



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 13, 2026 – 11:46 AM UTC

PDB ID : 5CA2 / pdb_00005ca2
Title : CONFORMATIONAL MOBILITY OF HIS-64 IN THE THR-200 (RIGHT ARROW) SER MUTANT OF HUMAN 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
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

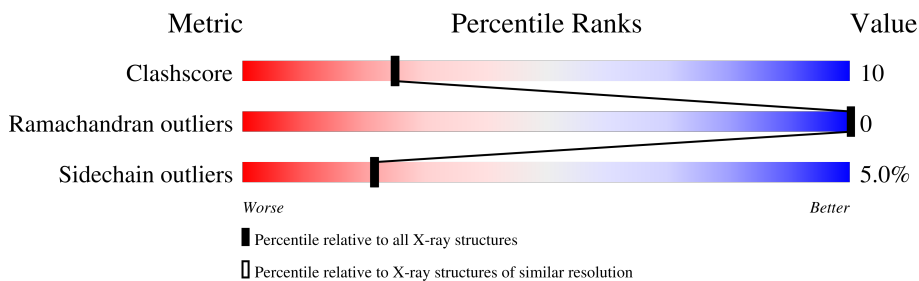
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.10 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	 46% 43% 8% ..

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 2149 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
			Total	C	N	O	S			
1	A	255	2028	1302	347	377	2	0	0	0

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	200	SER	THR	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.

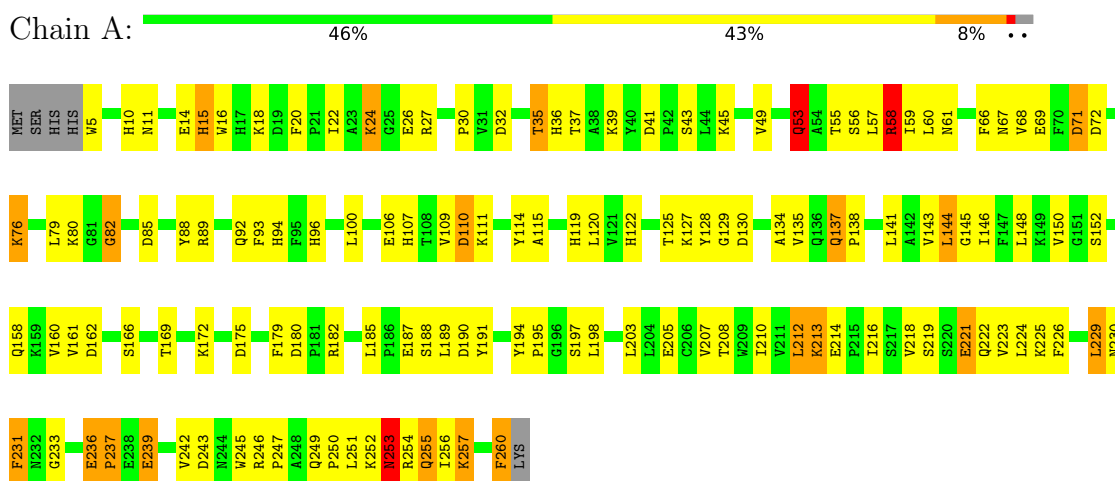
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	119	Total	O	0	0
			119	119		

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

Xtrriage (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	42.70Å 41.70Å 73.00Å 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}	0.160 , (Not available)	Depositor
Estimated twinning fraction	No twinning to report.	Xtrriage
Total number of atoms	2149	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	1.87	25/2087 (1.2%)	2.46	148/2831 (5.2%)

All (25) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	180	ASP	N-CA	7.23	1.54	1.45
1	A	198	LEU	N-CA	7.18	1.55	1.45
1	A	249	GLN	C-O	7.12	1.31	1.24
1	A	160	VAL	C-O	-6.12	1.17	1.24
1	A	5	TRP	N-CA	6.07	1.57	1.46
1	A	20	PHE	N-CA	5.99	1.53	1.46
1	A	10	HIS	CG-CD2	5.92	1.42	1.35
1	A	106	GLU	CA-C	-5.91	1.46	1.53
1	A	239	GLU	CD-OE2	5.85	1.36	1.25
1	A	236	GLU	CD-OE2	5.70	1.36	1.25
1	A	134	ALA	C-O	5.66	1.30	1.24
1	A	119	HIS	CE1-NE2	5.61	1.38	1.32
1	A	57	LEU	CA-C	5.57	1.57	1.52
1	A	172	LYS	C-O	5.52	1.30	1.23
1	A	115	ALA	N-CA	5.43	1.53	1.46
1	A	82	GLY	C-N	-5.32	1.28	1.34
1	A	107	HIS	CE1-NE2	5.28	1.37	1.32
1	A	76	LYS	C-O	5.26	1.30	1.24
1	A	194	TYR	C-N	-5.22	1.29	1.33
1	A	10	HIS	CA-CB	5.15	1.62	1.53
1	A	160	VAL	CA-C	5.10	1.59	1.52
1	A	249	GLN	CA-CB	-5.06	1.46	1.53
1	A	144	LEU	C-N	-5.05	1.29	1.33
1	A	198	LEU	CA-CB	-5.03	1.45	1.53
1	A	122	HIS	CE1-NE2	5.01	1.37	1.32

All (148) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	226	PHE	CA-CB-CG	13.57	127.38	113.80
1	A	93	PHE	CA-CB-CG	13.40	127.20	113.80
1	A	10	HIS	CA-CB-CG	-9.81	103.99	113.80
1	A	207	VAL	N-CA-C	9.29	122.56	108.71
1	A	253	ASN	CB-CG-ND2	9.06	129.99	116.40
1	A	246	ARG	CA-C-N	8.44	128.37	119.85
1	A	246	ARG	C-N-CA	8.44	128.37	119.85
1	A	144	LEU	CA-C-O	-8.02	111.45	120.43
1	A	58	ARG	NE-CZ-NH1	7.91	129.41	121.50
1	A	14	GLU	CB-CG-CD	7.82	125.90	112.60
1	A	158	GLN	CA-C-O	-7.82	112.26	120.55
1	A	89	ARG	NE-CZ-NH2	-7.69	112.28	119.20
1	A	15	HIS	ND1-CE1-NE2	7.66	116.06	108.40
1	A	236	GLU	CG-CD-OE1	7.60	135.88	118.40
1	A	94	HIS	ND1-CE1-NE2	7.45	115.85	108.40
1	A	208	THR	CA-C-O	-7.45	112.79	120.54
1	A	197	SER	N-CA-CB	-7.34	98.95	111.21
1	A	5	TRP	CA-C-N	7.12	130.31	121.83
1	A	5	TRP	C-N-CA	7.12	130.31	121.83
1	A	89	ARG	O-C-N	7.07	131.28	123.22
1	A	80	LYS	O-C-N	7.07	130.55	122.99
1	A	249	GLN	CA-C-N	7.05	127.45	119.83
1	A	249	GLN	C-N-CA	7.05	127.45	119.83
1	A	66	PHE	CA-CB-CG	7.05	120.85	113.80
1	A	187	GLU	CA-C-O	7.03	127.87	120.42
1	A	231	PHE	CA-CB-CG	7.01	120.81	113.80
1	A	96	HIS	CA-C-O	-6.96	112.60	120.32
1	A	89	ARG	CB-CA-C	-6.95	98.41	109.80
1	A	145	GLY	CA-C-N	6.89	132.76	122.98
1	A	145	GLY	C-N-CA	6.89	132.76	122.98
1	A	94	HIS	CA-CB-CG	-6.77	107.03	113.80
1	A	195	PRO	N-CA-CB	6.77	107.76	103.23
1	A	230	ASN	CA-CB-CG	6.75	119.35	112.60
1	A	246	ARG	CD-NE-CZ	6.75	133.85	124.40
1	A	158	GLN	OE1-CD-NE2	-6.64	115.96	122.60
1	A	36	HIS	ND1-CE1-NE2	6.62	115.02	108.40
1	A	114	TYR	O-C-N	6.62	130.51	122.84
1	A	224	LEU	CA-C-O	-6.62	113.54	120.55
1	A	197	SER	N-CA-C	6.58	117.82	108.74
1	A	169	THR	CA-CB-OG1	-6.55	99.77	109.60
1	A	255	GLN	CA-C-O	-6.54	113.30	120.36
1	A	256	ILE	N-CA-CB	6.51	117.82	110.72

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	39	LYS	N-CA-C	6.43	118.76	108.41
1	A	20	PHE	CA-C-N	6.39	126.89	119.47
1	A	20	PHE	C-N-CA	6.39	126.89	119.47
1	A	16	TRP	CA-C-O	-6.39	112.88	120.10
1	A	239	GLU	CA-C-O	-6.38	113.70	120.40
1	A	82	GLY	CA-C-N	6.35	127.26	120.47
1	A	82	GLY	C-N-CA	6.35	127.26	120.47
1	A	189	LEU	CA-C-O	-6.34	112.23	119.78
1	A	180	ASP	CA-C-N	6.32	126.00	119.56
1	A	180	ASP	C-N-CA	6.32	126.00	119.56
1	A	130	ASP	CA-C-O	-6.30	114.71	121.45
1	A	58	ARG	CB-CG-CD	6.30	125.79	111.30
1	A	106	GLU	CG-CD-OE2	-6.29	103.92	118.40
1	A	66	PHE	CB-CA-C	6.28	121.37	109.37
1	A	175	ASP	N-CA-C	-6.24	101.19	110.23
1	A	32	ASP	CA-C-O	-6.23	113.50	120.54
1	A	59	ILE	CB-CA-C	6.23	119.90	110.62
1	A	68	VAL	O-C-N	6.17	130.32	123.10
1	A	135	VAL	CA-C-O	-6.14	113.10	120.78
1	A	185	LEU	CA-C-N	6.11	127.47	119.84
1	A	185	LEU	C-N-CA	6.11	127.47	119.84
1	A	85	ASP	CA-CB-CG	6.08	118.68	112.60
1	A	194	TYR	O-C-N	6.07	127.23	121.71
1	A	180	ASP	CB-CA-C	6.03	116.14	110.17
1	A	197	SER	O-C-N	6.03	129.97	122.92
1	A	68	VAL	N-CA-C	-6.02	99.06	107.80
1	A	96	HIS	ND1-CE1-NE2	6.01	114.41	108.40
1	A	187	GLU	CA-C-N	6.01	130.99	122.09
1	A	187	GLU	C-N-CA	6.01	130.99	122.09
1	A	175	ASP	CA-CB-CG	6.00	118.60	112.60
1	A	68	VAL	CA-C-O	-5.99	114.12	120.53
1	A	233	GLY	N-CA-C	-5.98	103.52	113.02
1	A	221	GLU	CA-C-O	-5.96	113.11	119.97
1	A	49	VAL	CA-C-O	-5.95	114.16	120.53
1	A	158	GLN	N-CA-C	5.89	117.70	111.28
1	A	260	PHE	CA-CB-CG	-5.87	107.93	113.80
1	A	185	LEU	N-CA-C	5.82	117.15	109.93
1	A	107	HIS	ND1-CG-CD2	5.82	111.92	106.10
1	A	22	ILE	CA-C-N	5.80	128.63	120.28
1	A	22	ILE	C-N-CA	5.80	128.63	120.28
1	A	152	SER	CA-CB-OG	-5.78	99.53	111.10
1	A	216	ILE	N-CA-C	-5.77	100.03	108.97

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	122	HIS	CA-C-O	-5.75	114.38	121.11
1	A	189	LEU	O-C-N	5.75	129.42	122.35
1	A	36	HIS	CA-C-O	-5.71	112.59	119.27
1	A	141	LEU	N-CA-C	5.67	118.46	109.50
1	A	55	THR	CA-C-O	-5.65	113.45	120.57
1	A	226	PHE	N-CA-C	-5.62	105.15	111.28
1	A	210	ILE	O-C-N	5.62	129.59	122.57
1	A	53	GLN	CB-CG-CD	-5.58	103.11	112.60
1	A	237	PRO	N-CA-C	-5.56	102.46	111.14
1	A	137	GLN	OE1-CD-NE2	-5.56	117.04	122.60
1	A	239	GLU	CA-CB-CG	5.55	125.20	114.10
1	A	92	GLN	O-C-N	5.54	129.35	123.42
1	A	148	LEU	O-C-N	5.53	129.78	123.31
1	A	214	GLU	CB-CA-C	-5.50	101.47	109.38
1	A	175	ASP	CB-CG-OD1	5.47	130.98	118.40
1	A	144	LEU	N-CA-CB	5.46	119.34	110.17
1	A	11	ASN	OD1-CG-ND2	-5.44	117.16	122.60
1	A	14	GLU	CA-C-O	5.44	125.95	119.10
1	A	15	HIS	O-C-N	5.42	129.02	122.35
1	A	71	ASP	CA-C-O	-5.39	114.51	120.60
1	A	188	SER	CA-C-O	5.36	127.09	120.92
1	A	213	LYS	CB-CG-CD	5.36	123.63	111.30
1	A	182	ARG	CD-NE-CZ	-5.36	116.90	124.40
1	A	24	LYS	CG-CD-CE	-5.34	99.01	111.30
1	A	58	ARG	NH1-CZ-NH2	-5.34	112.35	119.30
1	A	61	ASN	CA-C-O	-5.34	114.98	120.54
1	A	96	HIS	ND1-CG-CD2	5.34	111.44	106.10
1	A	150	VAL	CB-CA-C	5.33	117.51	110.91
1	A	53	GLN	CG-CD-NE2	-5.32	108.42	116.40
1	A	203	LEU	N-CA-CB	-5.32	101.50	110.49
1	A	143	VAL	O-C-N	5.31	129.00	123.26
1	A	109	VAL	CB-CA-C	5.31	117.89	110.99
1	A	130	ASP	O-C-N	5.31	129.21	123.10
1	A	88	TYR	CA-C-O	-5.31	114.62	120.24
1	A	251	LEU	N-CA-C	-5.29	105.60	111.36
1	A	191	TYR	CA-C-O	5.27	127.09	121.45
1	A	26	GLU	CG-CD-OE1	5.26	130.51	118.40
1	A	158	GLN	O-C-N	5.25	127.68	122.12
1	A	218	VAL	CA-C-O	-5.25	116.44	121.63
1	A	56	SER	N-CA-C	-5.23	102.73	110.48
1	A	114	TYR	CA-C-O	-5.22	115.26	121.89
1	A	89	ARG	NE-CZ-NH1	5.22	126.72	121.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	56	SER	N-CA-CB	5.21	118.20	110.29
1	A	208	THR	O-C-N	5.20	129.24	123.05
1	A	10	HIS	O-C-N	5.20	129.23	122.42
1	A	53	GLN	OE1-CD-NE2	5.20	127.80	122.60
1	A	120	LEU	CB-CA-C	5.19	119.09	110.78
1	A	166	SER	O-C-N	5.16	129.96	122.43
1	A	253	ASN	CB-CG-OD1	-5.14	110.53	120.80
1	A	229	LEU	N-CA-CB	-5.13	103.02	110.36
1	A	107	HIS	ND1-CE1-NE2	5.13	113.53	108.40
1	A	110	ASP	OD1-CG-OD2	-5.12	110.60	122.90
1	A	72	ASP	OD1-CG-OD2	-5.11	110.64	122.90
1	A	35	THR	CA-C-O	-5.10	113.31	119.49
1	A	255	GLN	OE1-CD-NE2	-5.07	117.53	122.60
1	A	257	LYS	CA-C-N	5.04	130.49	122.94
1	A	257	LYS	C-N-CA	5.04	130.49	122.94
1	A	129	GLY	CA-C-O	-5.03	111.82	120.57
1	A	37	THR	CA-CB-OG1	-5.03	102.06	109.60
1	A	242	VAL	CA-C-O	-5.03	116.66	121.63
1	A	55	THR	O-C-N	5.02	130.59	122.96
1	A	247	PRO	N-CA-CB	5.02	108.00	103.33
1	A	67	ASN	CB-CG-ND2	5.00	123.91	116.40
1	A	179	PHE	N-CA-CB	5.00	118.58	110.43

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	2028	0	1979	38	1
2	A	1	0	0	0	0
3	A	1	0	0	0	0
4	A	119	0	0	2	1
All	All	2149	0	1979	38	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 10.

All (38) 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	1.61	0.99
1:A:125:THR:C	1:A:127:LYS:N	2.28	0.92
1:A:146:ILE:HG12	1:A:212:LEU:HD23	1.68	0.74
1:A:253:ASN:C	1:A:253:ASN:HD22	1.99	0.70
1:A:125:THR:C	1:A:127:LYS:CA	2.72	0.62
1:A:253:ASN:C	1:A:253:ASN:ND2	2.58	0.61
1:A:161:VAL:HG13	1:A:225:LYS:HD2	1.82	0.59
1:A:58:ARG:CD	1:A:69:GLU:OE1	2.46	0.57
1:A:27:ARG:HG3	1:A:205:GLU:HB3	1.87	0.56
1:A:213:LYS:HD3	1:A:260:PHE:CZ	2.40	0.56
1:A:15:HIS:ND1	1:A:18:LYS:NZ	2.37	0.56
1:A:253:ASN:HD22	1:A:254:ARG:N	2.04	0.56
1:A:71:ASP:OD2	1:A:76:LYS:NZ	2.39	0.54
1:A:250:PRO:HB2	1:A:252:LYS:HG3	1.89	0.54
1:A:252:LYS:O	1:A:253:ASN:CG	2.50	0.54
1:A:24:LYS:NZ	4:A:374:HOH:O	2.41	0.54
1:A:231:PHE:HD2	1:A:239:GLU:HG2	1.72	0.54
1:A:53:GLN:HG3	4:A:348:HOH:O	2.08	0.53
1:A:58:ARG:HD2	1:A:69:GLU:CD	2.32	0.53
1:A:110:ASP:O	1:A:111:LYS:HB2	2.10	0.52
1:A:161:VAL:CG1	1:A:225:LYS:HD2	2.41	0.51
1:A:128:TYR:CE1	1:A:137:GLN:HG3	2.47	0.49
1:A:41:ASP:OD1	1:A:43:SER:OG	2.23	0.47
1:A:219:SER:OG	1:A:222:GLN:HG3	2.15	0.46
1:A:35:THR:OG1	1:A:110:ASP:OD2	2.29	0.45
1:A:255:GLN:OE1	1:A:257:LYS:HE2	2.17	0.45
1:A:45:LYS:O	1:A:82:GLY:HA2	2.16	0.44
1:A:125:THR:C	1:A:127:LYS:HA	2.43	0.43
1:A:236:GLU:HB3	1:A:237:PRO:HD2	1.99	0.43
1:A:190:ASP:HB3	1:A:260:PHE:CD2	2.53	0.43
1:A:255:GLN:OE1	1:A:257:LYS:CE	2.66	0.43
1:A:243:ASP:HA	1:A:245:TRP:CD1	2.54	0.43
1:A:236:GLU:HB3	1:A:237:PRO:CD	2.49	0.42
1:A:213:LYS:HD3	1:A:260:PHE:CE1	2.53	0.42
1:A:144:LEU:HD22	1:A:212:LEU:HD21	2.01	0.42
1:A:137:GLN:HA	1:A:138:PRO:HD3	1.93	0.41
1:A:252:LYS:O	1:A:253:ASN:CB	2.68	0.41
1:A:253:ASN:ND2	1:A:254:ARG:N	2.68	0.41

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:343:HOH:O[2_445]	2.16	0.04

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	251/260 (96%)	238 (95%)	13 (5%)	0	100 100

There are no Ramachandran outliers to report.

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	220/225 (98%)	209 (95%)	11 (5%)	22 22

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

Mol	Chain	Res	Type
1	A	30	PRO
1	A	53	GLN
1	A	58	ARG
1	A	60	LEU
1	A	79	LEU
1	A	100	LEU

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Mol	Chain	Res	Type
1	A	212	LEU
1	A	221	GLU
1	A	223	VAL
1	A	229	LEU
1	A	253	ASN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (2) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	53	GLN
1	A	253	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](#)

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	2.28

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.