



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 27, 2014 – 10:35 AM GMT

PDB ID : 2HFW  
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 validation report for a publicly released PDB entry.  
We welcome your comments at [validation@mail.wwpdb.org](mailto:validation@mail.wwpdb.org)  
A user guide is available at <http://wwpdb.org/ValidationPDFNotes.html>

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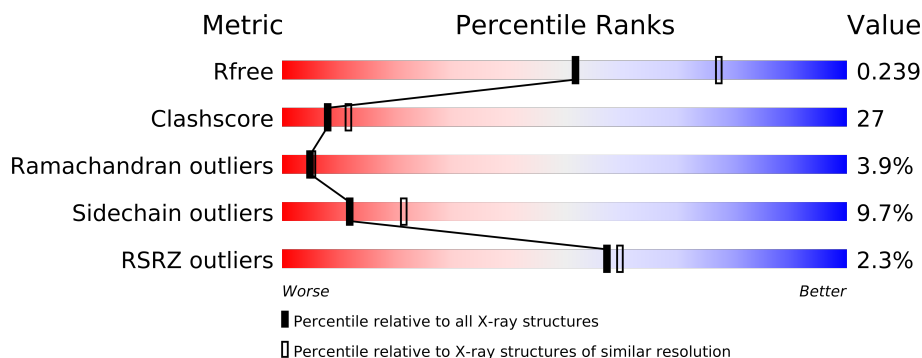
The following versions of software and data (see [references](#)) were used in the production of this report:

MolProbity : 4.02b-467  
Mogul : 1.15 2013  
Xtriage (Phenix) : dev-1323  
EDS : stable22639  
Percentile statistics : 21963  
Refmac : 5.8.0049  
CCP4 : 6.3.0 (Settle)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et. al. (1996)  
Validation Pipeline (wwPDB-VP) : stable22683

# 1 Overall quality at a glance


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))
$R_{free}$	66092	2784 (2.50-2.50)
Clashscore	79885	3562 (2.50-2.50)
Ramachandran outliers	78287	3480 (2.50-2.50)
Sidechain outliers	78261	3482 (2.50-2.50)
RSRZ outliers	66119	2785 (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 on the lower bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density.

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 hydrogen and 0 are deuterium.

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	UNP P07451
A	67	ASN	ARG	ENGINEERED	UNP P07451
A	182	SER	CYS	ENGINEERED	UNP P07451
A	188	SER	CYS	ENGINEERED	UNP P07451

- Molecule 2 is ZINC ION (three-letter code: ZN) (formula: Zn).

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

- Molecule 3 is water.

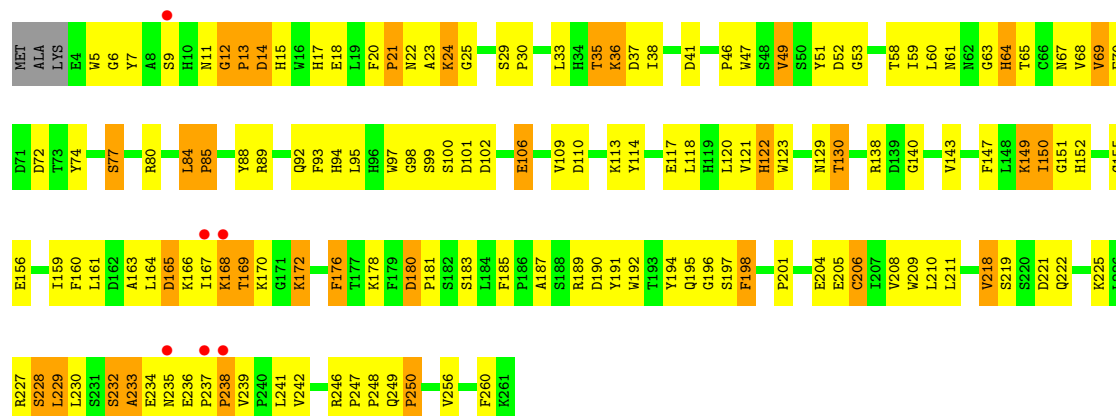
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	35	Total	O	0	0
			35	35		

### 3 Residue-property plots

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors 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

Chain A: 



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	42.37Å 51.67Å 117.66Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	20.00 – 2.50 19.61 – 2.50	Depositor EDS
% Data completeness (in resolution range)	(Not available) (20.00-2.50) 86.8 (19.61-2.50)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	0.10	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.58 (at 2.50Å)	Xtriage
Refinement program	CNS 1.1	Depositor
R, $R_{free}$	0.204 , 0.239 0.212 , 0.239	Depositor DCC
$R_{free}$ test set	448 reflections (5.49%)	DCC
Wilson B-factor (Å <sup>2</sup> )	39.9	Xtriage
Anisotropy	0.419	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.31 , 33.8	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.33$	Xtriage
Outliers	0 of 8508 reflections	Xtriage
$F_o, F_c$ correlation	0.94	EDS
Total number of atoms	2101	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	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.*

<sup>1</sup>Intensities estimated from amplitudes.

## 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	2.18	63/2134 (3.0%)	1.18	14/2905 (0.5%)

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 (63) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	191	TYR	CD1-CE1	-9.80	1.24	1.39
1	A	191	TYR	CE2-CZ	-9.57	1.26	1.38
1	A	218	VAL	CB-CG2	-7.86	1.36	1.52
1	A	117	GLU	CD-OE1	-7.72	1.17	1.25
1	A	206	CYS	CB-SG	-7.66	1.69	1.82
1	A	191	TYR	CE1-CZ	-7.57	1.28	1.38
1	A	114	TYR	CE1-CZ	-7.56	1.28	1.38
1	A	47	TRP	CE3-CZ3	-6.77	1.26	1.38
1	A	205	GLU	CD-OE2	-6.76	1.18	1.25
1	A	196	GLY	C-O	-6.76	1.12	1.23
1	A	192	TRP	CE3-CZ3	-6.75	1.26	1.38
1	A	187	ALA	CA-CB	-6.73	1.38	1.52
1	A	194	TYR	CE2-CZ	-6.71	1.29	1.38
1	A	106	GLU	CD-OE2	-6.64	1.18	1.25
1	A	69	VAL	CB-CG1	-6.63	1.39	1.52
1	A	205	GLU	CD-OE1	-6.52	1.18	1.25
1	A	117	GLU	CD-OE2	-6.24	1.18	1.25
1	A	121	VAL	CB-CG2	-6.23	1.39	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	97	TRP	CG-CD1	-6.23	1.28	1.36
1	A	191	TYR	CZ-OH	-6.21	1.27	1.37
1	A	121	VAL	CB-CG1	-6.09	1.40	1.52
1	A	47	TRP	CG-CD1	-6.08	1.28	1.36
1	A	93	PHE	CD1-CE1	-6.08	1.27	1.39
1	A	143	VAL	CB-CG1	-6.08	1.40	1.52
1	A	256	VAL	CB-CG2	-6.08	1.40	1.52
1	A	191	TYR	CD2-CE2	-6.01	1.30	1.39
1	A	140	GLY	C-O	-5.99	1.14	1.23
1	A	194	TYR	CD1-CE1	-5.97	1.30	1.39
1	A	160	PHE	CD1-CE1	-5.94	1.27	1.39
1	A	93	PHE	CD2-CE2	-5.82	1.27	1.39
1	A	147	PHE	CD2-CE2	-5.80	1.27	1.39
1	A	260	PHE	CE2-CZ	-5.79	1.26	1.37
1	A	204	GLU	CD-OE1	-5.78	1.19	1.25
1	A	208	VAL	CB-CG2	-5.76	1.40	1.52
1	A	185	PHE	CD1-CE1	-5.75	1.27	1.39
1	A	68	VAL	CB-CG1	-5.74	1.40	1.52
1	A	74	TYR	CD2-CE2	-5.72	1.30	1.39
1	A	114	TYR	CD2-CE2	-5.71	1.30	1.39
1	A	197	SER	CB-OG	-5.66	1.34	1.42
1	A	123	TRP	CG-CD1	-5.66	1.28	1.36
1	A	163	ALA	CA-CB	-5.65	1.40	1.52
1	A	7	TYR	CD1-CE1	-5.62	1.30	1.39
1	A	211	LEU	CG-CD2	-5.54	1.31	1.51
1	A	185	PHE	CD2-CE2	-5.53	1.28	1.39
1	A	176	PHE	CE1-CZ	-5.53	1.26	1.37
1	A	180	ASP	CB-CG	-5.49	1.40	1.51
1	A	25	GLY	C-O	-5.47	1.14	1.23
1	A	109	VAL	CB-CG1	-5.44	1.41	1.52
1	A	198	PHE	CE1-CZ	-5.40	1.27	1.37
1	A	106	GLU	CD-OE1	-5.38	1.19	1.25
1	A	185	PHE	CE2-CZ	-5.34	1.27	1.37
1	A	122	HIS	C-O	-5.30	1.13	1.23
1	A	176	PHE	CD2-CE2	-5.27	1.28	1.39
1	A	49	VAL	CB-CG1	-5.18	1.42	1.52
1	A	198	PHE	CD1-CE1	-5.14	1.28	1.39
1	A	191	TYR	CG-CD1	-5.11	1.32	1.39
1	A	192	TRP	CG-CD1	-5.10	1.29	1.36
1	A	88	TYR	CE2-CZ	-5.10	1.31	1.38
1	A	114	TYR	CG-CD2	-5.06	1.32	1.39
1	A	201	PRO	CB-CG	-5.05	1.24	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	160	PHE	CD2-CE2	-5.04	1.29	1.39
1	A	209	TRP	CG-CD1	-5.03	1.29	1.36
1	A	123	TRP	CE3-CZ3	-5.02	1.29	1.38

All (14) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	52	ASP	CB-CG-OD2	10.54	127.79	118.30
1	A	101	ASP	CB-CG-OD2	7.68	125.21	118.30
1	A	221	ASP	CB-CG-OD2	7.31	124.88	118.30
1	A	130	THR	N-CA-CB	7.25	124.08	110.30
1	A	84	LEU	C-N-CD	-6.63	106.01	120.60
1	A	190	ASP	CB-CG-OD2	6.57	124.21	118.30
1	A	206	CYS	CA-CB-SG	5.55	124.00	114.00
1	A	210	LEU	CB-CG-CD2	-5.49	101.67	111.00
1	A	164	LEU	CB-CG-CD1	-5.41	101.81	111.00
1	A	37	ASP	CB-CG-OD2	5.39	123.16	118.30
1	A	165	ASP	CB-CG-OD2	5.29	123.06	118.30
1	A	102	ASP	CB-CG-OD2	5.23	123.01	118.30
1	A	211	LEU	CA-CB-CG	5.17	127.19	115.30
1	A	155	GLY	N-CA-C	5.09	125.82	113.10

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 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 hydrogens added by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, and the number in parentheses is this value normalized per 1000 atoms of the molecule in the chain. The Symm-Clashes column gives symmetry related clashes, in the same way as for the Clashes column.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2065	0	1974	108	1

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	A	1	0	0	0	0
3	A	35	0	0	5	0
All	All	2101	0	1974	108	1

Clashscore is defined as the number of clashes calculated for the entry per 1000 atoms (including hydrogens) of the entry. The overall clashscore for this entry is 27.

All (108) close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(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:CD	1:A:36:LYS:H	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
1:A:6:GLY:HA3	1:A:11:ASN:HD22	1.51	0.74
1:A:169:THR:CG2	1:A:170:LYS:O	2.38	0.72
1:A:166:LYS:NZ	3:A:328:HOH:O	2.23	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:O	1:A:229:LEU:C	2.31	0.67
1:A:61:ASN:C	1:A:61:ASN:OD1	2.30	0.67
1:A:24:LYS:HG3	1:A:24:LYS:O	1.94	0.66
1:A:169:THR:HG22	1:A:170:LYS:O	1.97	0.65
1:A:22:ASN:O	1:A:24:LYS:N	2.30	0.65
1:A:35:THR:O	3:A:403:HOH:O	2.16	0.64
1:A:64:HIS:ND1	1:A:64:HIS:N	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: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:228:SER:C	1:A:229:LEU:O	2.34	0.62
1:A:167:ILE:O	1:A:168:LYS:C	2.37	0.61

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:22:ASN:C	1:A:24:LYS:H	2.04	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: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:169:THR:HG23	1:A:170:LYS:O	2.04	0.56
1:A:161:LEU:O	1:A:225:LYS:HE2	2.05	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:249:GLN:HB3	1:A:250:PRO:HD2	1.88	0.54
1:A:69:VAL:HG12	1:A:70:PHE:N	2.22	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:234:GLU:C	1:A:236:GLU:H	2.14	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:180:ASP:O	1:A:183:SER:OG	2.26	0.51
1:A:22:ASN:C	1:A:24:LYS:N	2.64	0.51
1:A:232:SER:O	1:A:233:ALA:O	2.30	0.50
1:A:237:PRO:O	1:A:238:PRO:O	2.30	0.50
1:A:169:THR:HG23	1:A:233:ALA:HA	1.94	0.49
1:A:65:THR:HG23	1:A:67:ASN:OD1	2.12	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:98:GLY:O	1:A:227:ARG:HD2	2.14	0.47
1:A:234:GLU:O	1:A:236:GLU:N	2.48	0.47
1:A:228:SER:O	1:A:230:LEU:CD2	2.58	0.47
1:A:166:LYS:O	1:A:172:LYS:CD	2.49	0.47
1:A:53:GLY:O	1:A:178:LYS:HA	2.15	0.47
1:A:5:TRP:CZ2	1:A:64:HIS:NE2	2.83	0.47
1:A:129:ASN:C	1:A:130:THR:CG2	2.84	0.46
1:A:94:HIS:O	1:A:95:LEU:HG	2.16	0.45
1:A:236:GLU:HB3	1:A:237:PRO:HD2	1.98	0.45
1:A:29:SER:HB3	1:A:30:PRO:HA	1.98	0.45
1:A:237:PRO:O	1:A:238:PRO:C	2.54	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

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:129:ASN:C	1:A:130:THR:HG23	2.36	0.45
1:A:46:PRO:HB3	3:A:348:HOH:O	2.17	0.45
1:A:150:ILE:HD12	1:A:150:ILE:HA	1.58	0.45
1:A:24:LYS:HE3	1:A:24:LYS:O	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:180:ASP:C	1:A:180:ASP:OD1	2.55	0.44
1:A:149:LYS:HG3	1:A:149:LYS:HZ3	1.53	0.44
1:A:150:ILE:N	1:A:150:ILE:HD13	2.33	0.44
1:A:180:ASP:HA	1:A:181:PRO:HD3	1.77	0.43
1:A:72:ASP:OD2	1:A:72:ASP:N	2.51	0.43
1:A:156:GLU:HA	1:A:159:ILE:HD12	2.00	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:237:PRO:HA	1:A:238:PRO:HD2	1.47	0.42
1:A:11:ASN:O	1:A:12:GLY:O	2.36	0.42
1:A:11:ASN:N	1:A:11:ASN:OD1	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:41:ASP:OD2	1:A:41:ASP:C	2.55	0.42
1:A:14:ASP:N	1:A:14:ASP:OD1	2.33	0.42
1:A:234:GLU:C	1:A:236:GLU:N	2.73	0.42
1:A:94:HIS:O	1:A:118:LEU:HD12	2.18	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:HD2	1:A:36:LYS:N	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:247:PRO:HA	1:A:248:PRO:HD3	1.78	0.41
1:A:64:HIS:C	1:A:241:LEU:HD21	2.38	0.41
1:A:84:LEU:HB3	1:A:85:PRO:HD2	2.01	0.41
1:A:65:THR:CG2	1:A:67:ASN:OD1	2.69	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	Distance(Å)	Clash(Å)
1:A:18:GLU:OE1	1:A:113:LYS:NZ[4_456]	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	255/260 (98%)	218 (86%)	27 (11%)	10 (4%)	5 5

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%)	204 (90%)	22 (10%)	12 21

All (22) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	24	LYS
1	A	33	LEU
1	A	35	THR
1	A	36	LYS

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
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	149	LYS
1	A	150	ILE
1	A	152	HIS
1	A	169	THR
1	A	172	LYS
1	A	189	ARG
1	A	228	SER
1	A	232	SER
1	A	235	ASN
1	A	242	VAL
1	A	250	PRO

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

Mol	Chain	Res	Type
1	A	64	HIS
1	A	94	HIS
1	A	253	ASN

### 5.3.3 RNA ⓘ

There are no RNA chains 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 carbohydrates 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.

## 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 ⓘ

### 6.1 Protein, DNA and RNA chains ⓘ

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, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	A	257/260 (98%)	-0.11	6 (2%) 57 60	16, 35, 63, 84	0

All (6) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	168	LYS	3.9
1	A	235	ASN	3.8
1	A	9	SER	2.7
1	A	237	PRO	2.5
1	A	167	ILE	2.2
1	A	238	PRO	2.2

### 6.2 Non-standard residues in protein, DNA, RNA chains ⓘ

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

### 6.3 Carbohydrates ⓘ

There are no carbohydrates in this entry.

### 6.4 Ligands ⓘ

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. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 95<sup>th</sup> 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	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
2	ZN	A	262	1/1	0.08	-2.01	26,26,26,26	0

## 6.5 Other polymers ⓘ

There are no such residues in this entry.