



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 11:07 AM UTC

PDB ID : 2HFW / pdb_00002hfw
Title : Structural and kinetic analysis of proton shuttle residues in the active site of human carbonic anhydrase III
Authors : Elder, I.; Fisher, S.Z.; Laipis, P.J.; Tu, C.K.; McKenna, R.; Silverman, D.N.
Deposited on : 2006-06-26
Resolution : 2.50 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)	:	2.0
EDS	:	3.0
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

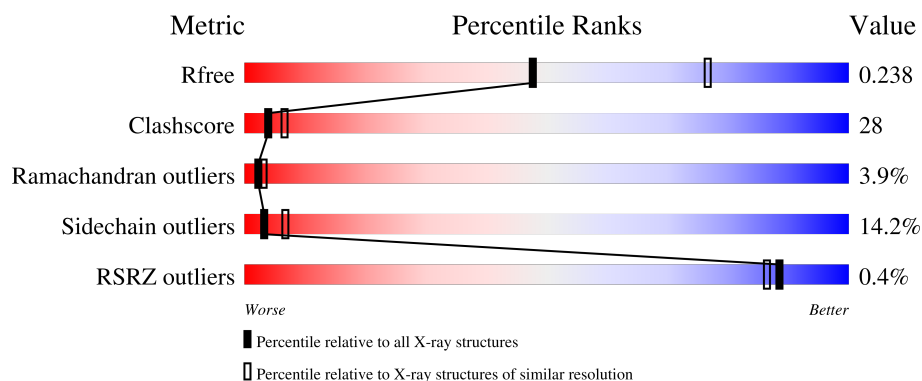
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.50 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))
R_{free}	180053	5829 (2.50-2.50)
Clashscore	190562	6492 (2.50-2.50)
Ramachandran outliers	187476	6378 (2.50-2.50)
Sidechain outliers	187428	6380 (2.50-2.50)
RSRZ outliers	180081	5833 (2.50-2.50)

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 $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	260	

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 2101 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 3.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	257	Total	C	N	O	S	0	0	0
			2065	1317	361	381	6			

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	64	HIS	LYS	engineered mutation	UNP P07451
A	67	ASN	ARG	engineered mutation	UNP P07451
A	182	SER	CYS	engineered mutation	UNP P07451
A	188	SER	CYS	engineered mutation	UNP P07451

- 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		

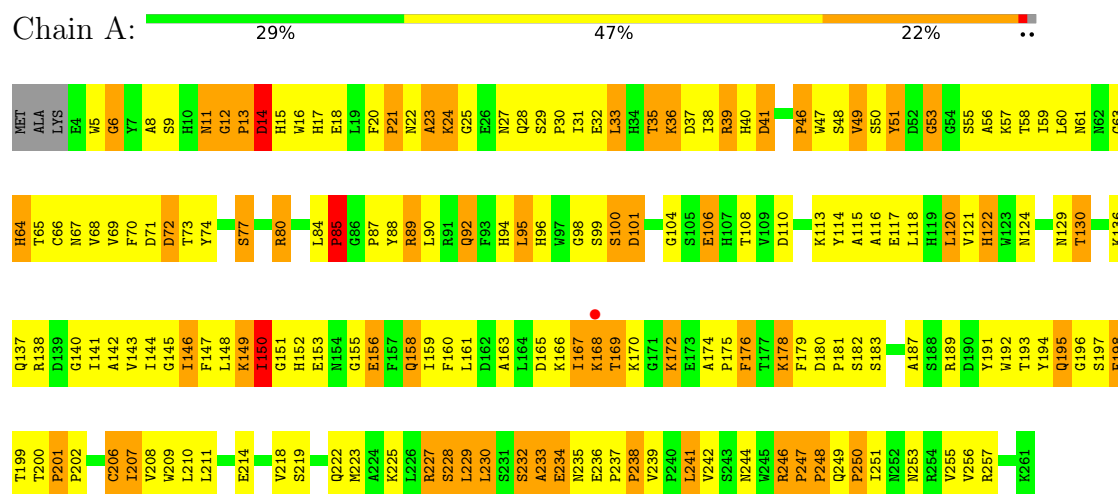
- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	35	Total	O	0	0
			35	35		

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 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.

• Molecule 1: Carbonic anhydrase 3



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	42.37Å 51.67Å 117.66Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	20.00 – 2.50 20.00 – 2.50	Depositor EDS
% Data completeness (in resolution range)	(Not available) (20.00-2.50) 86.6 (20.00-2.50)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.10	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.58 (at 2.50Å)	Xtriage
Refinement program	CNS	Depositor
R, R_{free}	0.204 , 0.239 0.212 , 0.238	Depositor DCC
R_{free} test set	448 reflections (5.27%)	wwPDB-VP
Wilson B-factor (Å ²)	39.9	Xtriage
Anisotropy	0.419	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.31 , 41.4	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	2101	wwPDB-VP
Average B, all atoms (Å ²)	38.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 10.91% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

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	2.58	105/2134 (4.9%)	1.49	34/2905 (1.2%)

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 (105) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	196	GLY	C-O	-13.56	1.12	1.24
1	A	25	GLY	C-O	-9.50	1.14	1.23
1	A	187	ALA	CA-CB	-9.50	1.38	1.53
1	A	150	ILE	CA-CB	-9.34	1.44	1.54
1	A	247	PRO	CA-C	-8.46	1.44	1.52
1	A	122	HIS	C-O	-8.36	1.13	1.23
1	A	208	VAL	C-O	-8.22	1.14	1.23
1	A	257	ARG	C-O	-8.14	1.14	1.23
1	A	163	ALA	CA-CB	-8.00	1.40	1.53
1	A	193	THR	C-O	-7.87	1.14	1.24
1	A	41	ASP	C-O	-7.75	1.18	1.25
1	A	256	VAL	C-O	-7.65	1.15	1.24
1	A	146	ILE	C-O	-7.54	1.16	1.24
1	A	121	VAL	C-O	-7.47	1.15	1.24
1	A	130	THR	N-CA	7.37	1.55	1.46
1	A	140	GLY	C-O	-7.30	1.14	1.23
1	A	210	LEU	C-O	-7.19	1.15	1.23
1	A	176	PHE	C-O	-7.16	1.16	1.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	90	LEU	C-O	-7.13	1.15	1.23
1	A	40	HIS	C-O	-7.12	1.15	1.23
1	A	187	ALA	C-O	-7.04	1.16	1.24
1	A	73	THR	CA-C	-7.00	1.43	1.52
1	A	194	TYR	C-O	-6.93	1.15	1.23
1	A	117	GLU	C-O	-6.87	1.15	1.24
1	A	46	PRO	CA-C	-6.71	1.44	1.52
1	A	137	GLN	N-CA	-6.70	1.38	1.45
1	A	49	VAL	C-O	-6.68	1.16	1.24
1	A	101	ASP	N-CA	-6.67	1.37	1.46
1	A	207	ILE	C-O	-6.66	1.16	1.24
1	A	56	ALA	CA-CB	-6.64	1.42	1.53
1	A	192	TRP	C-O	-6.63	1.16	1.23
1	A	23	ALA	CA-CB	-6.61	1.42	1.53
1	A	200	THR	N-CA	-6.56	1.38	1.45
1	A	90	LEU	CA-C	-6.54	1.44	1.52
1	A	209	TRP	C-O	-6.50	1.16	1.24
1	A	32	GLU	C-O	-6.45	1.16	1.23
1	A	211	LEU	CG-CD2	-6.43	1.31	1.52
1	A	87	PRO	C-O	-6.39	1.16	1.23
1	A	114	TYR	C-O	-6.38	1.15	1.23
1	A	114	TYR	CA-C	-6.32	1.45	1.52
1	A	89	ARG	C-O	-6.30	1.16	1.24
1	A	39	ARG	C-O	-6.30	1.16	1.23
1	A	68	VAL	C-O	-6.28	1.17	1.24
1	A	202	PRO	CB-CG	-6.26	1.26	1.51
1	A	201	PRO	C-O	-6.26	1.17	1.24
1	A	51	TYR	N-CA	-6.20	1.38	1.45
1	A	176	PHE	CA-C	-6.20	1.47	1.53
1	A	142	ALA	CA-CB	-6.18	1.44	1.53
1	A	195	GLN	C-O	-6.18	1.16	1.24
1	A	246	ARG	C-O	-6.16	1.16	1.24
1	A	28	GLN	C-O	-6.12	1.16	1.23
1	A	88	TYR	C-O	-6.08	1.16	1.23
1	A	179	PHE	C-O	-6.07	1.17	1.23
1	A	11	ASN	C-O	-6.01	1.16	1.24
1	A	50	SER	C-O	-5.99	1.17	1.23
1	A	16	TRP	C-O	-5.95	1.16	1.24
1	A	234	GLU	CA-C	-5.92	1.45	1.52
1	A	124	ASN	CA-C	-5.90	1.45	1.52
1	A	46	PRO	C-O	-5.88	1.16	1.23
1	A	174	ALA	CA-CB	-5.86	1.46	1.54

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	142	ALA	C-O	-5.82	1.17	1.24
1	A	244	ASN	C-O	-5.79	1.19	1.24
1	A	27	ASN	C-O	-5.77	1.16	1.23
1	A	246	ARG	CA-C	-5.76	1.44	1.53
1	A	248	PRO	C-O	-5.74	1.17	1.23
1	A	144	ILE	C-O	-5.73	1.18	1.24
1	A	158	GLN	C-O	-5.72	1.17	1.24
1	A	104	GLY	C-O	-5.68	1.16	1.23
1	A	14	ASP	C-O	-5.64	1.16	1.24
1	A	191	TYR	C-O	-5.64	1.17	1.23
1	A	143	VAL	C-O	-5.63	1.18	1.24
1	A	71	ASP	CA-C	-5.62	1.46	1.52
1	A	57	LYS	C-O	-5.58	1.17	1.24
1	A	53	GLY	C-O	-5.57	1.17	1.24
1	A	250	PRO	C-O	-5.57	1.17	1.23
1	A	115	ALA	CA-CB	-5.52	1.44	1.53
1	A	108	THR	C-O	-5.52	1.16	1.23
1	A	100	SER	C-O	-5.52	1.17	1.23
1	A	73	THR	C-O	-5.51	1.16	1.24
1	A	197	SER	C-O	-5.47	1.16	1.23
1	A	115	ALA	C-O	-5.47	1.16	1.24
1	A	148	LEU	C-O	-5.39	1.17	1.24
1	A	211	LEU	C-O	-5.39	1.17	1.24
1	A	255	VAL	C-O	-5.38	1.17	1.23
1	A	39	ARG	NE-CZ	-5.34	1.27	1.33
1	A	66	CYS	C-O	-5.34	1.17	1.24
1	A	6	GLY	C-O	-5.30	1.17	1.24
1	A	33	LEU	C-O	-5.28	1.17	1.24
1	A	198	PHE	C-O	-5.28	1.17	1.23
1	A	199	THR	C-O	-5.20	1.17	1.24
1	A	206	CYS	C-O	-5.17	1.17	1.24
1	A	163	ALA	C-O	-5.17	1.16	1.24
1	A	85	PRO	C-O	-5.15	1.17	1.24
1	A	47	TRP	C-O	-5.12	1.17	1.23
1	A	191	TYR	CZ-OH	-5.12	1.27	1.38
1	A	39	ARG	CZ-NH2	-5.11	1.26	1.33
1	A	120	LEU	C-O	-5.11	1.18	1.24
1	A	247	PRO	C-O	-5.11	1.18	1.24
1	A	255	VAL	CA-CB	-5.08	1.48	1.53
1	A	191	TYR	CE2-CZ	-5.06	1.26	1.38
1	A	33	LEU	CA-C	-5.06	1.46	1.52
1	A	92	GLN	C-O	-5.05	1.17	1.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	214	GLU	C-O	-5.05	1.17	1.24
1	A	241	LEU	CA-C	-5.05	1.46	1.53
1	A	74	TYR	C-O	-5.03	1.18	1.23

All (34) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	155	GLY	N-CA-C	9.29	125.82	113.37
1	A	182	SER	N-CA-C	8.98	122.04	111.71
1	A	207	ILE	N-CA-C	8.18	119.93	107.99
1	A	130	THR	N-CA-CB	8.04	124.08	110.49
1	A	244	ASN	N-CA-C	8.01	119.86	110.41
1	A	253	ASN	N-CA-C	7.90	122.99	112.25
1	A	121	VAL	N-CA-C	7.17	118.91	108.58
1	A	153	GLU	N-CA-C	6.98	120.09	110.24
1	A	55	SER	N-CA-C	6.92	120.82	112.38
1	A	92	GLN	N-CA-C	6.90	119.01	108.52
1	A	195	GLN	N-CA-C	6.90	119.93	108.96
1	A	48	SER	N-CA-C	6.82	119.81	109.23
1	A	80	ARG	N-CA-C	6.75	118.38	108.86
1	A	50	SER	N-CA-C	6.64	120.69	107.62
1	A	234	GLU	N-CA-C	-6.63	102.69	111.24
1	A	73	THR	N-CA-C	-6.59	105.06	113.23
1	A	106	GLU	N-CA-C	6.43	119.54	111.24
1	A	196	GLY	N-CA-C	6.31	122.27	111.16
1	A	253	ASN	N-CA-CB	-5.95	101.98	110.79
1	A	31	ILE	N-CA-C	5.91	118.71	108.95
1	A	255	VAL	N-CA-C	5.89	116.92	107.73
1	A	8	ALA	N-CA-C	5.68	117.86	108.48
1	A	160	PHE	N-CA-C	5.62	117.09	111.07
1	A	96	HIS	N-CA-C	-5.55	99.62	109.06
1	A	95	LEU	N-CA-C	5.49	117.14	108.96
1	A	178	LYS	N-CA-C	5.49	118.81	111.24
1	A	141	ILE	CB-CA-C	5.45	118.67	111.21
1	A	141	ILE	N-CA-C	5.41	117.09	108.87
1	A	156	GLU	N-CA-C	-5.40	106.20	112.89
1	A	146	ILE	N-CA-C	5.38	115.64	108.11
1	A	143	VAL	N-CA-C	5.36	115.58	107.80
1	A	147	PHE	N-CA-C	5.13	118.08	110.48
1	A	101	ASP	N-CA-C	5.02	118.51	112.38
1	A	72	ASP	N-CA-C	5.02	117.31	110.88

There are no chirality outliers.

All (3) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	13	PRO	Peptide
1	A	49	VAL	Peptide
1	A	85	PRO	Peptide

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	2065	0	1974	114	1
2	A	1	0	0	0	0
3	A	35	0	0	5	0
All	All	2101	0	1974	114	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 28.

All (114) 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:5:TRP:CH2	1:A:64:HIS:HD2	1.55	1.24
1:A:238:PRO:O	1:A:239:VAL:HG23	1.41	1.17
1:A:5:TRP:CH2	1:A:64:HIS:CD2	2.34	1.16
1:A:6:GLY:HA3	1:A:11:ASN:ND2	1.69	1.07
1:A:166:LYS:O	1:A:172:LYS:HD3	1.61	1.01
1:A:36:LYS:H	1:A:36:LYS:HD3	1.25	1.01
1:A:36:LYS:H	1:A:36:LYS:CD	1.76	0.97
1:A:17:HIS:HA	1:A:20:PHE:O	1.69	0.92
1:A:35:THR:OG1	1:A:110:ASP:OD1	1.86	0.92
1:A:64:HIS:O	1:A:241:LEU:HD21	1.74	0.88
1:A:5:TRP:CZ2	1:A:64:HIS:CD2	2.65	0.84
1:A:238:PRO:O	1:A:239:VAL:CG2	2.24	0.83
1:A:228:SER:O	1:A:230:LEU:HD23	1.79	0.82
1:A:228:SER:O	1:A:229:LEU:O	2.01	0.78
1:A:36:LYS:CD	1:A:36:LYS:N	2.49	0.75

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:6:GLY:HA3	1:A:11:ASN:HD22	1.51	0.74
1:A:228:SER:O	1:A:229:LEU:C	2.31	0.72
1:A:169:THR:CG2	1:A:170:LYS:O	2.38	0.72
1:A:61:ASN:C	1:A:61:ASN:OD1	2.30	0.71
1:A:150:ILE:CG2	1:A:151:GLY:N	2.54	0.68
1:A:92:GLN:OE1	1:A:94:HIS:HD2	1.75	0.68
1:A:228:SER:C	1:A:229:LEU:O	2.34	0.66
1:A:22:ASN:C	1:A:24:LYS:H	2.04	0.66
1:A:167:ILE:O	1:A:168:LYS:C	2.37	0.66
1:A:24:LYS:HG3	1:A:24:LYS:O	1.94	0.66
1:A:22:ASN:O	1:A:24:LYS:N	2.30	0.65
1:A:169:THR:HG22	1:A:170:LYS:O	1.97	0.65
1:A:35:THR:O	3:A:403:HOH:O	2.16	0.64
1:A:64:HIS:N	1:A:64:HIS:ND1	2.45	0.63
1:A:129:ASN:O	1:A:130:THR:HG22	1.98	0.63
1:A:129:ASN:O	1:A:130:THR:CG2	2.46	0.63
1:A:15:HIS:HD1	1:A:18:GLU:CD	2.06	0.62
1:A:167:ILE:O	1:A:169:THR:N	2.31	0.62
1:A:219:SER:OG	1:A:222:GLN:HG3	2.00	0.62
1:A:116:ALA:HB2	1:A:223:MET:HE1	1.81	0.61
1:A:15:HIS:ND1	1:A:18:GLU:OE2	2.35	0.60
1:A:156:GLU:N	1:A:156:GLU:OE2	2.35	0.59
1:A:166:LYS:NZ	3:A:328:HOH:O	2.23	0.59
1:A:5:TRP:CZ3	1:A:64:HIS:CD2	2.89	0.58
1:A:92:GLN:OE1	1:A:94:HIS:CD2	2.57	0.57
1:A:51:TYR:HA	1:A:77:SER:HB3	1.87	0.57
1:A:161:LEU:O	1:A:225:LYS:HE2	2.05	0.56
1:A:169:THR:HG23	1:A:170:LYS:O	2.04	0.56
1:A:234:GLU:C	1:A:236:GLU:H	2.14	0.56
1:A:150:ILE:HG23	1:A:151:GLY:N	2.20	0.56
1:A:63:GLY:HA3	1:A:170:LYS:HE2	1.87	0.55
1:A:35:THR:HG22	3:A:332:HOH:O	2.07	0.54
1:A:69:VAL:HG12	1:A:70:PHE:N	2.22	0.54
1:A:249:GLN:HB3	1:A:250:PRO:HD2	1.88	0.54
1:A:225:LYS:O	1:A:228:SER:OG	2.25	0.53
1:A:30:PRO:HG3	1:A:106:GLU:HB3	1.90	0.52
1:A:138:ARG:NH2	1:A:195:GLN:OE1	2.38	0.52
1:A:89:ARG:O	1:A:122:HIS:HA	2.10	0.52
1:A:129:ASN:C	1:A:130:THR:CG2	2.84	0.51
1:A:129:ASN:C	1:A:130:THR:HG23	2.36	0.50
1:A:232:SER:O	1:A:233:ALA:O	2.30	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:237:PRO:O	1:A:238:PRO:O	2.30	0.50
1:A:237:PRO:O	1:A:238:PRO:C	2.54	0.50
1:A:65:THR:HG23	1:A:67:ASN:OD1	2.12	0.49
1:A:169:THR:HG23	1:A:233:ALA:HA	1.94	0.49
1:A:218:VAL:HG22	1:A:219:SER:N	2.28	0.49
1:A:167:ILE:HA	1:A:172:LYS:HB3	1.95	0.48
1:A:69:VAL:CG1	1:A:70:PHE:N	2.76	0.48
1:A:156:GLU:HG2	1:A:183:SER:HB2	1.94	0.48
1:A:5:TRP:HH2	1:A:64:HIS:HD2	1.45	0.47
1:A:41:ASP:OD2	1:A:41:ASP:C	2.55	0.47
1:A:98:GLY:O	1:A:227:ARG:HD2	2.14	0.47
1:A:228:SER:O	1:A:230:LEU:CD2	2.58	0.47
1:A:234:GLU:O	1:A:236:GLU:N	2.48	0.47
1:A:53:GLY:O	1:A:178:LYS:HA	2.15	0.47
1:A:166:LYS:O	1:A:172:LYS:CD	2.49	0.47
1:A:5:TRP:CZ2	1:A:64:HIS:NE2	2.83	0.47
1:A:64:HIS:C	1:A:241:LEU:HD21	2.38	0.45
1:A:94:HIS:O	1:A:95:LEU:HG	2.16	0.45
1:A:29:SER:HB3	1:A:30:PRO:HA	1.98	0.45
1:A:236:GLU:HB3	1:A:237:PRO:HD2	1.98	0.45
1:A:180:ASP:OD1	1:A:180:ASP:C	2.55	0.45
1:A:61:ASN:OD1	1:A:61:ASN:O	2.34	0.45
1:A:84:LEU:HA	1:A:85:PRO:HD3	1.54	0.45
1:A:46:PRO:HB3	3:A:348:HOH:O	2.17	0.45
1:A:150:ILE:HA	1:A:150:ILE:HD12	1.58	0.45
1:A:24:LYS:O	1:A:24:LYS:HE3	2.16	0.44
1:A:95:LEU:HD11	1:A:118:LEU:HD13	2.00	0.44
1:A:246:ARG:HA	1:A:247:PRO:HD3	1.58	0.44
1:A:149:LYS:HZ3	1:A:149:LYS:HG3	1.53	0.44
1:A:150:ILE:N	1:A:150:ILE:HD13	2.33	0.44
1:A:72:ASP:OD2	1:A:72:ASP:N	2.51	0.43
1:A:180:ASP:HA	1:A:181:PRO:HD3	1.77	0.43
1:A:156:GLU:HA	1:A:159:ILE:HD12	2.00	0.43
1:A:234:GLU:C	1:A:236:GLU:N	2.73	0.43
1:A:20:PHE:HA	1:A:21:PRO:HD3	1.64	0.43
1:A:46:PRO:HA	3:A:348:HOH:O	2.18	0.43
1:A:11:ASN:O	1:A:12:GLY:O	2.36	0.42
1:A:11:ASN:OD1	1:A:11:ASN:N	2.52	0.42
1:A:59:ILE:HG22	1:A:176:PHE:HB2	2.01	0.42
1:A:198:PHE:CE1	1:A:206:CYS:SG	3.12	0.42
1:A:237:PRO:HA	1:A:238:PRO:HD2	1.47	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:14:ASP:OD1	1:A:14:ASP:N	2.33	0.42
1:A:94:HIS:O	1:A:118:LEU:HD12	2.18	0.42
1:A:158:GLN:O	1:A:159:ILE:C	2.63	0.42
1:A:151:GLY:N	1:A:218:VAL:O	2.53	0.42
1:A:95:LEU:HD11	1:A:118:LEU:CD1	2.50	0.41
1:A:36:LYS:N	1:A:36:LYS:HD2	2.33	0.41
1:A:120:LEU:HB3	1:A:122:HIS:HE1	1.85	0.41
1:A:12:GLY:HA2	1:A:13:PRO:HD3	1.78	0.41
1:A:38:ILE:HG21	1:A:38:ILE:HD13	1.79	0.41
1:A:180:ASP:O	1:A:183:SER:OG	2.26	0.41
1:A:247:PRO:HA	1:A:248:PRO:HD3	1.78	0.41
1:A:84:LEU:HB3	1:A:85:PRO:HD2	2.01	0.41
1:A:232:SER:C	1:A:233:ALA:O	2.64	0.41
1:A:145:GLY:C	1:A:146:ILE:HG13	2.46	0.40
1:A:167:ILE:C	1:A:169:THR:N	2.80	0.40
1:A:65:THR:CG2	1:A:67:ASN:OD1	2.69	0.40
1:A:136:LYS:HZ3	1:A:136:LYS:HG3	1.55	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:18:GLU:OE1	1:A:113:LYS:NZ[4_456]	1.80	0.40

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	255/260 (98%)	218 (86%)	27 (11%)	10 (4%)	2 3

All (10) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	14	ASP
1	A	168	LYS
1	A	229	LEU
1	A	233	ALA
1	A	238	PRO
1	A	12	GLY
1	A	23	ALA
1	A	165	ASP
1	A	9	SER
1	A	21	PRO

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	226/228 (99%)	194 (86%)	32 (14%)	3 7

All (32) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	14	ASP
1	A	24	LYS
1	A	33	LEU
1	A	35	THR
1	A	36	LYS
1	A	37	ASP
1	A	39	ARG
1	A	58	THR
1	A	60	LEU
1	A	64	HIS
1	A	77	SER
1	A	80	ARG
1	A	99	SER
1	A	100	SER
1	A	101	ASP
1	A	149	LYS
1	A	150	ILE

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Mol	Chain	Res	Type
1	A	152	HIS
1	A	167	ILE
1	A	169	THR
1	A	172	LYS
1	A	175	PRO
1	A	189	ARG
1	A	201	PRO
1	A	207	ILE
1	A	227	ARG
1	A	228	SER
1	A	230	LEU
1	A	232	SER
1	A	235	ASN
1	A	242	VAL
1	A	251	ILE

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	40	HIS
1	A	64	HIS
1	A	94	HIS
1	A	252	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

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 [i](#)

6.1 Protein, DNA and RNA chains [i](#)

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	257/260 (98%)	-0.03	1 (0%) 88 86	16, 35, 63, 84	0

All (1) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	168	LYS	4.9

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

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

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled ‘Q< 0.9’ lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
2	ZN	A	262	1/1	0.98	0.09	26,26,26,26	0

6.5 Other polymers [i](#)

There are no such residues in this entry.