



# Full wwPDB X-ray Structure Validation Report ⓘ

Mar 10, 2026 – 12:54 AM UTC

PDB ID : 2CAB / pdb\_00002cab  
Title : STRUCTURE, REFINEMENT AND FUNCTION OF CARBONIC ANHYDRASE ISOZYMES. REFINEMENT OF HUMAN CARBONIC ANHYDRASE I  
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Deposited on : 1983-10-05  
Resolution : 2.00 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](mailto: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>.

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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

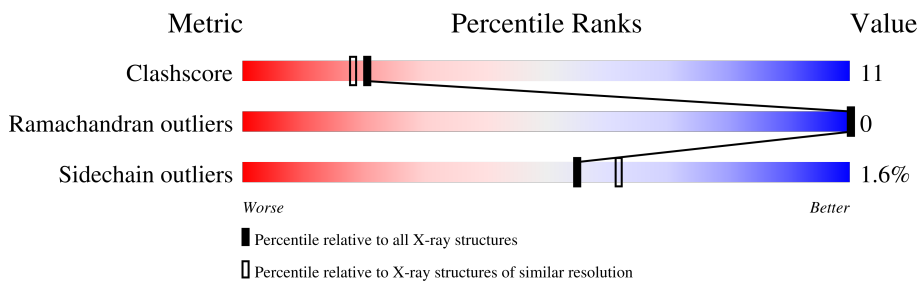
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.00 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	11152 (2.00-2.00)
Ramachandran outliers	187476	11031 (2.00-2.00)
Sidechain outliers	187428	11029 (2.00-2.00)

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  $\geq 3$ , 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	

## 2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 1722 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 FORM B.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	224	1721	1087	299	332	3	0	0	2

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	74	GLN	ASP	conflict	UNP P00915
A	75	ASP	ASN	conflict	UNP P00915

- 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		

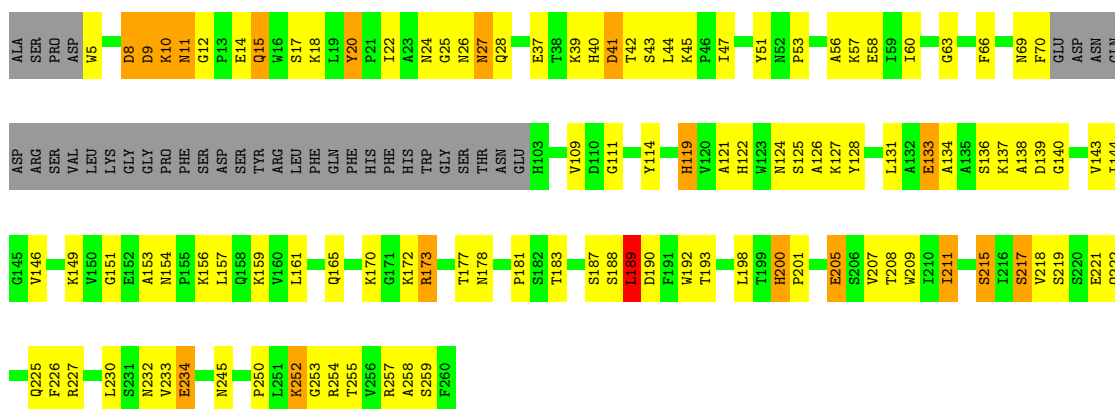
### 3 Residue-property plots [i](#)

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 FORM B

Chain A: 



## 4 Data and refinement statistics

Xtrriage (Phenix) and EDS were not executed - this section is therefore incomplete.

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	81.50Å 73.60Å 37.10Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	(Not available) – 2.00	Depositor
% Data completeness (in resolution range)	(Not available) ((Not available)-2.00)	Depositor
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
Refinement program	CORELS	Depositor
R, $R_{free}$	0.193 , (Not available)	Depositor
Estimated twinning fraction	No twinning to report.	Xtrriage
Total number of atoms	1722	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	14.0	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:  
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	1.73	16/1786 (0.9%)	2.17	64/2431 (2.6%)

All (16) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	144	ILE	C-N	-6.99	1.27	1.33
1	A	157	LEU	C-N	-6.27	1.26	1.33
1	A	121	ALA	N-CA	5.95	1.53	1.46
1	A	143	VAL	C-O	-5.88	1.18	1.24
1	A	230	LEU	N-CA	5.86	1.53	1.46
1	A	177	THR	CA-CB	5.84	1.62	1.53
1	A	245	ASN	N-CA	5.83	1.53	1.46
1	A	119	HIS	ND1-CE1	5.74	1.38	1.32
1	A	119	HIS	CD2-NE2	-5.69	1.31	1.37
1	A	227	ARG	CD-NE	-5.53	1.38	1.46
1	A	56	ALA	C-N	-5.39	1.26	1.33
1	A	207	VAL	CA-CB	5.34	1.61	1.54
1	A	125	SER	CB-OG	-5.31	1.31	1.42
1	A	20	TYR	N-CA	5.11	1.52	1.46
1	A	215	SER	N-CA	5.08	1.51	1.45
1	A	188	SER	N-CA	5.00	1.51	1.45

All (64) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	173	ARG	CA-CB-CG	11.63	137.36	114.10
1	A	133	GLU	CB-CG-CD	11.27	131.76	112.60
1	A	11	ASN	CA-C-N	10.71	135.07	121.36
1	A	11	ASN	C-N-CA	10.71	135.07	121.36
1	A	226	PHE	CA-CB-CG	9.43	123.23	113.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	227	ARG	CD-NE-CZ	8.12	135.77	124.40
1	A	9	ASP	CA-C-O	-8.05	109.60	119.18
1	A	221	GLU	CB-CG-CD	8.03	126.25	112.60
1	A	211	ILE	CB-CG1-CD1	7.90	130.39	113.80
1	A	234	GLU	CA-C-O	-7.47	113.48	120.95
1	A	198	LEU	N-CA-C	-7.43	100.02	110.50
1	A	124	ASN	CA-C-N	7.24	131.31	120.31
1	A	124	ASN	C-N-CA	7.24	131.31	120.31
1	A	66	PHE	O-C-N	6.95	131.75	123.27
1	A	57	LYS	CA-CB-CG	6.94	127.97	114.10
1	A	190	ASP	N-CA-C	-6.92	100.74	110.50
1	A	111	GLY	CA-C-N	6.90	131.00	122.37
1	A	111	GLY	C-N-CA	6.90	131.00	122.37
1	A	200	HIS	O-C-N	6.74	126.57	121.65
1	A	10	LYS	O-C-N	6.74	131.93	122.36
1	A	217	SER	CA-C-N	6.72	130.96	121.96
1	A	217	SER	C-N-CA	6.72	130.96	121.96
1	A	11	ASN	N-CA-CB	-6.69	98.28	111.60
1	A	9	ASP	CA-CB-CG	-6.54	106.06	112.60
1	A	28	GLN	OE1-CD-NE2	-6.52	116.08	122.60
1	A	125	SER	CA-CB-OG	6.47	124.04	111.10
1	A	15	GLN	CG-CD-NE2	-6.45	106.73	116.40
1	A	125	SER	N-CA-CB	-6.38	100.38	110.28
1	A	172	LYS	N-CA-CB	6.38	119.69	110.06
1	A	131	LEU	CA-C-O	6.18	127.10	120.55
1	A	27	ASN	CA-CB-CG	6.11	118.70	112.60
1	A	27	ASN	O-C-N	6.10	130.16	121.92
1	A	69	ASN	OD1-CG-ND2	-6.10	116.50	122.60
1	A	234	GLU	O-C-N	6.05	129.88	123.11
1	A	146	VAL	O-C-N	6.02	129.58	123.20
1	A	218	VAL	CA-C-O	-6.02	115.91	120.96
1	A	172	LYS	O-C-N	6.00	130.09	123.01
1	A	10	LYS	CA-C-O	-5.99	112.59	119.60
1	A	252	LYS	CA-C-N	5.94	132.56	120.80
1	A	252	LYS	C-N-CA	5.94	132.56	120.80
1	A	232	ASN	OD1-CG-ND2	-5.89	116.71	122.60
1	A	109	VAL	O-C-N	5.88	129.29	123.18
1	A	41	ASP	CA-C-O	-5.84	114.11	120.36
1	A	109	VAL	CA-C-O	-5.84	114.37	120.27
1	A	225	GLN	CA-C-O	5.84	126.61	120.42
1	A	9	ASP	O-C-N	5.81	130.66	122.41
1	A	192	TRP	N-CA-CB	5.70	119.97	110.85

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	58	GLU	CB-CG-CD	5.62	122.16	112.60
1	A	8	ASP	CA-CB-CG	-5.54	107.06	112.60
1	A	178	ASN	N-CA-CB	-5.48	103.59	111.70
1	A	27	ASN	CA-C-O	-5.45	115.68	121.78
1	A	225	GLN	OE1-CD-NE2	-5.43	117.17	122.60
1	A	119	HIS	CA-C-N	5.38	130.43	123.11
1	A	119	HIS	C-N-CA	5.38	130.43	123.11
1	A	143	VAL	CA-C-N	-5.32	115.72	122.37
1	A	143	VAL	C-N-CA	-5.32	115.72	122.37
1	A	161	LEU	O-C-N	5.22	127.66	122.12
1	A	15	GLN	CB-CG-CD	-5.20	103.76	112.60
1	A	151	GLY	O-C-N	5.19	129.45	122.70
1	A	205	GLU	CA-C-O	5.08	129.32	122.51
1	A	189	LEU	O-C-N	5.08	128.81	121.95
1	A	20	TYR	O-C-N	5.04	125.90	121.32
1	A	208	THR	N-CA-CB	5.03	118.81	110.47
1	A	165	GLN	OE1-CD-NE2	-5.00	117.59	122.60

There are no chirality outliers.

There are no planarity outliers.

## 5.2 Too-close contacts [i](#)

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	1721	0	1703	42	116
2	A	1	0	0	0	0
All	All	1722	0	1703	42	116

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 11.

All (42) 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:10:LYS:O	1:A:15:GLN:NE2	2.01	0.93

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:39:LYS:HE2	1:A:255:THR:HG21	1.52	0.91
1:A:10:LYS:C	1:A:15:GLN:HE22	1.84	0.85
1:A:9:ASP:O	1:A:15:GLN:OE1	1.95	0.84
1:A:128:TYR:CE1	1:A:137:LYS:HG3	2.14	0.82
1:A:10:LYS:C	1:A:15:GLN:NE2	2.52	0.63
1:A:47:ILE:HD11	1:A:189:LEU:HD23	1.80	0.63
1:A:70:PHE:CZ	1:A:181:PRO:HG3	2.36	0.60
1:A:60:ILE:HD12	1:A:173:ARG:HG2	1.83	0.60
1:A:200:HIS:HB2	1:A:201:PRO:HD2	1.84	0.59
1:A:134:ALA:O	1:A:140:GLY:HA3	2.03	0.58
1:A:114:TYR:HD1	1:A:149:LYS:HG2	1.68	0.58
1:A:39:LYS:HE2	1:A:255:THR:CG2	2.31	0.57
1:A:209:TRP:HB3	1:A:211:ILE:HD12	1.88	0.56
1:A:114:TYR:CD1	1:A:149:LYS:HG2	2.42	0.55
1:A:47:ILE:HD11	1:A:189:LEU:CD2	2.37	0.54
1:A:154:ASN:HB2	1:A:217:SER:O	2.07	0.54
1:A:63:GLY:HA3	1:A:170:LYS:HD3	1.89	0.54
1:A:41:ASP:HB3	1:A:44:LEU:HG	1.93	0.51
1:A:127:LYS:HE2	1:A:139:ASP:OD2	2.11	0.50
1:A:149:LYS:HG3	1:A:215:SER:OG	2.13	0.49
1:A:17:SER:HA	1:A:20:TYR:O	2.14	0.47
1:A:11:ASN:HA	1:A:15:GLN:NE2	2.29	0.47
1:A:47:ILE:HD12	1:A:47:ILE:C	2.39	0.46
1:A:5:TRP:CD2	1:A:201:PRO:HG2	2.51	0.46
1:A:156:LYS:HD3	1:A:183:THR:O	2.16	0.46
1:A:63:GLY:CA	1:A:170:LYS:HD3	2.45	0.46
1:A:47:ILE:CD1	1:A:189:LEU:HD23	2.46	0.45
1:A:219:SER:OG	1:A:222:GLN:HG3	2.17	0.44
1:A:45:LYS:HE2	1:A:45:LYS:HB2	1.74	0.43
1:A:39:LYS:HE3	1:A:257:ARG:HG2	2.00	0.43
1:A:250:PRO:HB2	1:A:252:LYS:HG3	2.00	0.43
1:A:27:ASN:HD22	1:A:254:ARG:HD3	1.84	0.42
1:A:153:ALA:HA	1:A:219:SER:HB3	2.01	0.42
1:A:8:ASP:O	1:A:12:GLY:HA3	2.19	0.42
1:A:193:THR:HA	1:A:209:TRP:O	2.21	0.41
1:A:209:TRP:HB3	1:A:211:ILE:CD1	2.51	0.41

All (116) 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:42:THR:CA	1:A:252:LYS:NZ[2_555]	0.52	1.68
1:A:26:ASN:ND2	1:A:258:ALA:O[2_554]	0.58	1.62
1:A:39:LYS:CD	1:A:205:GLU:CG[2_555]	0.59	1.61
1:A:26:ASN:CA	1:A:40:HIS:C[2_554]	0.63	1.57
1:A:14:GLU:CA	1:A:159:LYS:CE[3_655]	0.85	1.35
1:A:39:LYS:CG	1:A:205:GLU:CD[2_555]	0.86	1.34
1:A:26:ASN:N	1:A:41:ASP:N[2_554]	0.87	1.33
1:A:137:LYS:NZ	1:A:253:GLY:N[2_554]	0.89	1.31
1:A:39:LYS:CG	1:A:205:GLU:OE2[2_555]	0.92	1.28
1:A:9:ASP:OD1	1:A:53:PRO:CG[3_655]	0.96	1.24
1:A:39:LYS:CD	1:A:205:GLU:CD[2_555]	0.98	1.22
1:A:27:ASN:OD1	1:A:39:LYS:CA[2_554]	0.99	1.21
1:A:137:LYS:CE	1:A:253:GLY:N[2_554]	1.12	1.08
1:A:137:LYS:NZ	1:A:252:LYS:C[2_554]	1.12	1.08
1:A:25:GLY:C	1:A:41:ASP:CA[2_554]	1.13	1.07
1:A:126:ALA:CB	1:A:234:GLU:OE1[4_445]	1.13	1.07
1:A:24:ASN:CB	1:A:43:SER:CB[2_554]	1.20	1.00
1:A:26:ASN:C	1:A:40:HIS:O[2_554]	1.20	1.00
1:A:26:ASN:N	1:A:40:HIS:C[2_554]	1.22	0.98
1:A:26:ASN:CB	1:A:40:HIS:CA[2_554]	1.23	0.97
1:A:26:ASN:CA	1:A:40:HIS:O[2_554]	1.27	0.93
1:A:40:HIS:CD2	1:A:252:LYS:CB[2_555]	1.28	0.92
1:A:14:GLU:N	1:A:159:LYS:NZ[3_655]	1.31	0.89
1:A:136:SER:CB	1:A:253:GLY:O[2_554]	1.32	0.88
1:A:26:ASN:N	1:A:41:ASP:CA[2_554]	1.34	0.86
1:A:39:LYS:CB	1:A:205:GLU:OE2[2_555]	1.34	0.86
1:A:24:ASN:C	1:A:41:ASP:OD1[2_554]	1.35	0.85
1:A:136:SER:OG	1:A:253:GLY:O[2_554]	1.36	0.84
1:A:27:ASN:OD1	1:A:39:LYS:C[2_554]	1.42	0.78
1:A:14:GLU:OE2	1:A:159:LYS:CD[3_655]	1.43	0.77
1:A:24:ASN:O	1:A:41:ASP:OD1[2_554]	1.45	0.75
1:A:27:ASN:N	1:A:40:HIS:O[2_554]	1.45	0.75
1:A:40:HIS:NE2	1:A:252:LYS:CB[2_555]	1.45	0.75
1:A:26:ASN:C	1:A:40:HIS:C[2_554]	1.49	0.71
1:A:42:THR:CB	1:A:252:LYS:NZ[2_555]	1.50	0.70
1:A:26:ASN:CA	1:A:41:ASP:N[2_554]	1.52	0.68
1:A:24:ASN:O	1:A:43:SER:N[2_554]	1.56	0.64
1:A:14:GLU:CB	1:A:159:LYS:CE[3_655]	1.57	0.63
1:A:26:ASN:N	1:A:40:HIS:O[2_554]	1.58	0.62
1:A:42:THR:CB	1:A:252:LYS:CE[2_555]	1.58	0.62
1:A:18:LYS:NZ	1:A:156:LYS:CG[3_655]	1.60	0.60
1:A:26:ASN:CB	1:A:40:HIS:C[2_554]	1.60	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:14:GLU:CD	1:A:159:LYS:CD[3_655]	1.61	0.59
1:A:25:GLY:N	1:A:41:ASP:OD1[2_554]	1.62	0.58
1:A:42:THR:CG2	1:A:252:LYS:CE[2_555]	1.64	0.56
1:A:22:ILE:CG1	1:A:39:LYS:NZ[2_554]	1.67	0.53
1:A:26:ASN:OD1	1:A:40:HIS:ND1[2_554]	1.67	0.53
1:A:14:GLU:CA	1:A:159:LYS:NZ[3_655]	1.68	0.52
1:A:42:THR:N	1:A:252:LYS:NZ[2_555]	1.68	0.52
1:A:25:GLY:CA	1:A:41:ASP:CA[2_554]	1.69	0.51
1:A:14:GLU:N	1:A:159:LYS:CE[3_655]	1.70	0.50
1:A:42:THR:CG2	1:A:252:LYS:CD[2_555]	1.70	0.50
1:A:14:GLU:CG	1:A:159:LYS:NZ[3_655]	1.71	0.49
1:A:25:GLY:CA	1:A:41:ASP:CG[2_554]	1.71	0.49
1:A:14:GLU:CB	1:A:159:LYS:CD[3_655]	1.73	0.47
1:A:26:ASN:CA	1:A:40:HIS:CA[2_554]	1.73	0.47
1:A:26:ASN:O	1:A:40:HIS:CB[2_554]	1.74	0.46
1:A:14:GLU:CB	1:A:159:LYS:NZ[3_655]	1.76	0.44
1:A:26:ASN:ND2	1:A:258:ALA:C[2_554]	1.76	0.44
1:A:136:SER:OG	1:A:253:GLY:C[2_554]	1.76	0.44
1:A:126:ALA:CB	1:A:234:GLU:CD[4_445]	1.78	0.42
1:A:25:GLY:CA	1:A:41:ASP:CB[2_554]	1.79	0.41
1:A:26:ASN:CG	1:A:40:HIS:ND1[2_554]	1.79	0.41
1:A:39:LYS:CG	1:A:205:GLU:CG[2_555]	1.79	0.41
1:A:25:GLY:O	1:A:42:THR:N[2_554]	1.81	0.39
1:A:39:LYS:CG	1:A:205:GLU:OE1[2_555]	1.81	0.39
1:A:26:ASN:CG	1:A:258:ALA:O[2_554]	1.82	0.38
1:A:26:ASN:C	1:A:40:HIS:CA[2_554]	1.82	0.38
1:A:27:ASN:CG	1:A:40:HIS:N[2_554]	1.83	0.37
1:A:26:ASN:CB	1:A:40:HIS:CB[2_554]	1.86	0.34
1:A:27:ASN:OD1	1:A:40:HIS:N[2_554]	1.86	0.34
1:A:39:LYS:CD	1:A:205:GLU:OE1[2_555]	1.86	0.34
1:A:22:ILE:CD1	1:A:257:ARG:CD[2_554]	1.87	0.33
1:A:26:ASN:CB	1:A:41:ASP:N[2_554]	1.87	0.33
1:A:14:GLU:CG	1:A:159:LYS:CD[3_655]	1.88	0.32
1:A:39:LYS:CE	1:A:205:GLU:CD[2_555]	1.88	0.32
1:A:27:ASN:OD1	1:A:39:LYS:N[2_554]	1.91	0.29
1:A:40:HIS:NE2	1:A:252:LYS:CG[2_555]	1.92	0.28
1:A:25:GLY:N	1:A:41:ASP:CG[2_554]	1.93	0.27
1:A:39:LYS:CE	1:A:205:GLU:CG[2_555]	1.93	0.27
1:A:9:ASP:CG	1:A:53:PRO:CG[3_655]	1.94	0.26
1:A:26:ASN:OD1	1:A:41:ASP:O[2_554]	1.94	0.26
1:A:39:LYS:CD	1:A:205:GLU:OE2[2_555]	1.94	0.26

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:39:LYS:CD	1:A:205:GLU:CB[2_555]	1.94	0.26
1:A:42:THR:C	1:A:252:LYS:NZ[2_555]	1.94	0.26
1:A:136:SER:OG	1:A:253:GLY:CA[2_554]	1.94	0.26
1:A:40:HIS:NE2	1:A:252:LYS:CD[2_555]	1.98	0.22
1:A:42:THR:CA	1:A:252:LYS:CE[2_555]	1.98	0.22
1:A:25:GLY:C	1:A:41:ASP:N[2_554]	1.99	0.21
1:A:137:LYS:CE	1:A:252:LYS:C[2_554]	1.99	0.21
1:A:137:LYS:NZ	1:A:252:LYS:CA[2_554]	2.00	0.20
1:A:9:ASP:OD1	1:A:53:PRO:CD[3_655]	2.03	0.17
1:A:26:ASN:OD1	1:A:40:HIS:CE1[2_554]	2.03	0.17
1:A:37:GLU:CB	1:A:138:ALA:CB[2_555]	2.03	0.17
1:A:24:ASN:O	1:A:42:THR:N[2_554]	2.05	0.15
1:A:27:ASN:CG	1:A:39:LYS:CA[2_554]	2.05	0.15
1:A:133:GLU:OE1	1:A:259:SER:O[1_554]	2.05	0.15
1:A:137:LYS:NZ	1:A:253:GLY:CA[2_554]	2.05	0.15
1:A:25:GLY:C	1:A:41:ASP:C[2_554]	2.06	0.14
1:A:14:GLU:OE2	1:A:159:LYS:CG[3_655]	2.09	0.11
1:A:25:GLY:O	1:A:41:ASP:CA[2_554]	2.10	0.10
1:A:26:ASN:CB	1:A:40:HIS:CG[2_554]	2.10	0.10
1:A:137:LYS:CE	1:A:253:GLY:CA[2_554]	2.10	0.10
1:A:24:ASN:CB	1:A:43:SER:OG[2_554]	2.11	0.09
1:A:14:GLU:CA	1:A:159:LYS:CD[3_655]	2.12	0.08
1:A:14:GLU:CG	1:A:159:LYS:CE[3_655]	2.12	0.08
1:A:27:ASN:N	1:A:40:HIS:C[2_554]	2.12	0.08
1:A:137:LYS:NZ	1:A:252:LYS:O[2_554]	2.12	0.08
1:A:26:ASN:CB	1:A:40:HIS:ND1[2_554]	2.13	0.07
1:A:137:LYS:CD	1:A:253:GLY:N[2_554]	2.13	0.07
1:A:18:LYS:NZ	1:A:156:LYS:NZ[3_655]	2.14	0.06
1:A:25:GLY:CA	1:A:41:ASP:OD1[2_554]	2.16	0.04
1:A:9:ASP:OD1	1:A:53:PRO:CB[3_655]	2.17	0.03
1:A:25:GLY:C	1:A:40:HIS:O[2_554]	2.17	0.03
1:A:26:ASN:CG	1:A:41:ASP:N[2_554]	2.17	0.03
1:A:25:GLY:O	1:A:41:ASP:C[2_554]	2.19	0.01

## 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	26/260 (10%)	25 (96%)	1 (4%)	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	193/225 (86%)	190 (98%)	3 (2%)	55	62

All (3) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	187	SER
1	A	189	LEU
1	A	233	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (6) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	15	GLN
1	A	27	ASN
1	A	64	HIS
1	A	103	HIS
1	A	158	GLN
1	A	243	HIS

### 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 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.