



# Full wwPDB X-ray Structure Validation Report ⓘ

Mar 4, 2026 – 10:12 PM UTC

PDB ID : 4CMS / pdb\_00004cms  
Title : X-RAY ANALYSES OF ASPARTIC PROTEINASES IV. STRUCTURE AND REFINEMENT AT 2.2 ANGSTROMS RESOLUTION OF BOVINE CHYMOSIN  
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Deposited on : 1991-11-01  
Resolution : 2.20 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](mailto: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>.

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The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity : 4-5-2 with Phenix2.0  
Xtrriage (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

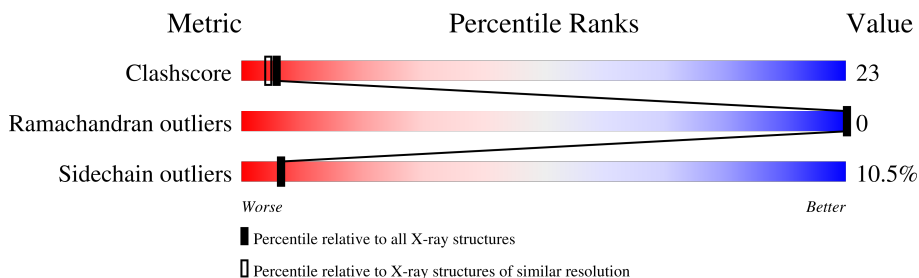
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.20 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	6851 (2.20-2.20)
Ramachandran outliers	187476	6768 (2.20-2.20)
Sidechain outliers	187428	6769 (2.20-2.20)

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  $\geq 3$ , 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	323	 37% 37% 23% ..

## 2 Entry composition [i](#)

There are 2 unique types of molecules in this entry. The entry contains 2618 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 CHYMOSIN B.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	320	2487	1585	395	493	14	0	0	0

- Molecule 2 is water.

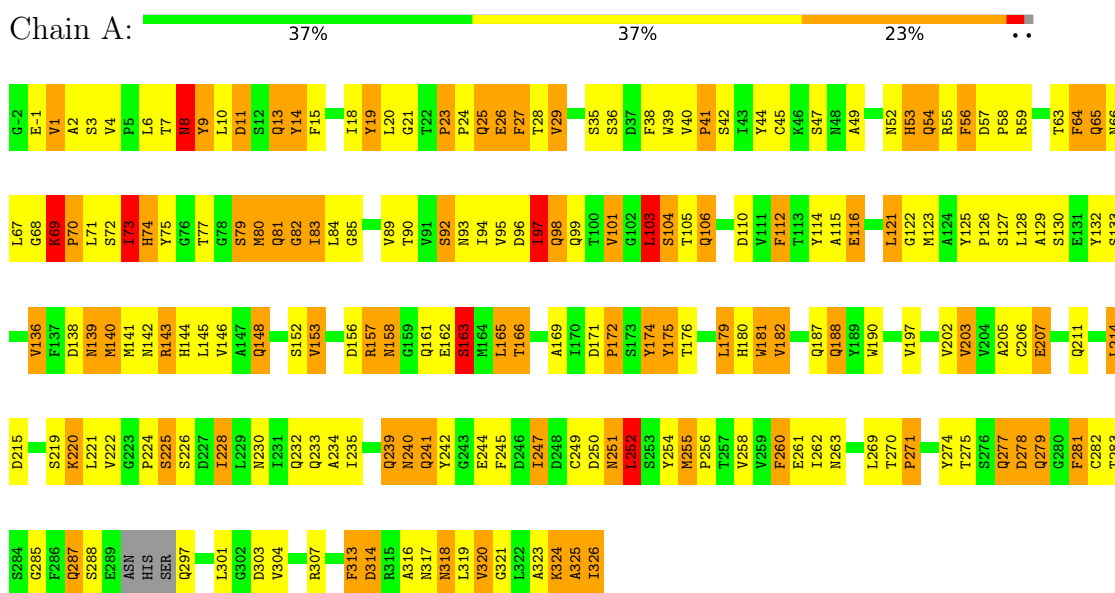
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	131	Total	O	0	0
			131	131		

### 3 Residue-property plots [i](#)

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

Note EDS was not executed.

- Molecule 1: CHYMOSIN B



## 4 Data and refinement statistics

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

Property	Value	Source
Space group	I 2 2 2	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	79.98Å 114.12Å 72.76Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	8.00 – 2.20	Depositor
% Data completeness (in resolution range)	(Not available) (8.00-2.20)	Depositor
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
Refinement program	RESTRAIN	Depositor
R, $R_{free}$	0.158 , (Not available)	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	2618	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	0.0	wwPDB-VP

## 5 Model quality i

### 5.1 Standard geometry i

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	1.59	42/2548 (1.6%)	2.56	231/3469 (6.7%)

All (42) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	144	HIS	CE1-NE2	8.32	1.40	1.32
1	A	74	HIS	ND1-CE1	7.89	1.40	1.32
1	A	74	HIS	CE1-NE2	7.83	1.40	1.32
1	A	180	HIS	ND1-CE1	7.74	1.40	1.32
1	A	180	HIS	CE1-NE2	7.72	1.40	1.32
1	A	4	VAL	N-CA	7.42	1.52	1.46
1	A	144	HIS	ND1-CE1	7.10	1.39	1.32
1	A	85	GLY	N-CA	7.01	1.52	1.45
1	A	80	MET	N-CA	6.98	1.54	1.45
1	A	180	HIS	N-CA	6.71	1.54	1.46
1	A	297	GLN	CD-OE1	6.19	1.35	1.23
1	A	181	TRP	NE1-CE2	-6.18	1.30	1.37
1	A	39	TRP	NE1-CE2	-6.16	1.30	1.37
1	A	106	GLN	CD-OE1	6.02	1.34	1.23
1	A	233	GLN	CD-OE1	5.99	1.34	1.23
1	A	81	GLN	CD-OE1	5.95	1.34	1.23
1	A	211	GLN	CD-OE1	5.92	1.34	1.23
1	A	129	ALA	N-CA	5.91	1.53	1.45
1	A	161	GLN	CD-OE1	5.90	1.34	1.23
1	A	230	ASN	CG-OD1	5.73	1.34	1.23
1	A	241	GLN	CD-OE1	5.71	1.34	1.23
1	A	13	GLN	CD-OE1	5.71	1.34	1.23
1	A	54	GLN	CD-OE1	5.69	1.34	1.23
1	A	279	GLN	CD-OE1	5.67	1.34	1.23
1	A	239	GLN	CD-OE1	5.65	1.34	1.23
1	A	188	GLN	CD-OE1	5.61	1.34	1.23
1	A	277	GLN	CD-OE1	5.60	1.34	1.23
1	A	25	GLN	CD-OE1	5.56	1.34	1.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	29	VAL	CA-CB	-5.52	1.47	1.54
1	A	148	GLN	CD-OE1	5.44	1.33	1.23
1	A	65	GLN	CD-OE1	5.37	1.33	1.23
1	A	82	GLY	N-CA	5.36	1.51	1.45
1	A	187	GLN	CD-OE1	5.29	1.33	1.23
1	A	142	ASN	CG-OD1	5.28	1.33	1.23
1	A	247	ILE	CA-CB	-5.20	1.47	1.54
1	A	52	ASN	CG-OD1	5.18	1.33	1.23
1	A	53	HIS	ND1-CE1	5.17	1.37	1.32
1	A	59	ARG	CD-NE	5.15	1.53	1.46
1	A	53	HIS	CE1-NE2	5.14	1.37	1.32
1	A	29	VAL	N-CA	-5.12	1.40	1.46
1	A	182	VAL	CA-C	-5.07	1.48	1.52
1	A	318	ASN	CG-OD1	5.05	1.33	1.23

All (231) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	121	LEU	CA-C-N	12.54	133.11	120.31
1	A	121	LEU	C-N-CA	12.54	133.11	120.31
1	A	240	ASN	CA-C-N	11.06	136.21	120.28
1	A	240	ASN	C-N-CA	11.06	136.21	120.28
1	A	106	GLN	OE1-CD-NE2	-10.08	112.52	122.60
1	A	80	MET	CA-C-O	-9.45	110.09	121.06
1	A	251	ASN	CA-CB-CG	-9.43	103.17	112.60
1	A	40	VAL	O-C-N	9.07	128.07	121.72
1	A	263	ASN	CA-CB-CG	8.79	121.39	112.60
1	A	27	PHE	CA-CB-CG	-8.77	105.03	113.80
1	A	158	ASN	CA-C-N	8.72	138.50	121.41
1	A	158	ASN	C-N-CA	8.72	138.50	121.41
1	A	141	MET	CG-SD-CE	8.67	119.97	100.90
1	A	1	VAL	CA-CB-CG1	8.63	125.08	110.40
1	A	179	LEU	CA-C-N	-8.58	110.89	122.99
1	A	179	LEU	C-N-CA	-8.58	110.89	122.99
1	A	74	HIS	CA-CB-CG	-8.46	105.34	113.80
1	A	80	MET	N-CA-C	-8.26	96.42	109.23
1	A	234	ALA	N-CA-C	8.24	121.18	111.71
1	A	29	VAL	CA-CB-CG1	8.09	124.15	110.40
1	A	59	ARG	CD-NE-CZ	-8.08	113.09	124.40
1	A	41	PRO	CA-C-N	8.01	137.02	122.92
1	A	41	PRO	C-N-CA	8.01	137.02	122.92
1	A	19	TYR	CA-CB-CG	-8.01	99.48	113.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	65	GLN	N-CA-C	7.76	120.20	107.23
1	A	-1	GLU	CA-C-O	7.69	130.41	121.49
1	A	252	LEU	CA-C-N	7.68	130.42	120.44
1	A	252	LEU	C-N-CA	7.68	130.42	120.44
1	A	29	VAL	O-C-N	-7.66	115.14	123.18
1	A	143	ARG	CD-NE-CZ	-7.54	113.84	124.40
1	A	138	ASP	CA-CB-CG	-7.43	105.17	112.60
1	A	176	THR	CA-CB-OG1	7.40	120.69	109.60
1	A	56	PHE	CA-CB-CG	-7.35	106.45	113.80
1	A	-1	GLU	N-CA-C	7.32	119.57	109.18
1	A	321	GLY	CA-C-O	-7.32	113.77	120.94
1	A	28	THR	CA-C-N	7.30	132.24	123.19
1	A	28	THR	C-N-CA	7.30	132.24	123.19
1	A	97	ILE	O-C-N	-7.28	113.63	122.59
1	A	97	ILE	CA-C-O	7.25	130.38	121.54
1	A	225	SER	O-C-N	7.22	129.60	122.09
1	A	202	VAL	CA-CB-CG2	7.21	122.65	110.40
1	A	258	VAL	CA-C-N	-7.19	113.54	123.10
1	A	258	VAL	C-N-CA	-7.19	113.54	123.10
1	A	139	ASN	CA-CB-CG	-7.18	105.42	112.60
1	A	69	LYS	CA-C-O	7.17	129.99	120.16
1	A	222	VAL	CA-CB-CG2	7.13	122.52	110.40
1	A	165	LEU	CA-C-N	7.10	133.19	123.11
1	A	165	LEU	C-N-CA	7.10	133.19	123.11
1	A	79	SER	CA-C-N	-7.06	110.64	122.29
1	A	79	SER	C-N-CA	-7.06	110.64	122.29
1	A	80	MET	O-C-N	7.04	131.44	123.27
1	A	101	VAL	CA-CB-CG2	7.01	122.32	110.40
1	A	278	ASP	CA-CB-CG	-6.99	105.61	112.60
1	A	301	LEU	CA-C-O	-6.98	113.44	120.98
1	A	21	GLY	CA-C-N	6.97	132.22	122.74
1	A	21	GLY	C-N-CA	6.97	132.22	122.74
1	A	172	PRO	CA-C-N	6.90	134.84	121.18
1	A	172	PRO	C-N-CA	6.90	134.84	121.18
1	A	55	ARG	CA-CB-CG	-6.89	100.32	114.10
1	A	40	VAL	CA-CB-CG2	6.89	122.11	110.40
1	A	98	GLN	CB-CG-CD	-6.85	100.96	112.60
1	A	73	ILE	O-C-N	-6.83	115.31	123.02
1	A	136	VAL	CA-CB-CG2	6.82	121.99	110.40
1	A	303	ASP	CA-CB-CG	-6.79	105.81	112.60
1	A	29	VAL	CA-C-O	6.73	127.61	120.48
1	A	47	SER	O-C-N	-6.68	114.27	122.82

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	54	GLN	CA-C-O	-6.67	113.08	120.69
1	A	8	ASN	N-CA-C	6.66	119.38	108.52
1	A	141	MET	CA-C-N	6.63	129.83	120.28
1	A	141	MET	C-N-CA	6.63	129.83	120.28
1	A	95	VAL	N-CA-C	6.63	117.39	107.51
1	A	157	ARG	CA-C-N	6.56	134.06	121.54
1	A	157	ARG	C-N-CA	6.56	134.06	121.54
1	A	162	GLU	N-CA-C	6.55	120.97	112.92
1	A	9	TYR	CA-C-N	6.51	132.11	122.74
1	A	9	TYR	C-N-CA	6.51	132.11	122.74
1	A	314	ASP	CB-CA-C	6.49	122.39	111.22
1	A	75	TYR	O-C-N	-6.45	114.60	123.12
1	A	122	GLY	CA-C-O	-6.45	115.77	121.58
1	A	166	THR	CB-CA-C	6.41	121.24	110.79
1	A	175	TYR	CA-C-N	6.41	131.57	122.09
1	A	175	TYR	C-N-CA	6.41	131.57	122.09
1	A	263	ASN	CB-CA-C	6.35	121.07	111.80
1	A	153	VAL	CA-CB-CG2	6.34	121.18	110.40
1	A	262	ILE	O-C-N	6.34	129.77	123.18
1	A	110	ASP	O-C-N	6.33	131.13	122.46
1	A	1	VAL	CA-C-O	6.32	126.65	120.27
1	A	171	ASP	CA-CB-CG	-6.32	106.28	112.60
1	A	225	SER	CA-C-N	6.27	128.59	120.44
1	A	225	SER	C-N-CA	6.27	128.59	120.44
1	A	3	SER	CA-C-N	-6.25	116.37	123.25
1	A	3	SER	C-N-CA	-6.25	116.37	123.25
1	A	81	GLN	OE1-CD-NE2	-6.25	116.35	122.60
1	A	260	PHE	CA-CB-CG	-6.25	107.55	113.80
1	A	40	VAL	CA-C-O	-6.25	113.45	121.13
1	A	241	GLN	CA-C-N	6.24	133.68	122.38
1	A	241	GLN	C-N-CA	6.24	133.68	122.38
1	A	176	THR	O-C-N	-6.22	115.95	123.16
1	A	211	GLN	OE1-CD-NE2	-6.21	116.39	122.60
1	A	121	LEU	CA-C-O	-6.20	113.89	120.40
1	A	65	GLN	N-CA-CB	6.19	120.88	110.79
1	A	230	ASN	CA-CB-CG	-6.14	106.46	112.60
1	A	180	HIS	CB-CG-CD2	-6.11	123.25	131.20
1	A	313	PHE	CA-CB-CG	-6.11	107.69	113.80
1	A	133	SER	CA-C-N	6.10	133.22	123.46
1	A	133	SER	C-N-CA	6.10	133.22	123.46
1	A	222	VAL	O-C-N	-6.08	116.49	122.93
1	A	169	ALA	N-CA-C	6.07	118.29	109.07

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	317	ASN	OD1-CG-ND2	-6.05	116.55	122.60
1	A	161	GLN	CA-C-N	6.04	132.31	122.65
1	A	161	GLN	C-N-CA	6.04	132.31	122.65
1	A	220	LYS	CA-C-N	6.03	131.28	122.41
1	A	220	LYS	C-N-CA	6.03	131.28	122.41
1	A	130	SER	O-C-N	-6.02	115.71	122.75
1	A	99	GLN	OE1-CD-NE2	-5.98	116.62	122.60
1	A	203	VAL	N-CA-CB	-5.98	105.06	111.46
1	A	7	THR	CA-C-N	-5.97	114.70	123.05
1	A	7	THR	C-N-CA	-5.97	114.70	123.05
1	A	79	SER	O-C-N	-5.95	115.92	123.24
1	A	80	MET	CA-C-N	5.95	131.56	122.93
1	A	80	MET	C-N-CA	5.95	131.56	122.93
1	A	176	THR	CA-CB-CG2	5.93	120.59	110.50
1	A	176	THR	CB-CA-C	5.93	119.31	109.53
1	A	318	ASN	CB-CA-C	-5.92	102.98	112.09
1	A	26	GLU	CB-CG-CD	-5.90	102.57	112.60
1	A	180	HIS	CA-CB-CG	-5.89	107.91	113.80
1	A	8	ASN	N-CA-CB	5.89	119.79	110.55
1	A	258	VAL	CB-CA-C	5.88	118.83	110.84
1	A	123	MET	CA-C-N	5.86	132.44	122.12
1	A	123	MET	C-N-CA	5.86	132.44	122.12
1	A	29	VAL	CA-C-N	-5.85	114.40	122.30
1	A	29	VAL	C-N-CA	-5.85	114.40	122.30
1	A	321	GLY	CA-C-N	5.84	132.15	122.33
1	A	321	GLY	C-N-CA	5.84	132.15	122.33
1	A	85	GLY	CA-C-O	-5.84	114.75	121.46
1	A	105	THR	N-CA-C	-5.83	106.70	113.88
1	A	1	VAL	CB-CA-C	5.83	118.29	110.42
1	A	112	PHE	CA-C-N	5.83	128.89	120.79
1	A	112	PHE	C-N-CA	5.83	128.89	120.79
1	A	271	PRO	CA-C-N	5.83	128.01	120.44
1	A	271	PRO	C-N-CA	5.83	128.01	120.44
1	A	1	VAL	O-C-N	-5.81	117.13	123.18
1	A	49	ALA	CA-C-N	5.81	128.34	120.44
1	A	49	ALA	C-N-CA	5.81	128.34	120.44
1	A	301	LEU	CA-C-N	5.81	128.94	122.55
1	A	301	LEU	C-N-CA	5.81	128.94	122.55
1	A	70	PRO	CA-N-CD	5.77	120.08	112.00
1	A	25	GLN	CA-C-N	-5.76	114.77	122.72
1	A	25	GLN	C-N-CA	-5.76	114.77	122.72
1	A	190	TRP	O-C-N	5.76	129.91	122.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	317	ASN	O-C-N	5.71	128.94	122.20
1	A	320	VAL	CA-C-N	-5.70	117.08	122.66
1	A	320	VAL	C-N-CA	-5.70	117.08	122.66
1	A	287	GLN	CB-CG-CD	-5.70	102.92	112.60
1	A	103	LEU	CA-C-O	-5.69	114.42	120.40
1	A	35	SER	CA-C-N	5.69	131.31	122.26
1	A	35	SER	C-N-CA	5.69	131.31	122.26
1	A	325	ALA	O-C-N	5.66	129.35	122.96
1	A	64	PHE	CA-CB-CG	-5.65	108.15	113.80
1	A	83	ILE	CA-C-O	-5.65	114.35	120.67
1	A	215	ASP	N-CA-C	5.64	119.68	107.49
1	A	161	GLN	OE1-CD-NE2	-5.64	116.96	122.60
1	A	106	GLN	CA-C-N	-5.64	116.65	122.85
1	A	106	GLN	C-N-CA	-5.64	116.65	122.85
1	A	182	VAL	N-CA-C	5.62	116.59	107.71
1	A	263	ASN	OD1-CG-ND2	-5.60	117.00	122.60
1	A	23	PRO	CA-C-N	5.59	126.45	120.13
1	A	23	PRO	C-N-CA	5.59	126.45	120.13
1	A	224	PRO	CA-C-N	5.52	127.99	120.54
1	A	224	PRO	C-N-CA	5.52	127.99	120.54
1	A	75	TYR	CA-C-O	5.51	126.28	120.33
1	A	245	PHE	CA-CB-CG	-5.45	108.35	113.80
1	A	104	SER	CA-C-O	5.44	127.18	121.19
1	A	35	SER	CA-C-O	-5.44	115.41	121.23
1	A	77	THR	CA-C-N	-5.44	117.33	122.66
1	A	77	THR	C-N-CA	-5.44	117.33	122.66
1	A	250	ASP	CA-C-N	5.41	131.06	120.99
1	A	250	ASP	C-N-CA	5.41	131.06	120.99
1	A	65	GLN	CA-C-O	5.38	126.94	120.27
1	A	66	ASN	O-C-N	5.37	129.44	122.89
1	A	320	VAL	CA-CB-CG2	5.37	119.52	110.40
1	A	207	GLU	CB-CA-C	5.36	117.88	110.16
1	A	14	TYR	CA-C-O	5.36	126.19	120.46
1	A	190	TRP	CA-C-O	-5.35	115.59	121.58
1	A	228	ILE	O-C-N	-5.35	116.47	121.87
1	A	277	GLN	CA-C-N	-5.33	115.53	123.11
1	A	277	GLN	C-N-CA	-5.33	115.53	123.11
1	A	92	SER	CA-C-N	-5.32	113.83	122.65
1	A	92	SER	C-N-CA	-5.32	113.83	122.65
1	A	66	ASN	CA-C-N	5.29	130.97	121.66
1	A	66	ASN	C-N-CA	5.29	130.97	121.66
1	A	174	TYR	CA-CB-CG	-5.29	104.39	113.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	233	GLN	OE1-CD-NE2	-5.27	117.33	122.60
1	A	320	VAL	O-C-N	-5.27	117.18	123.03
1	A	258	VAL	O-C-N	-5.26	117.19	123.03
1	A	45	CYS	CA-C-N	-5.26	114.40	122.60
1	A	45	CYS	C-N-CA	-5.26	114.40	122.60
1	A	97	ILE	CA-C-N	-5.25	115.04	122.34
1	A	97	ILE	C-N-CA	-5.25	115.04	122.34
1	A	97	ILE	CA-CB-CG2	5.25	119.43	110.50
1	A	96	ASP	CA-CB-CG	5.25	117.85	112.60
1	A	64	PHE	CA-C-N	5.22	129.76	121.72
1	A	64	PHE	C-N-CA	5.22	129.76	121.72
1	A	304	VAL	CA-CB-CG2	5.21	119.25	110.40
1	A	249	CYS	CA-C-N	5.19	129.38	120.71
1	A	249	CYS	C-N-CA	5.19	129.38	120.71
1	A	36	SER	O-C-N	-5.19	115.97	122.35
1	A	224	PRO	N-CA-C	5.18	119.22	111.14
1	A	206	CYS	N-CA-C	-5.18	104.75	111.74
1	A	38	PHE	O-C-N	-5.17	117.14	123.30
1	A	29	VAL	CA-CB-CG2	5.16	119.16	110.40
1	A	255	MET	CA-C-N	5.13	126.26	120.66
1	A	255	MET	C-N-CA	5.13	126.26	120.66
1	A	163	SER	N-CA-C	5.11	117.89	110.42
1	A	187	GLN	OE1-CD-NE2	-5.11	117.49	122.60
1	A	114	TYR	CA-C-N	5.11	128.46	120.75
1	A	114	TYR	C-N-CA	5.11	128.46	120.75
1	A	74	HIS	CA-C-N	5.11	130.11	122.86
1	A	74	HIS	C-N-CA	5.11	130.11	122.86
1	A	129	ALA	N-CA-C	-5.08	103.69	110.55
1	A	174	TYR	CA-C-O	5.08	125.36	119.32
1	A	44	TYR	N-CA-CB	5.06	118.62	110.42
1	A	148	GLN	N-CA-CB	5.06	120.35	111.55
1	A	140	MET	CA-C-N	5.05	127.31	120.44
1	A	140	MET	C-N-CA	5.05	127.31	120.44
1	A	66	ASN	N-CA-C	-5.04	102.82	110.28
1	A	44	TYR	CA-C-N	5.03	129.09	122.30
1	A	44	TYR	C-N-CA	5.03	129.09	122.30
1	A	163	SER	O-C-N	-5.00	117.51	123.11
1	A	261	GLU	CA-C-N	-5.00	115.88	122.98
1	A	261	GLU	C-N-CA	-5.00	115.88	122.98

There are no chirality outliers.

There are no planarity outliers.

## 5.2 Too-close contacts

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2487	0	2365	112	0
2	A	131	0	0	6	0
All	All	2618	0	2365	112	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 23.

All (112) 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:10:LEU:O	1:A:11:ASP:CB	2.06	1.03
1:A:10:LEU:O	1:A:11:ASP:HB2	1.22	1.02
1:A:278:ASP:HB2	1:A:281:PHE:CE2	1.98	0.97
1:A:69:LYS:HG2	1:A:132:TYR:CD2	1.99	0.97
1:A:73:ILE:HD13	2:A:1008:HOH:O	1.64	0.95
1:A:140:MET:HA	1:A:145:LEU:HD12	1.56	0.88
1:A:278:ASP:O	1:A:279:GLN:HG2	1.75	0.86
1:A:41:PRO:HA	1:A:104:SER:OG	1.79	0.82
1:A:251:ASN:ND2	1:A:254:TYR:HD1	1.79	0.79
1:A:2:ALA:HB1	1:A:92:SER:HB3	1.64	0.78
1:A:69:LYS:CG	1:A:132:TYR:CD2	2.66	0.78
1:A:247:ILE:O	1:A:282:CYS:HB2	1.84	0.77
1:A:20:LEU:HD13	1:A:89:VAL:HG22	1.65	0.77
1:A:270:THR:HB	1:A:271:PRO:HD2	1.66	0.76
1:A:25:GLN:HE22	1:A:57:ASP:H	1.31	0.75
1:A:277:GLN:HB2	1:A:282:CYS:SG	2.28	0.74
1:A:278:ASP:HB2	1:A:281:PHE:CD2	2.23	0.74
1:A:15:PHE:CE2	1:A:116:GLU:HB3	2.24	0.73
1:A:278:ASP:HB2	1:A:281:PHE:HE2	1.53	0.69
1:A:20:LEU:HD21	1:A:101:VAL:HG21	1.75	0.68
1:A:220:LYS:HG3	1:A:287:GLN:OE1	1.92	0.68
1:A:251:ASN:ND2	1:A:254:TYR:CD1	2.61	0.68
1:A:139:ASN:O	1:A:143:ARG:HD2	1.94	0.67
1:A:324:LYS:HE2	2:A:1105:HOH:O	1.94	0.67
1:A:270:THR:CB	1:A:271:PRO:HD2	2.29	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:228:ILE:O	1:A:232:GLN:HG2	2.00	0.61
1:A:203:VAL:HG12	1:A:207:GLU:HG2	1.82	0.61
1:A:278:ASP:O	1:A:281:PHE:HD2	1.84	0.59
1:A:2:ALA:HB1	1:A:92:SER:CB	2.30	0.59
1:A:316:ALA:HB3	2:A:1015:HOH:O	2.03	0.58
1:A:326:ILE:CG2	2:A:1064:HOH:O	2.52	0.58
1:A:69:LYS:HB3	1:A:84:LEU:HD12	1.85	0.57
1:A:203:VAL:CG1	1:A:207:GLU:HG2	2.34	0.57
1:A:15:PHE:CZ	1:A:116:GLU:HB3	2.39	0.57
1:A:9:TYR:HB2	1:A:15:PHE:CZ	2.40	0.56
1:A:6:LEU:HB2	1:A:163:SER:HB2	1.87	0.56
1:A:271:PRO:HA	1:A:274:TYR:CZ	2.41	0.56
1:A:69:LYS:HD2	1:A:69:LYS:N	2.19	0.55
1:A:11:ASP:O	1:A:307:ARG:NH2	2.40	0.55
1:A:127:SER:OG	1:A:188:GLN:HG2	2.07	0.55
1:A:97:ILE:O	1:A:98:GLN:C	2.50	0.54
1:A:156:ASP:OD2	1:A:158:ASN:HB2	2.07	0.54
1:A:42:SER:HB2	1:A:103:LEU:HD13	1.90	0.54
1:A:270:THR:HB	1:A:271:PRO:CD	2.37	0.54
1:A:239:GLN:HA	1:A:244:GLU:O	2.08	0.53
1:A:270:THR:CB	1:A:271:PRO:CD	2.87	0.53
1:A:19:TYR:HB2	1:A:90:THR:HB	1.91	0.52
1:A:19:TYR:HA	1:A:25:GLN:O	2.10	0.51
1:A:313:PHE:CD1	1:A:313:PHE:N	2.78	0.51
1:A:81:GLN:NE2	2:A:1033:HOH:O	2.44	0.50
1:A:19:TYR:CE1	1:A:26:GLU:HG3	2.46	0.50
1:A:220:LYS:HB3	1:A:285:GLY:O	2.12	0.50
1:A:20:LEU:CD1	1:A:89:VAL:HG22	2.38	0.50
1:A:172:PRO:HA	1:A:175:TYR:CE2	2.47	0.50
1:A:8:ASN:HB3	1:A:14:TYR:CD2	2.48	0.49
1:A:181:TRP:HB3	1:A:319:LEU:HD13	1.95	0.49
1:A:260:PHE:HE2	1:A:269:LEU:HD12	1.77	0.49
1:A:247:ILE:HG21	1:A:255:MET:HE1	1.93	0.48
1:A:225:SER:HA	1:A:288:SER:OG	2.14	0.48
1:A:153:VAL:HG23	1:A:313:PHE:HE1	1.79	0.47
1:A:2:ALA:CB	1:A:92:SER:HB3	2.41	0.47
1:A:68:GLY:O	1:A:83:ILE:HG23	2.15	0.47
1:A:69:LYS:HA	1:A:70:PRO:HD3	1.54	0.47
1:A:203:VAL:HG12	1:A:207:GLU:CG	2.44	0.47
1:A:271:PRO:O	1:A:275:THR:CB	2.65	0.45
1:A:314:ASP:O	1:A:318:ASN:CA	2.64	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:240:ASN:N	1:A:244:GLU:O	2.44	0.45
1:A:9:TYR:HB2	1:A:15:PHE:CE2	2.52	0.45
1:A:157:ARG:HH11	1:A:157:ARG:HD2	1.56	0.45
1:A:80:MET:HE2	1:A:104:SER:HA	1.98	0.45
1:A:69:LYS:HG3	1:A:132:TYR:CD2	2.50	0.45
1:A:81:GLN:HB3	1:A:106:GLN:HB2	1.98	0.45
1:A:324:LYS:HG3	1:A:325:ALA:N	2.30	0.44
1:A:271:PRO:HA	1:A:274:TYR:CE1	2.53	0.44
1:A:74:HIS:CE1	1:A:79:SER:OG	2.71	0.43
1:A:83:ILE:HG23	1:A:83:ILE:HD12	1.69	0.43
1:A:232:GLN:HA	1:A:232:GLN:OE1	2.18	0.43
1:A:314:ASP:O	1:A:318:ASN:HA	2.18	0.43
1:A:69:LYS:CG	1:A:132:TYR:CE2	3.01	0.43
1:A:252:LEU:HD11	1:A:275:THR:HG21	2.01	0.43
1:A:53:HIS:HE1	1:A:112:PHE:O	2.02	0.43
1:A:64:PHE:CG	1:A:65:GLN:N	2.86	0.43
1:A:278:ASP:C	1:A:279:GLN:HG2	2.41	0.43
1:A:197:VAL:HB	1:A:205:ALA:HB3	2.01	0.43
1:A:69:LYS:HG2	1:A:132:TYR:CG	2.51	0.43
1:A:56:PHE:O	1:A:58:PRO:HD3	2.19	0.42
1:A:82:GLY:O	1:A:83:ILE:HD13	2.18	0.42
1:A:214:LEU:HD12	1:A:214:LEU:HA	1.76	0.42
1:A:157:ARG:HG3	1:A:158:ASN:N	2.35	0.42
1:A:260:PHE:CD2	1:A:260:PHE:N	2.87	0.42
1:A:271:PRO:O	1:A:275:THR:HB	2.19	0.42
1:A:153:VAL:HG23	1:A:313:PHE:CE1	2.53	0.42
1:A:121:LEU:HD11	1:A:136:VAL:HG21	2.02	0.42
1:A:27:PHE:CE1	1:A:54:GLN:HB3	2.55	0.42
1:A:81:GLN:CB	1:A:106:GLN:HB2	2.50	0.42
1:A:219:SER:HB2	2:A:1104:HOH:O	2.19	0.42
1:A:182:VAL:N	1:A:320:VAL:O	2.45	0.42
1:A:9:TYR:HB3	1:A:13:GLN:HB2	2.01	0.41
1:A:19:TYR:CD2	1:A:19:TYR:N	2.88	0.41
1:A:174:TYR:HD2	1:A:174:TYR:HA	1.58	0.41
1:A:2:ALA:HB2	1:A:94:ILE:HG13	2.02	0.41
1:A:116:GLU:OE1	1:A:116:GLU:HA	2.20	0.41
1:A:152:SER:HB2	1:A:166:THR:HB	2.03	0.41
1:A:9:TYR:HB2	1:A:15:PHE:HZ	1.81	0.41
1:A:278:ASP:O	1:A:279:GLN:C	2.63	0.41
1:A:13:GLN:HE22	1:A:115:ALA:HA	1.84	0.40
1:A:179:LEU:HA	1:A:323:ALA:HB2	2.02	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:240:ASN:ND2	1:A:242:TYR:HB2	2.36	0.40
1:A:251:ASN:O	1:A:251:ASN:CG	2.63	0.40
1:A:235:ILE:HG22	1:A:256:PRO:HG2	2.03	0.40
1:A:125:TYR:HB3	1:A:126:PRO:HD2	2.04	0.40
1:A:23:PRO:HB2	1:A:24:PRO:HD2	2.03	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	316/323 (98%)	306 (97%)	10 (3%)	0	<b>100</b> <b>100</b>

There are no Ramachandran outliers to report.

#### 5.3.2 Protein sidechains [i](#)

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	277/280 (99%)	248 (90%)	29 (10%)	<b>6</b> <b>6</b>

All (29) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	1	VAL

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
1	A	8	ASN
1	A	11	ASP
1	A	18	ILE
1	A	29	VAL
1	A	63	THR
1	A	67	LEU
1	A	69	LYS
1	A	71	LEU
1	A	72	SER
1	A	73	ILE
1	A	93	ASN
1	A	97	ILE
1	A	103	LEU
1	A	116	GLU
1	A	128	LEU
1	A	146	VAL
1	A	148	GLN
1	A	163	SER
1	A	165	LEU
1	A	214	LEU
1	A	221	LEU
1	A	226	SER
1	A	241	GLN
1	A	252	LEU
1	A	281	PHE
1	A	283	THR
1	A	324	LYS
1	A	326	ILE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (6) such sidechains are listed below:

<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
1	A	25	GLN
1	A	54	GLN
1	A	99	GLN
1	A	139	ASN
1	A	142	ASN
1	A	251	ASN

### 5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

### 5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

### 5.6 Ligand geometry [i](#)

There are no ligands in this entry.

### 5.7 Other polymers [i](#)

There are no such residues in this entry.

### 5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

## 6 Fit of model and data [i](#)

### 6.1 Protein, DNA and RNA chains [i](#)

EDS was not executed - this section is therefore empty.

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

EDS was not executed - this section is therefore empty.

### 6.3 Carbohydrates [i](#)

EDS was not executed - this section is therefore empty.

### 6.4 Ligands [i](#)

EDS was not executed - this section is therefore empty.

### 6.5 Other polymers [i](#)

EDS was not executed - this section is therefore empty.