



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 09:39 PM UTC

PDB ID : 3CA2 / pdb_00003ca2
Title : CRYSTALLOGRAPHIC STUDIES OF INHIBITOR BINDING SITES IN HUMAN CARBONIC ANHYDRASE II. A PENTACOORDINATED BINDING OF THE SCN-ION TO THE ZINC AT HIGH P*H
Authors : Eriksson, A.E.; Jones, T.A.; Liljas, A.
Deposited on : 1989-10-02
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

<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)
Xtrriage (Phenix) : **NOT EXECUTED**
EDS : **NOT EXECUTED**
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
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

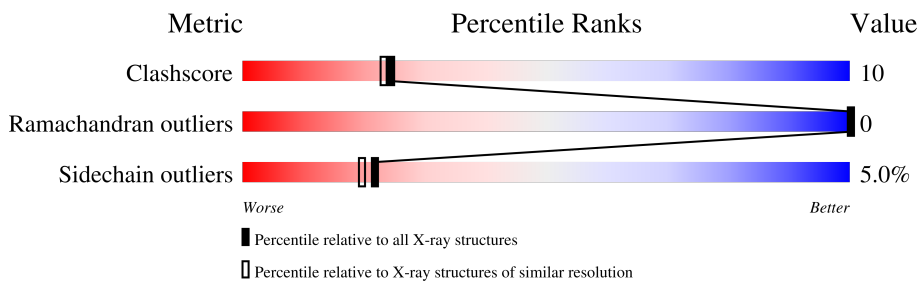
1 Overall quality at a glance

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 ≥ 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
4	AMS	A	265	-	X	-	-

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 2214 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
			Total	C	N	O	S			
1	A	256	2039	1309	350	378	2	0	0	0

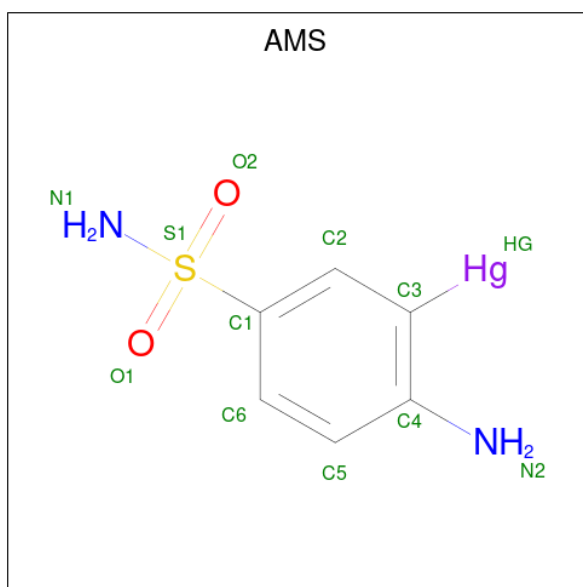
- Molecule 2 is MERCURY (II) ION (CCD ID: HG) (formula: Hg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	2	Total	Hg	0	0
			2	2		

- Molecule 3 is ZINC ION (CCD ID: ZN) (formula: Zn).

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

- Molecule 4 is 3-MERCURI-4-AMINOBENZENESULFONAMIDE (CCD ID: AMS) (formula: C₆H₇HgN₂O₂S).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	
			Total	C	Hg	N	O			S
4	A	1	12	6	1	2	2	1	0	0

- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	160	Total	O	0	0
			160	160		

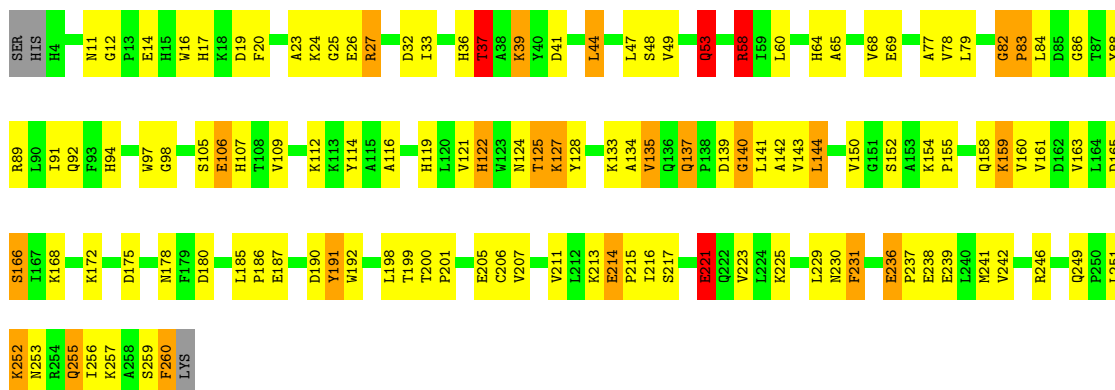
3 Residue-property plots [i](#)

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 II

Chain A:  51% 38% 8% ..



4 Data and refinement statistics

Xtrriage (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)	(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	PROLSQ	Depositor
R, R_{free}	0.192 , (Not available)	Depositor
Estimated twinning fraction	No twinning to report.	Xtrriage
Total number of atoms	2214	wwPDB-VP
Average B, all atoms (Å ²)	9.0	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: HG, AMS, 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	2.02	25/2100 (1.2%)	2.29	112/2851 (3.9%)

All (25) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	125	THR	C-N	32.04	1.83	1.33
1	A	94	HIS	CG-ND1	-9.43	1.27	1.38
1	A	246	ARG	CD-NE	8.30	1.57	1.46
1	A	98	GLY	N-CA	7.87	1.51	1.44
1	A	97	TRP	NE1-CE2	6.98	1.45	1.37
1	A	259	SER	N-CA	6.70	1.54	1.46
1	A	58	ARG	CD-NE	-6.58	1.37	1.46
1	A	64	HIS	ND1-CE1	-6.38	1.26	1.32
1	A	122	HIS	CE1-NE2	6.16	1.38	1.32
1	A	65	ALA	CA-CB	6.00	1.62	1.53
1	A	187	GLU	C-O	5.91	1.30	1.24
1	A	109	VAL	C-O	-5.85	1.17	1.24
1	A	125	THR	C-O	5.82	1.31	1.24
1	A	201	PRO	C-O	5.64	1.30	1.24
1	A	199	THR	C-O	5.58	1.31	1.23
1	A	150	VAL	N-CA	5.56	1.53	1.46
1	A	230	ASN	C-O	-5.33	1.17	1.24
1	A	121	VAL	CA-CB	5.30	1.60	1.54
1	A	49	VAL	C-O	5.26	1.29	1.24
1	A	144	LEU	CB-CG	-5.24	1.43	1.53
1	A	178	ASN	CA-CB	5.12	1.61	1.53
1	A	105	SER	N-CA	5.08	1.52	1.45
1	A	17	HIS	CE1-NE2	-5.08	1.27	1.32
1	A	107	HIS	CE1-NE2	-5.05	1.27	1.32
1	A	114	TYR	C-O	5.02	1.30	1.23

All (112) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	11	ASN	CA-C-N	10.15	137.81	121.87
1	A	11	ASN	C-N-CA	10.15	137.81	121.87
1	A	155	PRO	O-C-N	9.77	132.74	122.18
1	A	125	THR	CA-C-N	-9.51	99.26	121.52
1	A	125	THR	C-N-CA	-9.51	99.26	121.52
1	A	175	ASP	CA-CB-CG	9.47	122.07	112.60
1	A	231	PHE	CA-CB-CG	9.27	123.07	113.80
1	A	14	GLU	CB-CG-CD	8.79	127.54	112.60
1	A	185	LEU	CA-C-O	8.64	129.05	120.23
1	A	116	ALA	O-C-N	8.63	132.32	123.26
1	A	253	ASN	CA-CB-CG	8.60	121.20	112.60
1	A	180	ASP	CB-CA-C	8.38	118.47	110.17
1	A	36	HIS	CA-CB-CG	-8.24	105.56	113.80
1	A	58	ARG	CD-NE-CZ	8.11	135.75	124.40
1	A	252	LYS	CB-CA-C	-8.05	107.30	116.63
1	A	137	GLN	O-C-N	7.58	128.92	121.57
1	A	53	GLN	CB-CG-CD	-7.35	100.10	112.60
1	A	68	VAL	N-CA-C	-7.30	97.33	107.99
1	A	165	ASP	CA-C-N	7.29	132.90	120.72
1	A	165	ASP	C-N-CA	7.29	132.90	120.72
1	A	47	LEU	O-C-N	7.26	131.43	122.86
1	A	207	VAL	N-CA-C	7.25	118.92	108.48
1	A	200	THR	O-C-N	7.14	127.94	121.80
1	A	221	GLU	CB-CG-CD	7.04	124.57	112.60
1	A	47	LEU	CA-C-O	-6.87	114.07	121.56
1	A	172	LYS	CA-CB-CG	6.80	127.70	114.10
1	A	89	ARG	CD-NE-CZ	-6.80	114.89	124.40
1	A	187	GLU	CB-CG-CD	6.78	124.12	112.60
1	A	143	VAL	O-C-N	6.69	130.49	123.26
1	A	165	ASP	CA-CB-CG	6.66	119.26	112.60
1	A	236	GLU	O-C-N	6.62	125.91	121.14
1	A	142	ALA	CA-C-O	-6.50	113.35	120.24
1	A	64	HIS	N-CA-CB	6.46	119.50	110.98
1	A	64	HIS	CA-C-N	6.44	133.91	122.45
1	A	64	HIS	C-N-CA	6.44	133.91	122.45
1	A	97	TRP	CA-C-N	-6.40	115.03	122.77
1	A	97	TRP	C-N-CA	-6.40	115.03	122.77
1	A	84	LEU	O-C-N	6.37	130.12	122.85
1	A	89	ARG	CB-CA-C	-6.34	99.29	109.75
1	A	127	LYS	CA-C-O	-6.31	108.81	118.91
1	A	221	GLU	CA-CB-CG	6.29	126.68	114.10
1	A	86	GLY	O-C-N	6.22	129.08	122.86

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	175	ASP	N-CA-C	-6.21	101.23	110.23
1	A	152	SER	CA-CB-OG	-6.20	98.71	111.10
1	A	216	ILE	N-CA-C	-6.14	99.56	108.89
1	A	82	GLY	O-C-N	6.13	127.91	121.77
1	A	19	ASP	CA-C-O	-6.11	112.42	119.14
1	A	27	ARG	CA-CB-CG	6.11	126.31	114.10
1	A	158	GLN	OE1-CD-NE2	-6.11	116.50	122.60
1	A	186	PRO	N-CA-C	-6.11	102.67	111.22
1	A	16	TRP	O-C-N	6.10	129.35	122.22
1	A	114	TYR	O-C-N	-6.03	116.22	123.03
1	A	155	PRO	CA-C-O	-6.01	110.55	120.05
1	A	192	TRP	N-CA-C	-5.97	100.17	109.72
1	A	242	VAL	O-C-N	5.91	129.74	123.00
1	A	19	ASP	O-C-N	5.91	130.41	122.49
1	A	256	ILE	N-CA-CB	5.83	118.03	111.21
1	A	37	THR	CA-CB-OG1	-5.82	100.87	109.60
1	A	77	ALA	CB-CA-C	5.82	119.40	110.62
1	A	12	GLY	O-C-N	5.80	127.58	121.77
1	A	23	ALA	O-C-N	5.74	128.74	122.20
1	A	200	THR	CA-C-O	-5.72	114.00	120.46
1	A	175	ASP	CB-CG-OD1	5.69	131.49	118.40
1	A	112	LYS	O-C-N	5.69	129.69	123.04
1	A	166	SER	N-CA-C	5.68	119.47	112.54
1	A	26	GLU	CG-CD-OE1	5.65	131.40	118.40
1	A	26	GLU	CG-CD-OE2	-5.62	105.47	118.40
1	A	238	GLU	CG-CD-OE1	5.61	131.29	118.40
1	A	133	LYS	CA-CB-CG	5.57	125.24	114.10
1	A	191	TYR	O-C-N	5.54	129.47	123.10
1	A	68	VAL	CA-C-O	-5.53	114.56	120.59
1	A	58	ARG	CG-CD-NE	5.50	124.11	112.00
1	A	217	SER	CB-CA-C	5.50	118.79	109.50
1	A	58	ARG	NE-CZ-NH2	-5.49	114.26	119.20
1	A	141	LEU	O-C-N	5.47	130.44	123.11
1	A	158	GLN	CA-C-O	-5.47	114.75	120.55
1	A	246	ARG	CD-NE-CZ	-5.44	116.78	124.40
1	A	25	GLY	CA-C-N	5.43	132.16	122.06
1	A	25	GLY	C-N-CA	5.43	132.16	122.06
1	A	158	GLN	CA-C-N	5.42	127.55	120.28
1	A	158	GLN	C-N-CA	5.42	127.55	120.28
1	A	124	ASN	O-C-N	5.42	129.79	122.96
1	A	260	PHE	CA-C-O	-5.42	111.59	120.80
1	A	160	VAL	N-CA-C	-5.41	105.45	110.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	106	GLU	CG-CD-OE2	-5.40	105.97	118.40
1	A	211	VAL	O-C-N	5.38	129.40	123.10
1	A	77	ALA	O-C-N	5.38	130.22	123.12
1	A	140	GLY	CA-C-O	-5.36	114.98	120.66
1	A	20	PHE	CA-C-N	5.32	124.99	119.56
1	A	20	PHE	C-N-CA	5.32	124.99	119.56
1	A	107	HIS	N-CA-C	-5.32	102.61	110.48
1	A	39	LYS	N-CA-CB	-5.30	101.78	110.42
1	A	33	ILE	O-C-N	5.27	130.51	122.76
1	A	251	LEU	CB-CA-C	5.27	119.80	110.85
1	A	135	VAL	O-C-N	-5.25	115.17	122.31
1	A	48	SER	CA-C-O	-5.21	114.00	120.57
1	A	94	HIS	CB-CG-CD2	-5.21	124.43	131.20
1	A	78	VAL	O-C-N	5.20	128.82	123.04
1	A	214	GLU	N-CA-C	5.18	116.44	109.24
1	A	198	LEU	N-CA-C	-5.16	103.22	110.50
1	A	44	LEU	CB-CA-C	5.16	118.25	109.84
1	A	127	LYS	CA-CB-CG	-5.15	103.79	114.10
1	A	159	LYS	CA-C-O	5.14	126.00	120.55
1	A	190	ASP	N-CA-C	-5.12	102.70	110.28
1	A	249	GLN	O-C-N	5.11	125.80	121.20
1	A	77	ALA	CA-C-O	-5.10	114.82	120.33
1	A	154	LYS	CA-C-N	5.09	124.54	119.24
1	A	154	LYS	C-N-CA	5.09	124.54	119.24
1	A	238	GLU	CA-C-O	5.07	126.64	120.81
1	A	32	ASP	N-CA-C	-5.05	101.08	109.46
1	A	223	VAL	CG1-CB-CG2	-5.04	99.71	110.80
1	A	178	ASN	CA-CB-CG	-5.04	107.56	112.60

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	2039	0	1987	38	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	A	2	0	0	0	0
3	A	1	0	0	0	0
4	A	12	0	8	2	0
5	A	160	0	0	6	0
All	All	2214	0	1995	40	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 10.

All (40) 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:125:THR:C	1:A:127:LYS:N	1.83	1.36
1:A:58:ARG:HD2	1:A:69:GLU:OE1	1.42	1.18
4:A:265:AMS:HG	4:A:265:AMS:C3	1.78	0.91
1:A:125:THR:C	1:A:127:LYS:CA	2.50	0.85
4:A:265:AMS:HG	4:A:265:AMS:HG	0.84	0.83
1:A:252:LYS:NZ	5:A:362:HOH:O	2.22	0.73
1:A:135:VAL:O	1:A:206:CYS:SG	2.49	0.71
1:A:58:ARG:CD	1:A:69:GLU:OE1	2.31	0.70
1:A:161:VAL:CG1	1:A:225:LYS:HD2	2.23	0.68
1:A:213:LYS:HD3	1:A:260:PHE:CZ	2.30	0.67
1:A:159:LYS:HE3	5:A:423:HOH:O	1.95	0.65
1:A:168:LYS:NZ	5:A:403:HOH:O	2.23	0.63
1:A:159:LYS:CE	5:A:423:HOH:O	2.47	0.63
1:A:58:ARG:HD2	1:A:69:GLU:CD	2.23	0.61
1:A:255:GLN:OE1	1:A:257:LYS:HE2	2.05	0.57
1:A:44:LEU:HD11	1:A:83:PRO:HB3	1.88	0.56
1:A:236:GLU:HB3	1:A:237:PRO:CD	2.36	0.55
1:A:161:VAL:HG13	1:A:225:LYS:HD2	1.87	0.54
1:A:137:GLN:O	1:A:206:CYS:HB3	2.09	0.51
1:A:231:PHE:HD1	1:A:239:GLU:HG2	1.76	0.50
1:A:231:PHE:CE2	1:A:241:MET:HG3	2.47	0.49
1:A:27:ARG:HG3	1:A:205:GLU:HB3	1.95	0.49
1:A:128:TYR:CE2	1:A:137:GLN:HG3	2.48	0.48
1:A:24:LYS:NZ	5:A:425:HOH:O	2.49	0.46
1:A:134:ALA:O	1:A:140:GLY:HA3	2.17	0.45
1:A:163:VAL:O	1:A:166:SER:HB2	2.17	0.45
1:A:37:THR:HG22	5:A:375:HOH:O	2.17	0.45
1:A:139:ASP:OD2	1:A:139:ASP:N	2.49	0.44
1:A:53:GLN:HE21	1:A:53:GLN:HB2	1.42	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:88:TYR:HB3	1:A:122:HIS:HB3	2.00	0.44
1:A:236:GLU:HB3	1:A:237:PRO:HD2	2.00	0.42
1:A:41:ASP:C	1:A:41:ASP:OD2	2.61	0.42
1:A:125:THR:C	1:A:127:LYS:HA	2.40	0.42
1:A:82:GLY:HA2	1:A:191:TYR:OH	2.20	0.41
1:A:44:LEU:HG	1:A:191:TYR:OH	2.20	0.41
1:A:214:GLU:HA	1:A:215:PRO:HD3	1.81	0.41
1:A:255:GLN:CD	1:A:257:LYS:HE2	2.45	0.41
1:A:106:GLU:OE1	1:A:119:HIS:HE1	2.03	0.41
1:A:221:GLU:O	1:A:225:LYS:HG3	2.21	0.41
1:A:91:ILE:HG23	1:A:92:GLN:HG3	2.04	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	254/259 (98%)	244 (96%)	10 (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	221/224 (99%)	210 (95%)	11 (5%)	22 20

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

Mol	Chain	Res	Type
1	A	37	THR
1	A	39	LYS
1	A	53	GLN
1	A	58	ARG
1	A	60	LEU
1	A	79	LEU
1	A	83	PRO
1	A	144	LEU
1	A	221	GLU
1	A	229	LEU
1	A	255	GLN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (4) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	53	GLN
1	A	67	ASN
1	A	137	GLN
1	A	178	ASN

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

Of 4 ligands modelled in this entry, 3 are 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
4	AMS	A	265	1,3,5	9,12,12	2.68	5 (55%)	14,18,18	6.16	6 (42%)

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
4	AMS	A	265	1,3,5	-	4/6/6/6	0/1/1/1

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	265	AMS	C2-C1	4.73	1.47	1.39
4	A	265	AMS	C6-C5	4.09	1.45	1.38
4	A	265	AMS	C6-C1	3.38	1.44	1.38
4	A	265	AMS	C5-C4	2.60	1.46	1.40
4	A	265	AMS	C1-S1	2.35	1.80	1.77

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	265	AMS	O2-S1-O1	-12.85	99.04	118.80
4	A	265	AMS	O1-S1-C1	9.99	118.64	107.35
4	A	265	AMS	O2-S1-C1	9.67	118.27	107.35
4	A	265	AMS	C1-S1-N1	8.83	120.70	108.40
4	A	265	AMS	O1-S1-N1	-6.89	97.42	107.35
4	A	265	AMS	O2-S1-N1	-6.35	98.19	107.35

There are no chirality outliers.

All (4) torsion outliers are listed below:

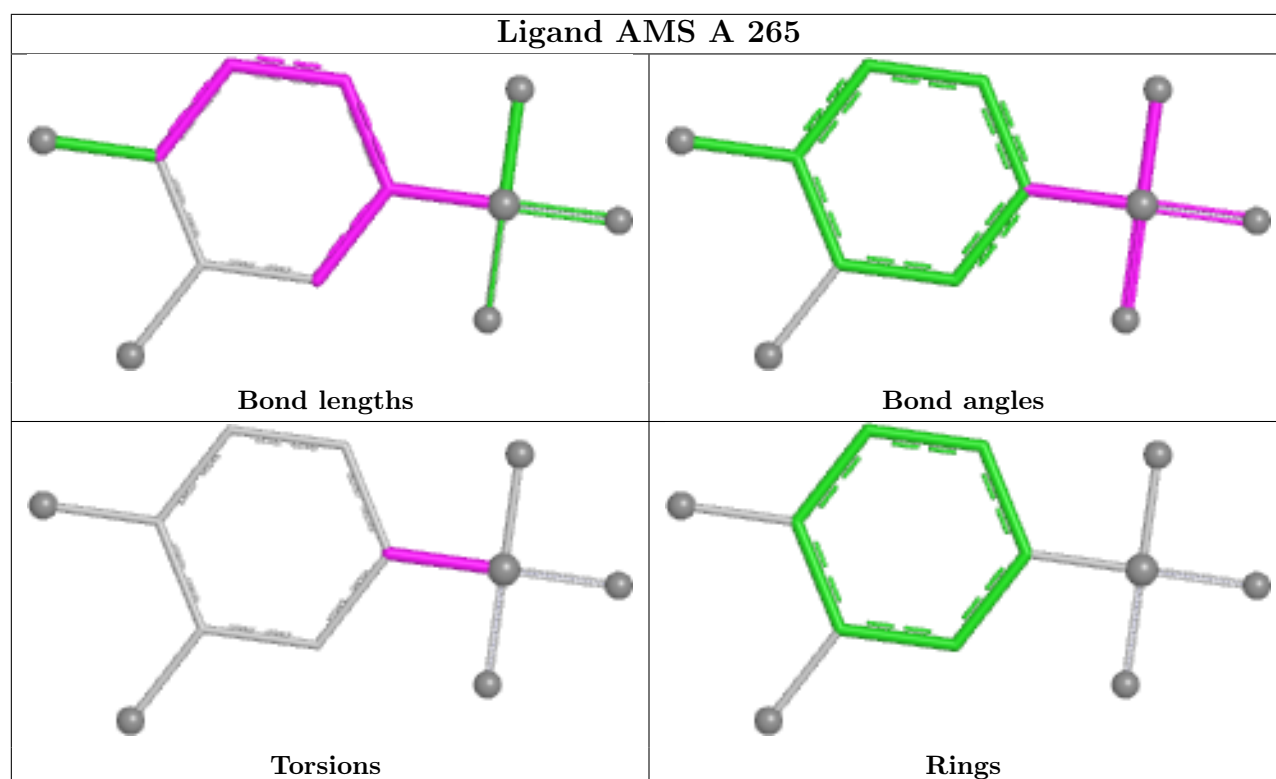
Mol	Chain	Res	Type	Atoms
4	A	265	AMS	C2-C1-S1-N1
4	A	265	AMS	C6-C1-S1-N1
4	A	265	AMS	C2-C1-S1-O2
4	A	265	AMS	C6-C1-S1-O2

There are no ring outliers.

1 monomer is involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	265	AMS	2	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.



5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
1	A	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	A	125:THR	C	127:LYS	N	1.83

6 Fit of model and data [i](#)

6.1 Protein, DNA and RNA chains [i](#)

EDS was not executed - this section is therefore empty.

6.2 Non-standard residues in protein, DNA, RNA chains [i](#)

EDS was not executed - this section is therefore empty.

6.3 Carbohydrates [i](#)

EDS was not executed - this section is therefore empty.

6.4 Ligands [i](#)

EDS was not executed - this section is therefore empty.

6.5 Other polymers [i](#)

EDS was not executed - this section is therefore empty.