



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 03:57 PM UTC

PDB ID : 1HEC / pdb_00001hec
Title : STRUCTURAL CONSEQUENCES OF HYDROPHILIC AMINO-ACID
SUBSTITUTIONS IN THE HYDROPHOBIC POCKET OF HUMAN CAR-
BONIC ANHYDRASE II
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

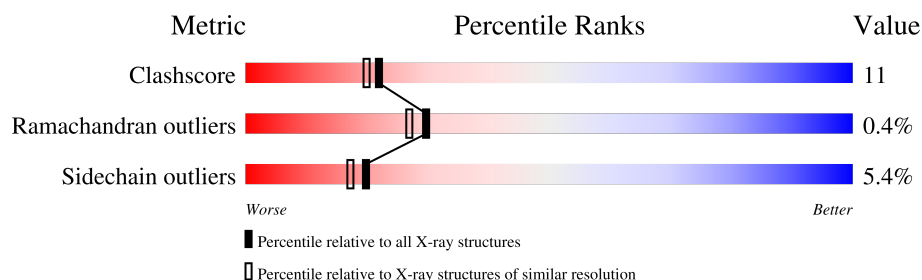
1 Overall quality at a glance

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	

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 2133 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
			2041	1309	352	378	2			

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	198	HIS	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 water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	91	Total	O	0	0
			91	91		

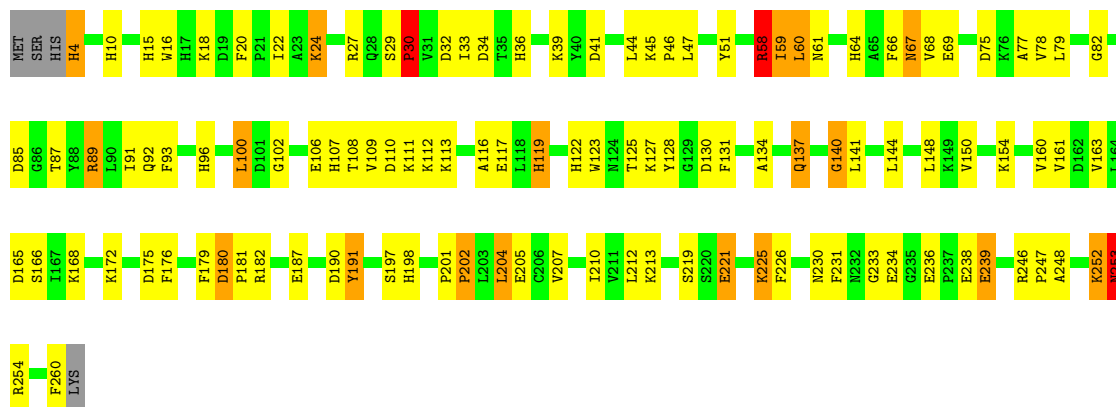
3 Residue-property plots

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)	(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	2133	wwPDB-VP
Average B, all atoms (Å ²)	13.0	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

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	1.90	33/2102 (1.6%)	2.16	78/2852 (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	1

All (33) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	64	HIS	CE1-NE2	7.83	1.40	1.32
1	A	107	HIS	CG-CD2	7.64	1.44	1.35
1	A	20	PHE	N-CA	7.52	1.55	1.46
1	A	36	HIS	CE1-NE2	6.58	1.39	1.32
1	A	108	THR	CA-C	6.56	1.60	1.52
1	A	59	ILE	C-O	6.33	1.30	1.24
1	A	109	VAL	N-CA	6.25	1.54	1.46
1	A	107	HIS	CE1-NE2	6.17	1.38	1.32
1	A	29	SER	CA-CB	6.08	1.62	1.53
1	A	29	SER	CA-C	-6.00	1.45	1.52
1	A	204	LEU	CA-C	-5.93	1.45	1.52
1	A	238	GLU	CD-OE1	5.83	1.36	1.25
1	A	77	ALA	N-CA	5.68	1.53	1.46
1	A	91	ILE	C-O	5.62	1.29	1.23
1	A	64	HIS	ND1-CE1	-5.52	1.27	1.32
1	A	100	LEU	CA-C	5.52	1.59	1.52
1	A	190	ASP	N-CA	5.43	1.52	1.46
1	A	22	ILE	N-CA	5.41	1.53	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	33	ILE	CA-C	5.41	1.58	1.52
1	A	4	HIS	ND1-CE1	-5.38	1.27	1.32
1	A	61	ASN	C-O	5.37	1.30	1.24
1	A	191	TYR	CA-CB	5.31	1.63	1.53
1	A	102	GLY	C-O	5.30	1.30	1.23
1	A	112	LYS	C-N	-5.30	1.25	1.33
1	A	140	GLY	N-CA	-5.26	1.39	1.45
1	A	89	ARG	N-CA	-5.19	1.39	1.46
1	A	33	ILE	C-N	-5.12	1.26	1.33
1	A	77	ALA	CA-CB	-5.12	1.45	1.53
1	A	16	TRP	C-N	-5.11	1.27	1.34
1	A	197	SER	C-N	5.08	1.40	1.33
1	A	234	GLU	CD-OE1	5.04	1.34	1.25
1	A	32	ASP	CA-C	5.01	1.58	1.52
1	A	239	GLU	N-CA	5.00	1.52	1.46

All (78) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	201	PRO	CA-C-O	-14.51	99.53	120.56
1	A	29	SER	CA-C-O	-14.47	103.19	120.41
1	A	201	PRO	O-C-N	11.55	135.09	121.46
1	A	165	ASP	CA-CB-CG	10.96	123.56	112.60
1	A	29	SER	O-C-N	10.54	131.79	121.57
1	A	202	PRO	N-CD-CG	10.13	115.96	103.80
1	A	226	PHE	CA-CB-CG	9.61	123.41	113.80
1	A	190	ASP	CA-CB-CG	9.20	121.80	112.60
1	A	130	ASP	CA-CB-CG	8.74	121.34	112.60
1	A	30	PRO	CA-N-CD	-8.42	99.71	111.50
1	A	207	VAL	N-CA-C	8.26	119.74	108.17
1	A	191	TYR	N-CA-C	8.18	121.15	108.96
1	A	202	PRO	CA-N-CD	-7.97	100.35	111.50
1	A	10	HIS	CA-CB-CG	-7.72	106.08	113.80
1	A	198	HIS	CA-CB-CG	7.50	121.30	113.80
1	A	93	PHE	CA-CB-CG	7.22	121.03	113.80
1	A	64	HIS	CE1-NE2-CD2	-7.18	101.82	109.00
1	A	198	HIS	N-CA-C	-7.08	101.18	110.53
1	A	30	PRO	N-CA-CB	6.97	110.27	102.60
1	A	68	VAL	N-CA-CB	6.95	120.10	111.41
1	A	67	ASN	CA-CB-CG	6.90	119.50	112.60
1	A	66	PHE	CA-CB-CG	6.71	120.52	113.80
1	A	233	GLY	N-CA-C	-6.50	103.85	112.82

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	179	PHE	CA-CB-CG	-6.46	107.34	113.80
1	A	131	PHE	CA-C-N	6.44	127.25	120.03
1	A	131	PHE	C-N-CA	6.44	127.25	120.03
1	A	154	LYS	O-C-N	6.44	127.65	120.83
1	A	30	PRO	N-CD-CG	6.39	111.47	103.80
1	A	187	GLU	CB-CG-CD	6.34	123.38	112.60
1	A	51	TYR	O-C-N	6.30	129.81	122.19
1	A	29	SER	N-CA-C	6.29	119.73	110.10
1	A	96	HIS	CA-C-O	-6.26	113.94	120.70
1	A	182	ARG	CD-NE-CZ	-6.17	115.75	124.40
1	A	150	VAL	CB-CA-C	6.14	118.39	110.96
1	A	230	ASN	CA-CB-CG	6.03	118.63	112.60
1	A	87	THR	CA-CB-OG1	-6.02	100.57	109.60
1	A	238	GLU	CB-CG-CD	5.90	122.63	112.60
1	A	122	HIS	CA-CB-CG	5.81	119.61	113.80
1	A	92	GLN	OE1-CD-NE2	-5.74	116.86	122.60
1	A	119	HIS	CA-CB-CG	5.70	119.50	113.80
1	A	24	LYS	CA-CB-CG	5.68	125.46	114.10
1	A	34	ASP	CA-CB-CG	5.67	118.27	112.60
1	A	175	ASP	O-C-N	5.64	130.05	122.82
1	A	202	PRO	N-CA-CB	5.63	108.79	102.60
1	A	122	HIS	ND1-CE1-NE2	5.62	114.02	108.40
1	A	253	ASN	CA-CB-CG	5.59	118.19	112.60
1	A	85	ASP	CA-CB-CG	5.58	118.18	112.60
1	A	41	ASP	CA-C-N	5.53	126.01	120.04
1	A	41	ASP	C-N-CA	5.53	126.01	120.04
1	A	78	VAL	O-C-N	5.51	128.90	123.00
1	A	18	LYS	O-C-N	5.47	127.92	122.12
1	A	252	LYS	N-CA-C	5.47	118.94	111.39
1	A	16	TRP	CA-C-O	-5.46	114.77	120.55
1	A	225	LYS	CA-CB-CG	-5.44	103.22	114.10
1	A	117	GLU	CA-C-N	5.41	130.18	122.72
1	A	117	GLU	C-N-CA	5.41	130.18	122.72
1	A	15	HIS	ND1-CE1-NE2	5.40	113.80	108.40
1	A	236	GLU	O-C-N	5.39	125.93	121.35
1	A	30	PRO	CB-CG-CD	-5.38	93.02	105.40
1	A	239	GLU	CA-C-O	-5.37	114.76	120.40
1	A	36	HIS	ND1-CG-CD2	5.34	111.44	106.10
1	A	207	VAL	CA-C-N	5.32	130.25	122.85
1	A	207	VAL	C-N-CA	5.32	130.25	122.85
1	A	180	ASP	CB-CA-C	5.31	115.43	110.17
1	A	166	SER	N-CA-C	5.29	119.00	112.54

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	89	ARG	O-C-N	5.27	129.23	123.27
1	A	137	GLN	CA-C-N	5.26	125.07	119.28
1	A	137	GLN	C-N-CA	5.26	125.07	119.28
1	A	60	LEU	N-CA-C	5.24	117.96	109.06
1	A	198	HIS	CA-C-O	-5.21	115.83	121.87
1	A	190	ASP	N-CA-C	-5.16	102.75	110.23
1	A	4	HIS	ND1-CE1-NE2	5.15	113.55	108.40
1	A	165	ASP	CA-C-N	5.13	129.29	120.72
1	A	165	ASP	C-N-CA	5.13	129.29	120.72
1	A	172	LYS	O-C-N	5.12	128.68	122.85
1	A	175	ASP	N-CA-C	-5.10	103.61	110.24
1	A	140	GLY	N-CA-C	5.06	119.25	112.77
1	A	32	ASP	O-C-N	5.06	128.99	123.22

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	58	ARG	Sidechain

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	2041	0	1984	43	0
2	A	1	0	0	0	0
3	A	91	0	0	2	0
All	All	2133	0	1984	43	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 (43) 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	2.05	1.14

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:58:ARG:HD2	1:A:69:GLU:OE1	1.55	1.04
1:A:161:VAL:HG13	1:A:225:LYS:HD2	1.58	0.84
1:A:161:VAL:CG1	1:A:225:LYS:HD2	2.08	0.83
1:A:213:LYS:HD3	1:A:260:PHE:CZ	2.18	0.78
1:A:253:ASN:C	1:A:253:ASN:HD22	1.93	0.76
1:A:253:ASN:HD22	1:A:254:ARG:N	1.92	0.68
1:A:27:ARG:HD3	1:A:205:GLU:HB3	1.78	0.66
1:A:231:PHE:HD2	1:A:239:GLU:HG2	1.60	0.65
1:A:253:ASN:ND2	1:A:254:ARG:N	2.46	0.64
1:A:253:ASN:C	1:A:253:ASN:ND2	2.58	0.62
1:A:58:ARG:HH11	1:A:69:GLU:CD	2.07	0.61
1:A:60:LEU:HD21	1:A:67:ASN:HB2	1.85	0.57
1:A:60:LEU:CD2	1:A:67:ASN:HB2	2.36	0.56
1:A:252:LYS:O	1:A:253:ASN:CG	2.49	0.56
1:A:45:LYS:O	1:A:82:GLY:HA2	2.07	0.54
1:A:59:ILE:HA	1:A:67:ASN:O	2.07	0.54
1:A:75:ASP:OD1	1:A:89:ARG:NE	2.35	0.52
1:A:44:LEU:HG	1:A:191:TYR:OH	2.09	0.52
1:A:202:PRO:HG2	1:A:204:LEU:HG	1.90	0.52
1:A:125:THR:C	1:A:127:LYS:CA	2.81	0.52
1:A:168:LYS:NZ	3:A:324:HOH:O	2.33	0.51
1:A:113:LYS:NZ	3:A:336:HOH:O	2.38	0.50
1:A:134:ALA:O	1:A:140:GLY:HA3	2.12	0.49
1:A:160:VAL:O	1:A:163:VAL:HG12	2.14	0.48
1:A:128:TYR:CE1	1:A:137:GLN:HG3	2.49	0.48
1:A:30:PRO:HG2	1:A:248:ALA:HA	1.96	0.47
1:A:27:ARG:HG3	1:A:27:ARG:O	2.14	0.47
1:A:27:ARG:CD	1:A:205:GLU:HB3	2.43	0.47
1:A:27:ARG:CG	1:A:205:GLU:HB3	2.46	0.46
1:A:58:ARG:HA	1:A:176:PHE:HB3	1.97	0.46
1:A:110:ASP:O	1:A:111:LYS:HB2	2.16	0.46
1:A:116:ALA:HB3	1:A:148:LEU:HB2	1.98	0.46
1:A:219:SER:OG	1:A:221:GLU:HG2	2.16	0.45
1:A:213:LYS:HD3	1:A:260:PHE:CE2	2.51	0.45
1:A:106:GLU:OE1	1:A:119:HIS:HE1	2.02	0.43
1:A:246:ARG:HA	1:A:247:PRO:HD3	1.82	0.43
1:A:123:TRP:CZ3	1:A:125:THR:HA	2.54	0.42
1:A:252:LYS:O	1:A:253:ASN:CB	2.68	0.42
1:A:180:ASP:HA	1:A:181:PRO:HD2	1.91	0.41
1:A:45:LYS:HA	1:A:46:PRO:HD3	1.90	0.41
1:A:47:LEU:HD11	1:A:210:ILE:HG21	2.03	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:221:GLU:CD	1:A:221:GLU:H	2.28	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%)	13 (5%)	1 (0%)	30 27

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	221/225 (98%)	209 (95%)	12 (5%)	20 17

All (12) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	4	HIS
1	A	24	LYS

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Mol	Chain	Res	Type
1	A	30	PRO
1	A	39	LYS
1	A	58	ARG
1	A	79	LEU
1	A	100	LEU
1	A	141	LEU
1	A	144	LEU
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 (2) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	136	GLN
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 1 ligands modelled in this entry, 1 is 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	2.05

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.