



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 7, 2026 – 03:05 AM UTC

PDB ID : 2CA2 / pdb_00002ca2
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
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Deposited on : 1989-02-06
Resolution : 1.90 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**
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

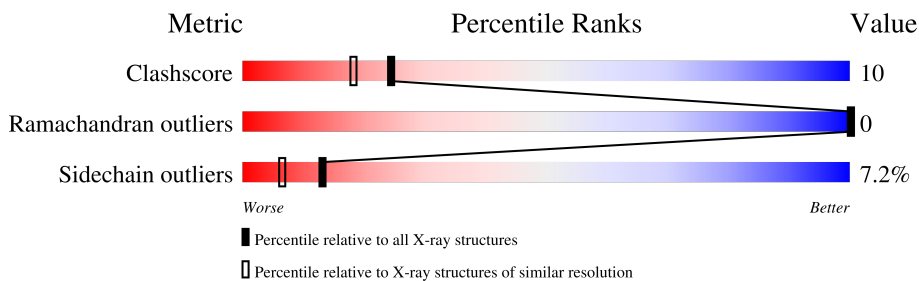
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.90 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	8410 (1.90-1.90)
Ramachandran outliers	187476	8333 (1.90-1.90)
Sidechain outliers	187428	8333 (1.90-1.90)

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	

2 Entry composition [i](#)

There are 5 unique types of molecules in this entry. The entry contains 2216 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.

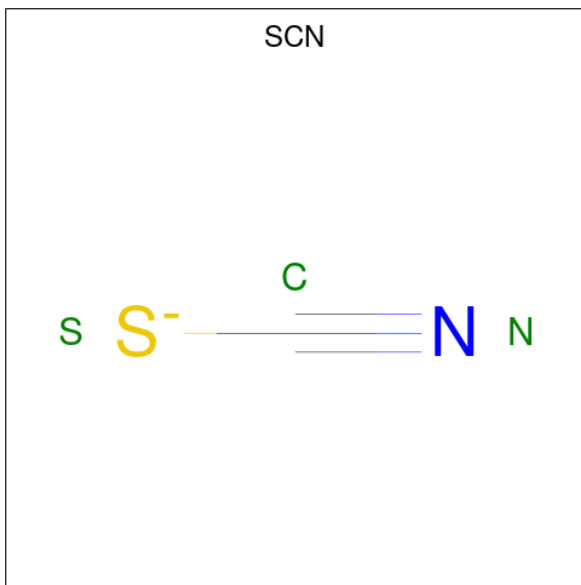
- Molecule 1 is a protein called CARBONIC ANHYDRASE II.

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	1	Total	Hg	0	0
			1	1		

- Molecule 3 is THIOCYANATE ION (CCD ID: SCN) (formula: CNS).



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

- Molecule 4 is ZINC ION (CCD ID: ZN) (formula: Zn).

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

- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	172	Total 172	O 172	0	0

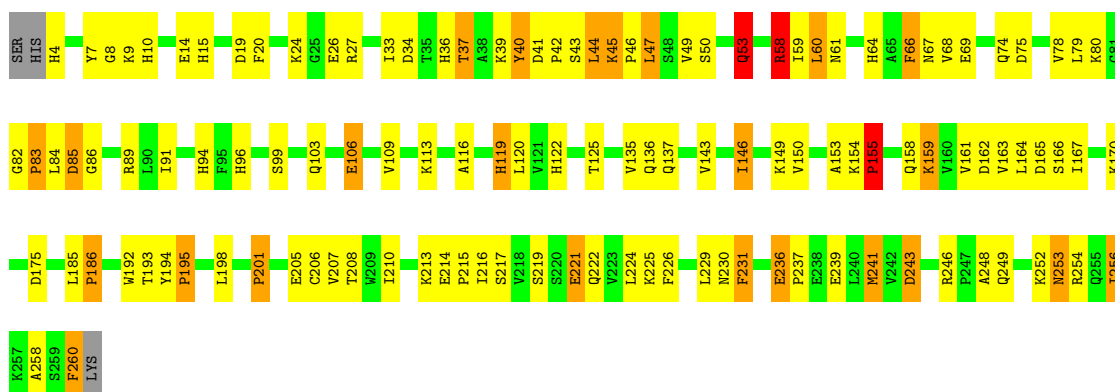
3 Residue-property plots

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:  51% 37% 9% ..



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) – 1.90	Depositor
% Data completeness (in resolution range)	(Not available) ((Not available)-1.90)	Depositor
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	PROLSQ	Depositor
R, R_{free}	0.176 , (Not available)	Depositor
Estimated twinning fraction	No twinning to report.	Xtrriage
Total number of atoms	2216	wwPDB-VP
Average B, all atoms (Å ²)	19.0	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, SCN, 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	1.71	14/2100 (0.7%)	2.36	118/2851 (4.1%)

All (14) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	125	THR	C-N	21.82	1.66	1.33
1	A	96	HIS	CG-ND1	-6.88	1.30	1.38
1	A	34	ASP	C-N	-5.99	1.25	1.33
1	A	94	HIS	CG-ND1	-5.92	1.31	1.38
1	A	193	THR	N-CA	5.71	1.53	1.45
1	A	158	GLN	N-CA	5.70	1.53	1.46
1	A	61	ASN	CA-C	5.41	1.59	1.52
1	A	120	LEU	C-O	5.41	1.30	1.24
1	A	15	HIS	C-O	5.27	1.31	1.24
1	A	8	GLY	N-CA	5.25	1.51	1.45
1	A	216	ILE	CA-C	5.18	1.58	1.52
1	A	193	THR	C-N	-5.17	1.27	1.33
1	A	80	LYS	N-CA	5.10	1.52	1.46
1	A	7	TYR	N-CA	5.05	1.51	1.46

All (118) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	36	HIS	CA-CB-CG	-13.53	100.27	113.80
1	A	155	PRO	CA-C-N	12.62	135.91	120.14
1	A	155	PRO	C-N-CA	12.62	135.91	120.14
1	A	230	ASN	CA-CB-CG	12.61	125.21	112.60
1	A	53	GLN	OE1-CD-NE2	11.70	134.30	122.60
1	A	125	THR	CA-C-N	-10.54	101.02	121.58
1	A	125	THR	C-N-CA	-10.54	101.02	121.58

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	231	PHE	CA-CB-CG	9.96	123.76	113.80
1	A	226	PHE	CA-CB-CG	9.34	123.14	113.80
1	A	103	GLN	CG-CD-NE2	9.27	130.31	116.40
1	A	4	HIS	CA-CB-CG	-8.60	105.20	113.80
1	A	136	GLN	OE1-CD-NE2	8.54	131.13	122.60
1	A	207	VAL	N-CA-C	8.52	120.88	108.53
1	A	14	GLU	CB-CG-CD	8.34	126.78	112.60
1	A	27	ARG	NE-CZ-NH2	7.86	126.27	119.20
1	A	53	GLN	CG-CD-NE2	-7.79	104.72	116.40
1	A	68	VAL	N-CA-C	-7.58	96.92	107.99
1	A	58	ARG	NE-CZ-NH1	7.52	129.02	121.50
1	A	166	SER	N-CA-C	7.51	121.70	112.54
1	A	66	PHE	CA-CB-CG	7.46	121.26	113.80
1	A	236	GLU	O-C-N	7.42	127.87	121.20
1	A	260	PHE	CA-C-O	-7.36	108.28	120.80
1	A	26	GLU	CG-CD-OE1	7.14	134.83	118.40
1	A	166	SER	CA-CB-OG	-7.11	96.89	111.10
1	A	175	ASP	CB-CG-OD1	7.06	134.64	118.40
1	A	85	ASP	CA-CB-CG	-7.05	105.55	112.60
1	A	47	LEU	CA-C-N	7.04	133.76	123.13
1	A	47	LEU	C-N-CA	7.04	133.76	123.13
1	A	53	GLN	CB-CG-CD	-7.00	100.70	112.60
1	A	78	VAL	CA-C-O	6.97	129.36	121.28
1	A	103	GLN	OE1-CD-NE2	-6.87	115.73	122.60
1	A	186	PRO	N-CA-C	-6.83	101.66	111.22
1	A	256	ILE	N-CA-CB	6.73	118.67	111.00
1	A	19	ASP	O-C-N	6.64	131.38	122.49
1	A	85	ASP	CB-CA-C	6.61	121.38	110.74
1	A	75	ASP	CA-CB-CG	6.60	119.20	112.60
1	A	116	ALA	CA-C-N	6.58	132.25	121.86
1	A	116	ALA	C-N-CA	6.58	132.25	121.86
1	A	96	HIS	CA-C-O	-6.43	113.18	120.32
1	A	64	HIS	CA-CB-CG	6.42	120.22	113.80
1	A	27	ARG	CA-CB-CG	6.41	126.91	114.10
1	A	195	PRO	N-CA-CB	6.35	108.63	103.36
1	A	198	LEU	CA-C-O	-6.35	114.64	121.56
1	A	45	LYS	N-CA-CB	6.33	118.52	109.78
1	A	208	THR	N-CA-CB	6.33	121.15	110.46
1	A	186	PRO	CA-C-N	6.26	128.58	120.44
1	A	186	PRO	C-N-CA	6.26	128.58	120.44
1	A	165	ASP	CA-C-O	6.20	127.53	120.90
1	A	10	HIS	CA-CB-CG	-6.15	107.65	113.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	119	HIS	O-C-N	6.06	130.36	123.27
1	A	19	ASP	CA-C-O	-6.04	112.50	119.14
1	A	253	ASN	CA-C-O	-6.03	111.89	120.51
1	A	44	LEU	CB-CA-C	6.00	119.62	109.84
1	A	137	GLN	OE1-CD-NE2	-6.00	116.60	122.60
1	A	159	LYS	N-CA-CB	6.00	118.94	110.12
1	A	137	GLN	CG-CD-NE2	5.95	125.33	116.40
1	A	84	LEU	O-C-N	5.92	129.69	123.06
1	A	99	SER	N-CA-C	-5.90	105.58	112.89
1	A	254	ARG	CA-C-N	5.86	131.26	123.05
1	A	254	ARG	C-N-CA	5.86	131.26	123.05
1	A	158	GLN	OE1-CD-NE2	-5.85	116.75	122.60
1	A	253	ASN	CA-CB-CG	5.84	118.44	112.60
1	A	207	VAL	CA-C-O	5.79	127.31	120.72
1	A	175	ASP	N-CA-C	-5.67	102.00	110.23
1	A	96	HIS	O-C-N	5.62	129.88	123.31
1	A	198	LEU	N-CA-C	-5.58	102.62	110.50
1	A	58	ARG	CD-NE-CZ	5.58	132.22	124.40
1	A	249	GLN	CA-C-N	5.58	125.85	119.83
1	A	249	GLN	C-N-CA	5.58	125.85	119.83
1	A	162	ASP	CA-C-O	-5.53	113.85	120.10
1	A	216	ILE	N-CA-C	-5.53	100.51	108.53
1	A	260	PHE	CA-CB-CG	-5.50	108.30	113.80
1	A	143	VAL	CB-CA-C	5.50	118.77	110.63
1	A	94	HIS	CB-CG-CD2	-5.49	124.06	131.20
1	A	224	LEU	CA-C-N	5.49	127.63	120.28
1	A	224	LEU	C-N-CA	5.49	127.63	120.28
1	A	24	LYS	CB-CG-CD	5.49	123.92	111.30
1	A	150	VAL	CB-CA-C	5.48	117.70	110.91
1	A	40	TYR	CA-C-O	-5.47	114.41	120.70
1	A	37	THR	CA-CB-CG2	5.43	119.74	110.50
1	A	58	ARG	N-CA-C	5.41	116.49	108.60
1	A	136	GLN	CA-CB-CG	-5.40	103.30	114.10
1	A	14	GLU	CA-CB-CG	5.38	124.87	114.10
1	A	86	GLY	CA-C-N	5.38	129.78	122.19
1	A	86	GLY	C-N-CA	5.38	129.78	122.19
1	A	33	ILE	N-CA-CB	5.38	118.13	111.41
1	A	74	GLN	CA-C-O	-5.35	115.55	121.33
1	A	44	LEU	CA-CB-CG	5.34	134.98	116.30
1	A	185	LEU	CA-C-O	5.33	124.67	120.19
1	A	61	ASN	N-CA-CB	5.33	118.68	110.21
1	A	49	VAL	CA-C-N	-5.32	115.10	123.13

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	49	VAL	C-N-CA	-5.32	115.10	123.13
1	A	164	LEU	O-C-N	5.31	128.25	122.20
1	A	252	LYS	CB-CA-C	-5.30	110.44	116.54
1	A	96	HIS	CB-CG-CD2	-5.30	124.31	131.20
1	A	201	PRO	N-CA-C	-5.29	104.24	110.70
1	A	91	ILE	CA-CB-CG2	5.29	119.50	110.50
1	A	158	GLN	CA-C-O	-5.29	114.94	120.55
1	A	37	THR	CB-CA-C	5.28	118.90	109.29
1	A	106	GLU	CG-CD-OE2	-5.26	106.29	118.40
1	A	258	ALA	N-CA-CB	5.20	119.16	110.85
1	A	34	ASP	CA-C-O	-5.17	115.05	120.58
1	A	243	ASP	CA-C-O	-5.17	115.55	121.54
1	A	205	GLU	N-CA-CB	-5.14	102.83	110.60
1	A	170	LYS	CA-C-N	5.13	130.35	122.20
1	A	170	LYS	C-N-CA	5.13	130.35	122.20
1	A	241	MET	CA-C-N	5.13	130.17	122.58
1	A	241	MET	C-N-CA	5.13	130.17	122.58
1	A	64	HIS	N-CA-CB	5.11	118.62	111.15
1	A	146	ILE	O-C-N	-5.08	117.78	123.26
1	A	239	GLU	CA-CB-CG	5.07	124.25	114.10
1	A	165	ASP	CA-C-N	5.07	129.19	120.72
1	A	165	ASP	C-N-CA	5.07	129.19	120.72
1	A	154	LYS	N-CA-CB	5.07	118.28	110.12
1	A	192	TRP	N-CA-C	-5.06	101.62	109.72
1	A	246	ARG	NE-CZ-NH2	-5.05	114.65	119.20
1	A	109	VAL	O-C-N	5.05	128.39	122.99
1	A	154	LYS	CA-C-O	5.04	124.38	119.99

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	2039	0	1988	40	0
2	A	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	A	3	0	0	0	0
4	A	1	0	0	0	0
5	A	172	0	0	9	0
All	All	2216	0	1988	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:248:ALA:HB2	5:A:308:HOH:O	1.21	1.25
1:A:58:ARG:HD2	1:A:69:GLU:OE1	1.49	1.12
1:A:45:LYS:HB3	1:A:46:PRO:CD	2.16	0.76
1:A:243:ASP:OD1	5:A:398:HOH:O	2.12	0.66
1:A:236:GLU:HB3	1:A:237:PRO:HD2	1.80	0.64
1:A:53:GLN:HG3	5:A:383:HOH:O	2.00	0.61
1:A:221:GLU:OE1	5:A:305:HOH:O	2.16	0.61
1:A:58:ARG:HD2	1:A:69:GLU:CD	2.26	0.58
1:A:85:ASP:O	5:A:339:HOH:O	2.18	0.56
1:A:146:ILE:HD13	1:A:186:PRO:HD3	1.88	0.56
1:A:40:TYR:HE1	1:A:42:PRO:HB3	1.71	0.55
1:A:113:LYS:HE3	5:A:299:HOH:O	2.05	0.55
1:A:45:LYS:HB3	1:A:46:PRO:HD2	1.88	0.55
1:A:225:LYS:HE3	5:A:435:HOH:O	2.06	0.55
1:A:59:ILE:HG12	1:A:167:ILE:HD13	1.90	0.54
1:A:161:VAL:CG1	1:A:225:LYS:HD2	2.39	0.53
1:A:159:LYS:HG3	5:A:301:HOH:O	2.10	0.52
1:A:41:ASP:HB3	1:A:44:LEU:HD22	1.93	0.49
1:A:40:TYR:CE1	1:A:42:PRO:HB3	2.47	0.49
1:A:219:SER:OG	1:A:221:GLU:HG2	2.13	0.49
1:A:45:LYS:O	1:A:82:GLY:HA2	2.14	0.48
1:A:58:ARG:CD	1:A:69:GLU:OE1	2.41	0.48
1:A:106:GLU:OE1	1:A:119:HIS:HE1	1.96	0.48
1:A:44:LEU:HD11	1:A:83:PRO:HB3	1.95	0.48
1:A:161:VAL:HG21	1:A:222:GLN:HG2	1.97	0.46
1:A:213:LYS:HD3	1:A:260:PHE:CZ	2.50	0.46
1:A:153:ALA:O	1:A:155:PRO:HD3	2.16	0.45
1:A:231:PHE:CE2	1:A:241:MET:HG3	2.52	0.44
1:A:213:LYS:HD3	1:A:260:PHE:CE2	2.52	0.44
1:A:149:LYS:O	1:A:217:SER:HA	2.16	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:225:LYS:CE	5:A:435:HOH:O	2.65	0.42
1:A:236:GLU:HB3	1:A:237:PRO:CD	2.47	0.42
1:A:60:LEU:O	1:A:66:PHE:HA	2.20	0.41
1:A:135:VAL:O	1:A:206:CYS:SG	2.78	0.41
1:A:20:PHE:CE2	1:A:201:PRO:HB3	2.55	0.41
1:A:214:GLU:HA	1:A:215:PRO:HD3	1.91	0.41
1:A:59:ILE:HA	1:A:67:ASN:O	2.20	0.41
1:A:89:ARG:O	1:A:122:HIS:HA	2.21	0.40
1:A:194:TYR:HA	1:A:195:PRO:HD3	1.91	0.40
1:A:47:LEU:HD11	1:A:210:ILE:HG21	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	254/259 (98%)	243 (96%)	11 (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%)	205 (93%)	16 (7%)	13 6

All (16) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	9	LYS
1	A	37	THR
1	A	39	LYS
1	A	43	SER
1	A	50	SER
1	A	53	GLN
1	A	58	ARG
1	A	60	LEU
1	A	79	LEU
1	A	83	PRO
1	A	155	PRO
1	A	163	VAL
1	A	221	GLU
1	A	229	LEU
1	A	253	ASN
1	A	256	ILE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (2) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	17	HIS
1	A	53	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](#)

Of 3 ligands modelled in this entry, 2 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
3	SCN	A	263	4	1,2,2	3.45	1 (100%)	0,1,1	-	-

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	263	SCN	C-N	3.45	1.27	1.15

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

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	1.66

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.