



Full wwPDB X-ray Structure Validation Report

Feb 28, 2014 – 12:01 AM GMT

PDB ID : 1CMS
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 validation report for a publicly released PDB entry.
We welcome your comments at validation@mail.wwpdb.org
A user guide is available at <http://wwpdb.org/ValidationPDFNotes.html>

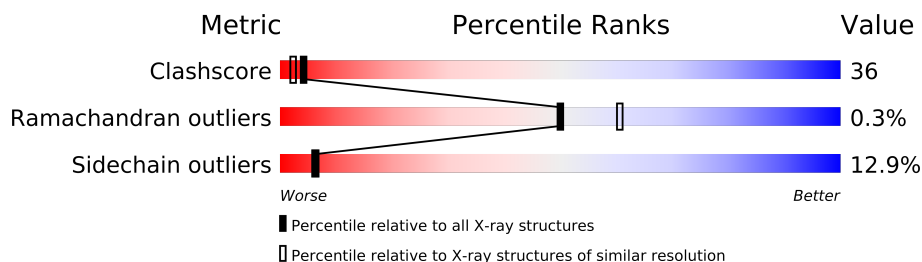
The following versions of software and data (see [references](#)) were used in the production of this report:

MolProbity : 4.02b-467
Mogul : 1.15 2013
Xtriage (Phenix) : **NOT EXECUTED**
EDS : **NOT EXECUTED**
Percentile statistics : 21963
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et. al. (1996)
Validation Pipeline (wwPDB-VP) : stable22683

1 Overall quality at a glance

The reported resolution of this entry is 2.30 Å.

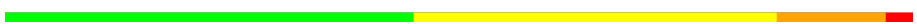
Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
Clashscore	79885	3679 (2.30-2.30)
Ramachandran outliers	78287	3642 (2.30-2.30)
Sidechain outliers	78261	3641 (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 on the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density.

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 hydrogen and 0 are deuterium.

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
1	A	323	Total	C	N	O	S	0	0	0
			2511	1598	401	498	14			

- Molecule 2 is water.

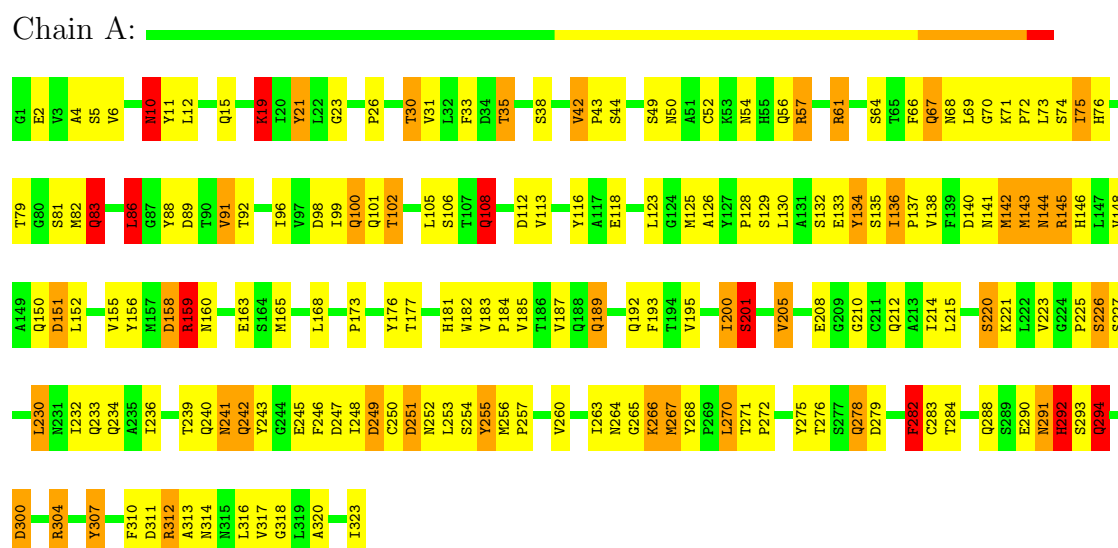
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	297	Total	O	0	0
			297	297		

3 Residue-property plots

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors 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.

Note EDS was not executed.

• Molecule 1: PROCHYMOSIN A/B PRECURSOR



4 Data and refinement statistics

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

Property	Value	Source
Space group	I 2 2 2	Depositor
Cell constants a, b, c, α , β , γ	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.	Xtriage
Total number of atoms	2808	wwPDB-VP
Average B, all atoms (Å ²)	24.0	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	1.22	5/2574 (0.2%)	2.13	76/3506 (2.2%)

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	3

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	312	ARG	CD-NE	11.44	1.65	1.46
1	A	208	GLU	CD-OE2	7.88	1.34	1.25
1	A	100	GLN	N-CA	6.74	1.59	1.46
1	A	292	HIS	N-CA	-5.83	1.34	1.46
1	A	99	ILE	C-O	5.10	1.33	1.23

All (76) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	312	ARG	NE-CZ-NH2	26.09	133.34	120.30
1	A	312	ARG	NE-CZ-NH1	-21.81	109.39	120.30
1	A	291	ASN	C-N-CA	17.97	166.62	121.70
1	A	57	ARG	NE-CZ-NH2	16.79	128.69	120.30
1	A	312	ARG	CD-NE-CZ	-15.71	101.60	123.60
1	A	159	ARG	NE-CZ-NH2	-13.66	113.47	120.30
1	A	61	ARG	CA-CB-CG	12.86	141.69	113.40
1	A	159	ARG	NE-CZ-NH1	11.99	126.30	120.30
1	A	145	ARG	NE-CZ-NH1	-11.72	114.44	120.30
1	A	292	HIS	N-CA-C	11.24	141.36	111.00
1	A	134	TYR	CB-CG-CD2	-10.36	114.79	121.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	57	ARG	NE-CZ-NH1	-10.09	115.26	120.30
1	A	112	ASP	CB-CG-OD1	9.00	126.40	118.30
1	A	255	TYR	CB-CG-CD1	-8.49	115.90	121.00
1	A	294	GLN	CA-C-O	8.40	137.75	120.10
1	A	249	ASP	N-CA-CB	8.34	125.61	110.60
1	A	61	ARG	CB-CA-C	7.96	126.31	110.40
1	A	100	GLN	CB-CA-C	7.86	126.13	110.40
1	A	145	ARG	CD-NE-CZ	-7.82	112.65	123.60
1	A	291	ASN	CB-CA-C	7.49	125.39	110.40
1	A	294	GLN	C-N-CA	7.29	139.93	121.70
1	A	112	ASP	CB-CG-OD2	-7.16	111.86	118.30
1	A	99	ILE	C-N-CA	-7.10	103.94	121.70
1	A	88	TYR	N-CA-CB	7.09	123.36	110.60
1	A	215	LEU	CB-CA-C	6.97	123.45	110.20
1	A	30	THR	N-CA-CB	6.85	123.32	110.30
1	A	304	ARG	NE-CZ-NH1	6.85	123.72	120.30
1	A	307	TYR	CB-CG-CD2	6.69	125.01	121.00
1	A	83	GLN	CB-CA-C	6.63	123.65	110.40
1	A	282	PHE	CB-CG-CD2	-6.53	116.23	120.80
1	A	21	TYR	CA-CB-CG	-6.51	101.03	113.40
1	A	200	ILE	C-N-CA	-6.38	105.74	121.70
1	A	116	TYR	CB-CG-CD1	-6.37	117.18	121.00
1	A	100	GLN	O-C-N	6.36	132.87	122.70
1	A	249	ASP	O-C-N	6.27	132.73	122.70
1	A	266	LYS	N-CA-CB	6.18	121.73	110.60
1	A	291	ASN	CA-C-O	6.17	133.06	120.10
1	A	220	SER	CB-CA-C	-6.16	98.39	110.10
1	A	320	ALA	N-CA-CB	6.11	118.66	110.10
1	A	253	LEU	CA-CB-CG	6.07	129.27	115.30
1	A	143	MET	CG-SD-CE	6.06	109.90	100.20
1	A	255	TYR	CA-CB-CG	-6.00	102.01	113.40
1	A	230	LEU	CB-CG-CD2	-5.99	100.82	111.00
1	A	42	VAL	CA-CB-CG2	5.97	119.85	110.90
1	A	201	SER	CB-CA-C	5.90	121.32	110.10
1	A	151	ASP	CB-CG-OD1	5.87	123.58	118.30
1	A	311	ASP	CB-CG-OD1	5.86	123.57	118.30
1	A	142	MET	CG-SD-CE	-5.79	90.94	100.20
1	A	52	CYS	CA-CB-SG	-5.78	103.60	114.00
1	A	291	ASN	O-C-N	-5.78	113.46	122.70
1	A	144	ASN	CA-CB-CG	-5.76	100.72	113.40
1	A	256	MET	CA-CB-CG	-5.67	103.66	113.30
1	A	66	PHE	N-CA-CB	5.65	120.77	110.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	158	ASP	CB-CG-OD2	5.56	123.31	118.30
1	A	49	SER	N-CA-CB	-5.53	102.20	110.50
1	A	300	ASP	CB-CG-OD1	5.51	123.26	118.30
1	A	42	VAL	N-CA-CB	-5.51	99.39	111.50
1	A	50	ASN	CB-CG-OD1	-5.48	110.64	121.60
1	A	243	TYR	N-CA-CB	5.46	120.43	110.60
1	A	42	VAL	CB-CA-C	5.46	121.76	111.40
1	A	35	THR	N-CA-CB	5.38	120.52	110.30
1	A	91	VAL	CA-CB-CG2	5.32	118.88	110.90
1	A	50	ASN	OD1-CG-ND2	5.31	134.11	121.90
1	A	134	TYR	CB-CG-CD1	5.29	124.17	121.00
1	A	100	GLN	CA-C-N	-5.26	105.62	117.20
1	A	294	GLN	CA-C-N	-5.26	105.63	117.20
1	A	86	LEU	C-N-CA	5.24	133.30	122.30
1	A	19	LYS	CB-CA-C	-5.22	99.97	110.40
1	A	205	VAL	N-CA-CB	-5.20	100.06	111.50
1	A	108	GLN	OE1-CD-NE2	5.20	133.85	121.90
1	A	304	ARG	NH1-CZ-NH2	-5.19	113.69	119.40
1	A	35	THR	CA-CB-CG2	5.15	119.61	112.40
1	A	292	HIS	CA-CB-CG	-5.11	104.91	113.60
1	A	133	GLU	CG-CD-OE1	5.11	128.51	118.30
1	A	10	ASN	CA-C-N	-5.05	106.08	117.20
1	A	108	GLN	CB-CG-CD	-5.02	98.55	111.60

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 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 hydrogens added by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, and the number in parentheses is this value normalized per 1000 atoms of the molecule in the chain. The Symm-Clashes column gives symmetry related clashes, in the same way as for the Clashes column.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2511	0	2383	178	2
2	A	297	0	0	38	2
All	All	2808	0	2383	178	2

Clashscore is defined as the number of clashes calculated for the entry per 1000 atoms (including hydrogens) of the entry. The overall clashscore for this entry is 36.

All (178) close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(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:247:ASP:HB2	1:A:282:PHE:HE1	1.15	0.93
1:A:33:PHE:HB3	1:A:125:MET:HE2	1.51	0.92
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
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:241:ASN:HB2	1:A:245:GLU:O	1.84	0.76
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:276:THR:CG2	1:A:278:GLN:HE21	2.01	0.72
1:A:19:LYS:HE2	1:A:30:THR:HG22	1.70	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

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
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:82:MET:HE2	1:A:106:SER:HB3	1.77	0.67
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:181:HIS:HB2	1:A:266:LYS:HZ2	1.60	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:76:HIS:CE1	1:A:81:SER:HG	2.16	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:91:VAL:CG2	1:A:101:GLN:HG2	2.29	0.62
1:A:83:GLN:HE21	1:A:108:GLN:HE21	1.47	0.62
1:A:156:TYR:HB2	1:A:307:TYR:HD2	1.65	0.61
1:A:230:LEU:O	1:A:234:GLN:HG3	2.00	0.60
1:A:195:VAL:O	1:A:210:GLY:HA2	2.01	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:260:VAL:CG1	1:A:267:MET:HG3	2.32	0.60
1:A:73:LEU:HD11	1:A:75:ILE:CD1	2.32	0.60
1:A:181:HIS:HB2	1:A:266:LYS:HZ1	1.64	0.60
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:260:VAL:HG11	1:A:267:MET:HG3	1.85	0.59
1:A:184:PRO:HA	1:A:316:LEU:HD12	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:181:HIS:HB2	1:A:266:LYS:CE	2.34	0.57
1:A:113:VAL:HB	2:A:492:HOH:O	2.04	0.57
1:A:272:PRO:HA	1:A:275:TYR:CZ	2.39	0.57
1:A:294:GLN:HE21	1:A:294:GLN:N	2.02	0.57
1:A:159:ARG:NH1	1:A:323:ILE:O	2.38	0.57
1:A:69:LEU:CD2	1:A:71:LYS:HG2	2.34	0.57
1:A:268:TYR:CE1	2:A:616:HOH:O	2.51	0.56
1:A:82:MET:CE	1:A:106:SER:HB3	2.35	0.56

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
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:200:ILE:HG22	1:A:201:SER:N	2.22	0.54
1:A:21:TYR:HB3	1:A:26:PRO:HB3	1.89	0.54
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:312:ARG:NH1	2:A:407:HOH:O	2.39	0.51
1:A:293:SER:H	1:A:294:GLN:NE2	2.09	0.51
1:A:21:TYR:HB2	1:A:92:THR:HB	1.92	0.51
1:A:132:SER:HB3	2:A:438:HOH:O	2.10	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:226:SER:HG	1:A:292:HIS:CE1	2.30	0.50
1:A:271:THR:HB	1:A:272:PRO:HD2	1.94	0.50
1:A:271:THR:HB	1:A:272:PRO:CD	2.42	0.49
1:A:83:GLN:NE2	1:A:108:GLN:HE21	2.10	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:247:ASP:CB	1:A:282:PHE:CD1	2.95	0.49
1:A:43:PRO:HA	1:A:106:SER:OG	2.12	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:98:ASP:CG	1:A:101:GLN:HE21	2.10	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:242:GLN:CD	2:A:686:HOH:O	2.48	0.48

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
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:159:ARG:HG2	1:A:160:ASN:N	2.30	0.47
1:A:10:ASN:H	1:A:10:ASN:HD22	1.62	0.47
1:A:252:ASN:ND2	1:A:255:TYR:CD2	2.79	0.46
1:A:44:SER:HB2	1:A:105:LEU:HD13	1.97	0.46
1:A:293:SER:C	1:A:294:GLN:HE21	2.18	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: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:143:MET:HG2	1:A:151:ASP:OD1	2.15	0.45
1:A:86:LEU:HD23	1:A:134:TYR:HB2	1.99	0.45
1:A:241:ASN:N	1:A:245:GLU:O	2.45	0.44
1:A:241:ASN:HB2	1:A:245:GLU:C	2.36	0.44
1:A:223:VAL:CG1	1:A:290:GLU:HG3	2.48	0.44
1:A:276:THR:HG22	1:A:278:GLN:HG3	1.98	0.44
1:A:241:ASN:HB3	1:A:245:GLU:H	1.83	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:314:ASN:C	2:A:452:HOH:O	2.57	0.43
1:A:138:VAL:CG1	1:A:142:MET:HE3	2.48	0.43
1:A:135:SER:C	1:A:136:ILE:HD12	2.39	0.43
1:A:138:VAL:CG1	1:A:142:MET:CE	2.96	0.43
1:A:220:SER:HA	1:A:300:ASP:OD2	2.18	0.43
1:A:272:PRO:HA	1:A:275:TYR:CE2	2.54	0.43
1:A:317:VAL:HG12	1:A:318:GLY:N	2.33	0.42
1:A:128:PRO:HA	1:A:137:PRO:HG2	2.00	0.42
1:A:181:HIS:ND1	2:A:616:HOH:O	2.35	0.42
1:A:73:LEU:CD1	1:A:75:ILE:CD1	2.96	0.42
1:A:240:GLN:HB3	2:A:545:HOH:O	2.19	0.42
1:A:38:SER:OG	1:A:126:ALA:HB3	2.20	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:35:THR:HG21	1:A:310:PHE:CZ	2.55	0.41
1:A:136:ILE:CD1	1:A:136:ILE:N	2.82	0.41

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:282:PHE:HD2	1:A:282:PHE:HA	1.33	0.41
1:A:263:ILE:HB	2:A:616:HOH:O	2.20	0.41
1:A:250:CYS:C	1:A:252:ASN:H	2.24	0.41
1:A:74:SER:O	1:A:75:ILE:HD12	2.20	0.41
1:A:165:MET:HB3	2:A:576:HOH:O	2.20	0.41
1:A:56:GLN:HG2	2:A:460:HOH:O	2.20	0.41
1:A:4:ALA:HB3	1:A:168:LEU:HB2	2.03	0.41
1:A:71:LYS:HA	1:A:72:PRO:HD3	1.89	0.41
1:A:10:ASN:N	1:A:10:ASN:HD22	2.17	0.41
1:A:69:LEU:HB3	1:A:86:LEU:O	2.21	0.41
1:A:123:LEU:HD23	1:A:123:LEU:C	2.42	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
1:A:225:PRO:HB3	1:A:292:HIS:O	2.20	0.40
1:A:152:LEU:HD12	1:A:152:LEU:C	2.42	0.40
1:A:250:CYS:C	1:A:251:ASP:CG	2.80	0.40
1:A:252:ASN:HA	1:A:252:ASN:HD22	1.62	0.40
1:A:129:SER:OG	1:A:189:GLN:HA	2.22	0.40

All (2) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:83:GLN:NE2	2:A:426:HOH:O[7_545]	2.07	0.13
1:A:187:VAL:CG2	2:A:581:HOH:O[8_455]	2.17	0.03

5.3 Torsion angles

5.3.1 Protein backbone ⓘ

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%)	50 60

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	291	ASN

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	280/280 (100%)	244 (87%)	36 (13%)	6 6

All (36) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
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	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	201	SER
1	A	226	SER
1	A	227	SER
1	A	233	GLN
1	A	239	THR
1	A	241	ASN
1	A	242	GLN
1	A	249	ASP

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Mol	Chain	Res	Type
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

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (13) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	50	ASN
1	A	68	ASN
1	A	76	HIS
1	A	83	GLN
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

5.3.3 RNA ⓘ

There are no RNA chains 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 ⓘ

There are no carbohydrates in this entry.

5.6 Ligand geometry ⓘ

There are no ligands in this entry.

5.7 Other polymers ⓘ

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 will therefore be empty.

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

EDS was not executed - this section will therefore be empty.

6.3 Carbohydrates ⓘ

EDS was not executed - this section will therefore be empty.

6.4 Ligands ⓘ

EDS was not executed - this section will therefore be empty.

6.5 Other polymers ⓘ

EDS was not executed - this section will therefore be empty.