



# wwPDB X-ray Structure Validation Summary Report ⓘ

Mar 18, 2026 – 07:02 AM UTC

PDB ID : 3MC2 / pdb\_00003mc2  
Title : Crystal Structure of the Murine Inhibitor of Carbonic Anhydrase  
Authors : Eckenroth, B.E.; Mason, A.B.; Everse, S.J.  
Deposited on : 2010-03-26  
Resolution : 2.40 Å(reported)

This is a wwPDB X-ray Structure Validation Summary 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  
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

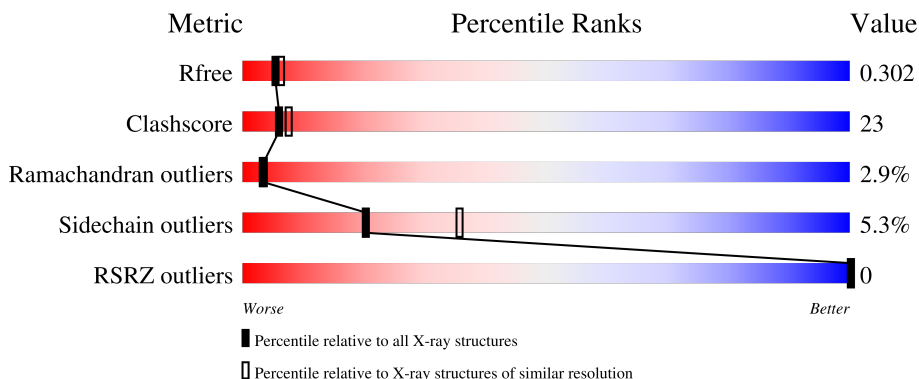
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.40 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	4912 (2.40-2.40)
Clashscore	190562	5391 (2.40-2.40)
Ramachandran outliers	187476	5320 (2.40-2.40)
Sidechain outliers	187428	5321 (2.40-2.40)
RSRZ outliers	180081	4916 (2.40-2.40)

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  $\leq 5\%$ . 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	687	 54% 39% 5% ..
1	B	687	 56% 38% ..
1	C	687	 57% 36% 5% ..
1	D	687	 58% 35% 5% ..

## 2 Entry composition [i](#)

There is only 1 type of molecule in this entry. The entry contains 20772 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 Inhibitor of Carbonic Anhydrase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	675	5193	3257	902	986	48	51	0	0
1	B	675	5193	3257	902	986	48	79	0	0
1	C	675	5193	3257	902	986	48	45	0	0
1	D	675	5193	3257	902	986	48	57	0	0

There are 32 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-5	HIS	-	expression tag	UNP Q9DBD0
A	-4	HIS	-	expression tag	UNP Q9DBD0
A	-3	HIS	-	expression tag	UNP Q9DBD0
A	-2	HIS	-	expression tag	UNP Q9DBD0
A	-1	HIS	-	expression tag	UNP Q9DBD0
A	0	HIS	-	expression tag	UNP Q9DBD0
A	470	ASP	ASN	engineered mutation	UNP Q9DBD0
A	645	ASP	ASN	engineered mutation	UNP Q9DBD0
B	-5	HIS	-	expression tag	UNP Q9DBD0
B	-4	HIS	-	expression tag	UNP Q9DBD0
B	-3	HIS	-	expression tag	UNP Q9DBD0
B	-2	HIS	-	expression tag	UNP Q9DBD0
B	-1	HIS	-	expression tag	UNP Q9DBD0
B	0	HIS	-	expression tag	UNP Q9DBD0
B	470	ASP	ASN	engineered mutation	UNP Q9DBD0
B	645	ASP	ASN	engineered mutation	UNP Q9DBD0
C	-5	HIS	-	expression tag	UNP Q9DBD0
C	-4	HIS	-	expression tag	UNP Q9DBD0
C	-3	HIS	-	expression tag	UNP Q9DBD0
C	-2	HIS	-	expression tag	UNP Q9DBD0
C	-1	HIS	-	expression tag	UNP Q9DBD0

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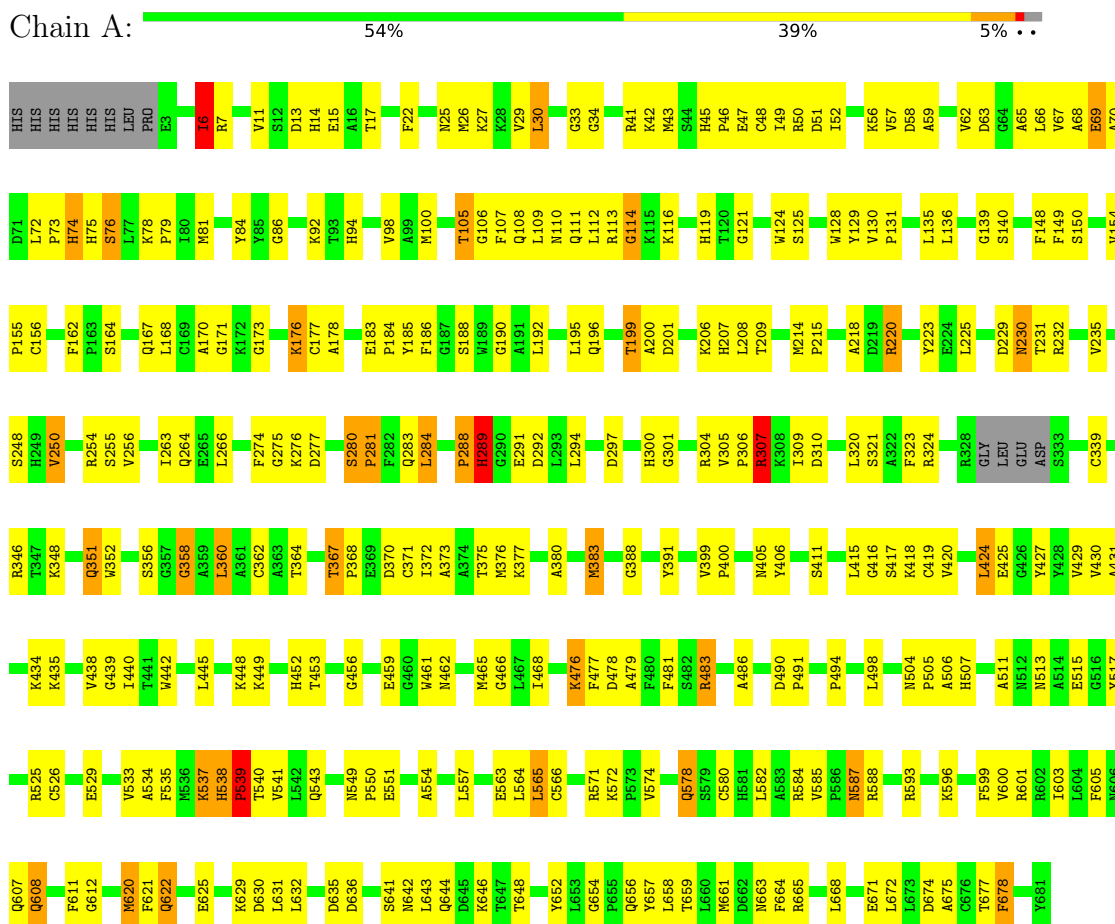
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Chain	Residue	Modelled	Actual	Comment	Reference
C	0	HIS	-	expression tag	UNP Q9DBD0
C	470	ASP	ASN	engineered mutation	UNP Q9DBD0
C	645	ASP	ASN	engineered mutation	UNP Q9DBD0
D	-5	HIS	-	expression tag	UNP Q9DBD0
D	-4	HIS	-	expression tag	UNP Q9DBD0
D	-3	HIS	-	expression tag	UNP Q9DBD0
D	-2	HIS	-	expression tag	UNP Q9DBD0
D	-1	HIS	-	expression tag	UNP Q9DBD0
D	0	HIS	-	expression tag	UNP Q9DBD0
D	470	ASP	ASN	engineered mutation	UNP Q9DBD0
D	645	ASP	ASN	engineered mutation	UNP Q9DBD0

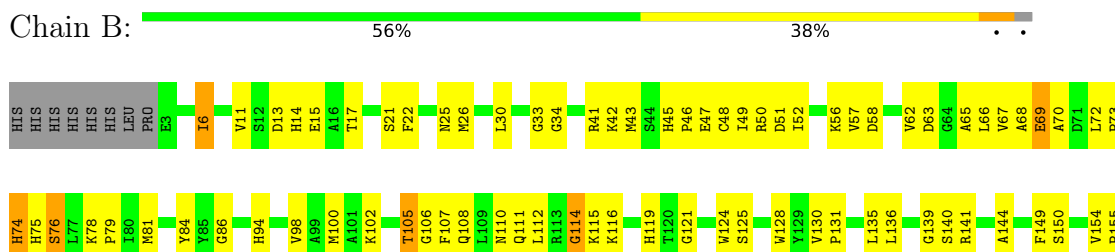
### 3 Residue-property plots

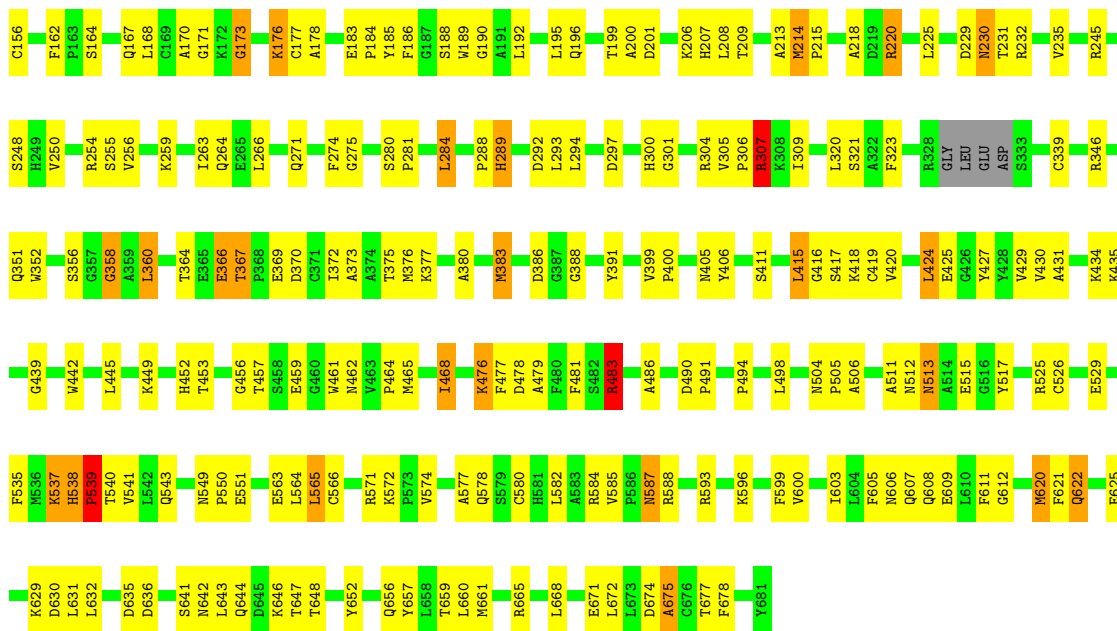
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. 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: Inhibitor of Carbonic Anhydrase

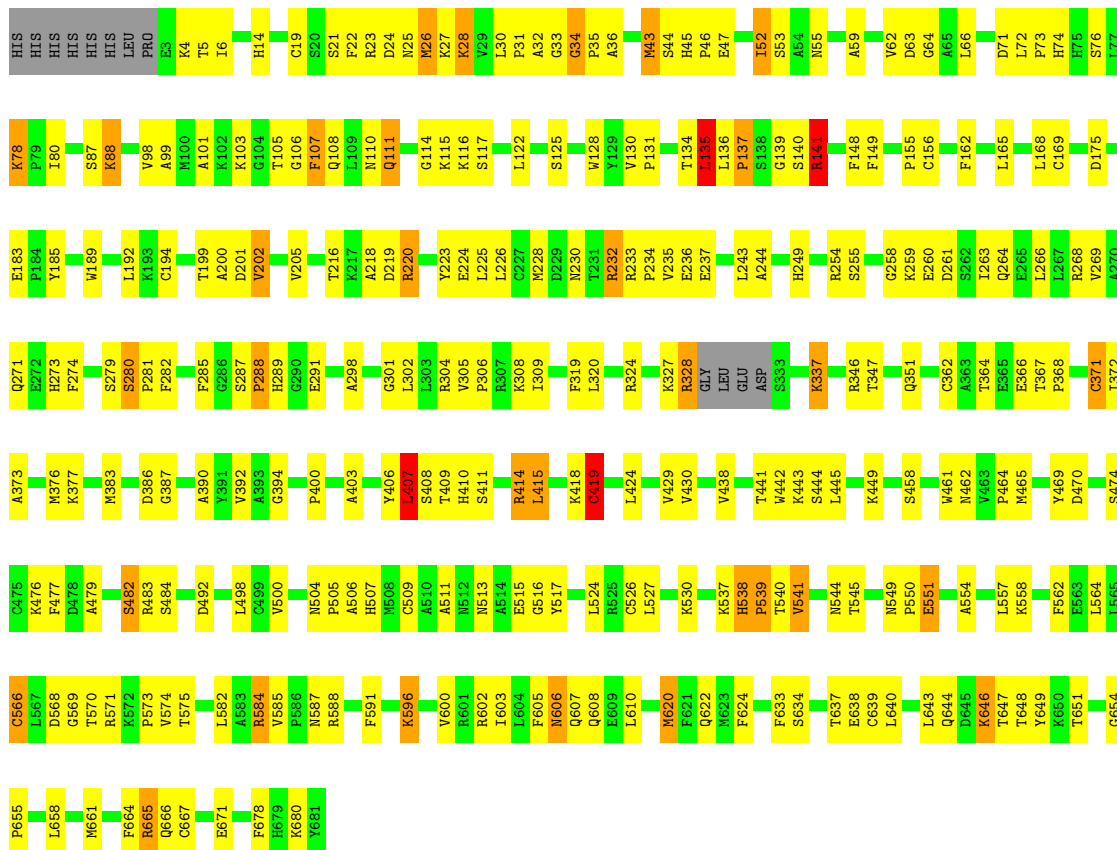


- Molecule 1: Inhibitor of Carbonic Anhydrase



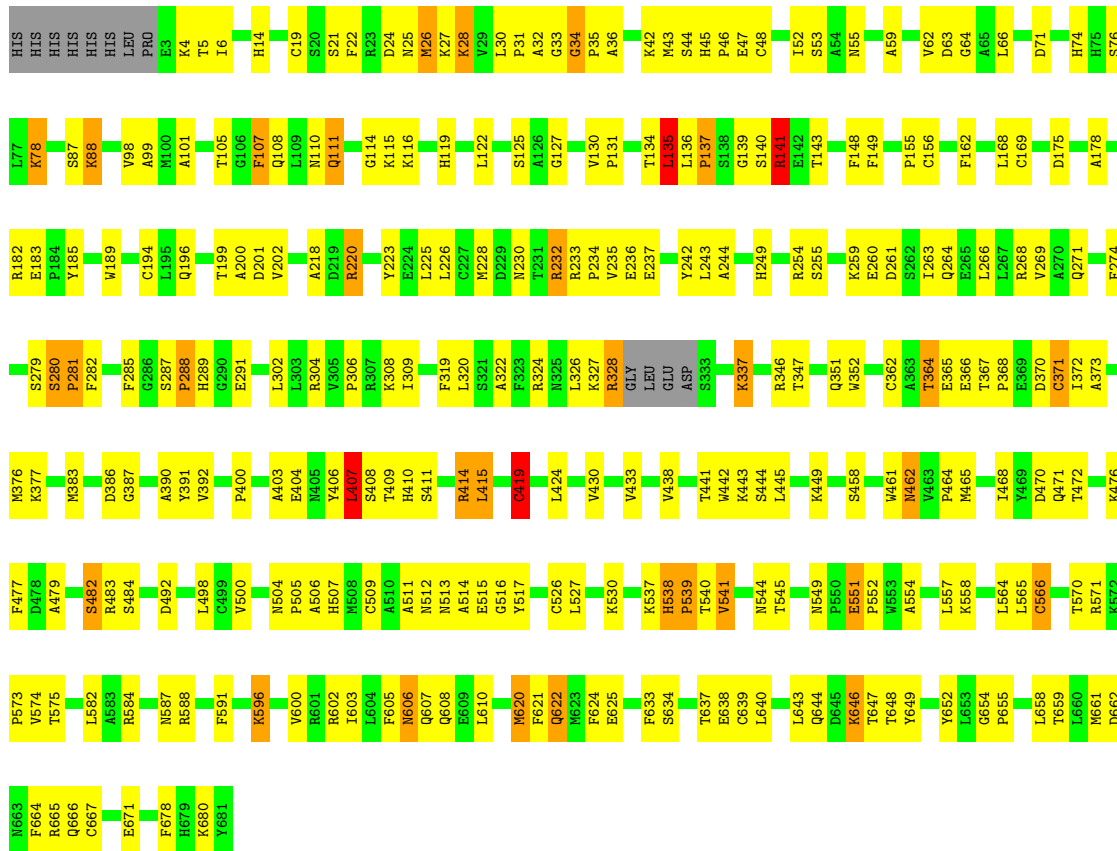


• Molecule 1: Inhibitor of Carbonic Anhydrase



• Molecule 1: Inhibitor of Carbonic Anhydrase

Chain D:  58% 35% 5% ..



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	68.56Å 136.93Å 155.57Å 90.00° 90.11° 90.00°	Depositor
Resolution (Å)	19.00 – 2.40 19.00 – 2.40	Depositor EDS
% Data completeness (in resolution range)	93.2 (19.00-2.40) 94.3 (19.00-2.40)	Depositor EDS
$R_{merge}$	0.07	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	3.12 (at 2.41Å)	Xtrriage
Refinement program	CNS, REFMAC	Depositor
R, $R_{free}$	0.239 , 0.301 0.240 , 0.302	Depositor DCC
$R_{free}$ test set	10093 reflections (9.56%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	52.1	Xtrriage
Anisotropy	0.797	Xtrriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.29 , 41.4	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.42$ , $\langle L^2 \rangle = 0.25$	Xtrriage
Estimated twinning fraction	0.478 for h,-k,-l	Xtrriage
Reported twinning fraction	0.500 for h,-k,-l	Depositor
Outliers	1 of 105600 reflections (0.001%)	Xtrriage
$F_o, F_c$ correlation	0.97	EDS
Total number of atoms	20772	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	75.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 47.58 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 9.7286e-05. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

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

<sup>2</sup>Theoretical 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 i

### 5.1 Standard geometry i

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	0.72	7/5312 (0.1%)	1.13	34/7179 (0.5%)
1	B	0.67	5/5312 (0.1%)	1.11	30/7179 (0.4%)
1	C	0.62	3/5312 (0.1%)	1.00	18/7179 (0.3%)
1	D	0.58	3/5312 (0.1%)	1.00	19/7179 (0.3%)
All	All	0.65	18/21248 (0.1%)	1.06	101/28716 (0.4%)

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
1	B	0	1
All	All	0	2

The worst 5 of 18 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	254	ARG	CZ-NH2	-13.75	1.15	1.33
1	B	307	ARG	CZ-NH2	-13.23	1.16	1.33
1	B	307	ARG	CZ-NH1	-12.90	1.14	1.32
1	A	307	ARG	CZ-NH1	-12.30	1.15	1.32
1	A	307	ARG	CZ-NH2	-12.23	1.17	1.33

The worst 5 of 101 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	307	ARG	NE-CZ-NH2	20.19	137.37	119.20
1	B	307	ARG	NH1-CZ-NH2	-19.96	93.36	119.30
1	A	254	ARG	NH1-CZ-NH2	-19.67	93.73	119.30
1	B	254	ARG	NH1-CZ-NH2	-19.33	94.17	119.30
1	A	307	ARG	NH1-CZ-NH2	-19.07	94.51	119.30

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	652	TYR	Sidechain
1	B	652	TYR	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	5193	0	5024	231	0
1	B	5193	0	5024	219	0
1	C	5193	0	5024	241	0
1	D	5193	0	5024	234	0
All	All	20772	0	20096	920	0

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 23.

The worst 5 of 920 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:C:414:ARG:HG2	1:C:415:LEU:H	1.21	1.05
1:D:414:ARG:HG2	1:D:415:LEU:H	1.21	1.03
1:A:572:LYS:HE2	1:A:580:CYS:HB2	1.43	0.99
1:B:587:ASN:N	1:B:587:ASN:HD22	1.57	0.98
1:C:218:ALA:HA	1:C:220:ARG:HE	1.27	0.96

There are no symmetry-related clashes.

## 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	671/687 (98%)	578 (86%)	74 (11%)	19 (3%)	4	3
1	B	671/687 (98%)	574 (86%)	78 (12%)	19 (3%)	4	3
1	C	671/687 (98%)	568 (85%)	83 (12%)	20 (3%)	3	3
1	D	671/687 (98%)	563 (84%)	87 (13%)	21 (3%)	3	3
All	All	2684/2748 (98%)	2283 (85%)	322 (12%)	79 (3%)	3	3

5 of 79 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	230	ASN
1	A	280	SER
1	A	289	HIS
1	A	539	PRO
1	A	620	MET

### 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	563/574 (98%)	532 (94%)	31 (6%)	19	34
1	B	563/574 (98%)	531 (94%)	32 (6%)	18	33
1	C	563/574 (98%)	535 (95%)	28 (5%)	22	38
1	D	563/574 (98%)	535 (95%)	28 (5%)	22	38
All	All	2252/2296 (98%)	2133 (95%)	119 (5%)	20	36

5 of 119 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	578	GLN
1	D	492	ASP
1	C	135	LEU

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Mol	Chain	Res	Type
1	D	482	SER
1	D	639	CYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 87 such sidechains are listed below:

Mol	Chain	Res	Type
1	C	606	ASN
1	D	283	GLN
1	C	608	GLN
1	D	119	HIS
1	D	446	GLN

### 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](#)

There are no ligands in this entry.

### 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 [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, 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	675/687 (98%)	-1.38	0 100 100	15, 63, 104, 116	18 (2%)
1	B	675/687 (98%)	-1.30	0 100 100	19, 77, 111, 128	25 (3%)
1	C	675/687 (98%)	-1.36	0 100 100	36, 67, 108, 125	16 (2%)
1	D	675/687 (98%)	-1.27	0 100 100	38, 82, 114, 134	19 (2%)
All	All	2700/2748 (98%)	-1.33	0 100 100	15, 73, 110, 134	78 (2%)

There are no RSRZ outliers to report.

### 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](#)

There are no ligands in this entry.

### 6.5 Other polymers [i](#)

There are no such residues in this entry.