



Full wwPDB X-ray Structure Validation Report ⓘ

Jan 31, 2016 – 06:27 PM GMT

PDB ID : 1AVN
Title : HUMAN CARBONIC ANHYDRASE II COMPLEXED WITH THE HISTAMINE ACTIVATOR
Authors : Briganti, F.; Mangani, S.; Orioli, P.; Scozzafava, A.; Vernaglione, G.; Supuran, C.T.
Deposited on : 1997-09-17
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
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) : **NOT EXECUTED**
EDS : **NOT EXECUTED**
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : trunk26865

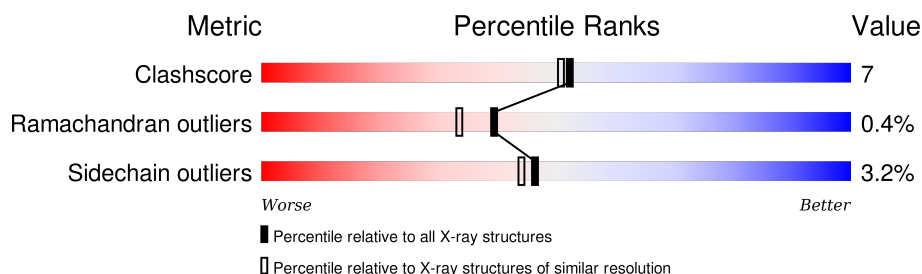
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.00 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	102246	7340 (2.00-2.00)
Ramachandran outliers	100387	7248 (2.00-2.00)
Sidechain outliers	100360	7247 (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 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.

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
5	HSM	A	264	-	-	X	-

2 Entry composition [i](#)

There are 6 unique types of molecules in this entry. The entry contains 2206 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	257	Total	C	N	O	S	0	0	0
			2038	1308	350	378	2			

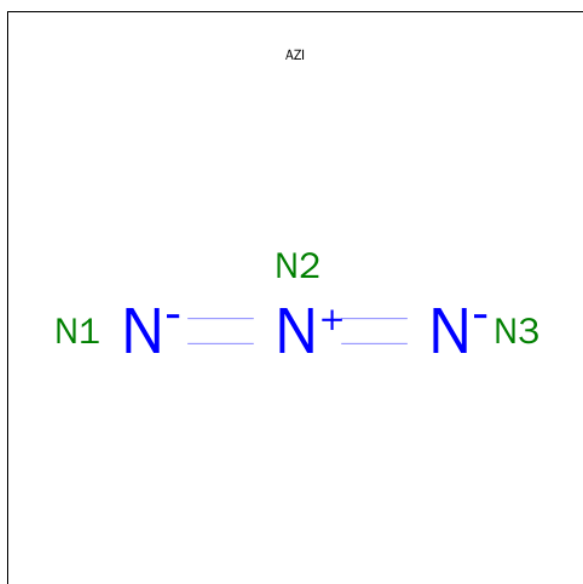
- Molecule 2 is ZINC ION (three-letter code: ZN) (formula: Zn).

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

- Molecule 3 is MERCURY (II) ION (three-letter code: HG) (formula: Hg).

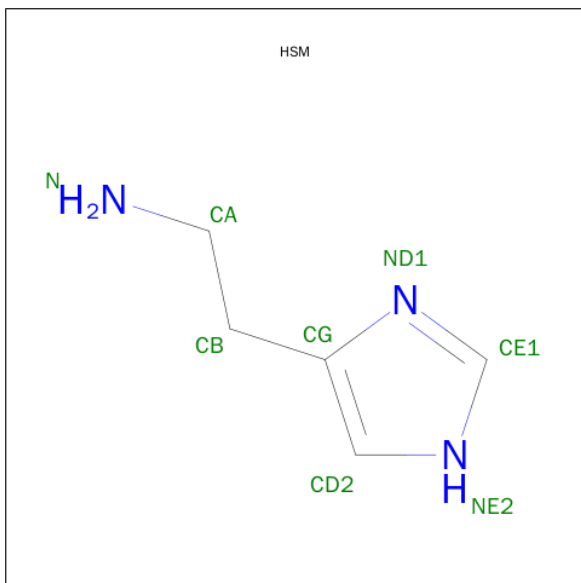
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	1	Total	Hg	0	0
			1	1		

- Molecule 4 is AZIDE ION (three-letter code: AZI) (formula: N₃).



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

- Molecule 5 is HISTAMINE (three-letter code: HSM) (formula: $C_5H_9N_3$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	1	Total C N 8 5 3	0	0

- Molecule 6 is water.

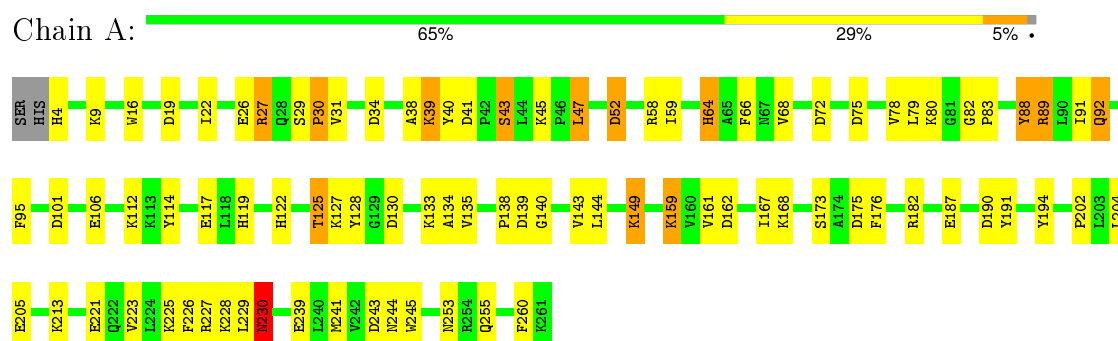
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	A	155	Total O 155 155	1	0

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.

Note EDS was not executed.

• Molecule 1: CARBONIC ANHYDRASE II



4 Data and refinement statistics

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

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	42.61 Å 41.69 Å 72.78 Å 90.00° 104.24° 90.00°	Depositor
Resolution (Å)	15.00 – 2.00	Depositor
% Data completeness (in resolution range)	80.6 (15.00-2.00)	Depositor
R_{merge}	0.08	Depositor
R_{sym}	0.09	Depositor
Refinement program	CCP4	Depositor
R, R_{free}	0.154 , (Not available)	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	2206	wwPDB-VP
Average B, all atoms (Å ²)	15.0	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: AZI, ZN, HG, HSM

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	0.98	4/2098 (0.2%)	2.34	94/2845 (3.3%)

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	125	THR	C-N	13.71	1.65	1.34
1	A	30	PRO	N-CD	9.88	1.61	1.47
1	A	4	HIS	N-CA	5.69	1.57	1.46
1	A	30	PRO	N-CA	-5.62	1.37	1.47

All (94) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	29	SER	O-C-N	20.71	160.45	121.10
1	A	30	PRO	N-CA-CB	20.32	127.68	103.30
1	A	30	PRO	CA-N-CD	-18.37	85.78	111.50
1	A	175	ASP	CB-CG-OD1	14.52	131.37	118.30
1	A	29	SER	C-N-CD	-14.30	89.14	120.60
1	A	191	TYR	CB-CG-CD2	13.64	129.19	121.00
1	A	182	ARG	NE-CZ-NH1	13.41	127.01	120.30
1	A	130	ASP	CB-CG-OD2	13.33	130.30	118.30
1	A	58	ARG	CD-NE-CZ	13.26	142.16	123.60
1	A	227	ARG	NE-CZ-NH2	13.19	126.89	120.30
1	A	27	ARG	NE-CZ-NH1	13.13	126.87	120.30
1	A	29	SER	C-N-CA	12.60	174.92	122.00
1	A	27	ARG	NE-CZ-NH2	-10.71	114.94	120.30
1	A	30	PRO	N-CD-CG	10.59	119.08	103.20
1	A	130	ASP	OD1-CG-OD2	-9.97	104.35	123.30
1	A	39	LYS	CA-CB-CG	9.48	134.26	113.40
1	A	175	ASP	CB-CG-OD2	-9.37	109.87	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	139	ASP	CB-CG-OD1	9.36	126.73	118.30
1	A	255	GLN	CA-CB-CG	9.25	133.74	113.40
1	A	26	GLU	OE1-CD-OE2	-8.71	112.85	123.30
1	A	226	PHE	CB-CG-CD1	8.66	126.86	120.80
1	A	34	ASP	CB-CG-OD1	8.65	126.09	118.30
1	A	29	SER	CA-C-N	-8.43	93.50	117.10
1	A	130	ASP	CB-CG-OD1	7.83	125.34	118.30
1	A	228	LYS	CB-CG-CD	7.70	131.63	111.60
1	A	19	ASP	CB-CG-OD2	-7.59	111.47	118.30
1	A	52	ASP	CB-CG-OD1	7.16	124.74	118.30
1	A	29	SER	CA-C-O	-7.12	105.14	120.10
1	A	162	ASP	CB-CG-OD2	-7.12	111.89	118.30
1	A	190	ASP	CB-CG-OD1	7.10	124.69	118.30
1	A	128	TYR	CB-CG-CD2	7.01	125.20	121.00
1	A	127	LYS	CA-CB-CG	6.78	128.32	113.40
1	A	43	SER	CA-CB-OG	6.76	129.47	111.20
1	A	75	ASP	C-N-CA	6.63	138.28	121.70
1	A	26	GLU	CB-CG-CD	6.61	132.04	114.20
1	A	58	ARG	NE-CZ-NH2	-6.45	117.07	120.30
1	A	187	GLU	O-C-N	-6.45	112.39	122.70
1	A	221	GLU	OE1-CD-OE2	-6.42	115.60	123.30
1	A	40	TYR	CB-CG-CD2	6.38	124.83	121.00
1	A	88	TYR	CB-CG-CD2	-6.35	117.19	121.00
1	A	83	PRO	N-CA-CB	-6.33	95.64	102.60
1	A	173	SER	N-CA-CB	6.30	119.95	110.50
1	A	101	ASP	CB-CG-OD1	6.24	123.92	118.30
1	A	16	TRP	O-C-N	6.21	132.63	122.70
1	A	41	ASP	CB-CG-OD1	6.16	123.85	118.30
1	A	112	LYS	CB-CG-CD	6.13	127.54	111.60
1	A	114	TYR	CB-CG-CD2	6.11	124.66	121.00
1	A	194	TYR	CB-CG-CD1	6.10	124.66	121.00
1	A	66	PHE	N-CA-CB	6.02	121.44	110.60
1	A	83	PRO	O-C-N	-6.02	113.07	122.70
1	A	91	ILE	O-C-N	-5.97	113.15	122.70
1	A	114	TYR	CB-CG-CD1	-5.97	117.42	121.00
1	A	187	GLU	N-CA-CB	-5.94	99.91	110.60
1	A	31	VAL	CA-CB-CG2	5.91	119.76	110.90
1	A	226	PHE	CB-CG-CD2	-5.87	116.69	120.80
1	A	191	TYR	CG-CD1-CE1	5.75	125.90	121.30
1	A	138	PRO	O-C-N	-5.72	113.54	122.70
1	A	117	GLU	OE1-CD-OE2	5.68	130.12	123.30
1	A	135	VAL	O-C-N	-5.63	113.69	122.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	41	ASP	CB-CG-OD2	5.60	123.34	118.30
1	A	241	MET	CG-SD-CE	5.59	109.14	100.20
1	A	41	ASP	OD1-CG-OD2	-5.58	112.69	123.30
1	A	91	ILE	CA-CB-CG1	-5.56	100.43	111.00
1	A	176	PHE	O-C-N	5.54	131.56	122.70
1	A	30	PRO	N-CA-C	-5.53	97.72	112.10
1	A	89	ARG	CB-CA-C	-5.50	99.39	110.40
1	A	162	ASP	CB-CG-OD1	5.49	123.24	118.30
1	A	135	VAL	C-N-CA	5.40	135.20	121.70
1	A	38	ALA	N-CA-CB	5.38	117.64	110.10
1	A	92	GLN	CA-C-O	-5.36	108.84	120.10
1	A	95	PHE	CB-CG-CD2	5.33	124.53	120.80
1	A	130	ASP	N-CA-CB	5.31	120.16	110.60
1	A	119	HIS	CA-CB-CG	5.30	122.61	113.60
1	A	31	VAL	CG1-CB-CG2	-5.30	102.42	110.90
1	A	64	HIS	N-CA-CB	5.28	120.10	110.60
1	A	58	ARG	N-CA-CB	-5.27	101.11	110.60
1	A	75	ASP	CA-CB-CG	5.27	125.00	113.40
1	A	75	ASP	O-C-N	-5.25	114.30	122.70
1	A	19	ASP	OD1-CG-OD2	5.24	133.25	123.30
1	A	149	LYS	CA-CB-CG	5.21	124.87	113.40
1	A	143	VAL	CG1-CB-CG2	-5.17	102.64	110.90
1	A	191	TYR	CD1-CG-CD2	-5.15	112.24	117.90
1	A	191	TYR	O-C-N	5.13	130.91	122.70
1	A	144	LEU	CA-C-N	5.12	126.44	116.20
1	A	244	ASN	O-C-N	-5.12	114.51	122.70
1	A	78	VAL	CA-CB-CG1	5.10	118.55	110.90
1	A	230	ASN	N-CA-CB	-5.10	101.42	110.60
1	A	106	GLU	OE1-CD-OE2	5.09	129.41	123.30
1	A	47	LEU	CB-CA-C	-5.07	100.58	110.20
1	A	221	GLU	CG-CD-OE1	5.06	128.42	118.30
1	A	223	VAL	CA-CB-CG1	-5.05	103.32	110.90
1	A	72	ASP	O-C-N	-5.03	114.64	122.70
1	A	68	VAL	O-C-N	-5.03	114.65	122.70
1	A	149	LYS	CB-CG-CD	5.02	124.65	111.60

There are no chirality outliers.

There are no planarity outliers.

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	2038	0	1991	26	0
2	A	1	0	0	0	0
3	A	1	0	0	0	0
4	A	3	0	0	0	0
5	A	8	0	9	4	0
6	A	155	0	0	6	0
All	All	2206	0	2000	27	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 7.

All (27) 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)
5:A:264:HSM:HE1	6:A:396:HOH:O	1.57	1.05
1:A:64:HIS:HD2	6:A:391:HOH:O	1.43	1.02
1:A:239:GLU:OE2	6:A:312:HOH:O	2.14	0.65
1:A:92:GLN:NE2	5:A:264:HSM:HE2	1.93	0.65
1:A:89:ARG:HG3	1:A:125:THR:HG22	1.78	0.65
1:A:59:ILE:HG12	1:A:167:ILE:HD13	1.82	0.61
1:A:134:ALA:O	1:A:140:GLY:HA3	2.07	0.54
1:A:22:ILE:HD11	1:A:205:GLU:HG3	1.92	0.52
1:A:243:ASP:HA	1:A:245:TRP:CD1	2.46	0.51
1:A:92:GLN:HE22	5:A:264:HSM:HE2	1.59	0.51
1:A:168:LYS:O	1:A:230:ASN:HB2	2.12	0.49
1:A:149:LYS:HE3	6:A:348:HOH:O	2.14	0.47
1:A:9:LYS:HD2	1:A:9:LYS:O	2.14	0.46
1:A:88:TYR:HB3	1:A:122:HIS:HB3	1.97	0.46
1:A:213:LYS:HD3	1:A:260:PHE:CZ	2.51	0.46
1:A:168:LYS:HA	1:A:229:LEU:HD23	1.98	0.46
1:A:27:ARG:HG3	1:A:205:GLU:HB3	1.98	0.45
1:A:133:LYS:HD2	6:A:324:HOH:O	2.16	0.45
1:A:22:ILE:CD1	1:A:205:GLU:HG3	2.46	0.44
1:A:27:ARG:CG	1:A:205:GLU:HB3	2.48	0.44
1:A:202:PRO:HG2	1:A:204:LEU:HG	1.99	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:89:ARG:HG3	1:A:125:THR:CG2	2.48	0.43
1:A:47:LEU:HD22	1:A:79:LEU:HD11	1.99	0.43
1:A:45:LYS:O	1:A:82:GLY:HA2	2.18	0.43
1:A:159:LYS:HB2	6:A:304:HOH:O	2.18	0.42
1:A:92:GLN:NE2	5:A:264:HSM:NE2	2.65	0.41
1:A:161:VAL:HG13	1:A:225:LYS:HB2	2.03	0.40

There are no symmetry-related clashes.

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	255/259 (98%)	242 (95%)	12 (5%)	1 (0%)	39 33

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	30	PRO

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%)	213 (97%)	7 (3%)	46 44

All (7) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	39	LYS
1	A	43	SER
1	A	52	ASP
1	A	80	LYS
1	A	159	LYS
1	A	230	ASN
1	A	253	ASN

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (1) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	64	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 carbohydrates in this entry.

5.6 Ligand geometry [i](#)

Of 4 ligands modelled in this entry, 2 are monoatomic - leaving 2 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
5	HSM	A	264	-	3,8,8	0.66	0	4,9,9	2.25	3 (75%)
4	AZI	A	265	2	0,2,2	0.00	-	0,1,1	0.00	-

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the chemical component dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	HSM	A	264	-	-	0/2/3/3	0/1/1/1
4	AZI	A	265	2	-	0/0/0/0	0/0/0/0

There are no bond length outliers.

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	A	264	HSM	CB-CG-CD2	2.16	132.88	129.55
5	A	264	HSM	CD2-NE2-CE1	2.65	109.89	105.71
5	A	264	HSM	CA-CB-CG	2.84	125.39	112.61

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

1 monomer is involved in 4 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	A	264	HSM	4	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 will therefore be empty.

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

EDS was not executed - this section will therefore be empty.

6.3 Carbohydrates ⓘ

EDS was not executed - this section will therefore be empty.

6.4 Ligands ⓘ

EDS was not executed - this section will therefore be empty.

6.5 Other polymers ⓘ

EDS was not executed - this section will therefore be empty.