



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 8, 2026 – 02:11 PM UTC

PDB ID : 1MUA / pdb_00001mua
Title : STRUCTURE AND ENERGETICS OF A NON-PROLINE CIS-PEPTIDYL
LINKAGE IN AN ENGINEERED PROTEIN
Authors : Nair, S.K.; Christianson, D.W.
Deposited on : 1993-06-18
Resolution : 1.70 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

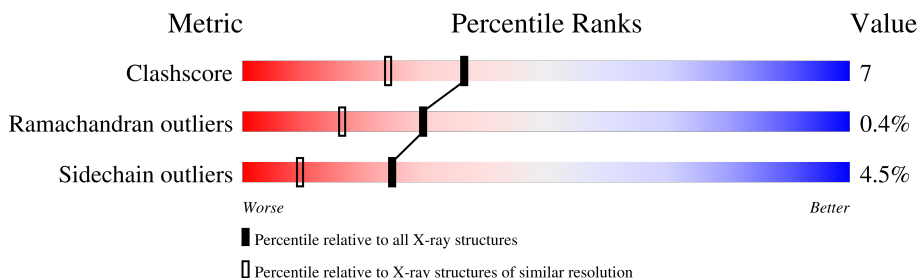
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.70 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	5924 (1.70-1.70)
Ramachandran outliers	187476	5846 (1.70-1.70)
Sidechain outliers	187428	5846 (1.70-1.70)

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	256	 64% 30% 5%

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 2130 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 CARBONIC ANHYDRASE II.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	256	Total	C	N	O	S	0	0	0
			2037	1307	350	378	2			

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	202	ALA	PRO	conflict	UNP P00918

- Molecule 2 is ZINC ION (CCD ID: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	1	Total	Zn	0	0
			1	1		

- Molecule 3 is MERCURY (II) ION (CCD ID: HG) (formula: Hg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	1	Total	Hg	0	0
			1	1		

- Molecule 4 is water.

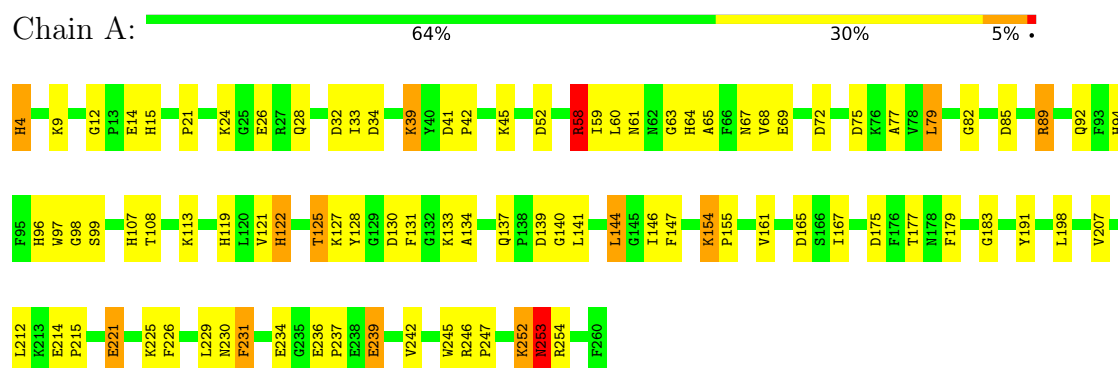
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	91	Total	O	0	0
			91	91		

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: CARBONIC ANHYDRASE II



4 Data and refinement statistics

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

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	42.70 Å 41.70 Å 73.00 Å 90.00° 104.60° 90.00°	Depositor
Resolution (Å)	(Not available) – 1.70	Depositor
% Data completeness (in resolution range)	(Not available) ((Not available)-1.70)	Depositor
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	PROLSQ	Depositor
R, R_{free}	0.188 , (Not available)	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	2130	wwPDB-VP
Average B, all atoms (Å ²)	12.0	wwPDB-VP

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: HG, ZN

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	1.95	26/2097 (1.2%)	2.00	64/2846 (2.2%)

All (26) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	125	THR	C-N	34.53	1.79	1.33
1	A	96	HIS	CE1-NE2	7.18	1.39	1.32
1	A	4	HIS	CE1-NE2	6.93	1.39	1.32
1	A	179	PHE	CA-C	6.66	1.61	1.52
1	A	64	HIS	CE1-NE2	6.55	1.39	1.32
1	A	252	LYS	C-N	-6.51	1.24	1.33
1	A	113	LYS	N-CA	6.50	1.53	1.46
1	A	139	ASP	CA-CB	-6.41	1.44	1.53
1	A	12	GLY	N-CA	6.22	1.51	1.43
1	A	107	HIS	CE1-NE2	6.19	1.38	1.32
1	A	64	HIS	CG-CD2	6.19	1.42	1.35
1	A	239	GLU	CD-OE2	6.09	1.36	1.25
1	A	253	ASN	C-O	6.07	1.31	1.24
1	A	28	GLN	C-N	5.94	1.40	1.32
1	A	99	SER	N-CA	5.89	1.53	1.46
1	A	144	LEU	C-N	-5.85	1.28	1.33
1	A	155	PRO	N-CD	5.55	1.55	1.47
1	A	72	ASP	N-CA	5.45	1.52	1.46
1	A	42	PRO	N-CD	5.42	1.55	1.47
1	A	97	TRP	C-N	-5.35	1.27	1.33
1	A	215	PRO	N-CD	5.30	1.55	1.47
1	A	146	ILE	C-O	-5.28	1.18	1.24
1	A	34	ASP	N-CA	5.28	1.53	1.46
1	A	131	PHE	C-O	5.18	1.30	1.24
1	A	79	LEU	C-N	-5.09	1.26	1.33
1	A	247	PRO	C-N	5.03	1.40	1.33

All (64) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	125	THR	CA-C-N	-9.44	103.44	120.99
1	A	125	THR	C-N-CA	-9.44	103.44	120.99
1	A	207	VAL	N-CA-C	7.97	119.76	108.36
1	A	230	ASN	CA-CB-CG	7.92	120.52	112.60
1	A	68	VAL	N-CA-CB	7.64	120.15	111.21
1	A	253	ASN	CA-CB-CG	7.44	120.04	112.60
1	A	231	PHE	CA-CB-CG	7.20	121.00	113.80
1	A	252	LYS	N-CA-C	6.83	120.80	111.17
1	A	14	GLU	CB-CG-CD	6.75	124.07	112.60
1	A	246	ARG	CA-C-N	6.70	127.09	119.92
1	A	246	ARG	C-N-CA	6.70	127.09	119.92
1	A	214	GLU	CA-C-N	6.69	126.86	120.31
1	A	214	GLU	C-N-CA	6.69	126.86	120.31
1	A	85	ASP	N-CA-C	-6.43	98.42	108.90
1	A	12	GLY	O-C-N	6.40	128.18	122.42
1	A	247	PRO	N-CA-CB	6.37	109.38	103.39
1	A	121	VAL	CA-C-O	-6.36	113.77	120.57
1	A	63	GLY	CA-C-O	-6.17	112.37	119.10
1	A	39	LYS	CA-CB-CG	6.13	126.36	114.10
1	A	98	GLY	O-C-N	6.00	129.75	123.09
1	A	52	ASP	CA-C-O	-5.94	113.39	120.10
1	A	154	LYS	CA-C-N	5.85	125.32	119.24
1	A	154	LYS	C-N-CA	5.85	125.32	119.24
1	A	191	TYR	N-CA-C	5.83	117.64	108.96
1	A	89	ARG	CD-NE-CZ	-5.77	116.33	124.40
1	A	175	ASP	N-CA-C	-5.73	101.56	110.10
1	A	34	ASP	CB-CA-C	5.68	120.95	111.30
1	A	33	ILE	O-C-N	5.67	129.80	122.77
1	A	65	ALA	O-C-N	5.62	129.01	122.99
1	A	119	HIS	CA-C-O	-5.62	114.44	120.46
1	A	15	HIS	CA-CB-CG	5.59	119.39	113.80
1	A	226	PHE	CA-CB-CG	5.55	119.35	113.80
1	A	122	HIS	ND1-CE1-NE2	5.53	113.93	108.40
1	A	58	ARG	O-C-N	5.50	129.04	123.26
1	A	21	PRO	O-C-N	5.50	128.83	122.17
1	A	147	PHE	O-C-N	5.48	129.20	123.06
1	A	61	ASN	CB-CA-C	5.47	119.84	110.81
1	A	165	ASP	CA-C-N	5.46	129.83	120.72
1	A	165	ASP	C-N-CA	5.46	129.83	120.72
1	A	242	VAL	CA-C-O	-5.40	116.28	121.63
1	A	94	HIS	ND1-CG-CD2	5.40	111.50	106.10
1	A	79	LEU	O-C-N	5.37	129.69	123.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	4	HIS	CA-C-N	5.31	128.77	120.75
1	A	4	HIS	C-N-CA	5.31	128.77	120.75
1	A	141	LEU	N-CA-CB	-5.30	102.61	111.20
1	A	231	PHE	N-CA-C	-5.30	105.55	112.23
1	A	64	HIS	CA-CB-CG	5.28	119.08	113.80
1	A	89	ARG	NE-CZ-NH2	-5.27	114.46	119.20
1	A	191	TYR	N-CA-CB	-5.26	103.24	111.56
1	A	177	THR	CA-CB-OG1	-5.25	101.73	109.60
1	A	24	LYS	CA-CB-CG	5.24	124.58	114.10
1	A	234	GLU	CA-CB-CG	5.20	124.50	114.10
1	A	32	ASP	CA-CB-CG	-5.13	107.47	112.60
1	A	34	ASP	O-C-N	5.12	129.18	122.68
1	A	125	THR	CA-C-O	5.12	125.68	119.49
1	A	26	GLU	N-CA-C	5.11	119.37	113.18
1	A	107	HIS	CA-CB-CG	-5.11	108.69	113.80
1	A	198	LEU	N-CA-C	-5.09	103.33	110.50
1	A	65	ALA	CA-C-O	-5.07	115.89	121.31
1	A	77	ALA	O-C-N	5.06	129.81	123.12
1	A	41	ASP	CB-CA-C	5.06	115.79	110.17
1	A	108	THR	O-C-N	5.03	129.43	123.24
1	A	245	TRP	CA-C-O	5.01	126.77	121.11
1	A	130	ASP	CA-CB-CG	5.00	117.60	112.60

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	2037	0	1985	29	0
2	A	1	0	0	0	0
3	A	1	0	0	0	0
4	A	91	0	0	0	0
All	All	2130	0	1985	29	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 7.

All (29) 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:125:THR:C	1:A:127:LYS:N	1.79	1.40
1:A:58:ARG:HD2	1:A:69:GLU:OE1	1.34	1.27
1:A:125:THR:C	1:A:127:LYS:CA	2.59	0.75
1:A:253:ASN:C	1:A:253:ASN:HD22	1.99	0.71
1:A:75:ASP:OD1	1:A:89:ARG:NE	2.28	0.64
1:A:45:LYS:O	1:A:82:GLY:HA2	2.00	0.60
1:A:127:LYS:HD2	1:A:128:TYR:CZ	2.38	0.59
1:A:231:PHE:HD2	1:A:239:GLU:HG2	1.68	0.58
1:A:221:GLU:H	1:A:221:GLU:CD	2.12	0.58
1:A:253:ASN:C	1:A:253:ASN:ND2	2.62	0.55
1:A:253:ASN:HD22	1:A:254:ARG:N	2.03	0.55
1:A:252:LYS:O	1:A:253:ASN:CG	2.53	0.52
1:A:60:LEU:CD2	1:A:67:ASN:HB2	2.38	0.52
1:A:253:ASN:ND2	1:A:254:ARG:N	2.57	0.52
1:A:60:LEU:HD21	1:A:67:ASN:HB2	1.92	0.52
1:A:154:LYS:HE3	1:A:183:GLY:O	2.10	0.50
1:A:252:LYS:O	1:A:253:ASN:CB	2.58	0.50
1:A:128:TYR:CE1	1:A:137:GLN:HG3	2.48	0.49
1:A:58:ARG:HD2	1:A:69:GLU:CD	2.27	0.49
1:A:134:ALA:O	1:A:140:GLY:HA3	2.14	0.48
1:A:59:ILE:HG12	1:A:167:ILE:HD13	1.97	0.46
1:A:60:LEU:HD22	1:A:69:GLU:OE2	2.15	0.46
1:A:236:GLU:HB3	1:A:237:PRO:HD2	2.00	0.44
1:A:89:ARG:O	1:A:122:HIS:HA	2.17	0.43
1:A:161:VAL:CG1	1:A:225:LYS:HD2	2.49	0.42
1:A:128:TYR:CZ	1:A:137:GLN:HG3	2.54	0.42
1:A:89:ARG:HG3	1:A:125:THR:CG2	2.50	0.42
1:A:9:LYS:HA	1:A:9:LYS:HD2	1.84	0.41
1:A:133:LYS:HD3	1:A:133:LYS:HA	1.95	0.41

There are no symmetry-related clashes.

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	254/256 (99%)	242 (95%)	11 (4%)	1 (0%)	30 16

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	253	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	220/220 (100%)	210 (96%)	10 (4%)	24 9

All (10) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	4	HIS
1	A	39	LYS
1	A	58	ARG
1	A	79	LEU
1	A	92	GLN
1	A	144	LEU
1	A	212	LEU
1	A	221	GLU
1	A	229	LEU
1	A	253	ASN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (5) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	10	HIS

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Mol	Chain	Res	Type
1	A	67	ASN
1	A	136	GLN
1	A	253	ASN
1	A	255	GLN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 2 ligands modelled in this entry, 2 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
1	A	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	A	125:THR	C	127:LYS	N	1.79

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.