



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 05:45 AM UTC

PDB ID : 1CVC / pdb_00001cvc
Title : REDESIGNING THE ZINC BINDING SITE OF HUMAN CARBONIC ANHYDRASE II: STRUCTURE OF A HIS2ASP-ZN²⁺ METAL COORDINATION POLYHEDRON
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Deposited on : 1993-09-22
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

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

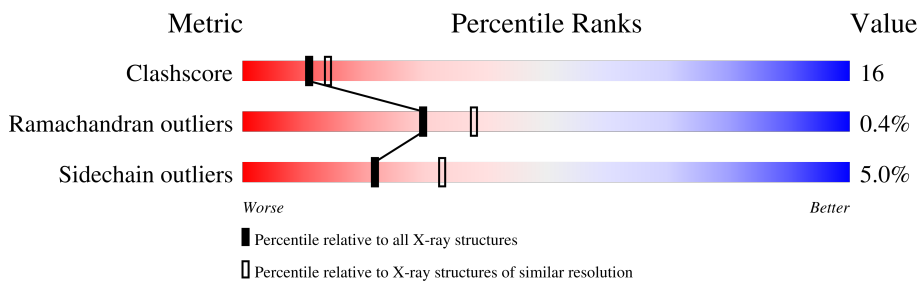
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.30 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 ≥ 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	259	

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 2140 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
			2027	1301	345	379	2			

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	94	ASP	HIS	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 water.

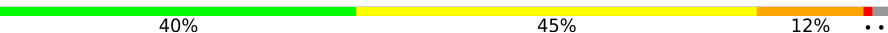
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	112	Total	O	0	0
			112	112		

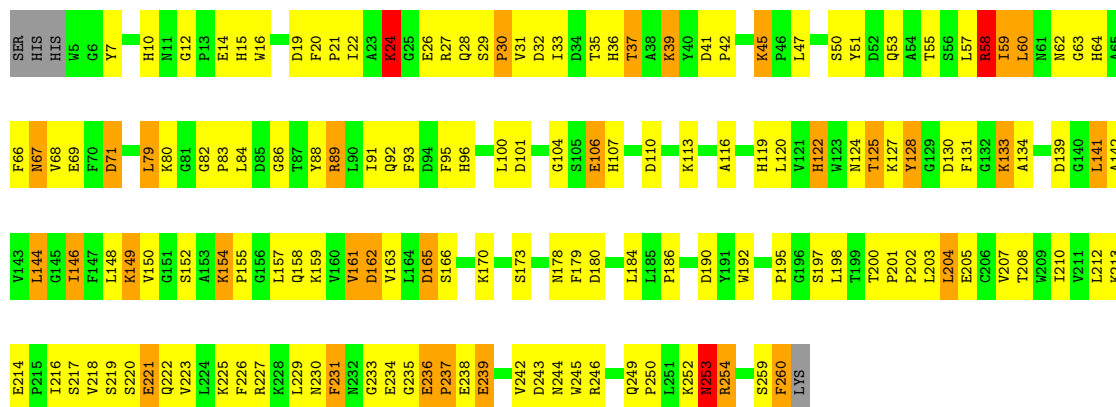
3 Residue-property plots

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

Chain A: 



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) – 2.30	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}	0.170 , (Not available)	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	2140	wwPDB-VP
Average B, all atoms (Å ²)	14.0	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: 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	1.77	26/2086 (1.2%)	2.40	137/2832 (4.8%)

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	1

All (26) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	30	PRO	C-N	-7.46	1.24	1.33
1	A	162	ASP	C-O	7.29	1.33	1.24
1	A	36	HIS	N-CA	6.52	1.54	1.46
1	A	104	GLY	C-N	-6.49	1.25	1.33
1	A	159	LYS	N-CA	6.26	1.53	1.46
1	A	7	TYR	N-CA	6.04	1.53	1.46
1	A	28	GLN	C-O	-5.99	1.16	1.23
1	A	235	GLY	N-CA	5.93	1.53	1.45
1	A	16	TRP	NE1-CE2	5.67	1.43	1.37
1	A	95	PHE	N-CA	5.62	1.53	1.45
1	A	201	PRO	C-O	5.60	1.30	1.24
1	A	130	ASP	C-N	-5.58	1.26	1.33
1	A	166	SER	C-N	-5.53	1.26	1.33
1	A	88	TYR	C-O	5.52	1.30	1.24
1	A	195	PRO	CA-C	-5.50	1.47	1.52
1	A	192	TRP	C-O	5.44	1.30	1.23
1	A	208	THR	CA-CB	5.43	1.60	1.53
1	A	89	ARG	C-N	-5.37	1.25	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	106	GLU	C-N	-5.28	1.26	1.33
1	A	86	GLY	N-CA	5.26	1.50	1.45
1	A	96	HIS	CE1-NE2	-5.18	1.27	1.32
1	A	59	ILE	CA-CB	5.14	1.62	1.54
1	A	203	LEU	N-CA	5.13	1.52	1.46
1	A	122	HIS	N-CA	5.13	1.52	1.45
1	A	125	THR	C-O	5.11	1.30	1.24
1	A	173	SER	C-O	5.02	1.29	1.23

All (137) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	95	PHE	CA-CB-CG	13.56	127.36	113.80
1	A	101	ASP	CA-CB-CG	10.61	123.21	112.60
1	A	93	PHE	CA-CB-CG	10.28	124.08	113.80
1	A	10	HIS	CA-CB-CG	-9.99	103.81	113.80
1	A	234	GLU	CB-CG-CD	9.72	129.12	112.60
1	A	26	GLU	CA-C-O	-9.48	107.56	119.31
1	A	226	PHE	CA-CB-CG	9.35	123.15	113.80
1	A	146	ILE	CA-C-N	9.27	134.67	121.42
1	A	146	ILE	C-N-CA	9.27	134.67	121.42
1	A	207	VAL	N-CA-C	9.17	122.37	108.71
1	A	80	LYS	CA-C-O	-9.14	111.53	121.31
1	A	154	LYS	CB-CA-C	9.01	119.52	110.33
1	A	179	PHE	CA-CB-CG	-8.98	104.82	113.80
1	A	230	ASN	CA-CB-CG	8.91	121.51	112.60
1	A	31	VAL	CA-C-O	8.90	130.44	121.63
1	A	144	LEU	CA-C-O	-8.89	111.07	120.58
1	A	244	ASN	CB-CG-ND2	8.68	129.42	116.40
1	A	80	LYS	O-C-N	8.56	132.15	122.99
1	A	122	HIS	CA-CB-CG	8.46	122.25	113.80
1	A	50	SER	CA-C-O	-8.04	111.22	121.11
1	A	244	ASN	OD1-CG-ND2	-7.87	114.73	122.60
1	A	68	VAL	N-CA-C	-7.87	97.15	108.17
1	A	158	GLN	CA-C-O	-7.64	112.45	120.55
1	A	203	LEU	N-CA-CB	-7.58	97.69	110.49
1	A	204	LEU	CA-C-O	7.44	129.40	120.92
1	A	207	VAL	CA-C-N	7.40	133.62	123.11
1	A	207	VAL	C-N-CA	7.40	133.62	123.11
1	A	190	ASP	N-CA-C	-7.39	99.34	110.28
1	A	58	ARG	N-CA-C	7.31	119.27	108.60
1	A	141	LEU	O-C-N	7.27	132.60	123.15

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	14	GLU	CB-CG-CD	7.23	124.89	112.60
1	A	253	ASN	O-C-N	7.10	132.03	122.59
1	A	96	HIS	CA-C-O	-7.06	112.48	120.32
1	A	67	ASN	O-C-N	6.96	132.28	123.23
1	A	223	VAL	CA-C-O	-6.95	113.72	120.95
1	A	222	GLN	CB-CG-CD	6.91	124.35	112.60
1	A	158	GLN	O-C-N	6.84	129.37	122.12
1	A	67	ASN	CA-C-O	-6.76	113.39	120.70
1	A	33	ILE	O-C-N	6.70	131.11	122.94
1	A	231	PHE	N-CA-C	-6.69	103.91	111.14
1	A	249	GLN	O-C-N	6.66	127.20	121.20
1	A	238	GLU	CG-CD-OE1	-6.59	103.24	118.40
1	A	253	ASN	CA-CB-CG	6.53	119.13	112.60
1	A	158	GLN	N-CA-C	6.50	118.37	111.28
1	A	60	LEU	CA-C-N	6.49	131.86	122.85
1	A	60	LEU	C-N-CA	6.49	131.86	122.85
1	A	12	GLY	O-C-N	6.48	128.25	122.42
1	A	238	GLU	CG-CD-OE2	6.30	132.89	118.40
1	A	120	LEU	O-C-N	6.29	130.69	123.27
1	A	26	GLU	O-C-N	6.29	131.14	122.46
1	A	71	ASP	CA-C-O	-6.25	113.54	120.60
1	A	82	GLY	CA-C-N	6.21	127.12	120.47
1	A	82	GLY	C-N-CA	6.21	127.12	120.47
1	A	244	ASN	N-CA-C	-6.20	103.06	111.55
1	A	19	ASP	O-C-N	6.18	131.13	122.36
1	A	26	GLU	CA-C-N	-6.18	112.55	122.62
1	A	26	GLU	C-N-CA	-6.18	112.55	122.62
1	A	107	HIS	N-CA-C	-6.17	101.35	110.48
1	A	142	ALA	CA-C-N	-6.16	115.07	123.14
1	A	142	ALA	C-N-CA	-6.16	115.07	123.14
1	A	197	SER	N-CA-C	6.12	117.49	108.86
1	A	162	ASP	CA-C-O	-6.09	113.21	120.10
1	A	51	TYR	CA-C-O	-6.05	112.34	119.48
1	A	144	LEU	CA-C-N	-6.04	116.46	122.20
1	A	144	LEU	C-N-CA	-6.04	116.46	122.20
1	A	35	THR	N-CA-C	6.04	119.91	112.54
1	A	260	PHE	CA-C-O	-6.02	110.56	120.80
1	A	139	ASP	CA-C-N	6.01	126.66	119.98
1	A	139	ASP	C-N-CA	6.01	126.66	119.98
1	A	236	GLU	CG-CD-OE2	-5.97	104.68	118.40
1	A	37	THR	CA-CB-OG1	-5.94	100.69	109.60
1	A	207	VAL	CA-C-O	5.92	127.71	120.84

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	67	ASN	CA-C-N	-5.91	115.86	123.19
1	A	67	ASN	C-N-CA	-5.91	115.86	123.19
1	A	223	VAL	O-C-N	5.90	127.59	121.87
1	A	208	THR	N-CA-CB	5.90	120.26	110.47
1	A	149	LYS	N-CA-C	-5.89	100.55	109.85
1	A	110	ASP	CB-CG-OD2	5.89	131.94	118.40
1	A	107	HIS	O-C-N	5.88	129.60	122.96
1	A	128	TYR	N-CA-C	5.86	120.43	113.16
1	A	93	PHE	N-CA-CB	5.85	121.60	111.13
1	A	125	THR	CA-CB-OG1	-5.85	100.83	109.60
1	A	238	GLU	N-CA-C	5.84	118.19	109.25
1	A	220	SER	CA-CB-OG	-5.83	99.45	111.10
1	A	253	ASN	CB-CG-ND2	5.79	125.08	116.40
1	A	149	LYS	N-CA-CB	5.76	120.53	111.20
1	A	242	VAL	O-C-N	5.68	129.01	122.82
1	A	180	ASP	O-C-N	5.67	127.58	121.12
1	A	214	GLU	CG-CD-OE2	5.63	131.34	118.40
1	A	42	PRO	N-CA-CB	5.61	108.89	103.51
1	A	142	ALA	CA-C-O	-5.54	114.37	120.24
1	A	221	GLU	O-C-N	5.53	129.07	122.27
1	A	200	THR	CA-CB-OG1	-5.49	101.36	109.60
1	A	227	ARG	NE-CZ-NH2	5.49	124.14	119.20
1	A	59	ILE	CB-CA-C	5.49	118.95	110.50
1	A	235	GLY	N-CA-C	-5.48	107.64	115.64
1	A	197	SER	N-CA-CB	-5.48	102.17	111.31
1	A	41	ASP	CA-C-N	5.47	125.08	119.56
1	A	41	ASP	C-N-CA	5.47	125.08	119.56
1	A	249	GLN	CA-C-O	-5.44	114.83	120.87
1	A	92	GLN	OE1-CD-NE2	-5.42	117.18	122.60
1	A	152	SER	CA-CB-OG	-5.42	100.26	111.10
1	A	22	ILE	CA-C-N	5.41	128.28	120.38
1	A	22	ILE	C-N-CA	5.41	128.28	120.38
1	A	139	ASP	N-CA-C	-5.41	105.37	112.41
1	A	239	GLU	CA-C-O	-5.40	114.73	120.40
1	A	15	HIS	O-C-N	5.40	129.01	122.48
1	A	259	SER	CA-C-O	-5.38	112.77	119.28
1	A	231	PHE	O-C-N	5.34	127.86	122.09
1	A	219	SER	CA-C-N	5.33	127.68	120.38
1	A	219	SER	C-N-CA	5.33	127.68	120.38
1	A	244	ASN	N-CA-CB	5.33	117.72	110.42
1	A	165	ASP	CA-CB-CG	5.27	117.87	112.60
1	A	53	GLN	OE1-CD-NE2	5.25	127.85	122.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	133	LYS	N-CA-CB	5.25	118.08	110.26
1	A	198	LEU	N-CA-C	-5.24	103.12	110.50
1	A	233	GLY	N-CA-C	-5.23	104.70	113.02
1	A	142	ALA	O-C-N	5.23	129.38	123.27
1	A	237	PRO	N-CA-C	-5.22	102.89	111.15
1	A	184	LEU	N-CA-CB	-5.21	102.75	110.61
1	A	178	ASN	OD1-CG-ND2	5.20	127.80	122.60
1	A	53	GLN	CG-CD-NE2	-5.18	108.63	116.40
1	A	93	PHE	N-CA-C	-5.17	100.26	109.06
1	A	24	LYS	O-C-N	5.17	128.82	122.20
1	A	161	VAL	CA-C-O	-5.15	116.06	121.41
1	A	45	LYS	CA-CB-CG	-5.14	103.82	114.10
1	A	134	ALA	CA-C-O	-5.13	115.11	120.55
1	A	190	ASP	CA-CB-CG	5.12	117.72	112.60
1	A	142	ALA	N-CA-CB	5.09	118.77	110.77
1	A	155	PRO	CB-CA-C	5.08	119.95	111.56
1	A	91	ILE	CA-C-O	-5.08	115.53	120.30
1	A	32	ASP	CA-CB-CG	-5.03	107.58	112.60
1	A	180	ASP	CB-CA-C	5.03	115.75	110.17
1	A	116	ALA	O-C-N	5.02	128.36	122.99
1	A	20	PHE	CA-C-N	5.02	124.68	119.56
1	A	20	PHE	C-N-CA	5.02	124.68	119.56
1	A	242	VAL	CA-C-O	-5.01	116.44	121.45

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	254	ARG	Sidechain

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	2027	0	1979	66	2
2	A	1	0	0	0	0
3	A	112	0	0	11	2

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
All	All	2140	0	1979	66	2

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 16.

All (66) 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:58:ARG:HD2	1:A:69:GLU:OE1	1.48	1.13
1:A:165:ASP:HB2	3:A:362:HOH:O	1.65	0.97
1:A:60:LEU:HD12	3:A:358:HOH:O	1.84	0.77
1:A:60:LEU:HB2	3:A:358:HOH:O	1.93	0.69
1:A:253:ASN:HD22	1:A:254:ARG:N	1.91	0.69
1:A:253:ASN:ND2	1:A:254:ARG:N	2.42	0.68
1:A:47:LEU:HD11	1:A:210:ILE:HG21	1.74	0.68
1:A:62:ASN:O	1:A:170:LYS:NZ	2.28	0.67
1:A:55:THR:HG23	3:A:288:HOH:O	1.97	0.65
1:A:106:GLU:OE1	1:A:119:HIS:HE1	1.80	0.64
1:A:253:ASN:HD22	1:A:253:ASN:C	2.06	0.63
1:A:161:VAL:HG13	1:A:225:LYS:HD2	1.79	0.62
1:A:202:PRO:HG2	1:A:204:LEU:HG	1.82	0.61
1:A:250:PRO:HB2	1:A:252:LYS:HG3	1.85	0.59
1:A:89:ARG:HG3	1:A:125:THR:CG2	2.35	0.57
1:A:60:LEU:HD21	1:A:67:ASN:HB2	1.87	0.56
1:A:146:ILE:HG12	1:A:212:LEU:HD22	1.89	0.55
1:A:253:ASN:ND2	1:A:253:ASN:C	2.64	0.54
1:A:89:ARG:HG3	1:A:125:THR:HG22	1.92	0.52
1:A:60:LEU:CD2	1:A:67:ASN:HB2	2.40	0.52
1:A:58:ARG:HD2	1:A:69:GLU:CD	2.28	0.52
1:A:57:LEU:HD11	1:A:71:ASP:HB2	1.93	0.51
1:A:79:LEU:HD13	1:A:84:LEU:HD11	1.93	0.51
1:A:29:SER:HB3	1:A:30:PRO:HA	1.92	0.50
1:A:47:LEU:HD22	1:A:79:LEU:HD21	1.92	0.50
1:A:113:LYS:NZ	3:A:343:HOH:O	2.45	0.50
1:A:39:LYS:HD3	3:A:314:HOH:O	2.12	0.49
1:A:149:LYS:O	1:A:217:SER:HA	2.12	0.49
1:A:252:LYS:O	1:A:253:ASN:CB	2.60	0.49
1:A:231:PHE:HD2	1:A:239:GLU:HG2	1.78	0.49
1:A:213:LYS:HD3	1:A:260:PHE:CZ	2.48	0.49
1:A:21:PRO:HD2	3:A:268:HOH:O	2.12	0.48
1:A:60:LEU:O	1:A:66:PHE:HA	2.13	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:24:LYS:CD	3:A:353:HOH:O	2.62	0.48
1:A:63:GLY:HA3	1:A:170:LYS:NZ	2.29	0.47
1:A:252:LYS:O	1:A:253:ASN:CG	2.57	0.47
1:A:131:PHE:CE1	1:A:141:LEU:HD21	2.51	0.46
1:A:144:LEU:CD2	1:A:212:LEU:HD11	2.45	0.46
1:A:64:HIS:NE2	3:A:344:HOH:O	2.36	0.45
1:A:59:ILE:HG21	1:A:163:VAL:HG11	1.99	0.45
1:A:24:LYS:CE	3:A:353:HOH:O	2.65	0.45
1:A:27:ARG:CG	1:A:205:GLU:HB3	2.46	0.45
1:A:124:ASN:HB3	1:A:128:TYR:CD2	2.53	0.44
1:A:47:LEU:HD11	1:A:210:ILE:CG2	2.46	0.44
1:A:154:LYS:O	1:A:157:LEU:HB3	2.18	0.44
1:A:148:LEU:HG	1:A:216:ILE:HG13	1.99	0.44
1:A:24:LYS:HD3	3:A:353:HOH:O	2.17	0.44
1:A:154:LYS:HG2	1:A:216:ILE:HD12	2.00	0.44
1:A:29:SER:O	1:A:246:ARG:NH1	2.50	0.43
1:A:150:VAL:HA	1:A:218:VAL:O	2.17	0.43
1:A:186:PRO:HG3	1:A:212:LEU:HD23	1.99	0.43
1:A:58:ARG:CD	1:A:69:GLU:OE1	2.41	0.43
1:A:243:ASP:HA	1:A:245:TRP:CD1	2.54	0.43
1:A:253:ASN:HD22	1:A:254:ARG:CA	2.32	0.42
1:A:186:PRO:CG	1:A:212:LEU:HD23	2.49	0.42
1:A:27:ARG:HG3	1:A:27:ARG:O	2.19	0.42
1:A:47:LEU:HD23	1:A:47:LEU:HA	1.88	0.41
1:A:89:ARG:O	1:A:122:HIS:HA	2.21	0.41
1:A:45:LYS:H	1:A:45:LYS:HG3	1.60	0.41
1:A:63:GLY:O	1:A:231:PHE:HD1	2.03	0.41
1:A:161:VAL:CG1	1:A:225:LYS:HD2	2.48	0.41
1:A:60:LEU:HD23	1:A:60:LEU:N	2.36	0.41
1:A:236:GLU:HB3	1:A:237:PRO:HD2	2.03	0.41
1:A:59:ILE:HA	1:A:67:ASN:O	2.22	0.40
1:A:63:GLY:HA3	1:A:170:LYS:HD2	2.03	0.40
1:A:79:LEU:HD13	1:A:84:LEU:CD1	2.50	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	Interatomic distance (Å)	Clash overlap (Å)
1:A:162:ASP:OD2	3:A:320:HOH:O[2_445]	1.85	0.35
1:A:133:LYS:CE	3:A:355:HOH:O[1_565]	2.10	0.10

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	253/259 (98%)	239 (94%)	13 (5%)	1 (0%)	30	38

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	253	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	220/224 (98%)	209 (95%)	11 (5%)	22	33

All (11) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	24	LYS
1	A	37	THR
1	A	39	LYS
1	A	58	ARG
1	A	79	LEU
1	A	83	PRO
1	A	100	LEU
1	A	127	LYS
1	A	221	GLU
1	A	229	LEU

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Mol	Chain	Res	Type
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	53	GLN
1	A	67	ASN
1	A	158	GLN
1	A	178	ASN
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 ⓘ

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

5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry ⓘ

Of 1 ligands modelled in this entry, 1 is 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](#)

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.