wwPDB X-ray Structure Validation Summary Report (i)

Jan 31, 2016 – 06:19 PM GMT

PDB ID	:	1A6E
Title	:	THERMOSOME-MG-ADP-ALF3 COMPLEX
Authors	:	Ditzel, L.; Loewe, J.; Stock, D.; Stetter, K.-O.; Huber, H.; Huber, R.; Steinbacher, S.
Deposited on	:	1998-02-24
Resolution	:	3.20 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
http://wwpdb.org/validation/2016/XrayValidationReportHelp
with specific help available everywhere you see the (i) symbol.

The following versions of software and data (see references (i)) were used in the production of this report:

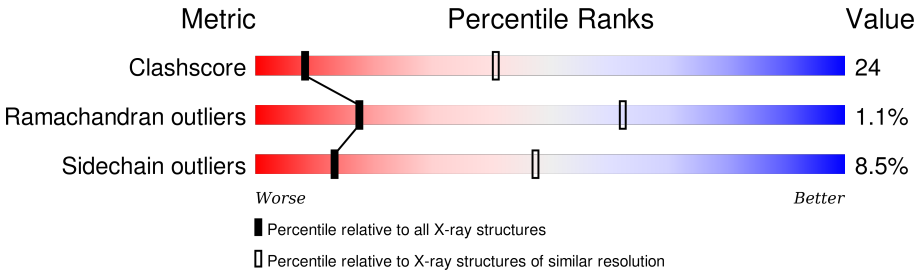
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	NOT EXECUTED
EDS	:	NOT EXECUTED
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	trunk26865

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 3.20 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	102246	1024 (3.22-3.18)
Ramachandran outliers	100387	1004 (3.22-3.18)
Sidechain outliers	100360	1003 (3.22-3.18)

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 <=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	545	49% 39% · 8%
2	B	543	49% 39% · 8%

2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 9390 atoms, of which 1742 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 THERMOSOME (ALPHA SUBUNIT).

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
			Total	C	H	N	O	S			
1	A	503	4668	2356	884	662	752	14	884	0	0

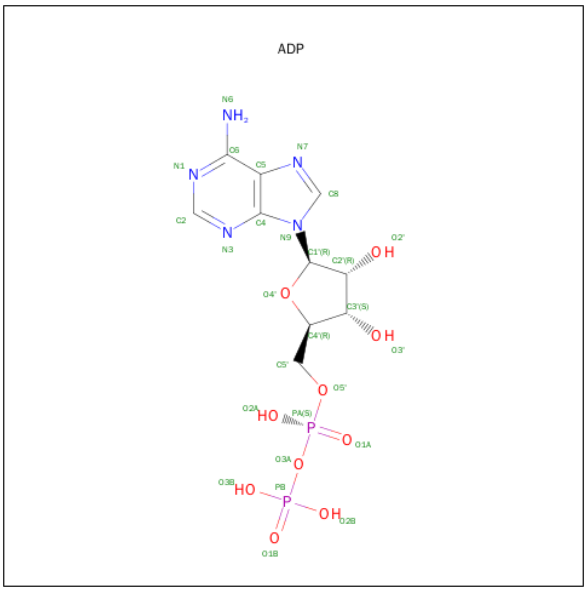
- Molecule 2 is a protein called THERMOSOME (BETA SUBUNIT).

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
			Total	C	H	N	O	S			
2	B	502	4656	2370	858	651	758	19	858	0	0

- Molecule 3 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

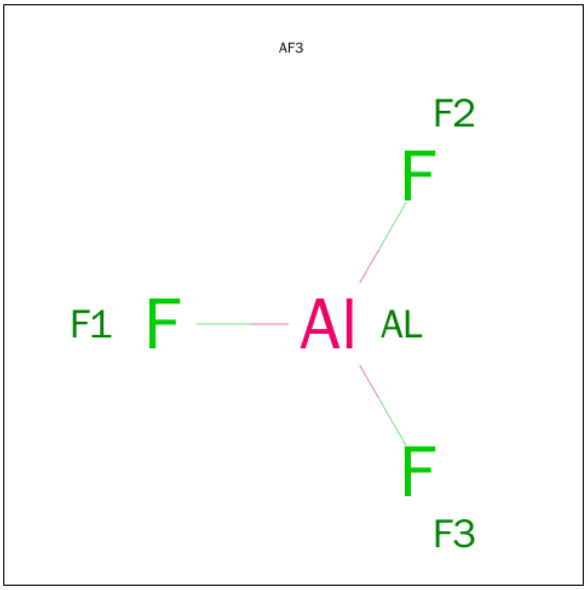
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	Mg		
3	B	1	1	1	0	0
			Total	Mg		
3	A	1	1	1	0	0

- Molecule 4 is ADENOSINE-5'-DIPHOSPHATE (three-letter code: ADP) (formula: $C_{10}H_{15}N_5O_{10}P_2$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
4	B	1	Total	C	N	O	P	0	0
			27	10	5	10	2		
4	A	1	Total	C	N	O	P	0	0
			27	10	5	10	2		

- Molecule 5 is ALUMINUM FLUORIDE (three-letter code: AF3) (formula: AlF_3).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
5	B	1	Total	Al	F		0	0
			4	1	3			
5	A	1	Total	Al	F		0	0
			4	1	3			

- Molecule 6 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	A	1	Total O 1 1	0	0
6	B	1	Total O 1 1	0	0

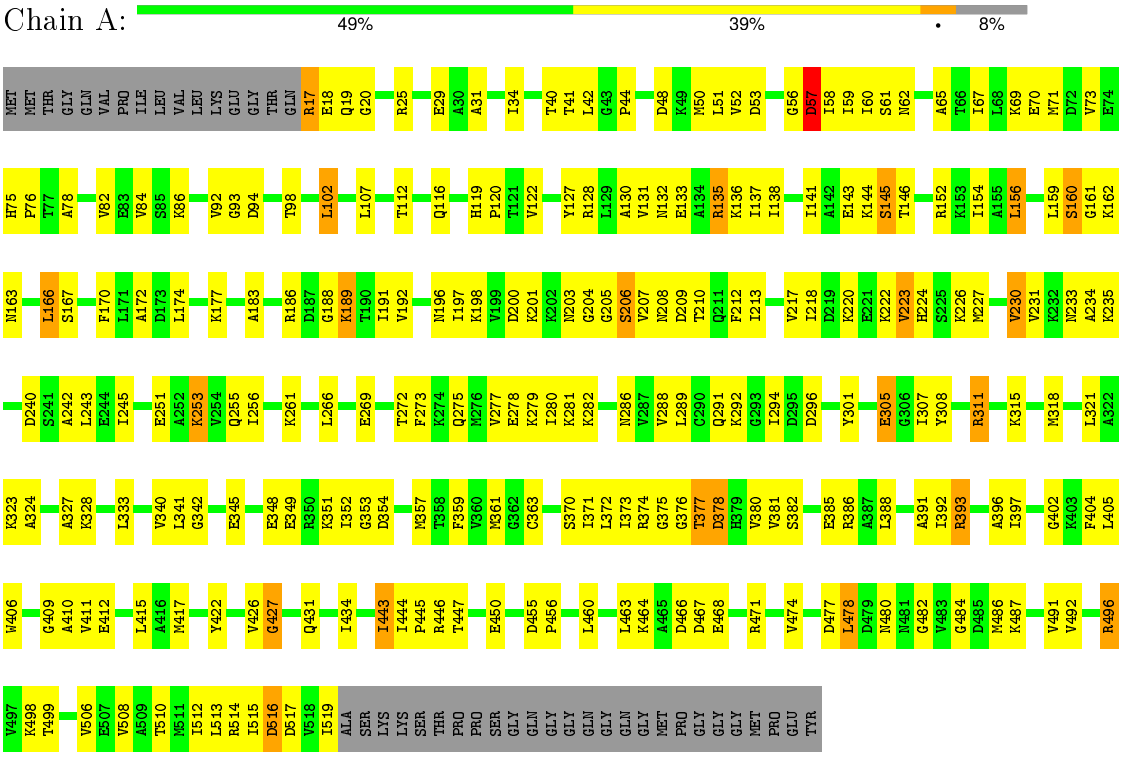
3 Residue-property plots (i)

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors 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.

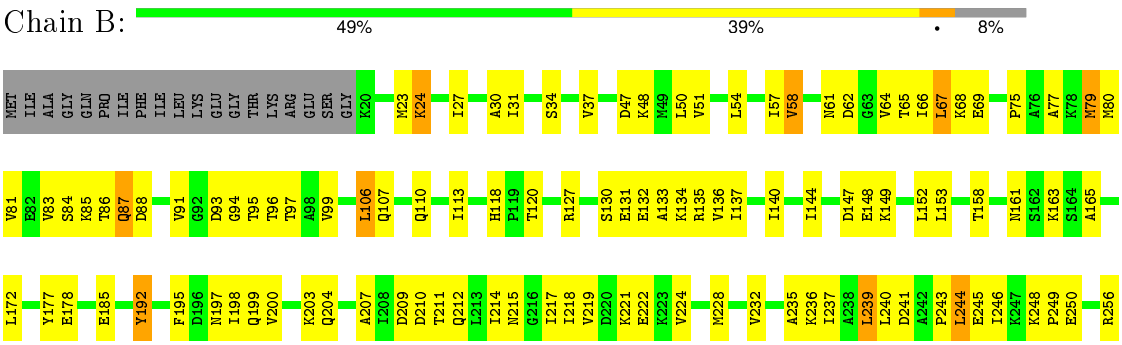
- Molecule 1: THERMOSOME (ALPHA SUBUNIT)

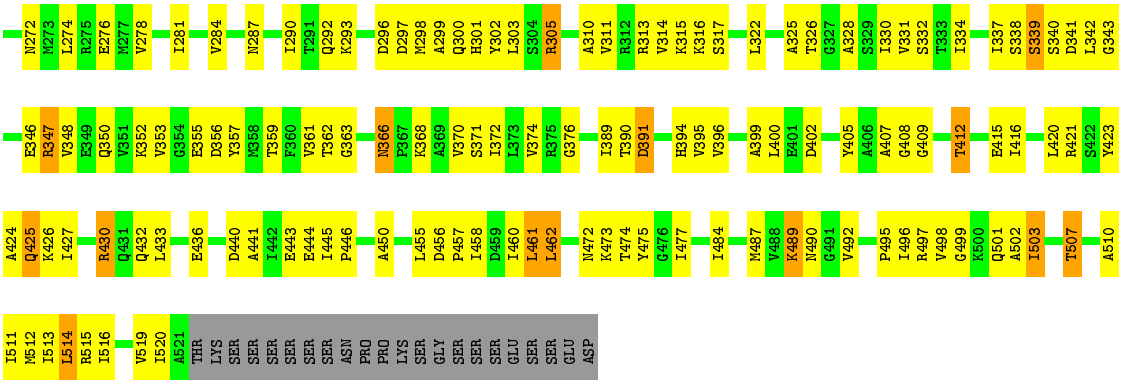
Chain A:



- Molecule 2: THERMOSOME (BETA SUBUNIT)

Chain B:




N272 M273 L274 R275 E276 M277 V278 I281 V284 N287 I290 T291 Q292 K293 D296 D297 M298 A299 Q300 H301 Y302 L303 S304 R305 A310 V311 R312 R313 V314 K315 K316 S317 L322 A325 T326 G327 A328 S329 I330 V331 S332 T333 I334 I337 S338 S339 S340 D341 L342 G343
E346 R347 V348 E349 Q350 V351 K352 V353 G354 E355 D356 Y357 M358 T359 F360 V361 T362 G363 N366 P367 K368 A369 V370 S371 I372 L373 V374 R375 G376 I389 T390 D391 H394 V395 V396 A399 L400 E401 D402 Y405 A406 A407 G408 G409 T412 E415 I416 L420 R421 S422 Y423
A424 Q425 K426 I427 R430 Q431 Q432 L433 E436 D440 A441 I442 E443 E444 I445 P446 A450 L455 D456 P457 I458 D459 I460 L461 L462 N472 K473 T474 Y475 G476 I477 I484 M487 V488 K489 N490 G491 V492 P495 I496 R497 V498 G499 K500 Q501 A502 I503 T507 A510
I511 M512 I513 L514 R515 I516 V519 I520 A521 THR LYS SER SER SER SER SER SER ASN PRO PRO LYS SER GLY SER SER SER GLU SER SER GLU ASP

4 Data and refinement statistics (i)

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

Property	Value	Source
Space group	I 4 2 2	Depositor
Cell constants a, b, c, α, β, γ	167.80Å 167.80Å 202.30Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	8.00 – 3.20	Depositor
% Data completeness (in resolution range)	92.5 (8.00-3.20)	Depositor
R_{merge}	(Not available)	Depositor
R_{sym}	0.11	Depositor
Refinement program	X-PLOR 3.851	Depositor
R, R_{free}	0.181 , 0.285	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	9390	wwPDB-VP
Average B, all atoms (Å^2)	31.0	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: MG, ADP, AF3

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	0.49	0/3812	0.74	2/5139 (0.0%)
2	B	0.52	0/3834	0.74	1/5166 (0.0%)
All	All	0.50	0/7646	0.74	3/10305 (0.0%)

There are no bond length outliers.

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	B	244	LEU	CA-CB-CG	5.21	127.28	115.30
1	A	57	ASP	N-CA-C	5.18	125.00	111.00
1	A	160	SER	N-CA-C	5.15	124.91	111.00

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	3784	884	3935	191	0
2	B	3798	858	3892	195	0
3	A	1	0	0	0	0
3	B	1	0	0	0	0
4	A	27	0	12	1	0
4	B	27	0	12	3	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
5	A	4	0	0	0	0
5	B	4	0	0	0	0
6	A	1	0	0	0	0
6	B	1	0	0	0	0
All	All	7648	1742	7851	374	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 24.

The worst 5 of 374 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:218:ILE:HD11	1:A:321:LEU:HD11	1.22	1.11
2:B:172:LEU:HD22	2:B:389:ILE:HD11	1.46	0.96
1:A:281:LYS:HD2	1:A:305:GLU:HG3	1.48	0.95
2:B:50:LEU:HB2	2:B:58:VAL:HG13	1.48	0.93
2:B:64:VAL:HG22	2:B:95:THR:HG21	1.49	0.93

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	501/545 (92%)	450 (90%)	41 (8%)	10 (2%)	9 48
2	B	500/543 (92%)	463 (93%)	36 (7%)	1 (0%)	52 88
All	All	1001/1088 (92%)	913 (91%)	77 (8%)	11 (1%)	17 62

5 of 11 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	57	ASP
1	A	145	SER
1	A	377	THR
1	A	378	ASP
1	A	160	SER

5.3.2 Protein sidechains

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	411/442 (93%)	375 (91%)	36 (9%)	12	45
2	B	410/446 (92%)	376 (92%)	34 (8%)	14	49
All	All	821/888 (92%)	751 (92%)	70 (8%)	13	47

5 of 70 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	467	ASP
2	B	67	LEU
2	B	462	LEU
1	A	478	LEU
1	A	516	ASP

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 26 such sidechains are listed below:

Mol	Chain	Res	Type
1	A	424	ASN
1	A	480	ASN
2	B	394	HIS
1	A	431	GLN
1	A	451	ASN

5.3.3 RNA

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 carbohydrates in this entry.

5.6 Ligand geometry (i)

Of 6 ligands modelled in this entry, 2 are monoatomic - leaving 4 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	$\#\|Z\| > 2$
4	ADP	A	898	3,5	22,29,29	1.20	3 (13%)	27,45,45	2.66	4 (14%)
5	AF3	A	899	3,4,6	0,3,3	0.00	-	0,3,3	0.00	-
4	ADP	B	998	3,5	22,29,29	1.16	3 (13%)	27,45,45	2.67	3 (11%)
5	AF3	B	999	3,4,6	0,3,3	0.00	-	0,3,3	0.00	-

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
4	ADP	A	898	3,5	-	0/12/32/32	0/3/3/3
5	AF3	A	899	3,4,6	-	0/0/0/0	0/0/0/0
4	ADP	B	998	3,5	-	0/12/32/32	0/3/3/3
5	AF3	B	999	3,4,6	-	0/0/0/0	0/0/0/0

The worst 5 of 6 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	898	ADP	C5-N7	-2.43	1.31	1.39
4	B	998	ADP	C5-N7	-2.22	1.31	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	898	ADP	O4'-C1'	2.42	1.44	1.41
4	B	998	ADP	O4'-C1'	2.66	1.44	1.41
4	B	998	ADP	PB-O2B	2.80	1.64	1.54

The worst 5 of 7 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	B	998	ADP	N3-C2-N1	-12.38	119.41	128.89
4	A	898	ADP	N3-C2-N1	-11.90	119.79	128.89
4	A	898	ADP	C2'-C1'-N9	-3.79	108.50	114.29
4	B	998	ADP	C2'-C1'-N9	-3.70	108.63	114.29
4	A	898	ADP	C4-C5-N7	-3.05	106.67	109.48

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

2 monomers are involved in 4 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	898	ADP	1	0
4	B	998	ADP	3	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 will therefore be empty.

6.2 Non-standard residues in protein, DNA, RNA chains

EDS was not executed - this section will therefore be empty.

6.3 Carbohydrates

EDS was not executed - this section will therefore be empty.

6.4 Ligands

EDS was not executed - this section will therefore be empty.

6.5 Other polymers

EDS was not executed - this section will therefore be empty.