	Type
1	A	395	SER
1	B	44	ALA
1	B	113	SER
1	B	137	LYS
1	A	43	GLY
1	A	45	THR
1	A	134	LYS
1	A	205	PRO
1	A	210	GLU
1	B	14	ARG
1	B	73	ASN
1	B	115	LYS
1	B	139	SER
1	B	151	LYS
1	B	154	THR
1	B	402	THR
1	B	407	ARG
1	B	419	ASN
1	A	73	ASN
1	A	139	SER
1	A	201	ASP
1	A	394	ARG
1	B	108	LYS
1	B	244	ASP
1	B	299	GLU
1	B	306	GLN
1	B	358	GLU
1	B	362	ASP
1	B	141	LEU
1	B	117	SER
1	B	241	TYR
1	B	112	ILE
1	B	210	GLU
1	A	165	VAL
1	A	264	VAL
1	B	352	LEU
1	B	264	VAL

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	374/383 (98%)	291 (78%)	83 (22%)	1	5
1	B	368/383 (96%)	299 (81%)	69 (19%)	1	9
All	All	742/766 (97%)	590 (80%)	152 (20%)	1	7

All (152) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	6	GLU
1	A	7	ASP
1	A	9	CYS
1	A	10	THR
1	A	12	LYS
1	A	14	ARG
1	A	15	ASP
1	A	19	ASN
1	A	22	CYS
1	A	32	THR
1	A	39	GLN
1	A	41	ILE
1	A	45	THR
1	A	47	ARG
1	A	48	ARG
1	A	52	LEU
1	A	61	THR
1	A	67	LEU
1	A	72	ASN
1	A	79	LEU
1	A	98	ASN
1	A	100	LEU
1	A	116	THR
1	A	130	ARG
1	A	134	LYS
1	A	138	SER
1	A	139	SER
1	A	140	GLU
1	A	142	VAL
1	A	147	LEU
1	A	160	GLN

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Mol	Chain	Res	Type
1	A	164	GLU
1	A	171	LEU
1	A	173	PRO
1	A	181	GLU
1	A	191	ILE
1	A	205	PRO
1	A	208	ILE
1	A	218	ASN
1	A	228	SER
1	A	232	PRO
1	A	236	ARG
1	A	242	LYS
1	A	264	VAL
1	A	266	GLU
1	A	268	THR
1	A	271	LEU
1	A	278	ASP
1	A	287	PRO
1	A	289	LEU
1	A	290	GLU
1	A	292	THR
1	A	293	LEU
1	A	299	GLU
1	A	301	THR
1	A	305	LEU
1	A	306	GLN
1	A	307	GLU
1	A	309	LEU
1	A	311	GLU
1	A	312	LEU
1	A	313	THR
1	A	314	GLU
1	A	316	LEU
1	A	318	VAL
1	A	327	GLU
1	A	329	SER
1	A	332	VAL
1	A	339	MET
1	A	352	LEU
1	A	360	ARG
1	A	378	GLU
1	A	379	GLU

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Mol	Chain	Res	Type
1	A	388	VAL
1	A	389	ILE
1	A	394	ARG
1	A	395	SER
1	A	400	ARG
1	A	412	LEU
1	A	419	ASN
1	A	420	THR
1	A	431	CYS
1	A	432	VAL
1	B	12	LYS
1	B	14	ARG
1	B	15	ASP
1	B	16	ILE
1	B	19	ASN
1	B	42	PRO
1	B	45	THR
1	B	49	VAL
1	B	72	ASN
1	B	73	ASN
1	B	79	LEU
1	B	82	LEU
1	B	84	ILE
1	B	85	SER
1	B	101	THR
1	B	124	PHE
1	B	129	CYS
1	B	131	LEU
1	B	133	ARG
1	B	136	ASN
1	B	152	SER
1	B	157	GLU
1	B	158	THR
1	B	171	LEU
1	B	172	GLN
1	B	179	ASN
1	B	184	ARG
1	B	191	ILE
1	B	198	ARG
1	B	203	ILE
1	B	204	PRO
1	B	210	GLU

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Mol	Chain	Res	Type
1	B	212	THR
1	B	213	VAL
1	B	214	LEU
1	B	219	THR
1	B	223	LYS
1	B	229	LYS
1	B	234	ASN
1	B	236	ARG
1	B	248	CYS
1	B	252	MET
1	B	270	VAL
1	B	281	THR
1	B	286	LEU
1	B	288	LYS
1	B	291	LYS
1	B	295	LYS
1	B	298	GLN
1	B	301	THR
1	B	305	LEU
1	B	308	TRP
1	B	312	LEU
1	B	316	LEU
1	B	330	PHE
1	B	333	LYS
1	B	334	GLU
1	B	337	GLN
1	B	350	SER
1	B	360	ARG
1	B	361	SER
1	B	363	LEU
1	B	377	ASN
1	B	388	VAL
1	B	412	LEU
1	B	414	ARG
1	B	427	VAL
1	B	432	VAL
1	B	433	ASP

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (18) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	19	ASN

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Mol	Chain	Res	Type
1	A	56	ASN
1	A	58	HIS
1	A	65	GLN
1	A	66	HIS
1	A	72	ASN
1	A	121	HIS
1	A	128	ASN
1	A	160	GLN
1	A	193	ASN
1	A	218	ASN
1	B	73	ASN
1	B	97	ASN
1	B	128	ASN
1	B	145	ASN
1	B	218	ASN
1	B	234	ASN
1	B	255	GLN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

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 ⓘ

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	421/429 (98%)	-0.35	6 (1%)	73 54	2, 13, 54, 66	0
1	B	411/429 (95%)	-0.32	7 (1%)	69 49	3, 23, 50, 69	0
All	All	832/858 (96%)	-0.34	13 (1%)	70 51	2, 20, 52, 69	0

All (13) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	11	ALA	6.4
1	A	359	GLY	6.4
1	B	136	ASN	3.2
1	B	13	PRO	2.9
1	B	12	LYS	2.8
1	A	13	PRO	2.6
1	B	138	SER	2.6
1	B	39	GLN	2.5
1	A	12	LYS	2.3
1	B	129	CYS	2.2
1	A	138	SER	2.1
1	B	135	ALA	2.1
1	A	14	ARG	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.