



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 6, 2026 – 07:24 AM UTC

PDB ID : 2ABX / pdb_00002abx
Title : THE CRYSTAL STRUCTURE OF ALPHA-BUNGAROTOXIN AT 2.5
ANGSTROMS RESOLUTION. RELATION TO SOLUTION STRUCTURE
AND BINDING TO ACETYLCHOLINE RECEPTOR
Authors : Love, R.; Stroud, R.
Deposited on : 1986-02-19
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

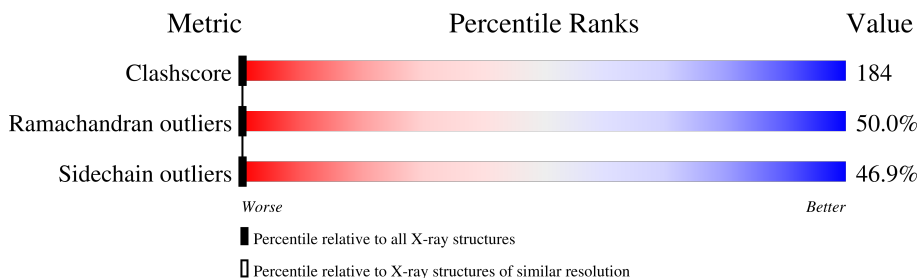
1 Overall quality at a glance

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	74	 • 9% 31% 58%
1	B	74	 • 12% 42% 45%

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 1118 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 ALPHA-BUNGAROTOXIN.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	74	Total	C	N	O	S	0	0	0
			551	338	97	105	11			
1	B	74	Total	C	N	O	S	0	0	0
			551	338	97	105	11			

There are 12 discrepancies between the modelled and reference sequences:

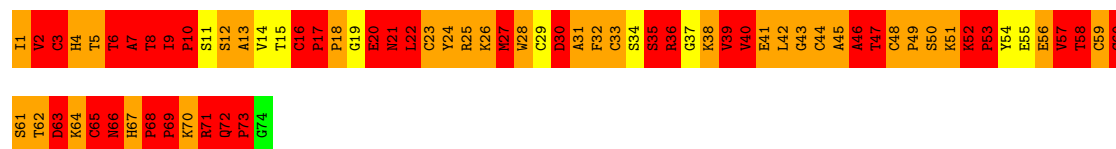
Chain	Residue	Modelled	Actual	Comment	Reference
A	9	ILE	SER	conflict	UNP P60615
A	11	SER	ILE	conflict	UNP P60615
A	67	HIS	PRO	conflict	UNP P60615
A	68	PRO	HIS	conflict	UNP P60615
A	71	ARG	GLN	conflict	UNP P60615
A	72	GLN	ARG	conflict	UNP P60615
B	9	ILE	SER	conflict	UNP P60615
B	11	SER	ILE	conflict	UNP P60615
B	67	HIS	PRO	conflict	UNP P60615
B	68	PRO	HIS	conflict	UNP P60615
B	71	ARG	GLN	conflict	UNP P60615
B	72	GLN	ARG	conflict	UNP P60615

- Molecule 2 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	10	Total	O	0	0
			10	10		
2	B	6	Total	O	0	0
			6	6		

Note EDS was not executed.

Chain A: 9% 31% 58%



4 Data and refinement statistics

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

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	67.80Å 78.40Å 22.40Å 90.00° 90.00° 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	PROLSQ	Depositor
R, R_{free}	0.240 , (Not available)	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	1118	wwPDB-VP
Average B, all atoms (Å ²)	15.0	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	2.00	13/565 (2.3%)	3.75	120/767 (15.6%)
1	B	2.08	20/565 (3.5%)	3.65	98/767 (12.8%)
All	All	2.04	33/1130 (2.9%)	3.70	218/1534 (14.2%)

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	2
All	All	0	3

All (33) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	64	LYS	N-CA	8.54	1.51	1.46
1	B	35	SER	N-CA	7.95	1.56	1.46
1	B	22	LEU	C-O	7.65	1.33	1.24
1	A	1	ILE	C-N	7.07	1.43	1.33
1	A	59	CYS	CB-SG	-6.85	1.58	1.81
1	B	69	PRO	C-O	6.37	1.32	1.24
1	B	55	GLU	CA-CB	-6.25	1.43	1.53
1	A	69	PRO	CA-CB	6.20	1.62	1.53
1	B	53	PRO	N-CA	-6.12	1.39	1.47
1	B	39	VAL	CA-C	6.12	1.60	1.52
1	B	3	CYS	CA-CB	6.08	1.63	1.53
1	A	73	PRO	N-CD	6.01	1.56	1.47
1	A	70	LYS	CA-CB	-5.99	1.43	1.53
1	B	35	SER	CA-C	5.89	1.60	1.52
1	A	69	PRO	N-CD	5.88	1.55	1.47
1	B	10	PRO	CA-CB	-5.71	1.45	1.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	36	ARG	N-CA	5.60	1.53	1.46
1	A	2	VAL	C-N	-5.57	1.25	1.33
1	B	13	ALA	N-CA	-5.51	1.39	1.46
1	B	28	TRP	NE1-CE2	-5.49	1.31	1.37
1	B	7	ALA	CA-CB	-5.45	1.44	1.53
1	A	72	GLN	CA-CB	5.44	1.62	1.53
1	B	57	VAL	C-O	5.42	1.30	1.24
1	A	33	CYS	N-CA	5.36	1.53	1.46
1	A	63	ASP	C-N	-5.32	1.28	1.33
1	B	57	VAL	CA-CB	-5.30	1.47	1.54
1	A	8	THR	C-N	-5.24	1.27	1.33
1	B	36	ARG	CZ-NH2	-5.18	1.26	1.33
1	A	36	ARG	C-O	5.17	1.30	1.24
1	B	2	VAL	C-N	-5.12	1.26	1.33
1	A	56	GLU	CD-OE2	5.04	1.34	1.25
1	B	57	VAL	N-CA	5.02	1.52	1.46
1	B	66	ASN	CA-CB	5.00	1.60	1.52

All (218) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	55	GLU	CA-CB-CG	18.31	150.72	114.10
1	A	33	CYS	CB-CA-C	18.02	134.75	111.50
1	B	64	LYS	CA-C-O	-17.87	107.58	117.94
1	B	57	VAL	CB-CA-C	17.53	140.04	111.29
1	A	54	TYR	CA-CB-CG	15.81	142.36	113.90
1	A	59	CYS	CA-CB-SG	15.36	149.73	114.40
1	A	66	ASN	N-CA-C	14.89	132.20	113.88
1	B	16	CYS	CA-C-N	14.12	134.93	120.38
1	B	16	CYS	C-N-CA	14.12	134.93	120.38
1	A	29	CYS	N-CA-C	13.85	131.76	111.81
1	B	17	PRO	N-CA-C	-13.36	94.40	110.70
1	A	31	ALA	O-C-N	12.85	139.68	122.59
1	A	18	PRO	CB-CA-C	-12.56	90.83	111.56
1	B	64	LYS	N-CA-C	-12.07	98.88	108.78
1	B	39	VAL	O-C-N	11.84	137.37	122.57
1	B	25	ARG	NE-CZ-NH2	11.78	129.80	119.20
1	B	53	PRO	N-CA-C	11.74	136.66	112.47
1	B	2	VAL	CA-C-N	11.74	143.96	121.54
1	B	2	VAL	C-N-CA	11.74	143.96	121.54
1	A	55	GLU	CA-C-N	11.65	142.12	121.97
1	A	55	GLU	C-N-CA	11.65	142.12	121.97

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	21	ASN	CA-C-N	11.28	143.09	121.54
1	B	21	ASN	C-N-CA	11.28	143.09	121.54
1	A	36	ARG	CD-NE-CZ	11.01	139.81	124.40
1	B	12	SER	CA-C-N	10.84	142.25	121.54
1	B	12	SER	C-N-CA	10.84	142.25	121.54
1	A	68	PRO	CA-C-N	10.82	133.36	119.84
1	A	68	PRO	C-N-CA	10.82	133.36	119.84
1	A	63	ASP	O-C-N	10.78	136.93	122.59
1	A	21	ASN	O-C-N	10.67	136.78	122.59
1	B	10	PRO	CB-CA-C	10.62	129.08	111.56
1	A	36	ARG	NE-CZ-NH2	10.26	128.43	119.20
1	B	40	VAL	CA-C-O	10.23	133.11	121.44
1	B	66	ASN	N-CA-CB	-10.23	96.41	110.42
1	B	33	CYS	O-C-N	10.23	136.39	122.48
1	A	25	ARG	CD-NE-CZ	9.79	138.11	124.40
1	A	2	VAL	O-C-N	9.75	134.76	122.57
1	B	40	VAL	N-CA-C	9.73	120.69	108.82
1	A	70	LYS	CA-C-O	-9.65	106.72	120.51
1	A	63	ASP	CA-CB-CG	9.53	122.13	112.60
1	B	66	ASN	N-CA-C	9.50	124.56	111.55
1	B	39	VAL	CA-C-N	9.45	137.16	123.27
1	B	39	VAL	C-N-CA	9.45	137.16	123.27
1	B	67	HIS	O-C-N	9.42	128.86	121.23
1	A	52	LYS	CA-C-N	9.35	131.53	119.84
1	A	52	LYS	C-N-CA	9.35	131.53	119.84
1	A	72	GLN	CA-C-N	8.96	131.03	119.84
1	A	72	GLN	C-N-CA	8.96	131.03	119.84
1	B	59	CYS	CA-CB-SG	8.74	134.51	114.40
1	A	40	VAL	CA-C-N	8.58	136.06	122.59
1	A	40	VAL	C-N-CA	8.58	136.06	122.59
1	B	17	PRO	O-C-N	8.57	131.58	121.46
1	B	17	PRO	CA-N-CD	-8.55	100.03	112.00
1	B	13	ALA	CA-C-O	-8.49	108.37	120.51
1	B	3	CYS	N-CA-CB	-8.38	96.32	110.49
1	A	67	HIS	O-C-N	8.36	130.93	121.32
1	B	57	VAL	CA-CB-CG2	8.30	124.51	110.40
1	A	25	ARG	NE-CZ-NH1	8.27	129.77	121.50
1	A	34	SER	N-CA-C	-8.18	104.30	112.97
1	B	72	GLN	O-C-N	8.18	130.72	121.32
1	B	8	THR	CA-C-O	8.12	132.13	120.51
1	A	70	LYS	N-CA-CB	8.09	124.16	110.49
1	A	72	GLN	OE1-CD-NE2	8.07	130.67	122.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	65	CYS	N-CA-C	8.07	127.98	110.80
1	B	13	ALA	CA-C-N	7.94	136.26	121.97
1	B	13	ALA	C-N-CA	7.94	136.26	121.97
1	B	8	THR	CA-C-N	7.90	136.74	122.13
1	B	8	THR	C-N-CA	7.90	136.74	122.13
1	B	59	CYS	O-C-N	7.82	132.44	122.28
1	A	39	VAL	CB-CA-C	7.80	124.08	111.29
1	B	46	ALA	O-C-N	7.79	132.95	122.59
1	A	29	CYS	CA-CB-SG	-7.78	96.50	114.40
1	B	72	GLN	CA-C-N	7.71	129.48	119.84
1	B	72	GLN	C-N-CA	7.71	129.48	119.84
1	B	3	CYS	CA-C-O	-7.70	109.49	120.51
1	B	4	HIS	CA-CB-CG	7.61	121.41	113.80
1	B	20	GLU	CB-CG-CD	7.59	125.51	112.60
1	B	26	LYS	CA-C-N	7.55	135.96	121.54
1	B	26	LYS	C-N-CA	7.55	135.96	121.54
1	A	62	THR	CA-C-N	7.54	135.94	121.54
1	A	62	THR	C-N-CA	7.54	135.94	121.54
1	B	52	LYS	CA-C-N	7.54	129.26	119.84
1	B	52	LYS	C-N-CA	7.54	129.26	119.84
1	A	58	THR	N-CA-CB	7.53	123.21	110.49
1	A	60	CYS	CA-C-O	-7.51	109.77	120.51
1	A	21	ASN	CA-C-N	7.51	135.88	121.54
1	A	21	ASN	C-N-CA	7.51	135.88	121.54
1	B	67	HIS	N-CA-CB	7.49	119.68	110.17
1	A	8	THR	O-C-N	7.34	132.35	122.59
1	A	58	THR	CA-C-N	7.32	135.52	121.54
1	A	58	THR	C-N-CA	7.32	135.52	121.54
1	A	55	GLU	N-CA-CB	7.30	122.83	110.49
1	B	67	HIS	CA-CB-CG	7.28	121.08	113.80
1	B	41	GLU	CA-C-N	7.22	134.45	122.33
1	B	41	GLU	C-N-CA	7.22	134.45	122.33
1	B	49	PRO	O-C-N	7.21	132.38	122.64
1	A	40	VAL	CA-C-O	7.18	129.76	120.78
1	A	33	CYS	CA-C-O	7.12	133.91	121.53
1	A	3	CYS	N-CA-CB	-7.05	98.92	110.41
1	B	69	PRO	CA-C-N	7.04	130.02	120.38
1	B	69	PRO	C-N-CA	7.04	130.02	120.38
1	A	54	TYR	N-CA-CB	7.00	122.31	110.49
1	A	10	PRO	CB-CA-C	6.98	123.07	111.56
1	A	34	SER	O-C-N	6.96	131.38	122.06
1	A	11	SER	N-CA-CB	-6.95	98.74	110.49

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	63	ASP	CA-C-O	-6.93	110.60	120.51
1	B	59	CYS	N-CA-C	-6.91	100.07	109.54
1	A	72	GLN	O-C-N	6.87	129.22	121.32
1	B	33	CYS	CB-CA-C	6.85	121.84	110.88
1	A	15	THR	N-CA-CB	6.80	121.98	110.49
1	B	20	GLU	CA-CB-CG	6.80	127.70	114.10
1	A	17	PRO	CB-CA-C	-6.74	102.69	110.92
1	A	1	ILE	CB-CA-C	6.72	125.03	111.60
1	A	22	LEU	O-C-N	6.71	131.51	122.59
1	A	9	ILE	N-CA-C	6.68	123.31	108.88
1	A	56	GLU	N-CA-C	6.62	120.43	110.64
1	A	69	PRO	CA-N-CD	-6.58	102.79	112.00
1	B	55	GLU	N-CA-CB	6.56	121.58	110.49
1	A	73	PRO	CB-CA-C	6.53	122.33	111.56
1	B	23	CYS	CA-C-O	-6.52	113.48	120.46
1	A	63	ASP	N-CA-CB	6.51	121.50	110.49
1	B	9	ILE	O-C-N	6.50	128.51	121.10
1	B	52	LYS	O-C-N	6.48	128.77	121.32
1	A	30	ASP	CA-CB-CG	6.45	119.05	112.60
1	A	36	ARG	NH1-CZ-NH2	-6.44	110.93	119.30
1	A	48	CYS	CA-CB-SG	6.39	129.11	114.40
1	A	41	GLU	CG-CD-OE2	-6.32	103.86	118.40
1	A	34	SER	N-CA-CB	6.30	119.60	110.65
1	A	30	ASP	CA-C-O	6.30	129.51	120.51
1	A	64	LYS	CA-C-O	-6.29	113.87	119.91
1	B	70	LYS	CB-CA-C	-6.29	99.98	110.68
1	A	23	CYS	O-C-N	-6.29	116.25	123.42
1	B	27	MET	CA-CB-CG	6.28	126.66	114.10
1	A	23	CYS	CA-C-N	6.25	132.29	122.17
1	A	23	CYS	C-N-CA	6.25	132.29	122.17
1	A	67	HIS	CA-C-O	-6.23	111.62	120.16
1	A	10	PRO	CA-C-N	-6.19	109.72	121.54
1	A	10	PRO	C-N-CA	-6.19	109.72	121.54
1	A	24	TYR	N-CA-C	6.14	118.79	108.23
1	A	69	PRO	CA-C-N	6.13	133.25	121.54
1	A	69	PRO	C-N-CA	6.13	133.25	121.54
1	B	6	THR	N-CA-C	-6.13	101.86	110.50
1	A	57	VAL	CA-C-N	6.11	133.21	121.54
1	A	57	VAL	C-N-CA	6.11	133.21	121.54
1	B	66	ASN	CA-CB-CG	-6.11	106.49	112.60
1	B	45	ALA	N-CA-C	-6.08	97.86	110.80
1	A	54	TYR	O-C-N	-6.07	114.51	122.59

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	15	THR	CA-C-O	6.03	129.13	120.51
1	B	3	CYS	CB-CA-C	-6.03	98.43	110.42
1	B	24	TYR	CB-CA-C	6.02	120.22	109.38
1	B	62	THR	N-CA-CB	-6.02	102.29	110.95
1	B	3	CYS	CA-CB-SG	-5.98	100.65	114.40
1	A	67	HIS	ND1-CE1-NE2	5.97	114.37	108.40
1	A	47	THR	N-CA-C	5.97	123.52	110.80
1	A	47	THR	CA-CB-OG1	-5.97	100.65	109.60
1	A	16	CYS	N-CA-C	5.93	122.91	109.81
1	A	22	LEU	N-CA-C	5.91	123.39	110.80
1	B	40	VAL	N-CA-CB	-5.90	105.84	112.45
1	B	10	PRO	CA-C-O	5.86	131.26	120.60
1	B	2	VAL	CA-CB-CG1	5.82	120.30	110.40
1	B	5	THR	O-C-N	5.82	130.33	122.59
1	A	33	CYS	N-CA-C	-5.81	103.44	111.81
1	A	8	THR	CA-C-N	5.77	132.81	122.13
1	A	8	THR	C-N-CA	5.77	132.81	122.13
1	A	69	PRO	N-CA-C	5.76	124.34	112.47
1	B	21	ASN	OD1-CG-ND2	5.76	128.36	122.60
1	B	65	CYS	N-CA-C	5.76	123.07	110.80
1	B	17	PRO	CA-C-O	-5.76	112.21	120.56
1	B	18	PRO	CB-CA-C	5.74	118.52	111.12
1	A	71	ARG	CA-C-O	5.73	128.70	120.51
1	B	35	SER	N-CA-C	5.72	122.99	110.80
1	A	54	TYR	CB-CA-C	5.70	121.76	110.42
1	A	58	THR	O-C-N	5.70	130.17	122.59
1	B	7	ALA	N-CA-C	-5.66	98.75	110.80
1	A	53	PRO	N-CA-C	5.65	124.11	112.47
1	A	65	CYS	CA-C-O	-5.65	112.43	120.51
1	A	31	ALA	CA-C-O	-5.65	112.43	120.51
1	B	66	ASN	CA-C-N	-5.64	114.29	121.74
1	B	66	ASN	C-N-CA	-5.64	114.29	121.74
1	B	46	ALA	CA-C-N	5.64	132.31	121.54
1	B	46	ALA	C-N-CA	5.64	132.31	121.54
1	B	73	PRO	CA-N-CD	-5.61	104.15	112.00
1	A	20	GLU	O-C-N	5.58	130.01	122.59
1	A	25	ARG	CA-C-O	-5.57	114.70	121.05
1	A	2	VAL	N-CA-C	5.56	120.90	109.34
1	B	59	CYS	CA-C-O	-5.53	112.65	121.94
1	A	13	ALA	N-CA-CB	-5.53	101.15	110.49
1	B	17	PRO	CB-CA-C	-5.52	104.18	110.92
1	A	48	CYS	N-CA-CB	-5.51	100.56	110.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	29	CYS	CA-C-N	5.49	132.02	121.54
1	A	29	CYS	C-N-CA	5.49	132.02	121.54
1	A	69	PRO	N-CD-CG	-5.47	94.99	103.20
1	A	12	SER	CA-C-O	5.46	128.32	120.51
1	B	7	ALA	O-C-N	5.42	129.79	122.59
1	B	64	LYS	O-C-N	5.42	125.53	121.47
1	B	8	THR	CB-CA-C	5.41	121.18	110.42
1	B	65	CYS	CA-C-N	5.40	132.24	122.62
1	B	65	CYS	C-N-CA	5.40	132.24	122.62
1	A	50	SER	CA-C-O	-5.38	112.82	120.51
1	B	41	GLU	CG-CD-OE2	-5.34	106.11	118.40
1	A	13	ALA	CA-C-O	5.27	128.05	120.51
1	B	68	PRO	CB-CA-C	5.23	117.30	110.92
1	B	62	THR	CA-CB-OG1	-5.21	101.79	109.60
1	A	64	LYS	CA-CB-CG	5.20	124.50	114.10
1	B	17	PRO	N-CD-CG	-5.17	95.45	103.20
1	A	21	ASN	CA-CB-CG	5.14	117.74	112.60
1	A	68	PRO	CB-CA-C	-5.12	104.67	110.92
1	A	24	TYR	CA-CB-CG	5.09	123.06	113.90
1	A	44	CYS	CA-CB-SG	5.08	126.08	114.40
1	B	43	GLY	N-CA-C	5.04	125.12	113.18
1	A	23	CYS	CA-C-O	5.04	126.28	120.14
1	A	32	PHE	CA-C-N	-5.03	112.96	122.27
1	A	32	PHE	C-N-CA	-5.03	112.96	122.27
1	A	58	THR	CA-CB-CG2	5.03	119.06	110.50
1	A	11	SER	CA-C-N	5.02	131.13	121.54
1	A	11	SER	C-N-CA	5.02	131.13	121.54
1	A	14	VAL	CA-C-N	5.00	131.09	121.54
1	A	14	VAL	C-N-CA	5.00	131.09	121.54

There are no chirality outliers.

All (3) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	71	ARG	Sidechain
1	B	36	ARG	Sidechain
1	B	71	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	551	0	532	230	6
1	B	551	0	532	168	7
2	A	10	0	0	2	3
2	B	6	0	0	0	0
All	All	1118	0	1064	398	9

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 184.

All (398) 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:16:CYS:HB2	1:A:17:PRO:CD	1.22	1.52
1:B:52:LYS:HB2	1:B:53:PRO:CD	1.06	1.52
1:A:42:LEU:CB	1:A:66:ASN:HD22	1.25	1.45
1:A:17:PRO:HB2	1:A:18:PRO:CD	1.31	1.40
1:A:42:LEU:HB2	1:A:66:ASN:ND2	1.12	1.39
1:A:4:HIS:CE1	1:A:13:ALA:HB1	1.60	1.35
1:B:52:LYS:CB	1:B:53:PRO:HD3	1.57	1.35
1:A:4:HIS:CD2	1:A:13:ALA:HB1	1.61	1.33
1:A:9:ILE:HB	1:A:10:PRO:CD	1.58	1.32
1:A:50:SER:O	1:A:51:LYS:HG3	1.32	1.28
1:A:24:TYR:CD1	1:A:51:LYS:HE2	1.66	1.27
1:B:52:LYS:CB	1:B:53:PRO:CD	2.00	1.27
1:A:4:HIS:NE2	1:A:13:ALA:HB1	1.47	1.26
1:B:16:CYS:CB	1:B:17:PRO:HD3	1.60	1.26
1:A:26:LYS:CG	1:A:57:VAL:HG13	1.68	1.24
1:A:4:HIS:CE1	1:A:13:ALA:CB	2.22	1.23
1:A:17:PRO:CB	1:A:18:PRO:CD	2.13	1.22
1:B:7:ALA:O	1:B:14:VAL:HG21	1.35	1.21
1:A:52:LYS:HB3	1:A:53:PRO:CD	1.71	1.21
1:A:16:CYS:CB	1:A:17:PRO:CD	2.14	1.20
1:A:3:CYS:O	1:A:15:THR:HG22	1.43	1.17
1:A:4:HIS:CG	1:A:13:ALA:HB1	1.79	1.17
1:A:9:ILE:CB	1:A:10:PRO:HD3	1.74	1.17

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:38:LYS:HD3	1:B:71:ARG:HG3	1.24	1.17
1:A:52:LYS:HB3	1:A:53:PRO:HD2	1.21	1.16
1:B:60:CYS:SG	1:B:61:SER:N	2.15	1.15
1:A:22:LEU:HD12	1:A:61:SER:HB2	1.26	1.14
1:A:16:CYS:HB2	1:A:17:PRO:HD2	1.23	1.13
1:A:16:CYS:CB	1:A:17:PRO:HD3	1.78	1.13
1:B:4:HIS:HB3	1:B:64:LYS:HZ3	1.13	1.12
1:A:26:LYS:HG3	1:A:57:VAL:CG1	1.79	1.12
1:B:38:LYS:CD	1:B:71:ARG:HG3	1.79	1.11
1:B:24:TYR:CZ	1:B:49:PRO:HG2	1.86	1.10
1:B:66:ASN:N	1:B:66:ASN:HD22	1.43	1.10
1:A:72:GLN:OE1	1:A:72:GLN:HA	1.42	1.09
1:A:22:LEU:HD12	1:A:61:SER:CB	1.81	1.09
1:B:66:ASN:ND2	1:B:66:ASN:H	1.33	1.08
1:A:2:VAL:HG11	1:A:22:LEU:N	1.68	1.08
1:A:6:THR:HA	1:A:11:SER:OG	1.53	1.08
1:B:9:ILE:HB	1:B:10:PRO:CD	1.84	1.08
1:B:41:GLU:C	1:B:42:LEU:HD12	1.78	1.06
1:A:29:CYS:O	1:A:33:CYS:SG	2.14	1.06
1:B:52:LYS:HB2	1:B:53:PRO:HD2	1.15	1.06
1:A:10:PRO:O	1:A:11:SER:HB2	1.28	1.05
1:B:17:PRO:HB2	1:B:18:PRO:HD2	1.37	1.05
1:A:2:VAL:HG11	1:A:22:LEU:CA	1.85	1.05
1:A:22:LEU:HD11	1:A:60:CYS:O	1.57	1.04
1:A:6:THR:HG22	1:A:7:ALA:H	1.21	1.03
1:A:22:LEU:CD1	1:A:61:SER:HB2	1.85	1.03
1:B:9:ILE:HB	1:B:10:PRO:HD2	1.04	1.03
1:B:9:ILE:O	1:B:11:SER:N	1.89	1.03
1:A:22:LEU:CD1	1:A:61:SER:CB	2.35	1.03
1:A:9:ILE:HB	1:A:10:PRO:HD3	1.04	1.02
1:B:16:CYS:HB3	1:B:17:PRO:CD	1.90	1.02
1:B:17:PRO:HD2	1:B:17:PRO:O	1.59	1.02
1:B:7:ALA:O	1:B:14:VAL:CG2	2.08	1.01
1:A:17:PRO:CB	1:A:18:PRO:HD2	1.81	1.00
1:A:27:MET:HG3	1:A:28:TRP:H	1.25	1.00
1:B:23:CYS:HB2	1:B:60:CYS:SG	2.01	1.00
1:B:16:CYS:CB	1:B:17:PRO:CD	2.40	0.99
1:A:4:HIS:NE2	1:A:13:ALA:CB	2.22	0.98
1:A:4:HIS:ND1	1:A:13:ALA:HB1	1.77	0.98
1:A:10:PRO:O	1:A:11:SER:CB	2.11	0.98
1:B:5:THR:HG23	1:B:64:LYS:HG3	1.43	0.97

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:53:PRO:O	1:A:54:TYR:O	1.83	0.96
1:B:9:ILE:CB	1:B:10:PRO:HD2	1.94	0.96
1:A:17:PRO:HD2	1:A:44:CYS:SG	2.06	0.96
1:B:4:HIS:HB3	1:B:64:LYS:NZ	1.81	0.96
1:A:50:SER:O	1:A:51:LYS:CG	2.15	0.95
1:A:42:LEU:CB	1:A:66:ASN:ND2	1.96	0.94
1:B:16:CYS:HB3	1:B:17:PRO:HD3	0.96	0.94
1:A:4:HIS:CD2	1:A:13:ALA:CB	2.50	0.94
1:B:30:ASP:O	1:B:31:ALA:HB2	1.68	0.93
1:A:41:GLU:C	1:A:42:LEU:HD22	1.94	0.93
1:A:3:CYS:O	1:A:15:THR:CG2	2.15	0.93
1:B:17:PRO:HB2	1:B:18:PRO:CD	1.99	0.93
1:B:42:LEU:HD12	1:B:42:LEU:N	1.81	0.93
1:A:48:CYS:O	1:A:50:SER:N	2.02	0.92
1:B:56:GLU:O	1:B:57:VAL:HB	1.67	0.92
1:A:27:MET:O	1:A:28:TRP:HB2	1.65	0.91
1:A:72:GLN:OE1	1:A:73:PRO:HD2	1.70	0.91
1:A:5:THR:OG1	1:A:66:ASN:OD1	1.89	0.90
1:A:41:GLU:C	1:A:42:LEU:CD2	2.44	0.90
1:A:72:GLN:OE1	1:A:72:GLN:CA	2.19	0.90
1:B:17:PRO:CD	1:B:17:PRO:O	2.15	0.90
1:A:16:CYS:HB2	1:A:17:PRO:HD3	0.90	0.90
1:A:17:PRO:HB2	1:A:18:PRO:HD2	0.90	0.88
1:B:25:ARG:HD2	1:B:66:ASN:HB3	1.55	0.88
1:A:16:CYS:CB	1:A:17:PRO:HD2	1.94	0.88
1:B:45:ALA:O	1:B:46:ALA:HB3	1.73	0.88
1:B:30:ASP:O	1:B:31:ALA:CB	2.19	0.88
1:A:12:SER:C	1:A:14:VAL:H	1.81	0.88
1:A:54:TYR:O	1:A:55:GLU:O	1.90	0.88
1:A:17:PRO:CB	1:A:18:PRO:HD3	2.02	0.88
1:B:66:ASN:N	1:B:66:ASN:ND2	2.09	0.88
1:A:6:THR:O	1:A:7:ALA:CB	2.22	0.86
1:B:9:ILE:O	1:B:10:PRO:C	2.19	0.86
1:A:48:CYS:C	1:A:50:SER:H	1.82	0.85
1:A:22:LEU:CD1	1:A:61:SER:HB3	2.04	0.85
1:A:2:VAL:CG1	1:A:22:LEU:N	2.39	0.85
1:A:44:CYS:O	1:A:45:ALA:HB2	1.77	0.84
1:A:24:TYR:CD1	1:A:51:LYS:CE	2.58	0.84
1:A:22:LEU:HD23	1:A:23:CYS:O	1.77	0.84
1:A:43:GLY:O	1:A:44:CYS:HB2	1.77	0.84
1:A:52:LYS:CB	1:A:53:PRO:CD	2.47	0.84

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:6:THR:CG2	1:B:42:LEU:HB2	2.08	0.83
1:B:4:HIS:CD2	1:B:13:ALA:HB2	2.14	0.83
1:A:26:LYS:O	1:A:27:MET:CB	2.25	0.82
1:B:66:ASN:HD22	1:B:66:ASN:H	0.85	0.82
1:A:27:MET:SD	1:A:54:TYR:OH	2.36	0.82
1:A:70:LYS:HB3	1:A:70:LYS:HZ2	1.44	0.82
1:B:4:HIS:CG	1:B:13:ALA:HB2	2.14	0.82
1:A:27:MET:HG3	1:A:28:TRP:N	1.94	0.82
1:A:53:PRO:HB3	2:A:217:HOH:O	1.78	0.82
1:A:2:VAL:HG11	1:A:22:LEU:HA	1.62	0.81
1:A:50:SER:C	1:A:51:LYS:HG3	2.06	0.81
1:B:42:LEU:N	1:B:42:LEU:CD1	2.44	0.81
1:B:28:TRP:HH2	1:B:69:PRO:HD2	1.46	0.80
1:B:45:ALA:O	1:B:46:ALA:CB	2.30	0.80
1:B:50:SER:O	1:B:51:LYS:HB2	1.80	0.80
1:B:60:CYS:O	1:B:61:SER:CB	2.28	0.80
1:A:70:LYS:O	1:A:71:ARG:HB2	1.81	0.79
1:A:66:ASN:O	1:A:67:HIS:C	2.25	0.79
1:A:14:VAL:HG12	1:A:16:CYS:N	1.98	0.79
1:A:19:GLY:O	1:A:20:GLU:CD	2.25	0.79
1:B:52:LYS:HB2	1:B:53:PRO:HD3	0.80	0.79
1:A:27:MET:CG	1:A:28:TRP:N	2.46	0.78
1:A:47:THR:O	1:A:48:CYS:C	2.25	0.78
1:A:42:LEU:O	1:A:66:ASN:ND2	2.14	0.78
1:B:66:ASN:O	1:B:68:PRO:HD3	1.83	0.78
1:B:47:THR:O	1:B:48:CYS:C	2.26	0.78
1:A:26:LYS:HG3	1:A:57:VAL:HG13	0.82	0.78
1:B:4:HIS:CD2	1:B:13:ALA:CB	2.67	0.78
1:B:52:LYS:CB	1:B:53:PRO:HD2	1.93	0.77
1:A:41:GLU:O	1:A:42:LEU:HB3	1.81	0.77
1:A:9:ILE:CG2	1:A:10:PRO:HD3	2.13	0.77
1:A:4:HIS:CG	1:A:13:ALA:CB	2.65	0.77
1:A:7:ALA:CB	1:A:43:GLY:HA2	2.15	0.76
1:A:34:SER:O	1:A:35:SER:HB2	1.83	0.76
1:A:6:THR:O	1:A:7:ALA:HB3	1.83	0.76
1:B:5:THR:CG2	1:B:64:LYS:CG	2.64	0.76
1:B:25:ARG:HH11	1:B:58:THR:HG21	1.51	0.76
1:B:5:THR:HG23	1:B:64:LYS:CG	2.14	0.76
1:A:64:LYS:HG3	1:A:65:CYS:N	2.01	0.75
1:A:6:THR:HB	1:A:42:LEU:HG	1.68	0.75
1:A:47:THR:O	1:A:49:PRO:N	2.18	0.75

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:4:HIS:ND1	1:A:13:ALA:O	2.18	0.75
1:B:2:VAL:HG12	1:B:3:CYS:SG	2.26	0.75
1:A:7:ALA:HA	1:A:43:GLY:HA2	1.69	0.75
1:A:48:CYS:C	1:A:50:SER:N	2.39	0.74
1:A:22:LEU:HD11	1:A:61:SER:HB3	1.68	0.74
1:B:43:GLY:O	1:B:44:CYS:HB3	1.88	0.74
1:A:22:LEU:HD23	1:A:23:CYS:H	1.53	0.74
1:A:42:LEU:CG	1:A:66:ASN:ND2	2.50	0.74
1:B:5:THR:CG2	1:B:64:LYS:HG3	2.18	0.73
1:A:19:GLY:O	1:A:20:GLU:CB	2.36	0.73
1:A:7:ALA:HA	1:A:43:GLY:CA	2.18	0.73
1:A:4:HIS:ND1	1:A:13:ALA:C	2.47	0.72
1:A:19:GLY:O	1:A:20:GLU:CG	2.38	0.72
1:A:52:LYS:HB3	1:A:53:PRO:HD3	1.71	0.72
1:A:4:HIS:CE1	1:A:13:ALA:C	2.68	0.72
1:B:72:GLN:CG	1:B:72:GLN:O	2.38	0.72
1:A:22:LEU:CG	1:A:61:SER:HB2	2.19	0.72
1:A:2:VAL:CG1	1:A:22:LEU:HA	2.20	0.72
1:B:28:TRP:CH2	1:B:69:PRO:HD2	2.24	0.71
1:A:6:THR:HG22	1:A:7:ALA:N	2.02	0.71
1:A:42:LEU:CG	1:A:66:ASN:HD22	2.04	0.71
1:B:60:CYS:O	1:B:61:SER:HB3	1.89	0.71
1:B:24:TYR:CZ	1:B:49:PRO:CG	2.72	0.70
1:B:16:CYS:HB2	1:B:17:PRO:HD3	1.70	0.70
1:B:23:CYS:O	1:B:60:CYS:HB3	1.92	0.70
1:B:35:SER:O	1:B:36:ARG:HG3	1.92	0.70
1:A:53:PRO:C	1:A:54:TYR:O	2.35	0.69
1:B:43:GLY:O	1:B:44:CYS:CB	2.41	0.68
1:A:17:PRO:CD	1:A:44:CYS:SG	2.79	0.68
1:A:3:CYS:C	1:A:15:THR:HG22	2.17	0.68
1:B:25:ARG:HD2	1:B:66:ASN:CB	2.23	0.68
1:A:52:LYS:CB	1:A:53:PRO:HD3	2.22	0.68
1:B:25:ARG:HD3	1:B:58:THR:HG21	1.74	0.68
1:B:30:ASP:N	1:B:30:ASP:OD1	2.27	0.68
1:A:47:THR:O	1:A:47:THR:OG1	2.08	0.68
1:A:19:GLY:O	1:A:20:GLU:HB2	1.94	0.68
1:A:19:GLY:O	1:A:20:GLU:OE1	2.13	0.67
1:B:1:ILE:O	1:B:1:ILE:HG13	1.94	0.67
1:B:24:TYR:OH	1:B:49:PRO:HG2	1.95	0.67
1:B:67:HIS:O	1:B:69:PRO:HD3	1.94	0.67
1:A:12:SER:O	1:A:13:ALA:HB3	1.95	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:26:LYS:O	1:A:27:MET:HB2	1.93	0.66
1:B:5:THR:O	1:B:13:ALA:HA	1.93	0.66
1:B:6:THR:CG2	1:B:42:LEU:HD22	2.25	0.66
1:A:30:ASP:O	1:A:31:ALA:HB2	1.94	0.66
1:B:41:GLU:CA	1:B:42:LEU:HD12	2.24	0.66
1:A:2:VAL:CG1	1:A:22:LEU:H	2.08	0.65
1:A:7:ALA:CA	1:A:43:GLY:HA2	2.26	0.65
1:A:32:PHE:C	1:A:34:SER:H	2.04	0.65
1:A:9:ILE:CB	1:A:10:PRO:CD	2.40	0.65
1:A:27:MET:HE2	1:A:39:VAL:O	1.97	0.65
1:B:40:VAL:HB	1:B:42:LEU:HD11	1.77	0.65
1:A:13:ALA:O	1:A:15:THR:N	2.30	0.65
1:B:25:ARG:CD	1:B:66:ASN:HB3	2.26	0.65
1:A:26:LYS:O	1:A:41:GLU:HB3	1.96	0.65
1:A:69:PRO:O	1:A:71:ARG:HG3	1.96	0.65
1:A:4:HIS:ND1	1:A:13:ALA:CB	2.48	0.65
1:A:64:LYS:HG3	1:A:65:CYS:H	1.61	0.65
1:A:4:HIS:CE1	1:A:13:ALA:HB3	2.26	0.64
1:B:38:LYS:HD2	1:B:71:ARG:HG3	1.78	0.64
1:B:38:LYS:CD	1:B:71:ARG:CG	2.69	0.64
1:A:41:GLU:O	1:A:42:LEU:CB	2.45	0.64
1:B:6:THR:HG22	1:B:42:LEU:HB2	1.80	0.63
1:A:58:THR:OG1	1:A:59:CYS:N	2.31	0.63
1:B:22:LEU:HA	1:B:61:SER:HB2	1.79	0.63
1:B:17:PRO:CB	1:B:18:PRO:CD	2.74	0.63
1:A:1:ILE:C	1:A:2:VAL:HG22	2.22	0.63
1:B:48:CYS:O	1:B:49:PRO:C	2.42	0.63
1:A:4:HIS:ND1	1:A:13:ALA:CA	2.62	0.63
1:A:68:PRO:O	1:A:71:ARG:HD2	1.98	0.63
1:B:48:CYS:O	1:B:50:SER:N	2.32	0.62
1:A:19:GLY:C	1:A:20:GLU:CD	2.68	0.62
1:A:24:TYR:CD1	1:A:24:TYR:O	2.52	0.62
1:A:20:GLU:O	1:A:21:ASN:HB3	1.99	0.61
1:B:68:PRO:HD2	1:B:73:PRO:HD2	1.82	0.61
1:B:64:LYS:O	1:B:65:CYS:CB	2.49	0.60
1:A:16:CYS:SG	1:A:23:CYS:SG	2.99	0.60
1:A:42:LEU:HD23	1:A:42:LEU:N	2.15	0.60
1:B:6:THR:HG21	1:B:42:LEU:HD22	1.82	0.60
1:A:17:PRO:HB3	1:A:18:PRO:HD3	1.82	0.60
1:A:22:LEU:HD11	1:A:60:CYS:C	2.27	0.60
1:A:6:THR:HG21	1:A:42:LEU:HD21	1.84	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:48:CYS:O	1:A:49:PRO:C	2.44	0.60
1:A:42:LEU:CD2	1:A:42:LEU:N	2.65	0.59
1:B:56:GLU:O	1:B:57:VAL:CB	2.45	0.59
1:A:27:MET:CG	1:A:28:TRP:H	2.00	0.59
1:B:8:THR:O	1:B:9:ILE:O	2.21	0.59
1:B:50:SER:O	1:B:51:LYS:CB	2.49	0.59
1:B:57:VAL:O	1:B:58:THR:HB	2.02	0.59
1:B:64:LYS:O	1:B:65:CYS:HB2	2.02	0.59
1:A:3:CYS:HA	1:A:64:LYS:HA	1.85	0.59
1:A:29:CYS:O	1:A:29:CYS:SG	2.61	0.59
1:A:5:THR:HG21	1:A:66:ASN:H	1.68	0.58
1:B:9:ILE:O	1:B:11:SER:CA	2.52	0.58
1:B:24:TYR:CE1	1:B:49:PRO:HG2	2.38	0.58
1:B:72:GLN:O	1:B:72:GLN:HG3	2.01	0.58
1:A:4:HIS:CE1	1:A:13:ALA:CA	2.86	0.58
1:A:26:LYS:CG	1:A:57:VAL:CG1	2.58	0.58
1:B:4:HIS:O	1:B:5:THR:CG2	2.53	0.57
1:A:24:TYR:HE1	1:A:41:GLU:CG	2.16	0.57
1:A:68:PRO:HG2	1:A:71:ARG:NH2	2.19	0.57
1:B:52:LYS:HB3	1:B:53:PRO:HD3	1.73	0.57
1:A:26:LYS:O	1:A:27:MET:HB3	2.03	0.57
1:B:48:CYS:C	1:B:50:SER:N	2.56	0.57
1:B:42:LEU:HB3	1:B:66:ASN:OD1	2.04	0.57
1:B:2:VAL:HB	1:B:16:CYS:SG	2.45	0.57
1:A:5:THR:C	1:A:6:THR:O	2.48	0.57
1:A:52:LYS:CG	1:A:53:PRO:HD3	2.35	0.57
1:A:9:ILE:C	1:A:11:SER:N	2.61	0.56
1:A:6:THR:CG2	1:A:7:ALA:N	2.65	0.56
1:A:51:LYS:O	1:A:52:LYS:HD2	2.06	0.56
1:A:14:VAL:HG12	1:A:16:CYS:H	1.68	0.56
1:B:60:CYS:O	1:B:61:SER:HB2	2.04	0.56
1:B:25:ARG:NH2	1:B:28:TRP:HZ3	2.04	0.56
1:A:8:THR:O	1:A:9:ILE:HD12	2.05	0.56
1:A:60:CYS:O	1:A:61:SER:HB3	2.06	0.55
1:B:5:THR:CG2	1:B:64:LYS:HG2	2.36	0.55
1:A:30:ASP:O	1:A:31:ALA:CB	2.52	0.55
1:B:4:HIS:HA	1:B:13:ALA:HB1	1.88	0.55
1:B:9:ILE:CB	1:B:10:PRO:CD	2.62	0.55
1:A:68:PRO:O	1:A:68:PRO:HG2	2.07	0.55
1:A:2:VAL:HG11	1:A:22:LEU:C	2.32	0.55
1:A:22:LEU:O	1:A:23:CYS:SG	2.65	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:6:THR:HG23	1:B:42:LEU:HB2	1.85	0.54
1:A:45:ALA:O	1:A:46:ALA:HB3	2.07	0.54
1:B:9:ILE:C	1:B:11:SER:N	2.62	0.54
1:B:1:ILE:O	1:B:1:ILE:CG1	2.56	0.54
1:A:12:SER:C	1:A:14:VAL:N	2.56	0.53
1:A:51:LYS:O	1:A:52:LYS:CD	2.56	0.53
1:A:33:CYS:C	1:A:35:SER:H	2.14	0.53
1:A:41:GLU:O	1:A:42:LEU:HD22	2.07	0.53
1:A:6:THR:O	1:A:7:ALA:HB2	2.08	0.53
1:A:32:PHE:C	1:A:34:SER:N	2.66	0.53
1:B:7:ALA:HB2	1:B:43:GLY:HA2	1.91	0.52
1:A:41:GLU:C	1:A:42:LEU:HD23	2.32	0.52
1:B:21:ASN:OD1	1:B:21:ASN:C	2.52	0.52
1:A:22:LEU:C	1:A:23:CYS:SG	2.93	0.52
1:A:3:CYS:SG	1:A:16:CYS:SG	3.08	0.51
1:B:48:CYS:C	1:B:50:SER:H	2.18	0.51
1:A:24:TYR:CE1	1:A:51:LYS:HE2	2.34	0.51
1:A:9:ILE:HB	1:A:10:PRO:HD2	1.78	0.51
1:A:23:CYS:HB3	1:A:43:GLY:O	2.11	0.51
1:A:45:ALA:O	1:A:46:ALA:CB	2.59	0.51
1:B:22:LEU:CB	1:B:61:SER:HB2	2.41	0.51
1:B:4:HIS:C	1:B:5:THR:HG23	2.36	0.50
1:A:64:LYS:O	1:A:65:CYS:CB	2.59	0.50
1:A:64:LYS:O	1:A:65:CYS:HB2	2.11	0.50
1:A:41:GLU:CA	1:A:42:LEU:HD22	2.41	0.50
1:A:70:LYS:HZ2	1:A:70:LYS:CB	2.10	0.50
1:B:4:HIS:CG	1:B:13:ALA:CB	2.88	0.50
1:A:24:TYR:CE1	1:A:41:GLU:CG	2.94	0.50
1:A:24:TYR:CG	1:A:51:LYS:HE2	2.35	0.50
1:B:25:ARG:HB2	1:B:58:THR:HG22	1.93	0.50
1:B:67:HIS:O	1:B:69:PRO:CD	2.59	0.49
1:B:22:LEU:HA	1:B:61:SER:CB	2.42	0.49
1:A:7:ALA:HB2	1:A:43:GLY:HA2	1.94	0.49
1:A:22:LEU:HG	1:A:61:SER:HB2	1.92	0.49
1:B:6:THR:HG22	1:B:42:LEU:HD22	1.93	0.49
1:B:22:LEU:C	1:B:22:LEU:CD2	2.86	0.49
1:A:54:TYR:O	1:A:55:GLU:C	2.47	0.49
1:B:19:GLY:O	1:B:20:GLU:HB2	2.12	0.49
1:A:22:LEU:HD23	1:A:23:CYS:C	2.37	0.48
1:A:6:THR:CG2	1:A:7:ALA:H	1.96	0.48
1:B:23:CYS:CB	1:B:60:CYS:SG	2.90	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:4:HIS:O	1:B:5:THR:HG23	2.14	0.48
1:B:24:TYR:CE2	1:B:49:PRO:HD2	2.48	0.48
1:B:22:LEU:C	1:B:22:LEU:HD23	2.38	0.48
1:A:7:ALA:HA	1:A:43:GLY:HA3	1.94	0.47
1:B:26:LYS:O	1:B:27:MET:HG3	2.14	0.47
1:B:21:ASN:OD1	1:B:22:LEU:HD13	2.14	0.47
1:B:47:THR:C	1:B:49:PRO:N	2.69	0.47
1:A:22:LEU:CD2	1:A:23:CYS:H	2.25	0.47
1:A:22:LEU:CD2	1:A:23:CYS:O	2.58	0.47
1:B:22:LEU:HG	1:B:48:CYS:HB2	1.95	0.47
1:B:25:ARG:CG	1:B:66:ASN:HB3	2.44	0.47
1:A:34:SER:O	1:A:35:SER:CB	2.56	0.47
1:A:16:CYS:SG	1:A:17:PRO:HD2	2.55	0.47
1:A:27:MET:HG2	1:A:39:VAL:O	2.14	0.47
1:A:41:GLU:HG3	1:A:42:LEU:N	2.30	0.47
1:A:54:TYR:C	1:A:55:GLU:O	2.58	0.47
1:B:16:CYS:HB2	1:B:17:PRO:CD	2.32	0.47
1:B:4:HIS:CB	1:B:64:LYS:NZ	2.66	0.47
1:B:51:LYS:C	1:B:52:LYS:HG2	2.40	0.47
1:A:8:THR:C	1:A:9:ILE:HD12	2.40	0.46
1:A:53:PRO:O	1:A:54:TYR:C	2.54	0.46
1:B:26:LYS:HB2	1:B:57:VAL:HG23	1.96	0.46
1:A:72:GLN:HA	1:A:73:PRO:HD2	1.67	0.46
1:A:5:THR:HG21	1:A:66:ASN:N	2.30	0.46
1:B:27:MET:SD	1:B:39:VAL:O	2.73	0.46
1:B:41:GLU:N	1:B:42:LEU:HD12	2.30	0.46
1:B:63:ASP:HB3	1:B:64:LYS:H	1.29	0.46
1:B:62:THR:O	1:B:63:ASP:CB	2.64	0.46
1:A:42:LEU:C	1:A:66:ASN:ND2	2.74	0.46
1:B:22:LEU:HD23	1:B:22:LEU:O	2.16	0.46
1:A:4:HIS:O	1:A:64:LYS:HD3	2.16	0.46
1:A:50:SER:C	1:A:51:LYS:CG	2.81	0.46
1:B:42:LEU:HD23	1:B:66:ASN:O	2.16	0.45
1:A:22:LEU:HD12	1:A:61:SER:HB3	1.70	0.45
1:B:24:TYR:CD2	1:B:49:PRO:HD2	2.52	0.45
1:B:7:ALA:HA	1:B:42:LEU:O	2.17	0.45
1:A:41:GLU:N	1:A:42:LEU:HD22	2.32	0.45
1:A:24:TYR:CG	1:A:51:LYS:CE	2.97	0.45
1:B:22:LEU:CD2	1:B:22:LEU:O	2.64	0.45
1:B:22:LEU:CA	1:B:61:SER:HB2	2.45	0.45
1:A:4:HIS:HA	1:A:13:ALA:HA	1.99	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:60:CYS:HB3	1:A:61:SER:H	1.62	0.45
1:B:4:HIS:O	1:B:64:LYS:NZ	2.37	0.45
1:B:28:TRP:O	1:B:37:GLY:HA2	2.17	0.44
1:A:13:ALA:O	1:A:14:VAL:C	2.60	0.44
1:A:39:VAL:HA	2:A:200:HOH:O	2.17	0.44
1:A:26:LYS:CD	1:A:57:VAL:HG13	2.43	0.44
1:A:22:LEU:HD23	1:A:23:CYS:N	2.26	0.44
1:A:26:LYS:HE2	1:A:54:TYR:CE2	2.52	0.44
1:B:67:HIS:HA	1:B:68:PRO:HD3	1.82	0.44
1:B:48:CYS:N	1:B:49:PRO:CD	2.78	0.44
1:B:25:ARG:CD	1:B:66:ASN:CB	2.91	0.44
1:A:24:TYR:O	1:A:42:LEU:HA	2.17	0.43
1:A:59:CYS:O	1:A:60:CYS:O	2.36	0.43
1:A:42:LEU:CA	1:A:66:ASN:ND2	2.77	0.43
1:B:57:VAL:O	1:B:58:THR:CB	2.66	0.43
1:B:25:ARG:HG2	1:B:66:ASN:HB3	2.01	0.43
1:B:47:THR:O	1:B:49:PRO:N	2.50	0.43
1:B:4:HIS:HA	1:B:13:ALA:CB	2.48	0.43
1:B:38:LYS:C	1:B:39:VAL:HG22	2.44	0.43
1:A:52:LYS:HG3	1:A:53:PRO:HD3	2.00	0.43
1:A:68:PRO:O	1:A:68:PRO:CG	2.65	0.43
1:A:12:SER:O	1:A:14:VAL:N	2.50	0.43
1:A:24:TYR:HD1	1:A:51:LYS:HE2	1.58	0.43
1:A:42:LEU:HB2	1:A:66:ASN:HD22	0.38	0.43
1:A:43:GLY:O	1:A:44:CYS:CB	2.58	0.43
1:B:4:HIS:O	1:B:64:LYS:HG3	2.19	0.43
1:B:29:CYS:O	1:B:31:ALA:N	2.51	0.43
1:A:42:LEU:HG	1:A:66:ASN:ND2	2.33	0.42
1:B:43:GLY:C	1:B:44:CYS:SG	3.02	0.42
1:B:14:VAL:HG12	1:B:16:CYS:N	2.34	0.42
1:B:71:ARG:HB3	1:B:72:GLN:H	1.36	0.42
1:B:19:GLY:O	1:B:20:GLU:CB	2.67	0.42
1:B:4:HIS:C	1:B:5:THR:CG2	2.92	0.42
1:B:27:MET:SD	1:B:40:VAL:HA	2.60	0.42
1:B:52:LYS:CG	1:B:53:PRO:HD2	2.49	0.42
1:A:5:THR:CG2	1:A:67:HIS:H	2.33	0.41
1:A:50:SER:O	1:A:51:LYS:CB	2.67	0.41
1:B:46:ALA:HB1	1:B:47:THR:HG23	2.03	0.41
1:A:22:LEU:HD11	1:A:61:SER:CB	2.30	0.41
1:B:72:GLN:O	1:B:72:GLN:HG2	2.16	0.41
1:B:59:CYS:C	1:B:60:CYS:O	2.64	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:2:VAL:HB	1:A:23:CYS:SG	2.60	0.41
1:B:38:LYS:HD2	1:B:71:ARG:CG	2.45	0.41
1:B:64:LYS:HE2	1:B:64:LYS:HB2	1.38	0.41
1:B:68:PRO:O	1:B:69:PRO:C	2.63	0.41
1:A:55:GLU:HB3	1:A:56:GLU:HG2	2.03	0.40
1:B:6:THR:HG23	1:B:42:LEU:O	2.22	0.40

All (9) 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:20:GLU:O	1:B:17:PRO:CA[4_467]	1.29	0.91
1:B:11:SER:OG	2:A:211:HOH:O[3_655]	1.51	0.69
1:B:51:LYS:NZ	1:B:69:PRO:O[1_556]	1.65	0.55
1:A:40:VAL:O	1:A:73:PRO:CG[1_556]	1.93	0.27
1:A:20:GLU:O	1:B:17:PRO:CB[4_467]	2.00	0.20
1:A:8:THR:O	1:B:9:ILE:CG2[3_646]	2.01	0.19
1:B:6:THR:OG1	2:A:211:HOH:O[3_655]	2.01	0.19
1:A:32:PHE:CZ	1:B:32:PHE:CE2[3_646]	2.11	0.09
1:A:73:PRO:O	2:A:209:HOH:O[1_554]	2.16	0.04

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	72/74 (97%)	10 (14%)	23 (32%)	39 (54%)	0	0
1	B	72/74 (97%)	15 (21%)	24 (33%)	33 (46%)	0	0
All	All	144/148 (97%)	25 (17%)	47 (33%)	72 (50%)	0	0

All (72) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	2	VAL
1	A	6	THR
1	A	7	ALA
1	A	9	ILE
1	A	14	VAL
1	A	16	CYS
1	A	20	GLU
1	A	21	ASN
1	A	27	MET
1	A	28	TRP
1	A	31	ALA
1	A	35	SER
1	A	42	LEU
1	A	44	CYS
1	A	45	ALA
1	A	46	ALA
1	A	49	PRO
1	A	50	SER
1	A	51	LYS
1	A	54	TYR
1	A	55	GLU
1	A	58	THR
1	A	60	CYS
1	A	61	SER
1	A	63	ASP
1	A	65	CYS
1	A	69	PRO
1	A	73	PRO
1	B	7	ALA
1	B	9	ILE
1	B	10	PRO
1	B	17	PRO
1	B	31	ALA
1	B	39	VAL
1	B	44	CYS
1	B	46	ALA
1	B	47	THR
1	B	50	SER
1	B	51	LYS
1	B	52	LYS
1	B	53	PRO
1	B	60	CYS
1	B	61	SER

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Mol	Chain	Res	Type
1	B	63	ASP
1	B	65	CYS
1	B	72	GLN
1	A	17	PRO
1	A	18	PRO
1	A	22	LEU
1	A	30	ASP
1	B	3	CYS
1	B	16	CYS
1	B	20	GLU
1	B	22	LEU
1	B	30	ASP
1	B	35	SER
1	B	36	ARG
1	B	58	THR
1	A	15	THR
1	A	36	ARG
1	B	8	THR
1	B	34	SER
1	B	56	GLU
1	B	69	PRO
1	A	52	LYS
1	A	68	PRO
1	B	68	PRO
1	B	73	PRO
1	A	37	GLY
1	A	48	CYS
1	A	67	HIS
1	B	48	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	65/65 (100%)	33 (51%)	32 (49%)	0 0
1	B	65/65 (100%)	36 (55%)	29 (45%)	0 0

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
All	All	130/130 (100%)	69 (53%)	61 (47%)	0 0

All (61) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	1	ILE
1	A	2	VAL
1	A	4	HIS
1	A	8	THR
1	A	9	ILE
1	A	12	SER
1	A	16	CYS
1	A	20	GLU
1	A	21	ASN
1	A	22	LEU
1	A	24	TYR
1	A	27	MET
1	A	30	ASP
1	A	38	LYS
1	A	39	VAL
1	A	41	GLU
1	A	42	LEU
1	A	47	THR
1	A	53	PRO
1	A	54	TYR
1	A	57	VAL
1	A	59	CYS
1	A	60	CYS
1	A	61	SER
1	A	62	THR
1	A	63	ASP
1	A	64	LYS
1	A	67	HIS
1	A	68	PRO
1	A	70	LYS
1	A	72	GLN
1	A	73	PRO
1	B	1	ILE
1	B	2	VAL
1	B	6	THR
1	B	9	ILE
1	B	12	SER

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Mol	Chain	Res	Type
1	B	15	THR
1	B	20	GLU
1	B	21	ASN
1	B	22	LEU
1	B	27	MET
1	B	30	ASP
1	B	32	PHE
1	B	33	CYS
1	B	38	LYS
1	B	39	VAL
1	B	40	VAL
1	B	42	LEU
1	B	47	THR
1	B	52	LYS
1	B	53	PRO
1	B	54	TYR
1	B	57	VAL
1	B	58	THR
1	B	60	CYS
1	B	63	ASP
1	B	65	CYS
1	B	66	ASN
1	B	70	LYS
1	B	71	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (2) such sidechains are listed below:

Mol	Chain	Res	Type
1	B	66	ASN
1	B	67	HIS

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.