



wwPDB X-ray Structure Validation Summary Report ⓘ

Feb 1, 2016 – 10:32 AM GMT

PDB ID : 3MC2
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
A user guide is available at
<http://wwpdb.org/validation/2016/XrayValidationReportHelp>
with specific help available everywhere you see the ⓘ symbol.

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

MolProbity : 4.02b-467
Mogul : 1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix) : 1.9-1692
EDS : rb-20026688
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac : 5.8.0135
CCP4 : 6.5.0
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : trunk26865

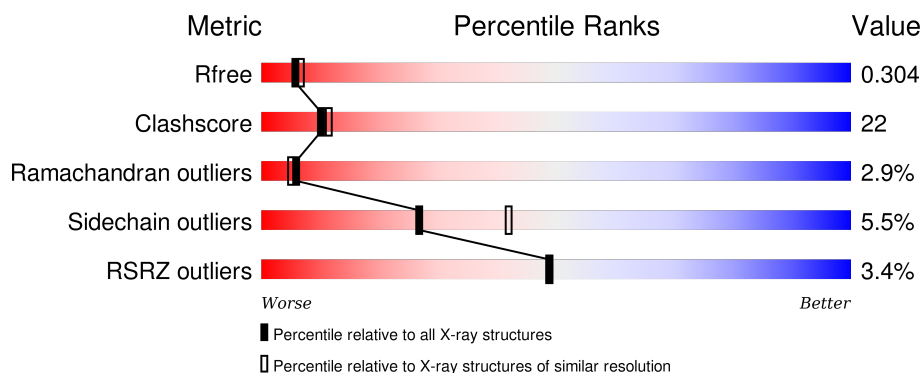
1 Overall quality at a glance

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}	91344	2919 (2.40-2.40)
Clashscore	102246	3407 (2.40-2.40)
Ramachandran outliers	100387	3351 (2.40-2.40)
Sidechain outliers	100360	3352 (2.40-2.40)
RSRZ outliers	91569	2928 (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 on the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria. 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	<div> <div>3%</div> <div>56% 38% . .</div> </div>
1	B	687	<div> <div>3%</div> <div>58% 37% . .</div> </div>
1	C	687	<div> <div>2%</div> <div>59% 35% . .</div> </div>
1	D	687	<div> <div>5%</div> <div>59% 34% . .</div> </div>

2 Entry composition

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
1	A	675	Total	C	N	O	S	51	0	0
			5193	3257	902	986	48			
1	B	675	Total	C	N	O	S	79	0	0
			5193	3257	902	986	48			
1	C	675	Total	C	N	O	S	45	0	0
			5193	3257	902	986	48			
1	D	675	Total	C	N	O	S	57	0	0
			5193	3257	902	986	48			

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	UNP Q9DBD0
A	645	ASP	ASN	ENGINEERED	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	UNP Q9DBD0
B	645	ASP	ASN	ENGINEERED	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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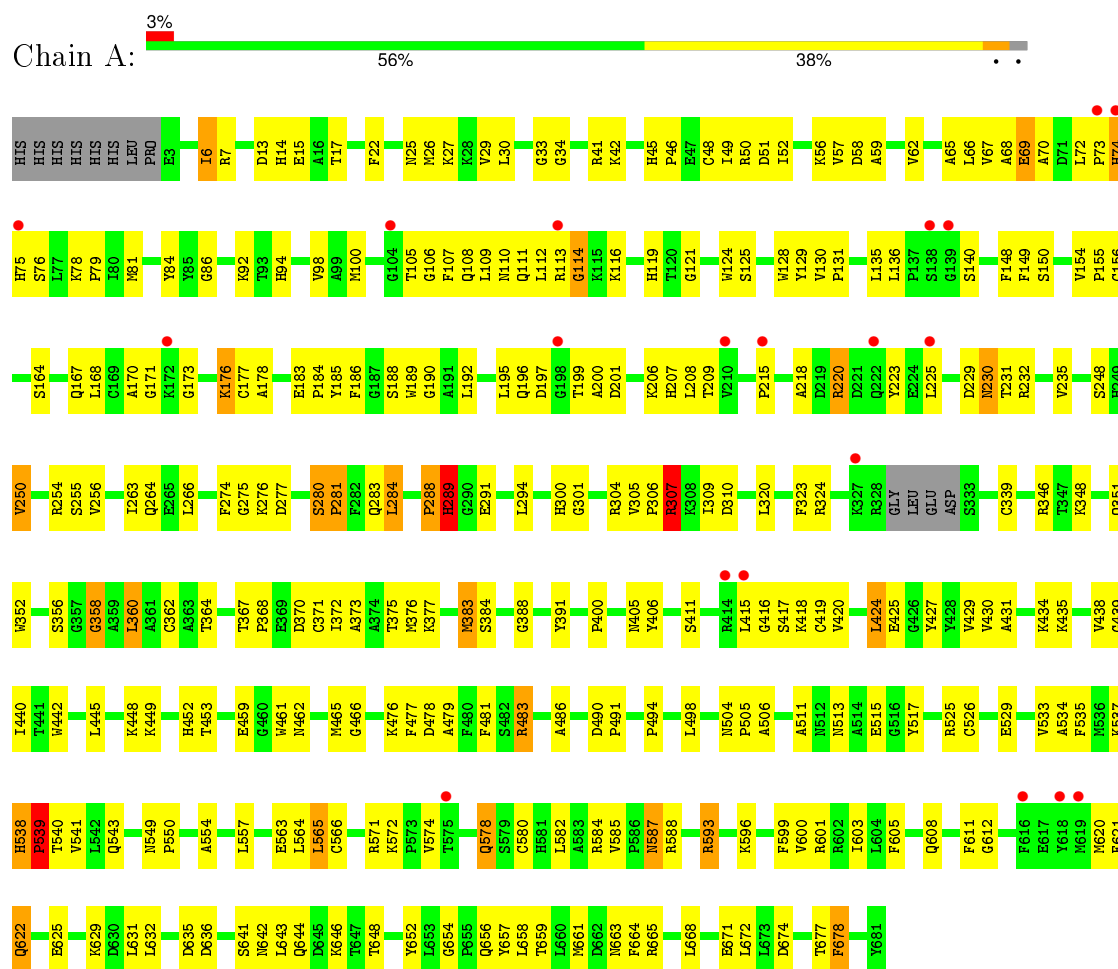
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Chain	Residue	Modelled	Actual	Comment	Reference
C	0	HIS	-	EXPRESSION TAG	UNP Q9DBD0
C	470	ASP	ASN	ENGINEERED	UNP Q9DBD0
C	645	ASP	ASN	ENGINEERED	UNP Q9DBD0
D	-5	HIS	-	EXPRESSION TAG	UNP Q9DBD0
D	-4	HIS	-	EXPRESSION TAG	UNP Q9DBD0
D	-3	HIS	-	EXPRESSION 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	UNP Q9DBD0
D	645	ASP	ASN	ENGINEERED	UNP Q9DBD0

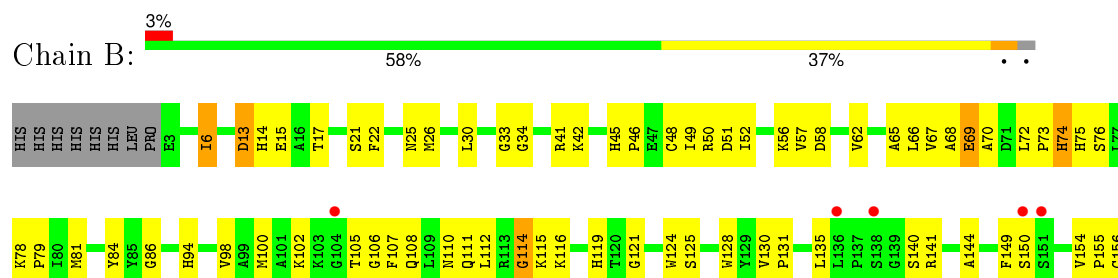
3 Residue-property plots

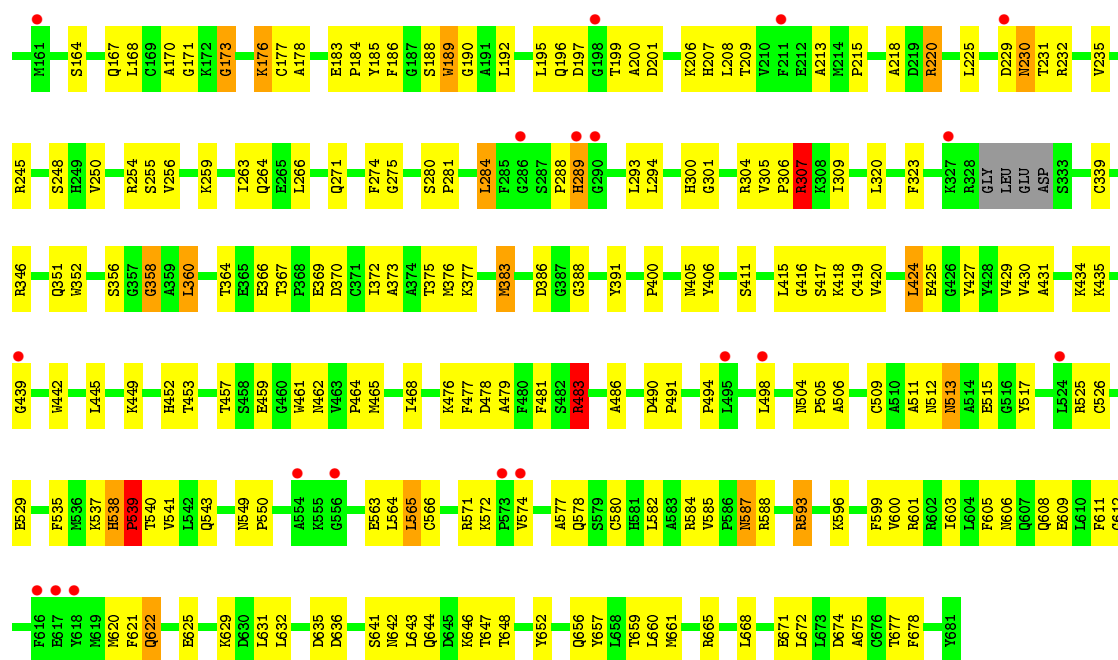
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according 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: Inhibitor of Carbonic Anhydrase

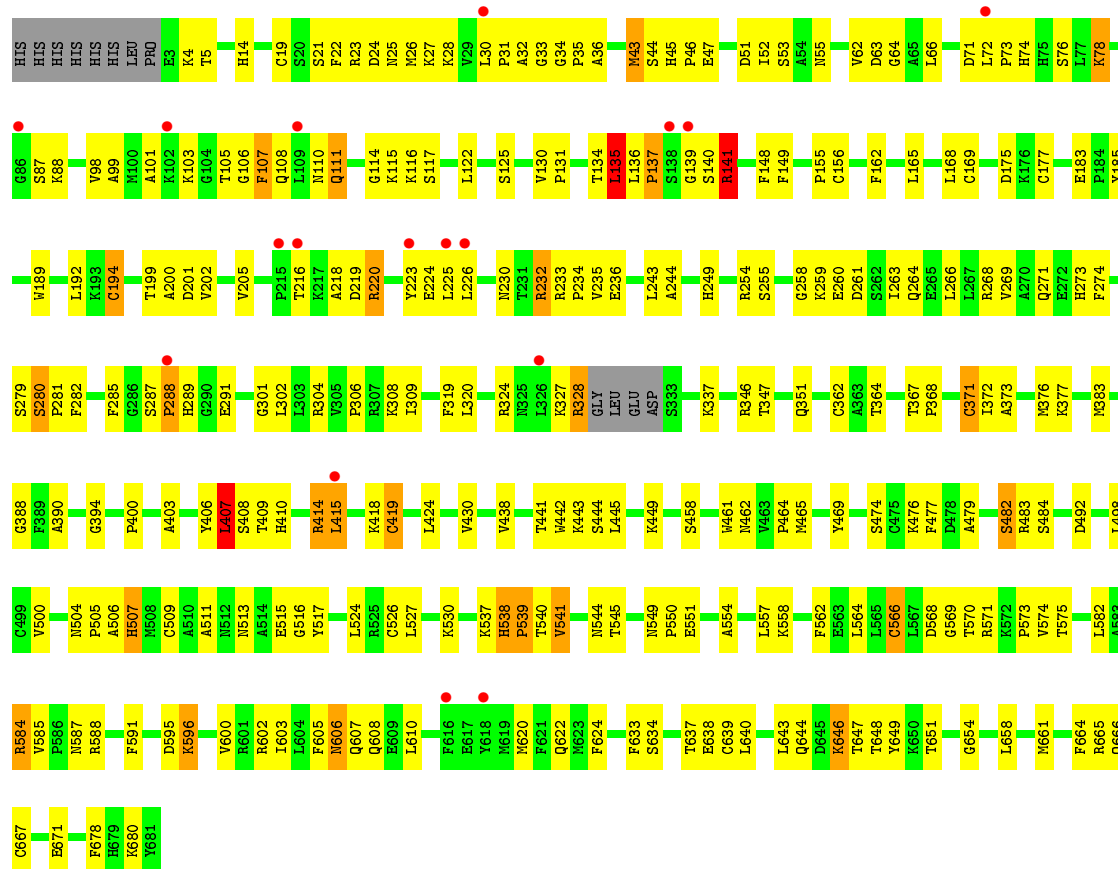


• Molecule 1: Inhibitor of Carbonic Anhydrase





• Molecule 1: Inhibitor of Carbonic Anhydrase



• Molecule 1: Inhibitor of Carbonic Anhydrase



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	68.56Å 136.93Å 155.57Å 90.00° 90.11° 90.00°	Depositor
Resolution (Å)	19.00 – 2.40 18.95 – 2.40	Depositor EDS
% Data completeness (in resolution range)	93.2 (19.00-2.40) 93.9 (18.95-2.40)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.12 (at 2.41Å)	Xtriage
Refinement program	CNS	Depositor
R, R_{free}	0.239 , 0.301 0.241 , 0.304	Depositor DCC
R_{free} test set	10093 reflections (10.57%)	DCC
Wilson B-factor (Å ²)	52.1	Xtriage
Anisotropy	0.797	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	(Not available) , (Not available)	EDS
Estimated twinning fraction	0.500 for h,-k,-l 0.478 for h,-k,-l	Xtriage
Reported twinning fraction	0.500 for h,-k,-l	Depositor
L-test for twinning ²	$\langle L \rangle = 0.42$, $\langle L^2 \rangle = 0.25$	Xtriage
Outliers	1 of 105600 reflections (0.001%)	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	20772	wwPDB-VP
Average B, all atoms (Å ²)	75.0	wwPDB-VP

Xtriage'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.*

¹ Intensities estimated from amplitudes.

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

5 Model quality

5.1 Standard geometry

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	0.61	4/5312 (0.1%)	1.04	10/7179 (0.1%)
1	B	0.58	4/5312 (0.1%)	0.99	8/7179 (0.1%)
1	C	0.51	3/5312 (0.1%)	0.75	8/7179 (0.1%)
1	D	0.47	3/5312 (0.1%)	0.73	7/7179 (0.1%)
All	All	0.55	14/21248 (0.1%)	0.89	33/28716 (0.1%)

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 14 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	307	ARG	CZ-NH1	-14.12	1.14	1.33
1	A	307	ARG	CZ-NH1	-13.47	1.15	1.33
1	A	254	ARG	CZ-NH2	-13.44	1.15	1.33
1	B	307	ARG	CZ-NH2	-12.93	1.16	1.33
1	A	307	ARG	CZ-NH2	-11.93	1.17	1.33

The worst 5 of 33 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	307	ARG	NE-CZ-NH2	34.14	137.37	120.30
1	B	254	ARG	NE-CZ-NH1	31.73	136.16	120.30
1	B	307	ARG	NE-CZ-NH1	29.80	135.20	120.30
1	A	254	ARG	NE-CZ-NH2	29.11	134.85	120.30
1	B	307	ARG	NH1-CZ-NH2	-23.68	93.36	119.40

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	224	0
1	B	5193	0	5024	210	0
1	C	5193	0	5024	233	0
1	D	5193	0	5024	222	0
All	All	20772	0	20096	884	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 22.

The worst 5 of 884 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:C:558:LYS:HB3	1:C:558:LYS:HZ2	1.22	1.02
1:D:558:LYS:HZ2	1:D:558:LYS:HB3	1.22	1.00
1:A:572:LYS:HE2	1:A:580:CYS:HB2	1.43	0.99

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%)	6	5
1	B	671/687 (98%)	574 (86%)	78 (12%)	19 (3%)	6	5
1	C	671/687 (98%)	568 (85%)	83 (12%)	20 (3%)	5	4
1	D	671/687 (98%)	563 (84%)	87 (13%)	21 (3%)	5	4
All	All	2684/2748 (98%)	2283 (85%)	322 (12%)	79 (3%)	6	5

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 ⓘ

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%)	27	42
1	B	563/574 (98%)	530 (94%)	33 (6%)	24	38
1	C	563/574 (98%)	535 (95%)	28 (5%)	30	48
1	D	563/574 (98%)	532 (94%)	31 (6%)	27	42
All	All	2252/2296 (98%)	2129 (94%)	123 (6%)	27	42

5 of 123 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	539	PRO
1	C	74	HIS
1	D	507	HIS

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Mol	Chain	Res	Type
1	B	566	CYS
1	B	648	THR

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 71 such sidechains are listed below:

Mol	Chain	Res	Type
1	B	656	GLN
1	C	264	GLN
1	D	606	ASN
1	B	663	ASN
1	C	167	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 carbohydrates 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, 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	675/687 (98%)	-0.09	20 (2%) 54 53	15, 64, 105, 116	18 (2%)
1	B	675/687 (98%)	0.09	24 (3%) 46 47	19, 79, 112, 128	25 (3%)
1	C	675/687 (98%)	-0.04	17 (2%) 61 60	36, 68, 109, 125	16 (2%)
1	D	675/687 (98%)	0.21	31 (4%) 36 37	48, 83, 114, 134	19 (2%)
All	All	2700/2748 (98%)	0.04	92 (3%) 49 49	15, 74, 110, 134	78 (2%)

The worst 5 of 92 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	215	PRO	7.1
1	D	290	GLY	6.5
1	D	326	LEU	6.1
1	D	170	ALA	5.3
1	D	618	TYR	5.3

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 carbohydrates 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.