



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 13, 2017 – 12:52 am GMT

PDB ID : 1B6T
Title : PHOSPHOPANTETHEINE ADENYLYLTRANSFERASE IN COMPLEX
WITH 3'-DEPHOSPHO-COA FROM ESCHERICHIA COLI
Authors : Izard, T.
Deposited on : 1999-01-18
Resolution : 1.80 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

<http://wwpdb.org/validation/2016/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 : 1.7.2 (RC1), CSD as538be (2017)
Xtriage (Phenix) : **NOT EXECUTED**
EDS : **NOT EXECUTED**
Percentile statistics : 20161228.v01 (using entries in the PDB archive December 28th 2016)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : recalc28949

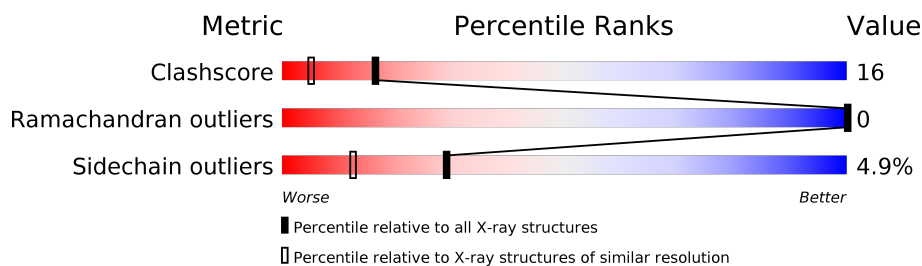
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.80 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	112137	5742 (1.80-1.80)
Ramachandran outliers	110173	5676 (1.80-1.80)
Sidechain outliers	110143	5675 (1.80-1.80)

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. 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 $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	159	 75% 23% ..
1	B	159	 75% 20% ..

2 Entry composition [i](#)

There are 4 unique types of molecules in this entry. The entry contains 2853 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 PROTEIN (PHOSPHOPANTETHEINE ADENYLYLTRANSFERASE).

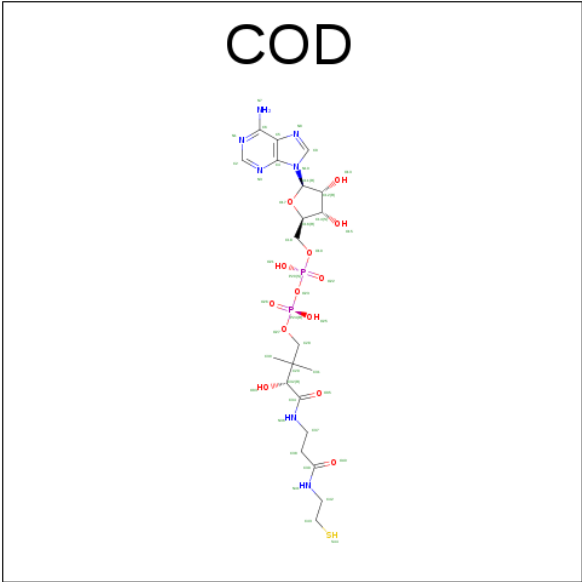
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	157	Total	C	N	O	S	0	0	0
			1236	787	219	222	8			
1	B	157	Total	C	N	O	S	0	0	0
			1236	787	219	222	8			

- Molecule 2 is SULFATE ION (three-letter code: SO4) (formula: O₄S).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	B	1	Total	O	S	0	0
			5	4	1		
2	A	1	Total	O	S	0	0
			5	4	1		
2	B	1	Total	O	S	0	0
			5	4	1		

- Molecule 3 is DEPHOSPHO COENZYME A (three-letter code: COD) (formula: C₂₁H₃₅N₇O₁₃P₂S).



Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
			Total	C	N	O	P	S		
3	B	1	44	21	7	13	2	1	0	0

- Molecule 4 is water.

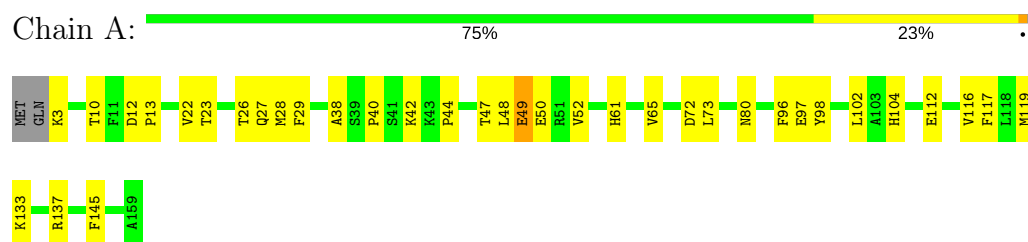
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	146	Total	O	0	0
			146	146		
4	B	176	Total	O	0	0
			176	176		

3 Residue-property plots [i](#)

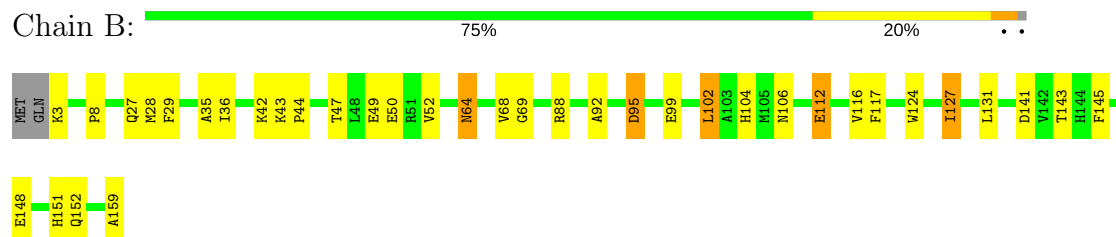
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are 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. A red dot above a residue indicates a poor fit to the electron density ($RSRZ > 2$). 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: PROTEIN (PHOSPHOPANTETHEINE ADENYLYLTRANSFERASE)



• Molecule 1: PROTEIN (PHOSPHOPANTETHEINE ADENYLYLTRANSFERASE)



4 Data and refinement statistics

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

Property	Value	Source
Space group	I 2 3	Depositor
Cell constants a, b, c, α , β , γ	135.50 Å 135.50 Å 135.50 Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	23.96 – 1.80	Depositor
% Data completeness (in resolution range)	97.6 (23.96-1.80)	Depositor
R_{merge}	0.09	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	CNS 1.0	Depositor
R, R_{free}	0.205 , 0.235	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	2853	wwPDB-VP
Average B, all atoms (Å ²)	25.0	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: COD, SO4

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	0.33	0/1264	0.57	0/1711
1	B	0.31	0/1264	0.55	0/1711
All	All	0.32	0/2528	0.56	0/3422

There are no bond length outliers.

There are no bond angle outliers.

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	1236	0	1234	39	1
1	B	1236	0	1234	49	0
2	A	5	0	0	0	0
2	B	10	0	0	0	0
3	B	44	0	33	7	0
4	A	146	0	0	4	0
4	B	176	0	0	9	1
All	All	2853	0	2501	80	1

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 16.

All (80) 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:49:GLU:CD	1:A:49:GLU:H	1.65	0.98
1:A:116:VAL:HG13	1:B:116:VAL:HG13	1.64	0.79
1:A:49:GLU:N	1:A:49:GLU:CD	2.38	0.77
1:A:48:LEU:HB3	1:A:49:GLU:OE2	1.88	0.72
1:B:88:ARG:HD2	4:B:3163:HOH:O	1.93	0.67
1:A:112:GLU:N	1:A:112:GLU:OE2	2.26	0.65
1:B:102:LEU:HD11	4:B:3146:HOH:O	1.94	0.65
1:B:102:LEU:HG	4:B:3118:HOH:O	1.98	0.64
1:B:49:GLU:CD	1:B:49:GLU:H	2.01	0.64
1:B:127:ILE:HD13	1:B:127:ILE:H	1.64	0.62
1:A:127:ILE:HG21	1:A:145:PHE:CE2	2.36	0.61
1:B:102:LEU:O	1:B:102:LEU:HD12	2.00	0.60
1:B:148:GLU:HG2	1:B:152:GLN:HE21	1.66	0.59
1:A:98:TYR:CE1	1:A:102:LEU:HD22	2.39	0.57
1:B:127:ILE:HG21	1:B:145:PHE:CD2	2.39	0.57
1:A:72:ASP:OD2	1:A:73:LEU:N	2.33	0.57
1:B:95:ASP:O	1:B:99:GLU:HG2	2.04	0.57
1:A:116:VAL:HG13	1:B:116:VAL:CG1	2.36	0.56
1:B:124:TRP:O	1:B:127:ILE:CD1	2.54	0.55
1:A:119:MET:SD	1:B:117:PHE:HE2	2.29	0.55
1:B:88:ARG:HB2	1:B:117:PHE:HD1	1.72	0.55
1:B:88:ARG:HB2	1:B:117:PHE:CD1	2.43	0.54
1:A:119:MET:SD	1:B:117:PHE:CE2	3.00	0.54
1:A:104:HIS:HE1	4:B:3020:HOH:O	1.90	0.54
1:A:22:VAL:O	1:A:26:THR:HG23	2.08	0.53
1:B:27:GLN:HB2	4:B:3170:HOH:O	2.08	0.52
1:A:133:LYS:O	1:A:137:ARG:HG3	2.10	0.52
1:B:42:LYS:HE3	4:B:3122:HOH:O	2.10	0.51
1:B:102:LEU:HD13	3:B:3000:COD:S44	2.51	0.51
1:A:61:HIS:HE1	4:A:540:HOH:O	1.93	0.51
1:B:127:ILE:H	1:B:127:ILE:CD1	2.25	0.50
1:A:10:THR:HG22	1:A:12:ASP:HB2	1.93	0.50
1:A:96:PHE:HE2	1:B:92:ALA:HA	1.76	0.50
1:A:49:GLU:N	1:A:49:GLU:OE2	2.43	0.49
1:A:38:ALA:HA	1:A:48:LEU:HD23	1.93	0.49
1:B:47:THR:OG1	1:B:50:GLU:HG3	2.13	0.49
1:B:127:ILE:HD11	3:B:3000:COD:HN71	1.78	0.48
1:A:28:MET:HG3	1:A:29:PHE:CD1	2.49	0.47
1:B:102:LEU:HD11	1:B:106:ASN:HD21	1.80	0.47
1:B:68:VAL:HG12	1:B:69:GLY:N	2.29	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:23:THR:O	1:A:27:GLN:HG3	2.15	0.46
1:A:40:PRO:HG2	1:A:42:LYS:O	2.15	0.46
4:A:517:HOH:O	1:B:104:HIS:HE1	1.99	0.46
1:B:102:LEU:CD1	3:B:3000:COD:S44	3.03	0.46
1:B:127:ILE:HD13	1:B:127:ILE:N	2.30	0.46
1:A:119:MET:CG	1:B:117:PHE:HE2	2.28	0.46
1:B:127:ILE:CD1	3:B:3000:COD:HN71	2.29	0.46
1:A:48:LEU:HD13	1:A:48:LEU:C	2.36	0.46
1:B:102:LEU:CD1	1:B:106:ASN:ND2	2.80	0.45
1:A:61:HIS:CD2	1:A:61:HIS:H	2.35	0.45
1:A:133:LYS:HB3	1:A:137:ARG:NH1	2.32	0.45
1:A:119:MET:HG3	1:B:117:PHE:HE2	1.82	0.45
1:A:26:THR:HG21	1:A:65:VAL:CG2	2.47	0.44
1:A:117:PHE:HB2	1:B:117:PHE:HB2	1.99	0.44
1:B:112:GLU:HB2	4:B:3120:HOH:O	2.18	0.43
1:A:127:ILE:HG13	1:A:127:ILE:O	2.19	0.43
1:B:43:LYS:N	1:B:44:PRO:HD3	2.34	0.43
1:A:104:HIS:HD2	4:B:3029:HOH:O	2.02	0.43
1:B:28:MET:HG3	1:B:29:PHE:CD1	2.54	0.43
1:A:40:PRO:HG2	1:A:44:PRO:HD3	2.01	0.42
1:A:48:LEU:O	1:A:52:VAL:HG23	2.19	0.42
1:B:64:ASN:HA	1:B:64:ASN:HD22	1.58	0.42
1:B:8:PRO:HA	1:B:35:ALA:O	2.19	0.42
1:A:27:GLN:HB2	4:A:606:HOH:O	2.19	0.42
1:A:127:ILE:HG23	4:A:532:HOH:O	2.20	0.42
1:B:141:ASP:OD2	1:B:143:THR:HG23	2.20	0.42
1:B:42:LYS:NZ	3:B:3000:COD:O26	2.52	0.42
1:B:159:ALA:HA	4:B:3172:HOH:O	2.20	0.42
1:B:102:LEU:C	1:B:102:LEU:HD12	2.40	0.41
1:B:127:ILE:CD1	3:B:3000:COD:N7	2.84	0.41
1:B:36:ILE:HD12	1:B:52:VAL:HA	2.02	0.41
1:B:28:MET:HG3	1:B:29:PHE:CE1	2.55	0.41
1:A:12:ASP:O	1:A:133:LYS:HD3	2.21	0.41
1:B:127:ILE:HD11	3:B:3000:COD:N7	2.35	0.41
1:B:143:THR:HG22	1:B:151:HIS:CE1	2.55	0.41
1:B:49:GLU:CD	1:B:49:GLU:N	2.71	0.41
1:A:112:GLU:CD	1:A:112:GLU:H	2.15	0.40
1:A:47:THR:OG1	1:A:50:GLU:HG3	2.21	0.40
1:A:28:MET:HG3	1:A:29:PHE:CE1	2.57	0.40
1:B:102:LEU:HD12	1:B:106:ASN:ND2	2.36	0.40

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the sym-

metry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:72:ASP:OD1	4:B:3140:HOH:O[24_555]	2.13	0.07

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	155/159 (98%)	152 (98%)	3 (2%)	0	100	100
1	B	155/159 (98%)	152 (98%)	3 (2%)	0	100	100
All	All	310/318 (98%)	304 (98%)	6 (2%)	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	132/134 (98%)	126 (96%)	6 (4%)	32	15
1	B	132/134 (98%)	125 (95%)	7 (5%)	26	11
All	All	264/268 (98%)	251 (95%)	13 (5%)	29	12

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

Mol	Chain	Res	Type
1	A	3	LYS

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Mol	Chain	Res	Type
1	A	13	PRO
1	A	49	GLU
1	A	80	ASN
1	A	97	GLU
1	A	131	LEU
1	B	3	LYS
1	B	64	ASN
1	B	95	ASP
1	B	102	LEU
1	B	112	GLU
1	B	127	ILE
1	B	131	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (16) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	16	ASN
1	A	56	GLN
1	A	61	HIS
1	A	80	ASN
1	A	104	HIS
1	A	138	HIS
1	A	152	GLN
1	B	16	ASN
1	B	27	GLN
1	B	56	GLN
1	B	64	ASN
1	B	80	ASN
1	B	81	GLN
1	B	104	HIS
1	B	106	ASN
1	B	152	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

There are no non-standard protein/DNA/RNA residues in this entry.

5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

5.6 Ligand geometry ⓘ

4 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$
2	SO4	A	502	-	4,4,4	0.29	0	6,6,6	0.11	0
3	COD	B	3000	-	39,46,46	1.76	11 (28%)	41,68,68	1.90	7 (17%)
2	SO4	B	501	-	4,4,4	0.32	0	6,6,6	0.09	0
2	SO4	B	503	-	4,4,4	0.32	0	6,6,6	0.10	0

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
2	SO4	A	502	-	-	0/0/0/0	0/0/0/0
3	COD	B	3000	-	-	0/39/59/59	0/3/3/3
2	SO4	B	501	-	-	0/0/0/0	0/0/0/0
2	SO4	B	503	-	-	0/0/0/0	0/0/0/0

All (11) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	3000	COD	C5-N8	-3.34	1.28	1.39
3	B	3000	COD	C43-S44	-2.16	1.73	1.80
3	B	3000	COD	C12-C11	2.06	1.56	1.53
3	B	3000	COD	O35-C34	2.10	1.27	1.23
3	B	3000	COD	C31-C29	2.38	1.59	1.53
3	B	3000	COD	C28-C29	2.69	1.56	1.52
3	B	3000	COD	C4-N3	3.03	1.40	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	3000	COD	C42-N41	3.06	1.53	1.46
3	B	3000	COD	C2-N1	3.33	1.40	1.33
3	B	3000	COD	C9-N8	3.92	1.42	1.34
3	B	3000	COD	C2-N3	4.03	1.38	1.32

All (7) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	3000	COD	N3-C2-N1	-7.99	121.90	128.86
3	B	3000	COD	O27-C28-C29	-3.39	105.10	110.55
3	B	3000	COD	C16-O17-C11	-2.22	107.41	109.77
3	B	3000	COD	C43-C42-N41	-2.13	107.85	112.50
3	B	3000	COD	C30-C29-C32	2.08	112.43	108.82
3	B	3000	COD	O17-C16-C14	2.49	110.13	105.17
3	B	3000	COD	C4-C5-N8	4.94	114.18	109.41

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

1 monomer is involved in 7 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	B	3000	COD	7	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.