



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 6, 2026 – 02:57 AM UTC

PDB ID : 1CVA / pdb_00001cva
Title : STRUCTURAL AND FUNCTIONAL IMPORTANCE OF A CONSERVED
HYDROGEN BOND NETWORK IN HUMAN CARBONIC ANHYDRASE
II
Authors : Ippolito, J.A.; Christianson, D.W.
Deposited on : 1993-02-04
Resolution : 2.25 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
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (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

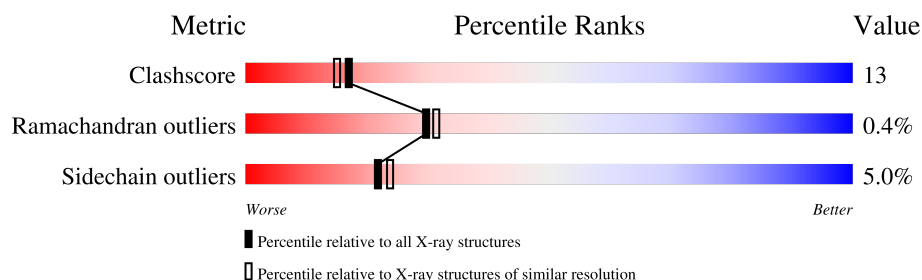
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.25 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	2005 (2.26-2.26)
Ramachandran outliers	187476	1965 (2.26-2.26)
Sidechain outliers	187428	1966 (2.26-2.26)

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 $\leq 5\%$.

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	259	

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
3	AZI	A	357	-	X	X	-

2 Entry composition [i](#)

There are 4 unique types of molecules in this entry. The entry contains 2127 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 II.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	255	Total	C	N	O	S	0	0	0
			2029	1304	347	376	2			

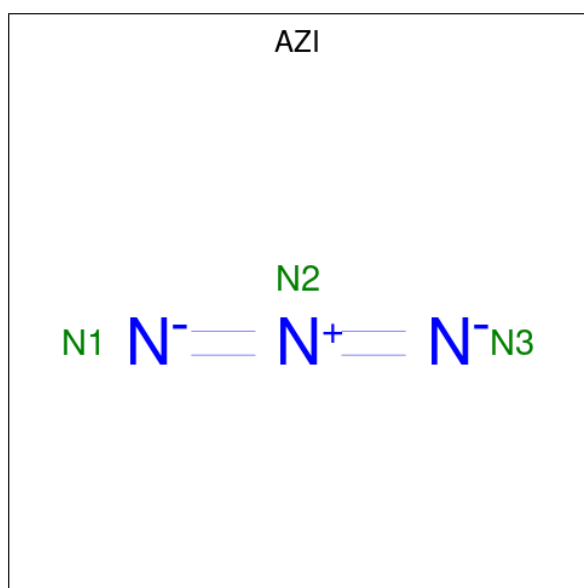
There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	199	VAL	THR	conflict	UNP P00918

- 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 AZIDE ION (CCD ID: AZI) (formula: N₃).



Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	1	Total	N	0	0
			3	3		

- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	94	Total	O	0	0
			94	94		

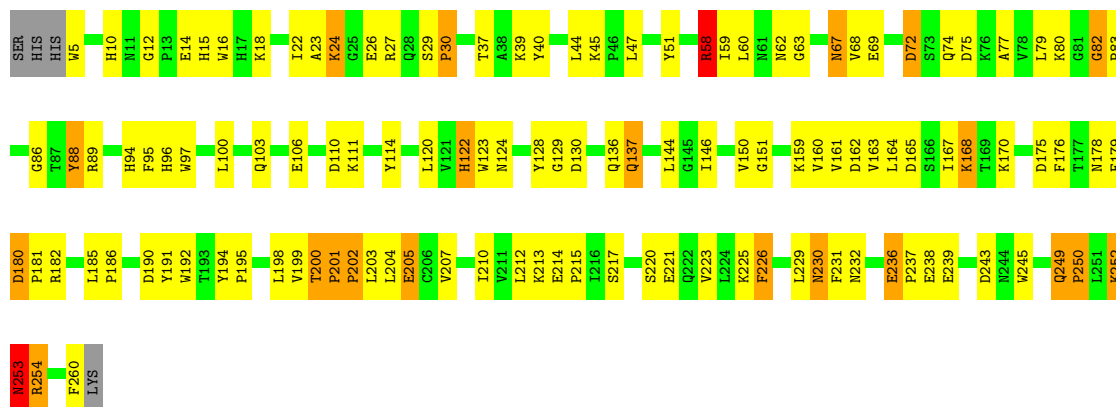
3 Residue-property plots

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. 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 II

Chain A: 



4 Data and refinement statistics

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

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	42.70Å 41.70Å 73.00Å 90.00° 104.60° 90.00°	Depositor
Resolution (Å)	6.50 – 2.25	Depositor
% Data completeness (in resolution range)	(Not available) (6.50-2.25)	Depositor
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	PROLSQ	Depositor
R, R_{free}	0.173 , (Not available)	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	2127	wwPDB-VP
Average B, all atoms (Å ²)	14.0	wwPDB-VP

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: ZN, AZI

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	1.89	29/2089 (1.4%)	2.08	77/2836 (2.7%)

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	2

All (29) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	217	SER	CA-C	7.37	1.61	1.52
1	A	10	HIS	CE1-NE2	6.55	1.39	1.32
1	A	129	GLY	N-CA	-6.52	1.35	1.45
1	A	194	TYR	C-O	6.38	1.32	1.24
1	A	39	LYS	N-CA	6.33	1.53	1.46
1	A	201	PRO	CA-C	-6.09	1.46	1.52
1	A	164	LEU	C-N	-6.07	1.26	1.33
1	A	94	HIS	CE1-NE2	6.06	1.38	1.32
1	A	24	LYS	CA-CB	-6.04	1.44	1.53
1	A	15	HIS	CG-CD2	6.02	1.42	1.35
1	A	151	GLY	CA-C	6.00	1.60	1.51
1	A	106	GLU	CA-C	-5.92	1.45	1.52
1	A	150	VAL	C-O	5.72	1.29	1.24
1	A	16	TRP	C-O	5.67	1.30	1.24
1	A	86	GLY	C-N	-5.49	1.25	1.33
1	A	97	TRP	C-O	5.49	1.30	1.24
1	A	150	VAL	N-CA	5.36	1.52	1.46
1	A	195	PRO	CA-C	-5.30	1.47	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	215	PRO	N-CD	5.26	1.55	1.47
1	A	88	TYR	N-CA	5.25	1.52	1.46
1	A	82	GLY	N-CA	5.24	1.51	1.44
1	A	194	TYR	C-N	-5.22	1.29	1.33
1	A	14	GLU	CD-OE1	5.16	1.35	1.25
1	A	16	TRP	C-N	-5.14	1.27	1.34
1	A	24	LYS	N-CA	5.14	1.52	1.46
1	A	22	ILE	N-CA	5.12	1.53	1.46
1	A	16	TRP	NE1-CE2	-5.07	1.31	1.37
1	A	72	ASP	C-O	5.06	1.30	1.23
1	A	238	GLU	CD-OE1	5.03	1.34	1.25

All (77) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	95	PHE	CA-CB-CG	10.46	124.25	113.80
1	A	201	PRO	CA-C-O	-10.45	105.41	120.56
1	A	226	PHE	CA-CB-CG	9.41	123.22	113.80
1	A	202	PRO	N-CA-CB	8.34	111.77	102.60
1	A	231	PHE	CA-CB-CG	8.32	122.12	113.80
1	A	180	ASP	CA-C-N	8.05	127.77	119.56
1	A	180	ASP	C-N-CA	8.05	127.77	119.56
1	A	29	SER	CA-C-O	-7.96	110.93	120.41
1	A	202	PRO	CA-N-CD	-7.82	100.55	111.50
1	A	136	GLN	OE1-CD-NE2	-7.79	114.81	122.60
1	A	23	ALA	O-C-N	7.52	130.77	122.20
1	A	68	VAL	CA-C-O	-7.43	112.12	120.74
1	A	67	ASN	CA-CB-CG	7.12	119.72	112.60
1	A	202	PRO	N-CD-CG	7.04	112.24	103.80
1	A	201	PRO	CB-CA-C	6.95	119.39	110.92
1	A	175	ASP	CB-CA-C	6.92	120.84	109.70
1	A	122	HIS	ND1-CE1-NE2	6.89	115.29	108.40
1	A	29	SER	O-C-N	6.86	128.23	121.57
1	A	130	ASP	CA-CB-CG	6.80	119.40	112.60
1	A	168	LYS	CA-C-O	-6.79	113.35	120.55
1	A	16	TRP	CA-C-O	-6.67	113.42	120.63
1	A	82	GLY	CA-C-N	6.48	127.04	120.04
1	A	82	GLY	C-N-CA	6.48	127.04	120.04
1	A	137	GLN	CA-C-N	6.45	126.03	119.19
1	A	137	GLN	C-N-CA	6.45	126.03	119.19
1	A	191	TYR	N-CA-C	6.42	118.52	108.96
1	A	201	PRO	O-C-N	6.41	129.03	121.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	180	ASP	CB-CA-C	6.40	116.51	110.17
1	A	18	LYS	O-C-N	6.40	130.14	122.27
1	A	198	LEU	N-CA-C	-6.39	101.49	110.50
1	A	253	ASN	CA-CB-CG	6.35	118.95	112.60
1	A	37	THR	CA-CB-OG1	-6.34	100.09	109.60
1	A	114	TYR	O-C-N	6.27	130.12	123.03
1	A	30	PRO	CA-N-CD	-6.10	102.96	111.50
1	A	207	VAL	O-C-N	6.08	129.38	122.93
1	A	186	PRO	O-C-N	6.08	130.40	122.86
1	A	15	HIS	ND1-CE1-NE2	6.00	114.40	108.40
1	A	200	THR	CA-CB-OG1	-5.96	100.66	109.60
1	A	239	GLU	CA-CB-CG	5.85	125.80	114.10
1	A	192	TRP	N-CA-C	-5.81	100.43	109.72
1	A	250	PRO	CA-C-O	-5.76	115.07	121.23
1	A	185	LEU	CA-C-N	5.75	125.73	120.21
1	A	185	LEU	C-N-CA	5.75	125.73	120.21
1	A	120	LEU	O-C-N	5.75	129.89	123.05
1	A	96	HIS	O-C-N	5.68	129.96	123.31
1	A	200	THR	O-C-N	5.66	125.97	121.55
1	A	182	ARG	CD-NE-CZ	-5.65	116.50	124.40
1	A	230	ASN	CA-CB-CG	5.61	118.21	112.60
1	A	94	HIS	CA-CB-CG	-5.59	108.21	113.80
1	A	249	GLN	CA-C-N	5.58	125.86	119.83
1	A	249	GLN	C-N-CA	5.58	125.86	119.83
1	A	214	GLU	CA-C-O	5.57	123.75	119.46
1	A	236	GLU	CB-CG-CD	5.55	122.03	112.60
1	A	10	HIS	ND1-CG-CD2	5.42	111.52	106.10
1	A	186	PRO	N-CA-C	-5.37	103.70	111.22
1	A	26	GLU	CA-C-O	-5.37	112.65	119.31
1	A	12	GLY	CA-C-N	5.34	125.67	119.47
1	A	12	GLY	C-N-CA	5.34	125.67	119.47
1	A	250	PRO	O-C-N	5.33	129.14	123.01
1	A	205	GLU	CA-C-N	5.33	130.60	122.29
1	A	205	GLU	C-N-CA	5.33	130.60	122.29
1	A	252	LYS	CA-C-O	-5.31	116.11	122.27
1	A	26	GLU	N-CA-C	5.28	119.44	112.89
1	A	231	PHE	N-CA-C	-5.27	105.20	111.69
1	A	30	PRO	N-CD-CG	5.26	110.11	103.80
1	A	114	TYR	CA-C-O	-5.22	115.30	121.66
1	A	190	ASP	CA-CB-CG	5.18	117.78	112.60
1	A	80	LYS	O-C-N	5.16	128.96	122.92
1	A	136	GLN	CG-CD-NE2	5.13	124.10	116.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	176	PHE	CB-CA-C	5.11	120.40	111.86
1	A	186	PRO	CA-C-O	-5.07	115.17	122.31
1	A	96	HIS	CA-C-N	-5.05	114.39	122.53
1	A	96	HIS	C-N-CA	-5.05	114.39	122.53
1	A	74	GLN	CA-C-O	-5.02	115.73	121.40
1	A	214	GLU	CA-C-N	5.01	125.22	120.31
1	A	214	GLU	C-N-CA	5.01	125.22	120.31
1	A	40	TYR	O-C-N	5.01	129.25	122.59

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	254	ARG	Sidechain
1	A	58	ARG	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	2029	0	1984	51	1
2	A	1	0	0	0	0
3	A	3	0	0	2	0
4	A	94	0	0	4	1
All	All	2127	0	1984	51	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 13.

All (51) 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:58:ARG:HD2	1:A:69:GLU:OE1	1.46	1.15
1:A:63:GLY:HA3	1:A:170:LYS:HZ3	1.34	0.90
1:A:253:ASN:HD22	1:A:254:ARG:N	1.77	0.82

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:253:ASN:HD22	1:A:253:ASN:C	1.94	0.75
1:A:165:ASP:HB2	4:A:304:HOH:O	1.86	0.75
1:A:161:VAL:CG1	1:A:225:LYS:HD2	2.17	0.74
1:A:253:ASN:ND2	1:A:254:ARG:N	2.35	0.73
1:A:63:GLY:HA3	1:A:170:LYS:NZ	2.03	0.72
1:A:161:VAL:HG13	1:A:225:LYS:HD2	1.75	0.67
1:A:213:LYS:HD3	1:A:260:PHE:CZ	2.31	0.66
1:A:250:PRO:HB2	1:A:252:LYS:HG3	1.82	0.61
1:A:236:GLU:HB3	1:A:237:PRO:HD2	1.84	0.60
1:A:62:ASN:O	1:A:170:LYS:NZ	2.33	0.60
1:A:110:ASP:O	1:A:111:LYS:HB2	2.02	0.59
1:A:128:TYR:CZ	1:A:137:GLN:HG3	2.38	0.59
1:A:128:TYR:CE1	1:A:137:GLN:HG3	2.40	0.56
1:A:249:GLN:HB3	1:A:250:PRO:CD	2.36	0.56
1:A:160:VAL:O	1:A:163:VAL:HG12	2.06	0.56
1:A:253:ASN:C	1:A:253:ASN:ND2	2.59	0.55
1:A:45:LYS:O	1:A:82:GLY:HA2	2.08	0.54
1:A:202:PRO:HG2	1:A:204:LEU:HG	1.90	0.54
1:A:159:LYS:HE2	1:A:179:PHE:HD1	1.72	0.53
1:A:103:GLN:NE2	1:A:243:ASP:OD1	2.44	0.51
1:A:201:PRO:HA	1:A:203:LEU:HG	1.93	0.51
1:A:213:LYS:HD3	1:A:260:PHE:CE2	2.46	0.50
1:A:27:ARG:HG3	1:A:205:GLU:HB3	1.94	0.50
1:A:47:LEU:HD11	1:A:210:ILE:HG21	1.94	0.49
1:A:249:GLN:HB3	1:A:250:PRO:HD2	1.94	0.49
1:A:75:ASP:OD1	1:A:89:ARG:NE	2.41	0.47
1:A:180:ASP:HA	1:A:181:PRO:HD2	1.76	0.47
1:A:27:ARG:CG	1:A:205:GLU:HB3	2.45	0.46
1:A:199:VAL:HG22	3:A:357:AZI:N3	2.31	0.46
1:A:168:LYS:NZ	4:A:353:HOH:O	2.29	0.46
1:A:243:ASP:HA	1:A:245:TRP:CD1	2.50	0.45
1:A:199:VAL:HG22	3:A:357:AZI:N2	2.31	0.45
1:A:72:ASP:OD2	1:A:123:TRP:NE1	2.42	0.45
1:A:159:LYS:HD2	4:A:308:HOH:O	2.17	0.45
1:A:58:ARG:HD2	1:A:69:GLU:CD	2.31	0.44
1:A:230:ASN:HB3	1:A:232:ASN:OD1	2.18	0.44
1:A:59:ILE:HA	1:A:67:ASN:O	2.18	0.44
1:A:58:ARG:CD	1:A:69:GLU:OE1	2.39	0.43
1:A:88:TYR:CE2	1:A:124:ASN:HB2	2.53	0.43
1:A:223:VAL:O	1:A:226:PHE:HB2	2.19	0.43
1:A:89:ARG:O	1:A:122:HIS:HA	2.20	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:60:LEU:HD21	1:A:67:ASN:HB2	2.02	0.42
1:A:51:TYR:CD1	1:A:77:ALA:HB1	2.55	0.42
1:A:167:ILE:O	1:A:167:ILE:HG13	2.19	0.41
1:A:144:LEU:HD23	1:A:144:LEU:HA	1.87	0.41
1:A:178:ASN:HB2	4:A:325:HOH:O	2.22	0.40
1:A:146:ILE:HG12	1:A:212:LEU:HD12	2.04	0.40
1:A:5:TRP:CH2	1:A:200:THR:HB	2.55	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:162:ASP:OD2	4:A:352:HOH:O[2_445]	2.00	0.20

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	253/259 (98%)	237 (94%)	15 (6%)	1 (0%)	30 31

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	253	ASN

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	220/224 (98%)	209 (95%)	11 (5%)	22	24

All (11) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	24	LYS
1	A	30	PRO
1	A	44	LEU
1	A	58	ARG
1	A	79	LEU
1	A	83	PRO
1	A	100	LEU
1	A	220	SER
1	A	221	GLU
1	A	229	LEU
1	A	253	ASN

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

Mol	Chain	Res	Type
1	A	10	HIS
1	A	67	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 [i](#)

Of 2 ligands modelled in this entry, 1 is monoatomic - leaving 1 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. 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 $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
3	AZI	A	357	2	2,2,2	3.47	2 (100%)	0,1,1	-	-

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	357	AZI	N1-N2	-3.65	1.15	1.23
3	A	357	AZI	N3-N2	3.29	1.29	1.23

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

1 monomer is involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	357	AZI	2	0

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.