



wwPDB X-ray Structure Validation Summary Report ⓘ

Aug 10, 2020 – 05:56 AM BST

PDB ID : 1NU8
Title : Crystal structure of human dipeptidyl peptidase IV (DPP-IV) in complex with Diprotin A (IPI)
Authors : Thoma, R.; Loeffler, B.; Stihle, M.; Huber, W.; Ruf, A.; Hennig, M.
Deposited on : 2003-01-31
Resolution : 2.50 Å(reported)

This is a wwPDB X-ray Structure Validation Summary 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 following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity : 4.02b-467
Mogul : 1.8.5 (274361), CSD as541be (2020)
Xtrriage (Phenix) : **NOT EXECUTED**
EDS : **NOT EXECUTED**
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.13.1

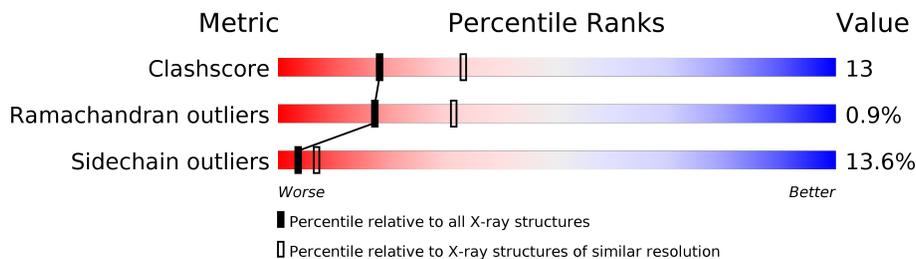
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.50 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	141614	5346 (2.50-2.50)
Ramachandran outliers	138981	5231 (2.50-2.50)
Sidechain outliers	138945	5233 (2.50-2.50)

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 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	728	
1	B	728	
2	D	3	

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
3	NAG	A	794	X	-	-	-

2 Entry composition [i](#)

There are 4 unique types of molecules in this entry. The entry contains 12335 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.

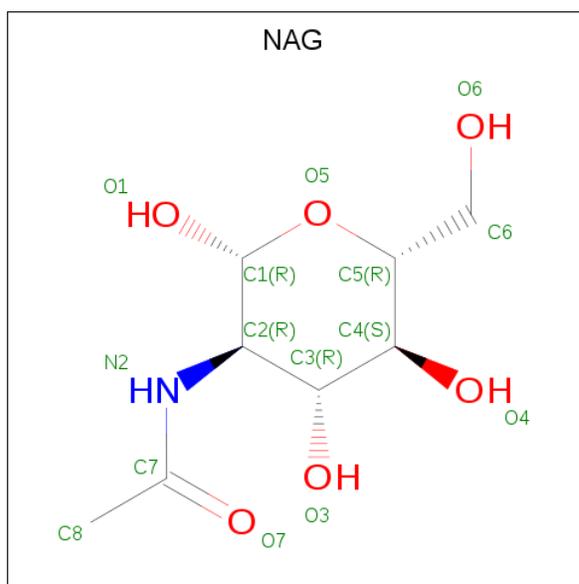
- Molecule 1 is a protein called Dipeptidyl peptidase IV.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	728	Total 5963	C 3827	N 982	O 1128	S 26	0	0	0
1	B	728	Total 5963	C 3827	N 982	O 1128	S 26	0	0	0

- Molecule 2 is a protein called 3-mer peptide.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
			Total	C	N	O			
2	D	3	Total 24	C 17	N 3	O 4	0	0	0

- Molecule 3 is 2-acetamido-2-deoxy-beta-D-glucopyranose (three-letter code: NAG) (formula: C₈H₁₅NO₆).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	C	N	O		
3	A	1	Total 14	C 8	N 1	O 5	0	0

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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	A	1	Total	C	N	O	0	0
			14	8	1	5		
3	A	1	Total	C	N	O	0	0
			14	8	1	5		
3	A	1	Total	C	N	O	0	0
			14	8	1	5		
3	B	1	Total	C	N	O	0	0
			14	8	1	5		
3	B	1	Total	C	N	O	0	0
			14	8	1	5		
3	B	1	Total	C	N	O	0	0
			14	8	1	5		

- Molecule 4 is water.

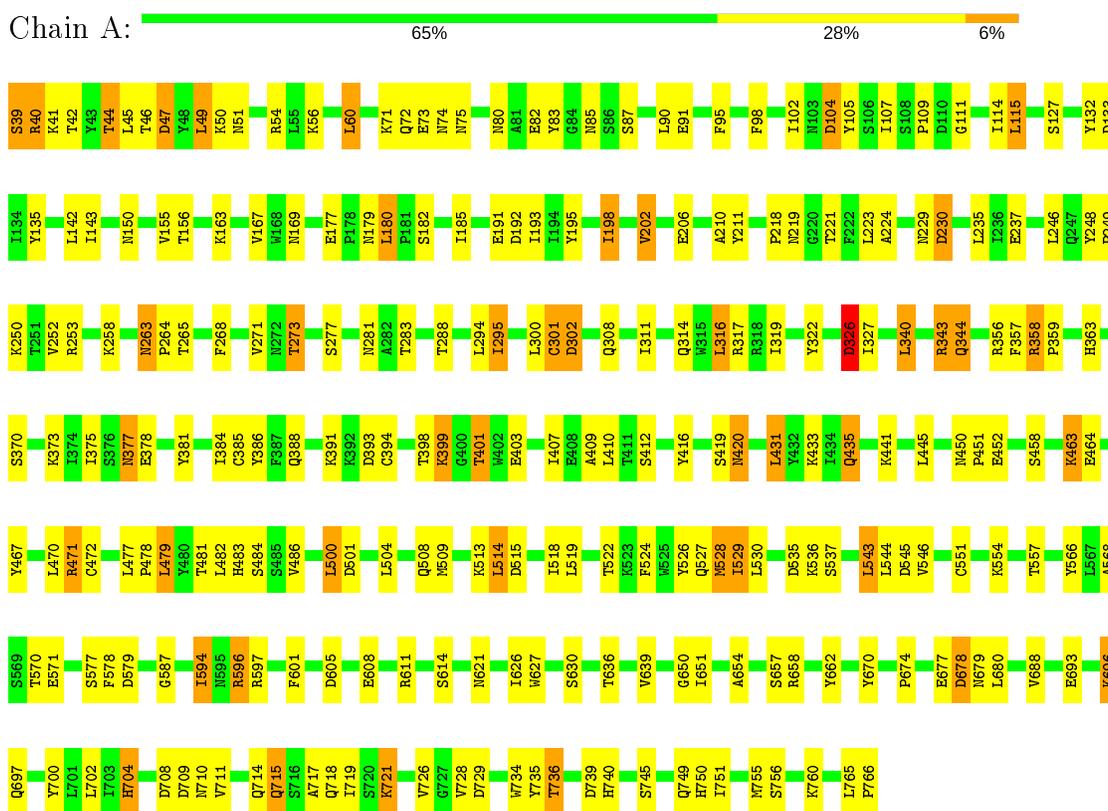
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	122	Total	O	0	0
			122	122		
4	B	150	Total	O	0	0
			150	150		
4	D	1	Total	O	0	0
			1	1		

3 Residue-property plots [i](#)

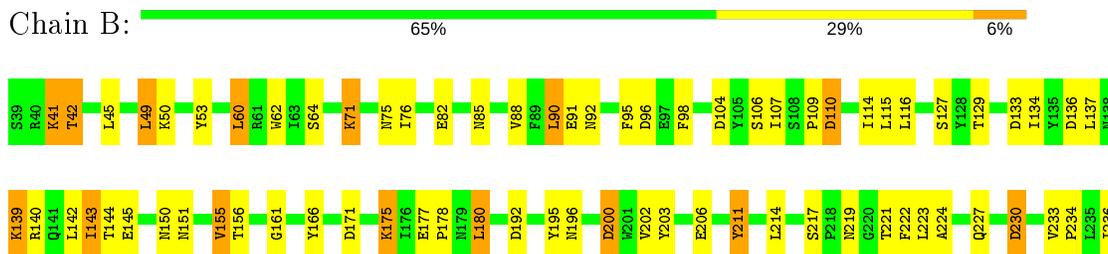
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry. Residues are color-coded 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.

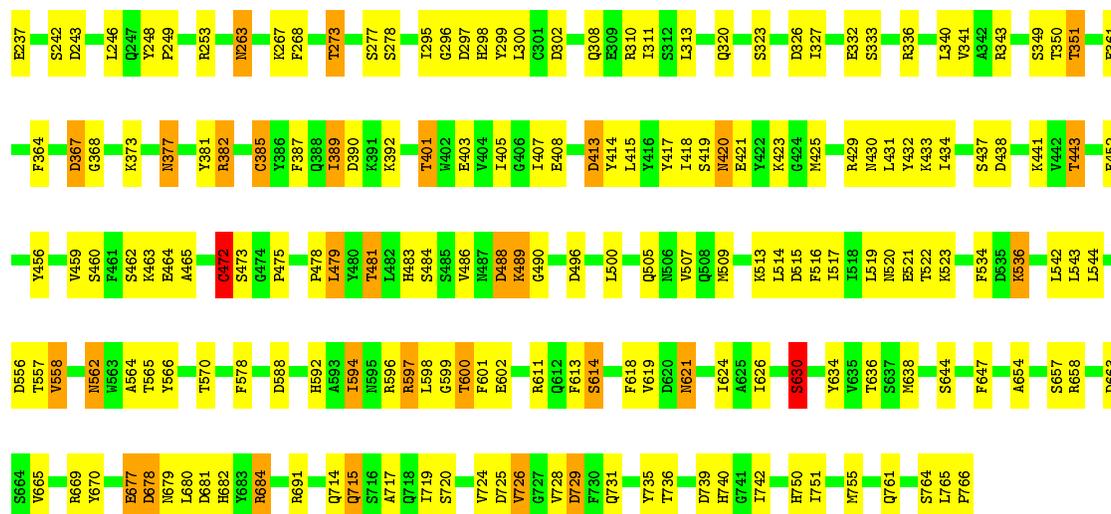
Note EDS was not executed.

- Molecule 1: Dipeptidyl peptidase IV



- Molecule 1: Dipeptidyl peptidase IV





- Molecule 2: 3-mer peptide

Chain D: 33% 67%

I1
P2
I3

4 Data and refinement statistics

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

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	65.14Å 67.07Å 419.63Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	12.00 – 2.50	Depositor
% Data completeness (in resolution range)	(Not available) (12.00-2.50)	Depositor
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	REFMAC 5.1	Depositor
R, R_{free}	0.225 , 0.282	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	12335	wwPDB-VP
Average B, all atoms (Å ²)	32.0	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:
NAG

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	0.67	0/6135	0.88	16/8344 (0.2%)
1	B	0.71	0/6135	0.90	21/8344 (0.3%)
2	D	1.89	2/24 (8.3%)	1.98	1/31 (3.2%)
All	All	0.69	2/12294 (0.0%)	0.90	38/16719 (0.2%)

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	B	0	1
2	D	0	1
All	All	0	2

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	2	PRO	C-O	6.24	1.35	1.23
2	D	2	PRO	C-N	5.85	1.47	1.34

The worst 5 of 38 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	630	SER	CA-CB-OG	8.62	134.49	111.20
2	D	2	PRO	CA-C-N	-8.41	98.70	117.20
1	B	60	LEU	CA-CB-CG	7.66	132.93	115.30
1	B	171	ASP	CB-CG-OD2	7.47	125.03	118.30
1	B	729	ASP	CB-CG-OD2	7.23	124.81	118.30

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	B	110	ASP	Peptide
2	D	2	PRO	Mainchain

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	5963	0	5683	157	0
1	B	5963	0	5683	164	2
2	D	24	0	31	3	0
3	A	56	0	52	11	0
3	B	56	0	52	8	0
4	A	122	0	0	15	0
4	B	150	0	0	6	3
4	D	1	0	0	0	0
All	All	12335	0	11501	314	3

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 13.

The worst 5 of 314 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:370:SER:HA	4:A:892:HOH:O	1.24	1.37
1:A:229:ASN:HD21	3:A:796:NAG:C1	1.43	1.32
1:B:92:ASN:HD21	3:B:797:NAG:C1	1.44	1.26
1:A:82:GLU:HG3	4:A:899:HOH:O	1.35	1.25
1:B:85:ASN:HD21	3:B:794:NAG:C1	1.52	1.22

All (3) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:82:GLU:O	4:B:1934:HOH:O[3_745]	1.84	0.36
1:B:437:SER:CB	4:B:1924:HOH:O[3_755]	1.93	0.27
4:B:1837:HOH:O	4:B:1884:HOH:O[1_455]	2.15	0.05

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	726/728 (100%)	666 (92%)	52 (7%)	8 (1%)	14 26
1	B	726/728 (100%)	677 (93%)	44 (6%)	5 (1%)	22 39
2	D	1/3 (33%)	1 (100%)	0	0	100 100
All	All	1453/1459 (100%)	1344 (92%)	96 (7%)	13 (1%)	17 31

5 of 13 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	111	GLY
1	B	486	VAL
1	A	40	ARG
1	B	465	ALA
1	A	210	ALA

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	653/653 (100%)	565 (86%)	88 (14%)	4 7

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	B	653/653 (100%)	564 (86%)	89 (14%)	3	7
2	D	3/3 (100%)	2 (67%)	1 (33%)	0	0
All	All	1309/1309 (100%)	1131 (86%)	178 (14%)	3	7

5 of 178 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	679	ASN
1	B	129	THR
1	B	614	SER
1	A	704	HIS
1	B	49	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 39 such sidechains are listed below:

Mol	Chain	Res	Type
1	A	697	GLN
1	A	750	HIS
1	B	715	GLN
1	A	715	GLN
1	A	731	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 monosaccharides in this entry.

5.6 Ligand geometry [i](#)

8 ligands are modelled in this entry.

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	NAG	A	795	-	14,14,15	0.54	0	17,19,21	1.02	2 (11%)
3	NAG	B	794	1	14,14,15	0.68	0	17,19,21	1.25	2 (11%)
3	NAG	A	796	-	14,14,15	0.50	0	17,19,21	1.31	3 (17%)
3	NAG	B	796	1	14,14,15	0.56	0	17,19,21	1.55	1 (5%)
3	NAG	B	797	1	14,14,15	0.64	0	17,19,21	0.75	0
3	NAG	B	1793	-	14,14,15	0.56	0	17,19,21	3.07	9 (52%)
3	NAG	A	793	-	14,14,15	0.62	0	17,19,21	1.89	4 (23%)
3	NAG	A	794	1	14,14,15	0.73	0	17,19,21	1.48	5 (29%)

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
3	NAG	A	795	-	-	3/6/23/26	0/1/1/1
3	NAG	B	794	1	-	0/6/23/26	0/1/1/1
3	NAG	A	796	-	-	2/6/23/26	0/1/1/1
3	NAG	B	796	1	-	2/6/23/26	0/1/1/1
3	NAG	B	797	1	-	2/6/23/26	0/1/1/1
3	NAG	B	1793	-	-	5/6/23/26	0/1/1/1
3	NAG	A	793	-	-	5/6/23/26	0/1/1/1
3	NAG	A	794	1	1/1/5/7	0/6/23/26	0/1/1/1

There are no bond length outliers.

The worst 5 of 26 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	1793	NAG	C2-N2-C7	6.07	131.55	122.90
3	B	1793	NAG	C1-O5-C5	5.61	119.80	112.19
3	B	796	NAG	C1-O5-C5	5.44	119.56	112.19

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	1793	NAG	C4-C3-C2	-5.08	103.58	111.02
3	B	1793	NAG	C1-C2-N2	5.01	119.05	110.49

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
3	A	794	NAG	C1

5 of 19 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	B	1793	NAG	C8-C7-N2-C2
3	B	1793	NAG	O7-C7-N2-C2
3	A	793	NAG	C3-C2-N2-C7
3	A	793	NAG	C8-C7-N2-C2
3	A	793	NAG	O7-C7-N2-C2

There are no ring outliers.

6 monomers are involved in 19 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	795	NAG	3	0
3	B	794	NAG	3	0
3	A	796	NAG	2	0
3	B	797	NAG	2	0
3	B	1793	NAG	3	0
3	A	793	NAG	6	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 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.