



# Full wwPDB X-ray Structure Validation Report ⓘ

Mar 6, 2026 – 11:29 AM UTC

PDB ID : 1CMS / pdb\_00001cms  
Title : THE THREE-DIMENSIONAL STRUCTURE OF RECOMBINANT BOVINE CHYMOSIN AT 2.3 ANGSTROMS RESOLUTION  
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Deposited on : 1989-10-12  
Resolution : 2.30 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

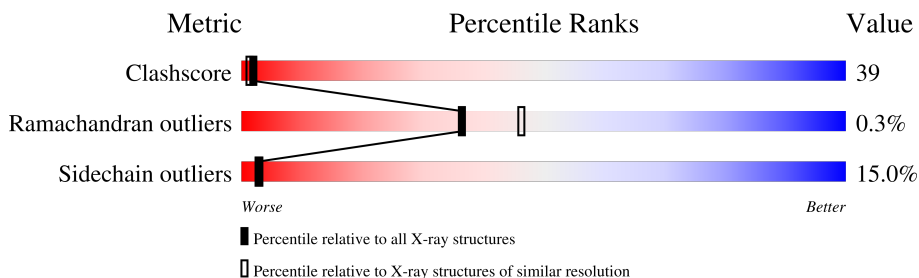
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.30 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	6919 (2.30-2.30)
Ramachandran outliers	187476	6854 (2.30-2.30)
Sidechain outliers	187428	6854 (2.30-2.30)

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	

## 2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 2808 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 PROCHYMOSIN A/B PRECURSOR.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	323	2511	1598	401	498	14	0	0	0

- Molecule 2 is water.

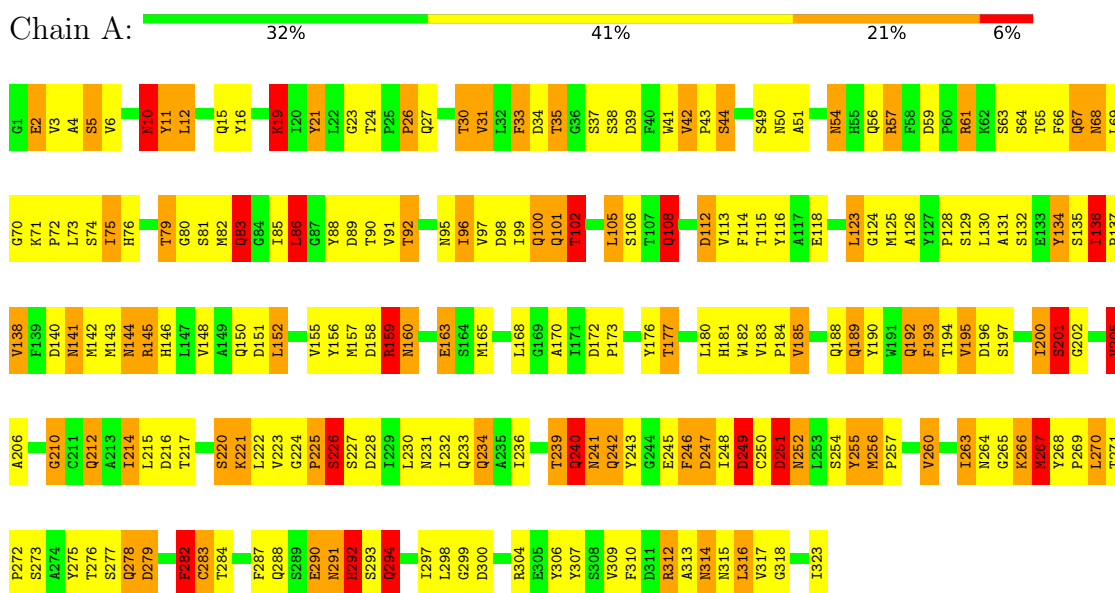
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	297	Total 297	O 297	0	0

### 3 Residue-property plots

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

Note EDS was not executed.

- Molecule 1: PROCHYMOSIN A/B PRECURSOR



## 4 Data and refinement statistics

Xtrriage (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, $\alpha$ , $\beta$ , $\gamma$	72.70Å 80.30Å 114.80Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	(Not available) – 2.30	Depositor
% Data completeness (in resolution range)	(Not available) ((Not available)-2.30)	Depositor
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
Refinement program	PROLSQ	Depositor
R, $R_{free}$	0.165 , (Not available)	Depositor
Estimated twinning fraction	No twinning to report.	Xtrriage
Total number of atoms	2808	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	24.0	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	1.56	16/2574 (0.6%)	2.65	207/3506 (5.9%)

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	3

All (16) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	312	ARG	CD-NE	14.03	1.65	1.46
1	A	292	HIS	N-CA	-8.92	1.34	1.46
1	A	99	ILE	C-O	7.97	1.33	1.24
1	A	100	GLN	N-CA	7.89	1.59	1.46
1	A	83	GLN	N-CA	6.25	1.53	1.46
1	A	90	THR	CA-CB	6.23	1.61	1.53
1	A	212	GLN	N-CA	6.16	1.53	1.45
1	A	292	HIS	CA-CB	6.05	1.63	1.53
1	A	201	SER	N-CA	5.93	1.55	1.46
1	A	24	THR	CA-CB	5.68	1.59	1.53
1	A	200	ILE	C-O	5.61	1.30	1.24
1	A	228	ASP	C-O	5.58	1.30	1.24
1	A	44	SER	N-CA	5.50	1.52	1.45
1	A	79	THR	N-CA	5.48	1.53	1.46
1	A	299	GLY	C-O	5.16	1.28	1.23
1	A	138	VAL	C-O	5.07	1.29	1.24

All (207) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	291	ASN	CA-C-N	23.60	166.62	121.54
1	A	291	ASN	C-N-CA	23.60	166.62	121.54
1	A	312	ARG	CD-NE-CZ	-16.28	101.60	124.40
1	A	312	ARG	NE-CZ-NH2	15.72	133.34	119.20
1	A	292	HIS	N-CA-C	14.35	141.36	110.80
1	A	99	ILE	CA-C-N	-14.25	103.94	123.03
1	A	99	ILE	C-N-CA	-14.25	103.94	123.03
1	A	61	ARG	CA-CB-CG	13.79	141.69	114.10
1	A	200	ILE	CA-C-N	-12.72	105.74	122.79
1	A	200	ILE	C-N-CA	-12.72	105.74	122.79
1	A	294	GLN	CA-C-N	12.58	139.93	122.19
1	A	294	GLN	C-N-CA	12.58	139.93	122.19
1	A	123	LEU	CA-C-N	12.23	131.66	119.92
1	A	123	LEU	C-N-CA	12.23	131.66	119.92
1	A	312	ARG	NE-CZ-NH1	-12.11	109.39	121.50
1	A	99	ILE	N-CA-C	12.09	121.89	110.53
1	A	294	GLN	CA-C-O	12.05	137.75	120.51
1	A	144	ASN	CA-CB-CG	-11.88	100.72	112.60
1	A	50	ASN	OD1-CG-ND2	11.51	134.11	122.60
1	A	108	GLN	OE1-CD-NE2	11.25	133.85	122.60
1	A	282	PHE	CA-CB-CG	-10.71	103.09	113.80
1	A	57	ARG	NE-CZ-NH2	10.55	128.69	119.20
1	A	249	ASP	N-CA-CB	10.10	125.61	109.95
1	A	100	GLN	CB-CA-C	9.71	126.13	111.85
1	A	112	ASP	CA-CB-CG	9.29	121.89	112.60
1	A	292	HIS	CA-CB-CG	-8.89	104.91	113.80
1	A	291	ASN	CA-C-O	8.78	133.06	120.51
1	A	282	PHE	N-CA-C	8.61	123.48	110.14
1	A	42	VAL	N-CA-CB	-8.45	99.39	111.21
1	A	145	ARG	CD-NE-CZ	-8.39	112.65	124.40
1	A	249	ASP	O-C-N	8.28	132.73	123.04
1	A	108	GLN	CB-CG-CD	-8.26	98.55	112.60
1	A	215	LEU	CB-CA-C	8.19	123.45	110.19
1	A	30	THR	N-CA-CB	8.12	123.32	110.57
1	A	144	ASN	OD1-CG-ND2	8.07	130.67	122.60
1	A	226	SER	O-C-N	7.99	130.59	122.12
1	A	220	SER	CB-CA-C	-7.92	98.39	110.90
1	A	61	ARG	CB-CA-C	7.91	126.31	110.17
1	A	12	LEU	N-CA-C	7.71	122.04	111.17
1	A	196	ASP	O-C-N	7.64	130.34	122.09
1	A	291	ASN	CB-CA-C	7.52	125.39	110.42
1	A	11	TYR	CA-C-N	7.39	133.32	122.82
1	A	11	TYR	C-N-CA	7.39	133.32	122.82

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	66	PHE	N-CA-CB	7.35	120.77	109.97
1	A	251	ASP	CA-CB-CG	7.24	119.83	112.60
1	A	83	GLN	CB-CA-C	7.22	123.65	109.35
1	A	21	TYR	CA-CB-CG	-7.15	101.03	113.90
1	A	170	ALA	CA-C-O	7.13	129.03	121.33
1	A	240	GLN	OE1-CD-NE2	7.12	129.72	122.60
1	A	145	ARG	NE-CZ-NH1	-7.06	114.44	121.50
1	A	54	ASN	CA-CB-CG	6.93	119.53	112.60
1	A	228	ASP	CA-C-O	-6.89	113.58	120.82
1	A	291	ASN	O-C-N	-6.87	113.46	122.59
1	A	247	ASP	CA-CB-CG	6.86	119.46	112.60
1	A	252	ASN	N-CA-C	-6.82	104.95	113.20
1	A	306	TYR	N-CA-C	6.81	119.94	108.02
1	A	205	VAL	N-CA-CB	-6.77	100.06	111.23
1	A	243	TYR	N-CA-CB	6.74	120.43	110.53
1	A	247	ASP	CA-C-N	6.69	132.29	122.99
1	A	247	ASP	C-N-CA	6.69	132.29	122.99
1	A	100	GLN	O-C-N	6.66	132.87	122.61
1	A	79	THR	CB-CA-C	6.62	121.92	110.01
1	A	255	TYR	CA-CB-CG	-6.61	102.01	113.90
1	A	88	TYR	N-CA-CB	6.59	123.36	111.37
1	A	115	THR	O-C-N	6.55	128.90	122.09
1	A	190	TYR	O-C-N	6.55	130.68	122.43
1	A	102	THR	CB-CA-C	6.52	120.08	109.90
1	A	10	ASN	OD1-CG-ND2	6.43	129.03	122.60
1	A	197	SER	N-CA-C	6.40	118.28	108.42
1	A	27	GLN	OE1-CD-NE2	-6.40	116.20	122.60
1	A	217	THR	CA-CB-OG1	-6.38	100.03	109.60
1	A	34	ASP	N-CA-C	6.38	120.18	107.62
1	A	159	ARG	NE-CZ-NH2	-6.37	113.47	119.20
1	A	33	PHE	CA-C-N	6.36	132.55	123.14
1	A	33	PHE	C-N-CA	6.36	132.55	123.14
1	A	80	GLY	N-CA-C	6.33	121.24	112.37
1	A	172	ASP	O-C-N	6.31	128.87	121.10
1	A	294	GLN	N-CA-C	6.28	124.18	110.80
1	A	2	GLU	CB-CG-CD	6.28	123.27	112.60
1	A	201	SER	CB-CA-C	6.27	121.32	111.72
1	A	57	ARG	NE-CZ-NH1	-6.24	115.26	121.50
1	A	136	ILE	O-C-N	6.23	128.20	120.66
1	A	279	ASP	CA-CB-CG	6.23	118.83	112.60
1	A	195	VAL	CB-CA-C	6.23	119.51	110.98
1	A	266	LYS	N-CA-CB	6.23	121.73	111.08

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	202	GLY	N-CA-C	-6.22	107.09	115.36
1	A	97	VAL	CB-CA-C	6.20	120.02	110.96
1	A	263	ILE	O-C-N	6.19	129.77	123.20
1	A	283	CYS	O-C-N	6.13	130.59	123.30
1	A	141	ASN	N-CA-C	-6.12	104.52	111.07
1	A	260	VAL	N-CA-C	6.12	116.73	108.17
1	A	39	ASP	CA-CB-CG	6.11	118.71	112.60
1	A	114	PHE	N-CA-C	6.10	118.01	111.36
1	A	190	TYR	N-CA-C	-6.09	100.98	110.17
1	A	27	GLN	CB-CA-C	6.07	119.76	109.75
1	A	86	LEU	CA-C-N	6.07	133.30	121.41
1	A	86	LEU	C-N-CA	6.07	133.30	121.41
1	A	96	ILE	CB-CA-C	6.05	119.01	111.15
1	A	163	GLU	CB-CG-CD	6.03	122.86	112.60
1	A	314	ASN	CA-CB-CG	-6.03	106.57	112.60
1	A	19	LYS	N-CA-C	6.02	119.45	109.46
1	A	277	SER	CA-C-O	6.01	126.93	120.32
1	A	292	HIS	CA-C-O	-6.01	111.92	120.51
1	A	19	LYS	CB-CA-C	-6.00	99.97	109.80
1	A	108	GLN	CA-C-O	5.98	127.63	120.28
1	A	61	ARG	N-CA-C	-5.97	105.84	113.01
1	A	26	PRO	N-CA-C	5.96	124.74	112.47
1	A	190	TYR	CA-C-N	-5.95	113.24	122.16
1	A	190	TYR	C-N-CA	-5.95	113.24	122.16
1	A	68	ASN	CA-CB-CG	5.93	118.53	112.60
1	A	234	GLN	CA-C-N	5.92	130.08	120.60
1	A	234	GLN	C-N-CA	5.92	130.08	120.60
1	A	267	MET	N-CA-C	5.92	119.28	109.46
1	A	269	PRO	CA-C-N	5.88	131.29	123.00
1	A	269	PRO	C-N-CA	5.88	131.29	123.00
1	A	141	ASN	O-C-N	5.88	128.12	122.07
1	A	92	THR	CA-CB-OG1	-5.86	100.81	109.60
1	A	243	TYR	N-CA-C	-5.85	106.31	113.50
1	A	5	SER	CA-C-O	-5.84	114.05	120.30
1	A	193	PHE	CA-C-O	5.83	127.69	121.45
1	A	152	LEU	O-C-N	5.83	129.89	123.25
1	A	214	ILE	O-C-N	5.81	129.22	123.00
1	A	35	THR	N-CA-CB	5.79	120.52	110.39
1	A	2	GLU	CA-C-O	5.78	128.22	121.46
1	A	215	LEU	CA-C-N	5.74	131.07	122.47
1	A	215	LEU	C-N-CA	5.74	131.07	122.47
1	A	42	VAL	CB-CA-C	5.72	121.76	111.36

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	63	SER	CA-C-O	5.71	126.61	120.38
1	A	210	GLY	CA-C-O	5.70	126.91	122.29
1	A	256	MET	CB-CA-C	5.70	117.07	108.86
1	A	188	GLN	CA-C-N	5.68	132.38	121.54
1	A	188	GLN	C-N-CA	5.68	132.38	121.54
1	A	31	VAL	N-CA-CB	-5.62	102.22	111.44
1	A	99	ILE	CA-C-O	-5.60	114.84	121.05
1	A	309	VAL	O-C-N	5.60	129.31	123.26
1	A	134	TYR	O-C-N	5.59	127.86	121.88
1	A	102	THR	N-CA-CB	-5.59	101.14	109.69
1	A	243	TYR	O-C-N	5.59	129.98	122.49
1	A	42	VAL	CA-CB-CG2	5.56	119.85	110.40
1	A	177	THR	N-CA-CB	5.55	119.73	110.85
1	A	225	PRO	O-C-N	5.55	129.74	123.03
1	A	226	SER	CA-C-O	-5.53	114.66	120.63
1	A	10	ASN	CA-C-O	5.52	126.67	120.70
1	A	49	SER	O-C-N	-5.52	116.50	123.12
1	A	287	PHE	N-CA-CB	5.52	119.26	110.16
1	A	59	ASP	CB-CA-C	-5.50	104.92	110.65
1	A	101	GLN	CA-C-O	5.50	126.59	120.43
1	A	239	THR	CB-CA-C	-5.50	98.87	109.37
1	A	314	ASN	CA-C-N	-5.43	114.69	122.68
1	A	314	ASN	C-N-CA	-5.43	114.69	122.68
1	A	249	ASP	CA-CB-CG	5.43	118.03	112.60
1	A	222	LEU	CB-CA-C	5.41	118.96	110.19
1	A	51	ALA	CA-C-O	-5.39	114.83	120.55
1	A	247	ASP	CB-CA-C	5.38	118.59	109.50
1	A	215	LEU	N-CA-C	-5.38	99.97	108.73
1	A	298	LEU	CA-C-N	5.37	129.76	122.04
1	A	298	LEU	C-N-CA	5.37	129.76	122.04
1	A	35	THR	CA-CB-CG2	5.36	119.61	110.50
1	A	200	ILE	N-CA-CB	5.34	120.05	111.23
1	A	290	GLU	N-CA-CB	5.34	118.99	110.65
1	A	273	SER	O-C-N	5.33	128.23	122.15
1	A	65	THR	CA-C-O	5.33	125.88	119.59
1	A	131	ALA	CA-C-O	5.33	127.19	121.55
1	A	96	ILE	N-CA-C	5.32	115.91	108.89
1	A	49	SER	N-CA-C	5.32	117.79	110.35
1	A	194	THR	O-C-N	5.29	129.21	123.13
1	A	283	CYS	N-CA-CB	5.28	119.55	110.68
1	A	231	ASN	O-C-N	5.27	127.50	122.07
1	A	299	GLY	CA-C-N	5.26	127.59	120.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	299	GLY	C-N-CA	5.26	127.59	120.38
1	A	216	ASP	CA-CB-CG	-5.26	107.34	112.60
1	A	297	ILE	O-C-N	5.26	128.78	123.20
1	A	234	GLN	CB-CG-CD	-5.25	103.67	112.60
1	A	5	SER	O-C-N	5.25	129.36	123.27
1	A	105	LEU	CA-C-O	-5.25	114.68	120.30
1	A	194	THR	N-CA-C	5.25	117.31	108.96
1	A	59	ASP	O-C-N	5.25	126.40	120.68
1	A	79	THR	CA-C-N	5.25	125.90	120.60
1	A	79	THR	C-N-CA	5.25	125.90	120.60
1	A	85	ILE	O-C-N	5.22	128.84	123.20
1	A	256	MET	CA-CB-CG	-5.22	103.66	114.10
1	A	66	PHE	O-C-N	5.20	129.23	122.89
1	A	79	THR	N-CA-C	-5.19	106.72	113.16
1	A	160	ASN	CA-C-N	5.18	129.78	120.77
1	A	160	ASN	C-N-CA	5.18	129.78	120.77
1	A	224	GLY	O-C-N	5.18	126.95	121.77
1	A	221	LYS	N-CA-C	5.17	118.37	110.36
1	A	42	VAL	O-C-N	5.16	126.98	121.10
1	A	206	ALA	O-C-N	5.13	129.00	123.10
1	A	273	SER	CA-C-O	-5.12	114.99	120.42
1	A	185	VAL	N-CA-CB	5.12	116.11	110.53
1	A	96	ILE	N-CA-CB	-5.11	104.96	110.53
1	A	188	GLN	OE1-CD-NE2	5.10	127.70	122.60
1	A	306	TYR	CA-CB-CG	-5.09	104.73	113.90
1	A	50	ASN	CB-CG-OD1	-5.08	110.64	120.80
1	A	246	PHE	N-CA-CB	5.08	118.90	110.47
1	A	108	GLN	CA-C-N	5.07	128.42	122.85
1	A	108	GLN	C-N-CA	5.07	128.42	122.85
1	A	214	ILE	N-CA-CB	5.06	121.28	111.93
1	A	124	GLY	CA-C-O	-5.05	116.97	121.41
1	A	37	SER	CA-C-O	-5.05	115.83	121.23
1	A	172	ASP	CA-C-N	5.05	124.66	119.56
1	A	172	ASP	C-N-CA	5.05	124.66	119.56
1	A	116	TYR	CA-C-O	-5.04	113.18	119.18
1	A	200	ILE	CA-C-O	-5.04	114.48	120.78
1	A	63	SER	CB-CA-C	5.01	118.39	109.72
1	A	180	LEU	O-C-N	5.00	128.93	123.22

There are no chirality outliers.

All (3) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	159	ARG	Sidechain
1	A	304	ARG	Sidechain
1	A	57	ARG	Sidechain

## 5.2 Too-close contacts [i](#)

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	2511	0	2383	189	0
2	A	297	0	0	38	0
All	All	2808	0	2383	189	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 39.

All (189) 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:247:ASP:HB2	1:A:282:PHE:CE1	1.64	1.31
1:A:267:MET:HG2	2:A:634:HOH:O	1.60	1.01
1:A:183:VAL:HG23	2:A:498:HOH:O	1.57	1.00
1:A:278:GLN:HG2	1:A:283:CYS:SG	2.02	0.99
1:A:150:GLN:NE2	2:A:596:HOH:O	1.96	0.98
1:A:33:PHE:HB3	1:A:125:MET:HE2	1.48	0.95
1:A:82:MET:HE2	1:A:106:SER:HB3	1.48	0.94
1:A:247:ASP:HB2	1:A:282:PHE:HE1	1.15	0.93
1:A:247:ASP:CB	1:A:282:PHE:CE1	2.52	0.92
1:A:181:HIS:HB2	1:A:266:LYS:NZ	1.83	0.92
1:A:33:PHE:HB3	1:A:125:MET:CE	2.01	0.90
1:A:234:GLN:NE2	2:A:443:HOH:O	1.98	0.88
1:A:279:ASP:HB3	2:A:511:HOH:O	1.72	0.88
1:A:98:ASP:OD1	1:A:101:GLN:NE2	2.07	0.87
1:A:276:THR:HG22	1:A:278:GLN:HE21	1.39	0.87
1:A:67:GLN:NE2	2:A:663:HOH:O	2.07	0.84
1:A:54:ASN:HB2	2:A:581:HOH:O	1.77	0.83
1:A:192:GLN:HG2	2:A:562:HOH:O	1.78	0.83
1:A:247:ASP:CB	1:A:282:PHE:HE1	1.92	0.80

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:11:TYR:CG	1:A:118:GLU:HG3	2.18	0.79
1:A:11:TYR:CD2	1:A:118:GLU:HG3	2.19	0.78
1:A:138:VAL:CG1	1:A:142:MET:HE3	2.14	0.78
1:A:181:HIS:HB2	1:A:266:LYS:HZ1	1.47	0.77
1:A:241:ASN:HB2	1:A:245:GLU:O	1.84	0.76
1:A:82:MET:HE2	1:A:106:SER:CB	2.16	0.75
1:A:282:PHE:CD2	1:A:283:CYS:N	2.55	0.75
1:A:293:SER:N	1:A:294:GLN:NE2	2.34	0.75
1:A:248:ILE:O	1:A:283:CYS:HB2	1.88	0.74
1:A:242:GLN:NE2	2:A:686:HOH:O	2.21	0.73
1:A:11:TYR:HA	2:A:515:HOH:O	1.88	0.72
1:A:102:THR:HG21	1:A:136:ILE:H	1.54	0.72
1:A:19:LYS:HE2	1:A:30:THR:HG22	1.70	0.72
1:A:276:THR:CG2	1:A:278:GLN:HE21	2.01	0.72
1:A:4:ALA:HB2	1:A:96:ILE:HD12	1.71	0.70
1:A:12:LEU:CD2	2:A:570:HOH:O	2.38	0.70
1:A:181:HIS:CE1	2:A:616:HOH:O	2.45	0.69
1:A:272:PRO:O	1:A:276:THR:HB	1.93	0.69
1:A:212:GLN:OE1	2:A:562:HOH:O	2.11	0.69
1:A:293:SER:N	1:A:294:GLN:HE22	1.91	0.68
1:A:278:GLN:CG	1:A:283:CYS:SG	2.82	0.68
1:A:252:ASN:ND2	1:A:255:TYR:HD2	1.92	0.67
1:A:76:HIS:CE1	1:A:81:SER:OG	2.48	0.67
1:A:102:THR:HG21	1:A:135:SER:HA	1.79	0.65
1:A:293:SER:OG	2:A:680:HOH:O	2.13	0.64
1:A:134:TYR:HD1	2:A:467:HOH:O	1.80	0.64
1:A:173:PRO:O	2:A:426:HOH:O	2.15	0.63
1:A:193:PHE:N	2:A:562:HOH:O	2.31	0.63
1:A:221:LYS:HD3	1:A:288:GLN:HB2	1.80	0.63
1:A:294:GLN:NE2	1:A:294:GLN:N	2.47	0.62
1:A:156:TYR:HB2	1:A:307:TYR:CD2	2.34	0.62
1:A:83:GLN:HE21	1:A:108:GLN:HE21	1.47	0.62
1:A:91:VAL:CG2	1:A:101:GLN:HG2	2.29	0.62
1:A:138:VAL:HG12	1:A:142:MET:HE3	1.81	0.61
1:A:156:TYR:HB2	1:A:307:TYR:HD2	1.65	0.61
1:A:195:VAL:O	1:A:210:GLY:HA2	2.01	0.60
1:A:230:LEU:O	1:A:234:GLN:HG3	2.00	0.60
1:A:173:PRO:HA	1:A:176:TYR:CE1	2.36	0.60
1:A:232:ILE:O	1:A:236:ILE:HG12	2.02	0.60
1:A:73:LEU:HD11	1:A:75:ILE:CD1	2.32	0.60
1:A:260:VAL:CG1	1:A:267:MET:HG3	2.32	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:41:TRP:CE3	1:A:82:MET:HE3	2.36	0.59
1:A:73:LEU:HD11	1:A:75:ILE:HD11	1.84	0.59
1:A:276:THR:HG22	1:A:278:GLN:NE2	2.16	0.59
1:A:136:ILE:HD12	1:A:136:ILE:N	2.18	0.59
1:A:184:PRO:HA	1:A:316:LEU:HD12	1.85	0.59
1:A:260:VAL:HG11	1:A:267:MET:HG3	1.85	0.59
1:A:141:ASN:O	1:A:145:ARG:HG3	2.04	0.58
1:A:6:VAL:HG11	1:A:33:PHE:CZ	2.39	0.58
1:A:240:GLN:HG3	1:A:246:PHE:CZ	2.37	0.58
1:A:236:ILE:HG22	1:A:257:PRO:HG2	1.85	0.58
1:A:113:VAL:HB	2:A:492:HOH:O	2.04	0.57
1:A:181:HIS:HB2	1:A:266:LYS:CE	2.34	0.57
1:A:272:PRO:HA	1:A:275:TYR:CZ	2.39	0.57
1:A:159:ARG:NH1	1:A:323:ILE:O	2.38	0.57
1:A:294:GLN:N	1:A:294:GLN:HE21	2.02	0.57
1:A:69:LEU:CD2	1:A:71:LYS:HG2	2.34	0.57
1:A:242:GLN:CD	2:A:686:HOH:O	2.48	0.56
1:A:268:TYR:CE1	2:A:616:HOH:O	2.51	0.56
1:A:177:THR:HG23	1:A:323:ILE:HG12	1.86	0.56
1:A:268:TYR:HE1	2:A:616:HOH:O	1.86	0.56
1:A:146:HIS:HA	2:A:585:HOH:O	2.06	0.55
1:A:44:SER:HB3	1:A:105:LEU:HB3	1.88	0.55
1:A:282:PHE:CG	1:A:283:CYS:N	2.75	0.55
1:A:11:TYR:CD2	1:A:118:GLU:CG	2.89	0.55
1:A:21:TYR:HB3	1:A:26:PRO:HB3	1.89	0.54
1:A:200:ILE:HG22	1:A:201:SER:N	2.22	0.54
1:A:98:ASP:CG	1:A:101:GLN:HE21	2.10	0.53
1:A:138:VAL:HG13	1:A:142:MET:HE3	1.88	0.53
1:A:200:ILE:HD12	1:A:205:VAL:HG21	1.90	0.53
1:A:264:ASN:HB2	2:A:548:HOH:O	2.09	0.53
1:A:155:VAL:HG23	1:A:310:PHE:HE1	1.73	0.52
1:A:236:ILE:HD12	1:A:248:ILE:HD11	1.92	0.52
1:A:272:PRO:O	1:A:276:THR:CB	2.58	0.52
1:A:294:GLN:NE2	2:A:680:HOH:O	2.43	0.52
1:A:247:ASP:HB2	1:A:282:PHE:CD1	2.35	0.52
1:A:181:HIS:CG	1:A:266:LYS:HE3	2.45	0.52
1:A:182:TRP:HA	1:A:317:VAL:O	2.10	0.51
1:A:293:SER:C	1:A:294:GLN:HE21	2.18	0.51
1:A:312:ARG:NH1	2:A:407:HOH:O	2.39	0.51
1:A:21:TYR:HB2	1:A:92:THR:HB	1.92	0.51
1:A:293:SER:H	1:A:294:GLN:NE2	2.09	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:132:SER:HB3	2:A:438:HOH:O	2.10	0.51
1:A:16:TYR:CG	1:A:157:MET:HE2	2.45	0.51
1:A:2:GLU:O	1:A:148:VAL:HA	2.11	0.50
1:A:241:ASN:HD22	1:A:242:GLN:H	1.60	0.50
1:A:271:THR:HB	1:A:272:PRO:HD2	1.94	0.50
1:A:250:CYS:C	1:A:251:ASP:CG	2.80	0.49
1:A:83:GLN:NE2	1:A:108:GLN:HE21	2.10	0.49
1:A:271:THR:HB	1:A:272:PRO:CD	2.42	0.49
1:A:181:HIS:HE1	1:A:264:ASN:HB3	1.77	0.49
1:A:181:HIS:CE1	1:A:264:ASN:HB3	2.47	0.49
1:A:43:PRO:HA	1:A:106:SER:OG	2.12	0.49
1:A:241:ASN:HB2	1:A:245:GLU:C	2.36	0.49
1:A:247:ASP:CB	1:A:282:PHE:CD1	2.95	0.49
1:A:250:CYS:O	1:A:251:ASP:CB	2.61	0.49
1:A:158:ASP:OD1	1:A:160:ASN:HB2	2.12	0.49
1:A:10:ASN:HA	1:A:15:GLN:O	2.13	0.49
1:A:130:LEU:HD13	1:A:189:GLN:CG	2.43	0.49
1:A:69:LEU:HD23	1:A:71:LYS:HG2	1.93	0.48
1:A:11:TYR:CG	1:A:118:GLU:CG	2.94	0.48
1:A:23:GLY:HA2	1:A:89:ASP:OD2	2.13	0.48
1:A:294:GLN:CB	2:A:624:HOH:O	2.62	0.48
1:A:91:VAL:HG21	1:A:101:GLN:HG2	1.95	0.48
1:A:314:ASN:C	2:A:452:HOH:O	2.57	0.48
1:A:135:SER:C	1:A:136:ILE:HD12	2.39	0.47
1:A:294:GLN:HB3	2:A:624:HOH:O	2.14	0.47
1:A:68:ASN:ND2	1:A:70:GLY:H	2.13	0.47
1:A:100:GLN:NE2	2:A:630:HOH:O	2.27	0.47
1:A:181:HIS:HB2	1:A:266:LYS:HZ2	1.77	0.47
1:A:159:ARG:HG2	1:A:160:ASN:N	2.30	0.47
1:A:10:ASN:HD22	1:A:10:ASN:H	1.62	0.47
1:A:44:SER:HB2	1:A:105:LEU:HD13	1.97	0.46
1:A:252:ASN:ND2	1:A:255:TYR:CD2	2.79	0.46
1:A:151:ASP:HB2	1:A:313:ALA:HB2	1.98	0.46
1:A:265:GLY:HA2	2:A:517:HOH:O	2.15	0.46
1:A:250:CYS:C	1:A:252:ASN:H	2.24	0.46
1:A:181:HIS:O	1:A:318:GLY:HA2	2.15	0.46
1:A:155:VAL:HG23	1:A:310:PHE:CE1	2.50	0.46
1:A:123:LEU:C	1:A:123:LEU:HD23	2.42	0.45
1:A:143:MET:HG2	1:A:151:ASP:OD1	2.15	0.45
1:A:152:LEU:C	1:A:152:LEU:HD12	2.42	0.45
1:A:86:LEU:HD23	1:A:134:TYR:HB2	1.99	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:241:ASN:N	1:A:245:GLU:O	2.45	0.44
1:A:223:VAL:CG1	1:A:290:GLU:HG3	2.48	0.44
1:A:241:ASN:HB3	1:A:245:GLU:H	1.83	0.44
1:A:276:THR:HG22	1:A:278:GLN:HG3	1.98	0.44
1:A:158:ASP:OD1	1:A:158:ASP:C	2.61	0.44
1:A:68:ASN:HD22	1:A:69:LEU:H	1.66	0.43
1:A:270:LEU:HD12	1:A:270:LEU:HA	1.84	0.43
1:A:152:LEU:HA	1:A:310:PHE:O	2.19	0.43
1:A:192:GLN:HG3	1:A:214:ILE:HG22	1.99	0.43
1:A:240:GLN:HG3	1:A:246:PHE:CE2	2.54	0.43
1:A:220:SER:HA	1:A:300:ASP:OD2	2.18	0.43
1:A:23:GLY:HA2	1:A:89:ASP:CG	2.44	0.43
1:A:272:PRO:HA	1:A:275:TYR:CE2	2.54	0.43
1:A:128:PRO:HA	1:A:137:PRO:HG2	2.00	0.42
1:A:317:VAL:HG12	1:A:318:GLY:N	2.33	0.42
1:A:73:LEU:CD1	1:A:75:ILE:CD1	2.96	0.42
1:A:181:HIS:ND1	2:A:616:HOH:O	2.35	0.42
1:A:38:SER:OG	1:A:126:ALA:HB3	2.20	0.42
1:A:240:GLN:HB3	2:A:545:HOH:O	2.19	0.42
1:A:177:THR:HG23	1:A:323:ILE:CG1	2.50	0.42
1:A:144:ASN:ND2	2:A:474:HOH:O	2.07	0.42
1:A:145:ARG:HH11	1:A:145:ARG:HD2	1.37	0.42
1:A:140:ASP:HA	1:A:143:MET:CE	2.50	0.42
1:A:249:ASP:C	1:A:250:CYS:O	2.62	0.42
1:A:35:THR:HG21	1:A:310:PHE:CZ	2.55	0.41
1:A:136:ILE:N	1:A:136:ILE:CD1	2.82	0.41
1:A:140:ASP:HA	1:A:143:MET:HE2	2.02	0.41
1:A:256:MET:HE2	1:A:272:PRO:HB3	2.02	0.41
1:A:282:PHE:HD2	1:A:282:PHE:HA	1.33	0.41
1:A:74:SER:O	1:A:75:ILE:HD12	2.20	0.41
1:A:263:ILE:HB	2:A:616:HOH:O	2.20	0.41
1:A:112:ASP:O	1:A:113:VAL:C	2.63	0.41
1:A:56:GLN:HG2	2:A:460:HOH:O	2.20	0.41
1:A:165:MET:HB3	2:A:576:HOH:O	2.20	0.41
1:A:4:ALA:HB3	1:A:168:LEU:HB2	2.03	0.41
1:A:10:ASN:HD22	1:A:10:ASN:N	2.17	0.41
1:A:71:LYS:HA	1:A:72:PRO:HD3	1.89	0.41
1:A:69:LEU:HB3	1:A:86:LEU:O	2.21	0.41
1:A:226:SER:HG	1:A:292:HIS:CE1	2.39	0.41
1:A:76:HIS:HE1	1:A:81:SER:OG	2.00	0.40
1:A:292:HIS:ND1	2:A:476:HOH:O	2.37	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:41:TRP:CD2	1:A:82:MET:HE3	2.56	0.40
1:A:225:PRO:HB3	1:A:292:HIS:O	2.20	0.40
1:A:292:HIS:C	1:A:294:GLN:HE22	2.27	0.40
1:A:314:ASN:O	1:A:315:ASN:C	2.63	0.40
1:A:129:SER:OG	1:A:189:GLN:HA	2.22	0.40
1:A:252:ASN:HD22	1:A:252:ASN:HA	1.62	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	321/323 (99%)	302 (94%)	18 (6%)	1 (0%)	36 46

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	291	ASN

### 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	280/280 (100%)	238 (85%)	42 (15%)	3 3

All (42) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	3	VAL
1	A	5	SER
1	A	10	ASN
1	A	19	LYS
1	A	31	VAL
1	A	42	VAL
1	A	61	ARG
1	A	64	SER
1	A	67	GLN
1	A	75	ILE
1	A	79	THR
1	A	83	GLN
1	A	86	LEU
1	A	95	ASN
1	A	102	THR
1	A	108	GLN
1	A	136	ILE
1	A	159	ARG
1	A	163	GLU
1	A	185	VAL
1	A	189	GLN
1	A	192	GLN
1	A	201	SER
1	A	205	VAL
1	A	226	SER
1	A	227	SER
1	A	233	GLN
1	A	239	THR
1	A	240	GLN
1	A	241	ASN
1	A	242	GLN
1	A	249	ASP
1	A	251	ASP
1	A	254	SER
1	A	267	MET
1	A	270	LEU
1	A	278	GLN
1	A	282	PHE
1	A	284	THR
1	A	292	HIS
1	A	294	GLN
1	A	316	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (16) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	10	ASN
1	A	50	ASN
1	A	68	ASN
1	A	76	HIS
1	A	83	GLN
1	A	146	HIS
1	A	150	GLN
1	A	188	GLN
1	A	192	GLN
1	A	233	GLN
1	A	234	GLN
1	A	240	GLN
1	A	252	ASN
1	A	278	GLN
1	A	294	GLN
1	A	314	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

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.