



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 07:50 AM UTC

PDB ID : 1HEA / pdb_00001hea
Title : CARBONIC ANHYDRASE II (CARBONATE DEHYDRATASE) (HCA II)
(E.C.4.2.1.1) MUTANT WITH LEU 198 REPLACED BY ARG (L198R)
Authors : Nair, S.K.; Christianson, D.W.
Deposited on : 1992-07-16
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
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

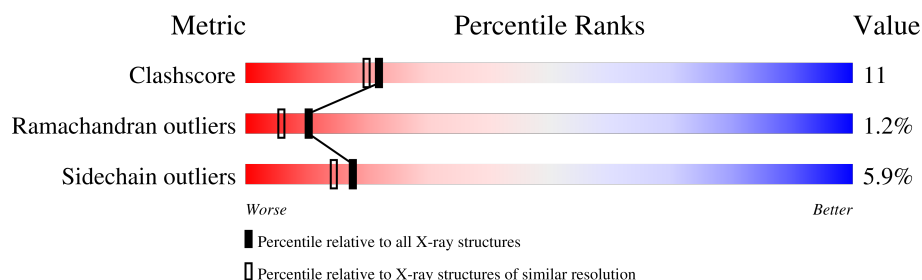
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.00 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	260	 54% 35% 8% . .

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 2154 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	256	Total	C	N	O	S	0	0	0
			2042	1309	353	378	2			

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	198	ARG	LEU	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 MERCURY (II) ION (CCD ID: HG) (formula: Hg).

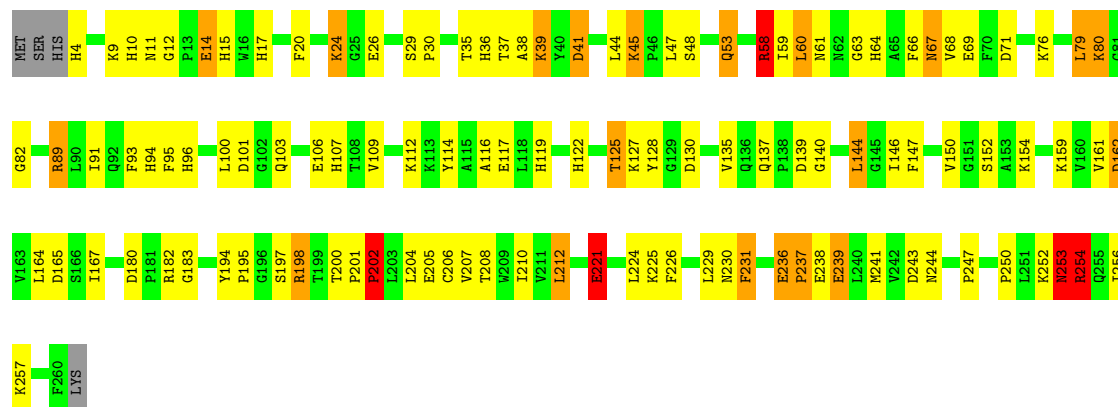
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	1	Total	Hg	0	0
			1	1		

- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	110	Total	O	0	0
			110	110		

Note EDS was not executed.

Chain A: 54% 35% 8%



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	42.70 Å 41.70 Å 73.00 Å 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}	0.182 , (Not available)	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	2154	wwPDB-VP
Average B, all atoms (Å ²)	12.0	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, HG

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	1.85	32/2102 (1.5%)	2.26	97/2851 (3.4%)

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	3

All (32) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	4	HIS	CE1-NE2	10.25	1.42	1.32
1	A	144	LEU	C-N	-7.44	1.29	1.33
1	A	106	GLU	CA-C	6.58	1.60	1.52
1	A	205	GLU	CA-C	-6.36	1.46	1.53
1	A	41	ASP	C-O	-6.18	1.19	1.25
1	A	205	GLU	C-O	6.08	1.30	1.23
1	A	48	SER	CA-C	6.08	1.60	1.52
1	A	257	LYS	C-O	6.04	1.30	1.23
1	A	64	HIS	CA-C	6.02	1.60	1.52
1	A	91	ILE	C-O	5.88	1.29	1.23
1	A	101	ASP	N-CA	5.85	1.53	1.46
1	A	109	VAL	N-CA	5.82	1.54	1.46
1	A	165	ASP	N-CA	5.81	1.53	1.46
1	A	117	GLU	N-CA	5.78	1.53	1.46
1	A	36	HIS	C-O	5.73	1.31	1.24
1	A	61	ASN	N-CA	5.54	1.53	1.46
1	A	236	GLU	CD-OE2	5.50	1.35	1.25
1	A	119	HIS	CE1-NE2	5.48	1.38	1.32

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	17	HIS	ND1-CE1	-5.45	1.27	1.32
1	A	94	HIS	ND1-CE1	5.43	1.38	1.32
1	A	253	ASN	C-O	5.41	1.30	1.24
1	A	35	THR	CA-C	5.38	1.60	1.52
1	A	224	LEU	N-CA	5.35	1.52	1.46
1	A	247	PRO	C-N	-5.32	1.26	1.33
1	A	58	ARG	C-O	5.28	1.29	1.23
1	A	4	HIS	C-N	-5.26	1.26	1.33
1	A	139	ASP	C-N	-5.18	1.27	1.33
1	A	107	HIS	CG-CD2	5.17	1.41	1.35
1	A	58	ARG	NE-CZ	5.07	1.38	1.33
1	A	241	MET	N-CA	5.07	1.53	1.46
1	A	253	ASN	N-CA	5.02	1.52	1.46
1	A	17	HIS	CE1-NE2	5.01	1.37	1.32

All (97) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	29	SER	O-C-N	13.75	133.63	121.80
1	A	201	PRO	CA-C-O	-13.12	101.53	120.56
1	A	201	PRO	O-C-N	12.06	135.69	121.46
1	A	29	SER	CA-C-O	-10.64	108.43	120.46
1	A	30	PRO	N-CA-CB	10.60	114.25	102.60
1	A	30	PRO	N-CD-CG	10.47	116.37	103.80
1	A	30	PRO	CA-N-CD	-9.51	98.18	111.50
1	A	201	PRO	CB-CA-C	9.32	122.30	110.92
1	A	93	PHE	CA-CB-CG	9.10	122.90	113.80
1	A	4	HIS	CA-CB-CG	-9.03	104.77	113.80
1	A	14	GLU	CB-CG-CD	8.47	127.00	112.60
1	A	122	HIS	CA-CB-CG	8.31	122.11	113.80
1	A	67	ASN	CA-CB-CG	8.25	120.85	112.60
1	A	63	GLY	O-C-N	8.16	132.31	122.60
1	A	35	THR	O-C-N	8.13	133.32	122.43
1	A	197	SER	CA-C-O	-8.12	112.39	121.40
1	A	207	VAL	N-CA-C	8.10	119.94	108.36
1	A	236	GLU	CB-CG-CD	8.03	126.25	112.60
1	A	165	ASP	CA-CB-CG	-8.03	104.57	112.60
1	A	101	ASP	CA-CB-CG	8.01	120.61	112.60
1	A	125	THR	CA-C-O	7.73	128.86	120.20
1	A	230	ASN	CA-CB-CG	7.62	120.22	112.60
1	A	94	HIS	CA-CB-CG	-7.59	106.21	113.80
1	A	202	PRO	N-CD-CG	7.56	112.87	103.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	58	ARG	CD-NE-CZ	-7.37	114.08	124.40
1	A	200	THR	CA-CB-OG1	-7.34	98.59	109.60
1	A	147	PHE	CA-CB-CG	7.28	121.08	113.80
1	A	95	PHE	CA-C-N	7.25	133.91	122.74
1	A	95	PHE	C-N-CA	7.25	133.91	122.74
1	A	89	ARG	CB-CA-C	-7.23	97.82	109.75
1	A	45	LYS	CA-C-N	7.13	126.89	119.76
1	A	45	LYS	C-N-CA	7.13	126.89	119.76
1	A	202	PRO	CA-N-CD	-7.13	101.52	111.50
1	A	10	HIS	CA-CB-CG	-7.01	106.79	113.80
1	A	197	SER	N-CA-C	6.88	118.56	108.86
1	A	63	GLY	CA-C-O	-6.82	111.44	119.07
1	A	26	GLU	N-CA-C	6.72	121.31	113.18
1	A	24	LYS	CA-CB-CG	6.64	127.38	114.10
1	A	198	ARG	N-CA-C	-6.51	101.94	110.53
1	A	231	PHE	CA-C-O	6.45	127.25	120.42
1	A	226	PHE	CA-CB-CG	6.40	120.20	113.80
1	A	250	PRO	O-C-N	6.38	130.35	123.01
1	A	94	HIS	ND1-CG-CD2	6.38	112.48	106.10
1	A	244	ASN	OD1-CG-ND2	-6.33	116.27	122.60
1	A	231	PHE	CA-CB-CG	6.32	120.11	113.80
1	A	230	ASN	CB-CG-ND2	6.21	125.71	116.40
1	A	48	SER	CA-C-O	-6.15	113.88	120.46
1	A	254	ARG	CD-NE-CZ	-6.15	115.79	124.40
1	A	80	LYS	O-C-N	6.09	129.66	123.26
1	A	194	TYR	CA-C-N	6.05	126.97	120.13
1	A	194	TYR	C-N-CA	6.05	126.97	120.13
1	A	66	PHE	CA-CB-CG	6.01	119.81	113.80
1	A	11	ASN	O-C-N	5.95	130.08	122.04
1	A	80	LYS	CA-C-O	-5.93	115.09	121.38
1	A	195	PRO	N-CA-CB	5.91	108.26	103.36
1	A	53	GLN	N-CA-C	5.87	120.45	112.88
1	A	236	GLU	CG-CD-OE1	5.85	131.86	118.40
1	A	162	ASP	CA-CB-CG	5.82	118.42	112.60
1	A	236	GLU	O-C-N	5.81	126.43	121.20
1	A	194	TYR	O-C-N	5.76	126.32	121.83
1	A	106	GLU	N-CA-C	-5.74	105.04	112.68
1	A	208	THR	N-CA-C	-5.72	99.41	108.73
1	A	68	VAL	N-CA-CB	5.70	117.88	111.21
1	A	182	ARG	NE-CZ-NH2	5.70	124.33	119.20
1	A	238	GLU	CB-CG-CD	5.67	122.25	112.60
1	A	243	ASP	CA-C-O	-5.66	115.28	121.84

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	96	HIS	N-CA-CB	5.65	120.57	110.80
1	A	150	VAL	CB-CA-C	5.63	117.89	110.91
1	A	180	ASP	CB-CA-C	5.58	116.36	110.17
1	A	119	HIS	CE1-NE2-CD2	-5.51	103.49	109.00
1	A	122	HIS	CE1-NE2-CD2	-5.50	103.50	109.00
1	A	237	PRO	O-C-N	5.50	129.34	123.01
1	A	12	GLY	CA-C-N	5.49	126.70	119.84
1	A	12	GLY	C-N-CA	5.49	126.70	119.84
1	A	237	PRO	CA-C-O	-5.37	115.48	121.23
1	A	256	ILE	N-CA-CB	5.36	117.48	111.21
1	A	71	ASP	CA-CB-CG	5.35	117.95	112.60
1	A	221	GLU	O-C-N	5.32	128.82	122.27
1	A	89	ARG	O-C-N	5.31	129.27	123.27
1	A	17	HIS	CE1-NE2-CD2	-5.25	103.75	109.00
1	A	239	GLU	CB-CG-CD	5.22	121.47	112.60
1	A	39	LYS	CA-CB-CG	5.21	124.53	114.10
1	A	38	ALA	N-CA-C	-5.21	102.57	110.28
1	A	197	SER	O-C-N	5.19	129.69	122.78
1	A	103	GLN	CA-C-O	-5.19	115.90	121.45
1	A	11	ASN	CA-C-O	-5.19	113.74	119.08
1	A	61	ASN	CB-CA-C	5.13	119.28	110.81
1	A	20	PHE	CA-C-N	5.12	124.78	119.56
1	A	20	PHE	C-N-CA	5.12	124.78	119.56
1	A	140	GLY	O-C-N	5.11	127.15	122.19
1	A	107	HIS	ND1-CG-CD2	5.10	111.20	106.10
1	A	17	HIS	ND1-CE1-NE2	5.05	113.45	108.40
1	A	116	ALA	O-C-N	5.04	128.89	123.10
1	A	122	HIS	ND1-CE1-NE2	5.02	113.42	108.40
1	A	130	ASP	CA-C-N	5.01	127.00	120.28
1	A	130	ASP	C-N-CA	5.01	127.00	120.28
1	A	35	THR	CA-C-O	-5.00	113.23	119.38

There are no chirality outliers.

All (3) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	254	ARG	Sidechain
1	A	58	ARG	Sidechain
1	A	89	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	2042	0	1990	42	0
2	A	1	0	0	0	0
3	A	1	0	0	0	0
4	A	110	0	0	5	0
All	All	2154	0	1990	42	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 11.

All (42) 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	2.01	1.19
1:A:252:LYS:O	1:A:253:ASN:CG	2.41	0.64
1:A:14:GLU:OE2	4:A:349:HOH:O	2.15	0.63
1:A:253:ASN:C	1:A:253:ASN:ND2	2.56	0.63
1:A:253:ASN:C	1:A:253:ASN:HD22	2.08	0.62
1:A:162:ASP:OD2	4:A:295:HOH:O	2.16	0.60
1:A:146:ILE:HG12	1:A:212:LEU:HD23	1.85	0.57
1:A:252:LYS:O	1:A:253:ASN:CB	2.53	0.56
1:A:41:ASP:CG	1:A:44:LEU:HD13	2.31	0.55
1:A:202:PRO:HG2	1:A:204:LEU:HG	1.87	0.55
1:A:253:ASN:ND2	1:A:254:ARG:N	2.54	0.54
1:A:112:LYS:HE3	1:A:114:TYR:CE2	2.43	0.53
1:A:252:LYS:O	1:A:253:ASN:OD1	2.27	0.53
1:A:236:GLU:HB3	1:A:237:PRO:CD	2.39	0.52
1:A:60:LEU:HD22	1:A:69:GLU:OE2	2.10	0.52
1:A:58:ARG:HD2	1:A:69:GLU:OE1	2.09	0.52
1:A:137:GLN:O	1:A:206:CYS:HB3	2.10	0.52
1:A:164:LEU:HB3	1:A:229:LEU:HD11	1.92	0.51
1:A:154:LYS:HE3	1:A:183:GLY:O	2.10	0.51
1:A:58:ARG:CG	1:A:69:GLU:OE1	2.58	0.51
1:A:125:THR:C	1:A:127:LYS:CA	2.81	0.51
1:A:45:LYS:O	1:A:82:GLY:HA2	2.12	0.50
1:A:9:LYS:HD2	4:A:349:HOH:O	2.10	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:58:ARG:CD	1:A:69:GLU:OE1	2.59	0.50
1:A:236:GLU:HB3	1:A:237:PRO:HD2	1.92	0.50
1:A:161:VAL:HG13	1:A:225:LYS:HD2	1.94	0.49
1:A:161:VAL:CG1	1:A:225:LYS:HD2	2.43	0.49
1:A:128:TYR:CE1	1:A:137:GLN:HG3	2.47	0.49
1:A:231:PHE:HD2	1:A:239:GLU:HG2	1.79	0.47
1:A:128:TYR:CZ	1:A:137:GLN:HG3	2.49	0.47
1:A:47:LEU:HD11	1:A:210:ILE:HG21	1.95	0.47
1:A:47:LEU:HD22	1:A:79:LEU:HD21	1.97	0.47
1:A:53:GLN:HB3	1:A:76:LYS:O	2.16	0.45
1:A:159:LYS:HB3	1:A:159:LYS:HE2	1.46	0.45
1:A:47:LEU:HD21	1:A:210:ILE:HD13	1.99	0.45
1:A:60:LEU:HD23	1:A:67:ASN:HB2	1.99	0.44
1:A:127:LYS:HD2	1:A:128:TYR:CZ	2.53	0.44
1:A:14:GLU:HG2	1:A:15:HIS:CD2	2.54	0.42
1:A:59:ILE:HG12	1:A:167:ILE:HD13	2.00	0.42
1:A:221:GLU:O	1:A:225:LYS:HG3	2.20	0.42
1:A:252:LYS:HD2	4:A:270:HOH:O	2.20	0.41
1:A:80:LYS:NZ	4:A:353:HOH:O	2.54	0.41

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	252/260 (97%)	238 (94%)	11 (4%)	3 (1%)	10 6

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	253	ASN
1	A	254	ARG

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Mol	Chain	Res	Type
1	A	135	VAL

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	221/225 (98%)	208 (94%)	13 (6%)	18	14

All (13) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	24	LYS
1	A	37	THR
1	A	39	LYS
1	A	60	LEU
1	A	79	LEU
1	A	100	LEU
1	A	144	LEU
1	A	152	SER
1	A	198	ARG
1	A	202	PRO
1	A	212	LEU
1	A	221	GLU
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	53	GLN
1	A	67	ASN
1	A	253	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 [i](#)

Of 2 ligands modelled in this entry, 2 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

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	2.01

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.