



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 8, 2026 – 04:27 PM UTC

PDB ID : 4CA2 / pdb_00004ca2
Title : ENGINEERING THE HYDROPHOBIC POCKET OF CARBONIC ANHYDRASE II
Authors : Alexander, R.S.; Christianson, D.W.
Deposited on : 1991-06-08
Resolution : 2.10 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

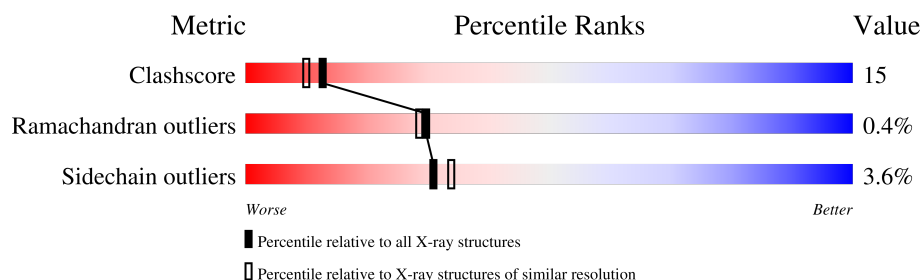
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.10 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	7164 (2.10-2.10)
Ramachandran outliers	187476	7099 (2.10-2.10)
Sidechain outliers	187428	7100 (2.10-2.10)

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	260	 34% 47% 15% . .

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 2133 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	255	Total	C	N	O	S	0	0	0
			2029	1303	347	377	2			

- 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.

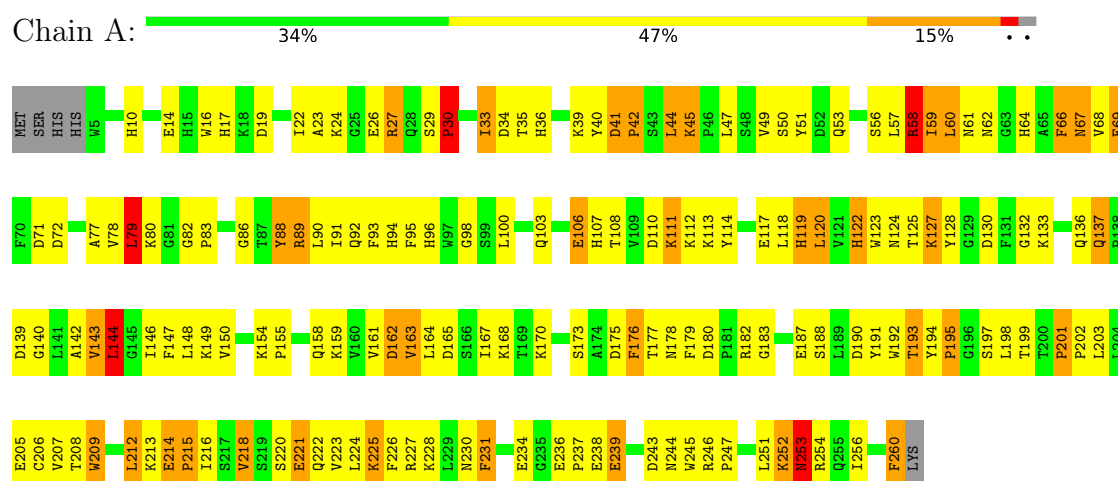
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	102	Total	O	0	0
			102	102		

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: 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) – 2.10	Depositor
% Data completeness (in resolution range)	(Not available) ((Not available)-2.10)	Depositor
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	PROLSQ	Depositor
R, R_{free}	0.180 , (Not available)	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	2133	wwPDB-VP
Average B, all atoms (Å ²)	12.0	wwPDB-VP

5 Model quality [i](#)

5.1 Standard geometry [i](#)

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	2.21	73/2088 (3.5%)	2.89	223/2833 (7.9%)

All (73) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	24	LYS	N-CA	11.06	1.60	1.46
1	A	117	GLU	C-O	-10.14	1.12	1.23
1	A	36	HIS	CE1-NE2	9.83	1.42	1.32
1	A	245	TRP	NE1-CE2	8.86	1.47	1.37
1	A	201	PRO	CA-C	-8.85	1.47	1.51
1	A	165	ASP	N-CA	8.81	1.57	1.46
1	A	201	PRO	C-O	8.48	1.32	1.25
1	A	59	ILE	C-O	8.09	1.32	1.24
1	A	190	ASP	CA-C	8.05	1.63	1.52
1	A	148	LEU	N-CA	-7.68	1.37	1.46
1	A	198	LEU	C-O	7.58	1.33	1.23
1	A	107	HIS	ND1-CE1	7.42	1.40	1.32
1	A	236	GLU	CD-OE2	7.27	1.39	1.25
1	A	36	HIS	C-N	-7.17	1.23	1.33
1	A	16	TRP	C-N	-7.12	1.24	1.34
1	A	146	ILE	C-O	7.10	1.31	1.24
1	A	202	PRO	N-CD	7.09	1.57	1.47
1	A	61	ASN	C-N	7.05	1.43	1.33
1	A	122	HIS	CG-CD2	6.71	1.43	1.35
1	A	58	ARG	CZ-NH1	-6.52	1.23	1.32
1	A	64	HIS	CE1-NE2	6.51	1.39	1.32
1	A	163	VAL	C-O	6.51	1.31	1.24
1	A	80	LYS	N-CA	6.47	1.54	1.46
1	A	173	SER	CB-OG	-6.38	1.29	1.42
1	A	96	HIS	C-O	-6.37	1.16	1.24
1	A	79	LEU	C-N	-6.28	1.25	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	238	GLU	CD-OE1	6.20	1.37	1.25
1	A	231	PHE	CA-C	6.19	1.61	1.52
1	A	227	ARG	NE-CZ	6.15	1.39	1.33
1	A	42	PRO	CA-CB	6.14	1.62	1.53
1	A	58	ARG	C-N	6.13	1.42	1.33
1	A	133	LYS	CA-C	-6.13	1.44	1.52
1	A	45	LYS	C-O	6.12	1.31	1.23
1	A	260	PHE	C-O	6.07	1.35	1.23
1	A	88	TYR	C-O	6.03	1.31	1.24
1	A	24	LYS	CA-CB	-6.03	1.45	1.53
1	A	98	GLY	N-CA	6.00	1.50	1.44
1	A	234	GLU	CD-OE1	5.98	1.36	1.25
1	A	218	VAL	C-O	5.77	1.29	1.23
1	A	59	ILE	C-N	-5.70	1.25	1.33
1	A	252	LYS	C-N	-5.63	1.25	1.33
1	A	230	ASN	C-N	5.61	1.42	1.33
1	A	221	GLU	N-CA	5.56	1.53	1.46
1	A	89	ARG	CA-CB	5.55	1.61	1.53
1	A	227	ARG	CA-C	5.54	1.62	1.52
1	A	192	TRP	N-CA	5.52	1.52	1.45
1	A	119	HIS	ND1-CE1	-5.51	1.27	1.32
1	A	231	PHE	C-N	-5.46	1.26	1.33
1	A	22	ILE	C-O	5.38	1.31	1.24
1	A	215	PRO	N-CD	5.33	1.55	1.47
1	A	207	VAL	CA-C	5.31	1.59	1.52
1	A	60	LEU	C-O	-5.30	1.17	1.23
1	A	41	ASP	C-O	-5.28	1.20	1.25
1	A	58	ARG	NE-CZ	5.25	1.38	1.33
1	A	243	ASP	C-N	-5.24	1.27	1.33
1	A	35	THR	CB-OG1	-5.23	1.35	1.43
1	A	122	HIS	CA-C	5.23	1.58	1.52
1	A	195	PRO	CA-CB	-5.21	1.47	1.53
1	A	45	LYS	CA-C	-5.20	1.46	1.53
1	A	34	ASP	N-CA	5.19	1.53	1.46
1	A	92	GLN	CG-CD	-5.19	1.39	1.52
1	A	209	TRP	NE1-CE2	-5.18	1.31	1.37
1	A	161	VAL	C-O	5.18	1.30	1.24
1	A	193	THR	N-CA	5.15	1.52	1.45
1	A	188	SER	C-N	-5.14	1.27	1.33
1	A	34	ASP	CA-CB	-5.12	1.46	1.52
1	A	51	TYR	CA-C	5.10	1.59	1.52
1	A	195	PRO	CA-C	5.08	1.57	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	62	ASN	N-CA	5.08	1.52	1.46
1	A	195	PRO	C-O	5.05	1.28	1.23
1	A	180	ASP	N-CA	-5.04	1.39	1.45
1	A	119	HIS	C-O	5.02	1.30	1.24
1	A	244	ASN	CA-C	5.02	1.59	1.52

All (223) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	165	ASP	CA-CB-CG	21.63	134.23	112.60
1	A	58	ARG	CB-CG-CD	21.47	160.68	111.30
1	A	92	GLN	CB-CG-CD	16.28	140.28	112.60
1	A	226	PHE	CA-CB-CG	13.76	127.56	113.80
1	A	24	LYS	CA-CB-CG	13.60	141.29	114.10
1	A	51	TYR	CA-CB-CG	13.15	137.57	113.90
1	A	221	GLU	CA-CB-CG	12.26	138.61	114.10
1	A	231	PHE	CA-CB-CG	11.88	125.68	113.80
1	A	207	VAL	CA-C-N	11.33	138.59	122.85
1	A	207	VAL	C-N-CA	11.33	138.59	122.85
1	A	91	ILE	CA-C-O	-11.07	110.27	120.34
1	A	93	PHE	CA-CB-CG	10.93	124.73	113.80
1	A	253	ASN	CA-CB-CG	10.28	122.88	112.60
1	A	190	ASP	CA-CB-CG	10.15	122.75	112.60
1	A	207	VAL	N-CA-C	9.61	123.03	108.71
1	A	142	ALA	CA-C-O	-9.60	108.48	120.20
1	A	24	LYS	CB-CA-C	9.46	127.64	111.46
1	A	178	ASN	CB-CG-ND2	9.28	130.32	116.40
1	A	14	GLU	CB-CG-CD	9.15	128.15	112.60
1	A	49	VAL	CA-C-O	-8.92	110.39	120.74
1	A	230	ASN	CA-CB-CG	8.77	121.37	112.60
1	A	182	ARG	NE-CZ-NH2	8.55	126.89	119.20
1	A	91	ILE	N-CA-C	-8.52	104.96	112.12
1	A	118	LEU	CA-C-N	-8.50	111.00	122.99
1	A	118	LEU	C-N-CA	-8.50	111.00	122.99
1	A	223	VAL	O-C-N	8.50	130.12	121.87
1	A	39	LYS	CB-CG-CD	8.49	130.83	111.30
1	A	89	ARG	NE-CZ-NH2	-8.47	111.58	119.20
1	A	158	GLN	CA-C-O	-8.46	111.59	120.55
1	A	67	ASN	CA-C-N	-8.44	112.15	123.12
1	A	67	ASN	C-N-CA	-8.44	112.15	123.12
1	A	207	VAL	CA-C-O	8.38	130.56	120.84
1	A	107	HIS	CB-CG-CD2	-8.32	120.39	131.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	59	ILE	CA-C-N	8.12	135.29	122.62
1	A	59	ILE	C-N-CA	8.12	135.29	122.62
1	A	24	LYS	N-CA-CB	-7.92	99.72	111.43
1	A	198	LEU	CA-C-O	-7.84	113.01	121.56
1	A	223	VAL	CA-C-O	-7.84	112.80	120.95
1	A	119	HIS	CB-CG-CD2	-7.82	121.04	131.20
1	A	10	HIS	CA-CB-CG	-7.82	105.98	113.80
1	A	120	LEU	N-CA-CB	7.76	123.18	110.37
1	A	119	HIS	CA-CB-CG	7.75	121.55	113.80
1	A	119	HIS	ND1-CE1-NE2	7.67	116.06	108.40
1	A	106	GLU	CG-CD-OE2	-7.66	100.78	118.40
1	A	95	PHE	CA-CB-CG	7.65	121.45	113.80
1	A	124	ASN	CA-CB-CG	-7.58	105.02	112.60
1	A	16	TRP	CA-C-O	-7.55	111.57	120.10
1	A	118	LEU	O-C-N	7.50	131.77	123.22
1	A	53	GLN	CB-CA-C	7.50	123.32	110.94
1	A	220	SER	O-C-N	7.50	130.07	122.12
1	A	71	ASP	CA-C-O	-7.34	111.89	120.62
1	A	107	HIS	ND1-CG-CD2	7.33	113.43	106.10
1	A	93	PHE	N-CA-CB	7.32	125.14	111.53
1	A	39	LYS	N-CA-C	7.26	120.57	108.73
1	A	16	TRP	O-C-N	7.22	130.66	122.22
1	A	179	PHE	CA-CB-CG	-7.22	106.58	113.80
1	A	175	ASP	CA-CB-CG	7.17	119.77	112.60
1	A	208	THR	CA-C-O	-7.14	113.13	120.84
1	A	67	ASN	CB-CG-ND2	7.11	127.06	116.40
1	A	149	LYS	N-CA-CB	7.09	121.26	110.70
1	A	143	VAL	O-C-N	7.08	130.83	123.18
1	A	17	HIS	CA-CB-CG	7.08	120.88	113.80
1	A	14	GLU	CA-C-N	7.06	133.69	122.11
1	A	14	GLU	C-N-CA	7.06	133.69	122.11
1	A	92	GLN	OE1-CD-NE2	-7.02	115.58	122.60
1	A	127	LYS	CB-CG-CD	6.95	127.28	111.30
1	A	177	THR	CA-C-N	6.95	132.00	122.07
1	A	177	THR	C-N-CA	6.95	132.00	122.07
1	A	260	PHE	CA-C-O	-6.90	109.06	120.80
1	A	36	HIS	CA-C-N	6.84	133.76	121.92
1	A	36	HIS	C-N-CA	6.84	133.76	121.92
1	A	144	LEU	N-CA-C	-6.81	97.42	108.52
1	A	119	HIS	CB-CG-ND1	6.80	132.91	122.70
1	A	253	ASN	CB-CG-ND2	6.80	126.60	116.40
1	A	78	VAL	O-C-N	6.79	130.27	123.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	51	TYR	O-C-N	6.78	130.40	122.19
1	A	243	ASP	CA-C-O	-6.77	114.42	122.27
1	A	107	HIS	ND1-CE1-NE2	6.76	115.16	108.40
1	A	227	ARG	O-C-N	6.76	133.23	122.41
1	A	133	LYS	CA-C-N	6.75	129.33	120.28
1	A	133	LYS	C-N-CA	6.75	129.33	120.28
1	A	91	ILE	O-C-N	6.73	128.84	121.97
1	A	208	THR	O-C-N	6.69	131.10	122.87
1	A	224	LEU	N-CA-CB	6.68	120.08	110.06
1	A	148	LEU	CA-C-O	-6.65	113.18	120.30
1	A	89	ARG	CB-CA-C	-6.64	98.90	109.80
1	A	23	ALA	CA-C-N	-6.64	112.03	123.25
1	A	23	ALA	C-N-CA	-6.64	112.03	123.25
1	A	50	SER	CA-C-N	-6.60	112.21	122.37
1	A	50	SER	C-N-CA	-6.60	112.21	122.37
1	A	206	CYS	CA-C-O	6.55	126.91	119.18
1	A	72	ASP	CA-CB-CG	-6.46	106.14	112.60
1	A	80	LYS	O-C-N	6.46	130.48	122.92
1	A	207	VAL	O-C-N	-6.46	116.09	122.93
1	A	106	GLU	CG-CD-OE1	6.43	133.19	118.40
1	A	94	HIS	ND1-CG-CD2	6.40	112.50	106.10
1	A	149	LYS	N-CA-C	-6.39	100.75	110.14
1	A	86	GLY	CA-C-N	6.38	131.53	122.72
1	A	86	GLY	C-N-CA	6.38	131.53	122.72
1	A	68	VAL	N-CA-C	-6.38	98.55	107.80
1	A	252	LYS	CB-CA-C	-6.36	102.29	112.09
1	A	146	ILE	CB-CG1-CD1	6.34	127.12	113.80
1	A	231	PHE	N-CA-CB	6.32	119.61	110.20
1	A	91	ILE	CB-CA-C	6.28	117.06	110.91
1	A	58	ARG	N-CA-CB	-6.28	101.03	111.57
1	A	236	GLU	CG-CD-OE1	6.27	132.82	118.40
1	A	78	VAL	CA-CB-CG1	6.26	121.05	110.40
1	A	238	GLU	CB-CG-CD	6.26	123.24	112.60
1	A	225	LYS	CA-C-N	6.26	128.67	120.28
1	A	225	LYS	C-N-CA	6.26	128.67	120.28
1	A	164	LEU	O-C-N	6.25	128.59	122.09
1	A	39	LYS	N-CA-CB	-6.25	100.24	110.42
1	A	252	LYS	N-CA-C	6.24	119.85	111.24
1	A	178	ASN	OD1-CG-ND2	-6.22	116.38	122.60
1	A	140	GLY	N-CA-C	6.22	120.19	112.73
1	A	162	ASP	CA-C-O	-6.21	111.98	119.49
1	A	14	GLU	CA-CB-CG	6.19	126.49	114.10

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	10	HIS	CB-CG-CD2	-6.17	123.18	131.20
1	A	50	SER	CA-C-O	-6.14	113.70	120.70
1	A	239	GLU	CA-CB-CG	6.13	126.37	114.10
1	A	103	GLN	CA-C-O	-6.07	114.77	121.33
1	A	51	TYR	CA-C-O	-6.04	112.35	119.48
1	A	33	ILE	O-C-N	6.03	131.62	122.76
1	A	119	HIS	CE1-NE2-CD2	-6.02	102.98	109.00
1	A	194	TYR	CA-C-N	6.02	129.31	120.46
1	A	194	TYR	C-N-CA	6.02	129.31	120.46
1	A	58	ARG	CD-NE-CZ	-6.01	115.99	124.40
1	A	175	ASP	O-C-N	6.00	130.28	122.97
1	A	148	LEU	O-C-N	6.00	130.22	123.27
1	A	92	GLN	CA-CB-CG	5.96	126.02	114.10
1	A	66	PHE	CA-C-O	5.95	127.13	120.70
1	A	69	GLU	CB-CG-CD	-5.95	102.48	112.60
1	A	214	GLU	CA-C-N	5.93	126.12	120.31
1	A	214	GLU	C-N-CA	5.93	126.12	120.31
1	A	58	ARG	CA-C-N	-5.92	114.89	123.06
1	A	58	ARG	C-N-CA	-5.92	114.89	123.06
1	A	45	LYS	N-CA-CB	-5.90	102.08	110.04
1	A	209	TRP	O-C-N	5.89	129.99	123.16
1	A	80	LYS	CA-C-O	-5.87	115.14	121.36
1	A	26	GLU	CG-CD-OE1	5.87	131.90	118.40
1	A	111	LYS	N-CA-CB	-5.86	104.66	114.27
1	A	136	GLN	CG-CD-NE2	-5.84	107.64	116.40
1	A	118	LEU	CA-C-O	-5.84	114.11	120.36
1	A	222	GLN	N-CA-C	-5.84	104.83	111.14
1	A	251	LEU	CB-CA-C	5.82	120.75	110.85
1	A	23	ALA	O-C-N	5.82	128.83	122.20
1	A	243	ASP	CA-CB-CG	-5.81	106.79	112.60
1	A	192	TRP	CA-CB-CG	5.79	124.60	113.60
1	A	253	ASN	OD1-CG-ND2	-5.77	116.83	122.60
1	A	107	HIS	CG-ND1-CE1	-5.77	99.49	109.30
1	A	142	ALA	O-C-N	5.76	130.65	123.28
1	A	27	ARG	O-C-N	5.72	129.43	121.83
1	A	139	ASP	CA-C-N	5.70	126.31	119.98
1	A	139	ASP	C-N-CA	5.70	126.31	119.98
1	A	191	TYR	N-CA-C	5.70	117.64	109.14
1	A	228	LYS	CB-CG-CD	-5.67	98.27	111.30
1	A	216	ILE	O-C-N	5.64	129.12	122.69
1	A	50	SER	O-C-N	5.63	130.32	123.01
1	A	130	ASP	O-C-N	5.62	129.56	123.10

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	53	GLN	N-CA-CB	-5.61	102.34	110.70
1	A	95	PHE	O-C-N	5.60	130.43	123.15
1	A	124	ASN	CB-CA-C	5.60	118.66	110.26
1	A	60	LEU	N-CA-C	5.57	118.30	109.50
1	A	56	SER	N-CA-C	-5.56	102.25	110.48
1	A	192	TRP	CA-C-O	-5.56	114.82	121.11
1	A	147	PHE	CA-C-N	5.56	130.83	123.00
1	A	147	PHE	C-N-CA	5.56	130.83	123.00
1	A	182	ARG	NH1-CZ-NH2	-5.55	112.08	119.30
1	A	208	THR	N-CA-CB	5.55	119.55	110.39
1	A	77	ALA	O-C-N	5.54	130.44	123.12
1	A	39	LYS	CA-C-O	5.53	126.27	120.36
1	A	158	GLN	OE1-CD-NE2	-5.52	117.08	122.60
1	A	34	ASP	CA-C-O	-5.52	115.18	120.92
1	A	19	ASP	CA-CB-CG	5.50	118.10	112.60
1	A	58	ARG	CA-CB-CG	5.49	125.08	114.10
1	A	188	SER	CA-CB-OG	-5.45	100.21	111.10
1	A	237	PRO	CB-CA-C	5.39	118.29	111.39
1	A	106	GLU	O-C-N	5.37	129.23	122.19
1	A	120	LEU	O-C-N	5.37	129.44	123.05
1	A	234	GLU	CA-C-O	-5.35	114.55	120.70
1	A	68	VAL	CA-C-O	-5.31	114.84	120.53
1	A	45	LYS	CA-C-N	5.29	125.23	119.78
1	A	45	LYS	C-N-CA	5.29	125.23	119.78
1	A	120	LEU	CA-C-N	-5.29	116.26	122.93
1	A	120	LEU	C-N-CA	-5.29	116.26	122.93
1	A	180	ASP	O-C-N	5.29	126.16	121.19
1	A	44	LEU	N-CA-CB	5.28	118.48	109.87
1	A	60	LEU	O-C-N	5.28	129.73	123.24
1	A	238	GLU	N-CA-C	5.27	117.34	108.96
1	A	108	THR	CA-C-O	-5.27	115.27	121.44
1	A	190	ASP	O-C-N	5.27	129.49	122.95
1	A	202	PRO	CA-C-N	5.26	131.60	121.54
1	A	202	PRO	C-N-CA	5.26	131.60	121.54
1	A	136	GLN	N-CA-C	-5.24	105.76	113.61
1	A	40	TYR	CA-CB-CG	-5.22	104.50	113.90
1	A	175	ASP	CB-CG-OD1	5.22	130.41	118.40
1	A	30	PRO	CB-CG-CD	-5.17	93.51	105.40
1	A	127	LYS	O-C-N	5.16	129.97	122.43
1	A	132	GLY	CA-C-O	-5.16	115.18	120.45
1	A	137	GLN	CA-C-N	5.16	124.96	119.28
1	A	137	GLN	C-N-CA	5.16	124.96	119.28

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	40	TYR	CA-C-O	-5.16	114.77	120.70
1	A	51	TYR	CB-CG-CD2	5.16	128.54	120.80
1	A	197	SER	O-C-N	5.13	129.60	122.78
1	A	67	ASN	O-C-N	5.12	129.72	123.21
1	A	117	GLU	CA-C-N	5.12	129.58	122.77
1	A	117	GLU	C-N-CA	5.12	129.58	122.77
1	A	236	GLU	CA-C-N	5.12	125.11	119.89
1	A	236	GLU	C-N-CA	5.12	125.11	119.89
1	A	90	LEU	CA-C-N	5.11	128.14	122.77
1	A	90	LEU	C-N-CA	5.11	128.14	122.77
1	A	251	LEU	CA-C-N	5.11	130.19	122.68
1	A	251	LEU	C-N-CA	5.11	130.19	122.68
1	A	60	LEU	CA-C-O	5.11	127.08	121.11
1	A	100	LEU	CA-CB-CG	5.10	134.15	116.30
1	A	103	GLN	CG-CD-NE2	5.10	124.05	116.40
1	A	180	ASP	CA-C-O	-5.09	115.08	119.36
1	A	19	ASP	CA-C-O	-5.09	113.54	119.14
1	A	187	GLU	CA-C-O	5.08	125.80	120.42
1	A	137	GLN	O-C-N	5.07	126.48	121.57
1	A	176	PHE	CA-CB-CG	5.05	118.85	113.80
1	A	216	ILE	CA-C-N	-5.04	114.07	122.64
1	A	216	ILE	C-N-CA	-5.04	114.07	122.64

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	2029	0	1981	61	1
2	A	1	0	0	0	0
3	A	1	0	0	0	0
4	A	102	0	0	3	1
All	All	2133	0	1981	61	1

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 15.

All (61) 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	2.07	1.11
1:A:144:LEU:CD2	1:A:212:LEU:HD21	1.96	0.95
1:A:144:LEU:HD21	1:A:212:LEU:HD21	1.57	0.87
1:A:110:ASP:O	1:A:111:LYS:HB2	1.91	0.70
1:A:60:LEU:O	1:A:66:PHE:HA	1.92	0.69
1:A:213:LYS:HD3	1:A:260:PHE:CZ	2.29	0.67
1:A:58:ARG:CD	1:A:69:GLU:OE1	2.43	0.67
1:A:144:LEU:HD22	1:A:212:LEU:HD21	1.78	0.66
1:A:125:THR:C	1:A:127:LYS:CA	2.70	0.64
1:A:58:ARG:HD3	1:A:69:GLU:OE1	1.97	0.64
1:A:144:LEU:CD2	1:A:212:LEU:CD2	2.75	0.64
1:A:60:LEU:HD21	1:A:69:GLU:OE2	2.00	0.62
1:A:60:LEU:CD2	1:A:69:GLU:OE2	2.50	0.60
1:A:253:ASN:HD22	1:A:254:ARG:N	2.00	0.59
1:A:144:LEU:HD22	1:A:212:LEU:CD2	2.32	0.59
1:A:225:LYS:HE3	4:A:345:HOH:O	2.03	0.58
1:A:213:LYS:HD3	1:A:260:PHE:CE2	2.40	0.57
1:A:89:ARG:HG3	1:A:125:THR:CG2	2.36	0.56
1:A:253:ASN:ND2	1:A:254:ARG:N	2.54	0.55
1:A:252:LYS:O	1:A:253:ASN:CG	2.50	0.54
1:A:58:ARG:HD2	1:A:69:GLU:OE1	2.08	0.53
1:A:59:ILE:HA	1:A:67:ASN:O	2.08	0.53
1:A:231:PHE:HD2	1:A:239:GLU:HG2	1.73	0.53
1:A:113:LYS:NZ	4:A:360:HOH:O	2.41	0.53
1:A:33:ILE:HG12	1:A:256:ILE:HD13	1.93	0.51
1:A:212:LEU:CD2	1:A:212:LEU:N	2.72	0.51
1:A:29:SER:HB3	1:A:30:PRO:HA	1.93	0.50
1:A:112:LYS:HE3	1:A:114:TYR:CE2	2.47	0.50
1:A:88:TYR:HA	1:A:123:TRP:O	2.11	0.49
1:A:45:LYS:O	1:A:82:GLY:HA2	2.14	0.48
1:A:88:TYR:HB3	1:A:122:HIS:HB3	1.96	0.48
1:A:128:TYR:CE1	1:A:137:GLN:HG3	2.49	0.48
1:A:106:GLU:OE1	1:A:199:THR:OG1	2.23	0.47
1:A:119:HIS:HB3	1:A:143:VAL:CG1	2.44	0.47
1:A:154:LYS:HE3	1:A:183:GLY:O	2.15	0.47
1:A:246:ARG:HA	1:A:247:PRO:HD3	1.74	0.47
1:A:58:ARG:HA	1:A:176:PHE:HB3	1.98	0.46
1:A:59:ILE:HG12	1:A:167:ILE:HD13	1.96	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:168:LYS:NZ	4:A:343:HOH:O	2.41	0.46
1:A:193:THR:HA	1:A:209:TRP:O	2.15	0.46
1:A:170:LYS:HB2	1:A:231:PHE:O	2.16	0.46
1:A:214:GLU:HA	1:A:215:PRO:HD3	1.75	0.45
1:A:41:ASP:HA	1:A:42:PRO:HD2	1.89	0.45
1:A:167:ILE:HG13	1:A:167:ILE:O	2.16	0.45
1:A:201:PRO:HA	1:A:203:LEU:HG	1.99	0.45
1:A:41:ASP:OD2	1:A:44:LEU:CD1	2.65	0.45
1:A:154:LYS:HA	1:A:155:PRO:HD2	1.83	0.44
1:A:57:LEU:O	1:A:58:ARG:HB3	2.18	0.43
1:A:45:LYS:H	1:A:45:LYS:HG3	1.64	0.42
1:A:159:LYS:HE2	1:A:159:LYS:HB3	1.75	0.42
1:A:41:ASP:CG	1:A:44:LEU:HD13	2.45	0.42
1:A:252:LYS:O	1:A:253:ASN:CB	2.68	0.42
1:A:47:LEU:HD22	1:A:79:LEU:HD21	2.01	0.42
1:A:27:ARG:HG3	1:A:205:GLU:HB3	2.01	0.42
1:A:89:ARG:HG3	1:A:125:THR:HG22	2.02	0.42
1:A:163:VAL:HG11	1:A:176:PHE:CE1	2.55	0.41
1:A:212:LEU:N	1:A:212:LEU:HD22	2.36	0.40
1:A:195:PRO:O	1:A:254:ARG:NH1	2.47	0.40
1:A:89:ARG:O	1:A:122:HIS:HA	2.22	0.40
1:A:120:LEU:N	1:A:120:LEU:HD12	2.36	0.40
1:A:150:VAL:HA	1:A:218:VAL:O	2.22	0.40

All (1) 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:162:ASP:OD2	4:A:330:HOH:O[2_445]	1.80	0.40

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	251/260 (96%)	239 (95%)	11 (4%)	1 (0%)	30	28

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	220/225 (98%)	212 (96%)	8 (4%)	31	34

All (8) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	30	PRO
1	A	58	ARG
1	A	79	LEU
1	A	83	PRO
1	A	144	LEU
1	A	212	LEU
1	A	221	GLU
1	A	253	ASN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (3) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	53	GLN
1	A	136	GLN
1	A	253	ASN

5.3.3 RNA ⓘ

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	2.07

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.