



# wwPDB X-ray Structure Validation Summary Report

Feb 28, 2014 – 12:41 PM GMT

PDB ID : 1A6E  
Title : THERMOSOME-MG-ADP-ALF3COMPLEX  
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 validation summary report for a publicly released PDB entry.

We welcome your comments at [validation@mail.wwpdb.org](mailto:validation@mail.wwpdb.org)

A user guide is available at <http://wwpdb.org/ValidationPDFNotes.html>

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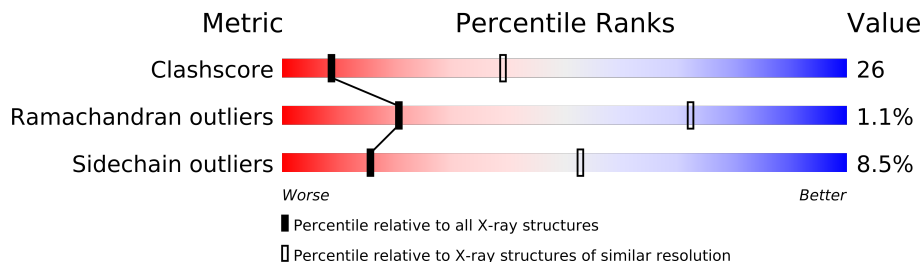
The following versions of software and data (see [references](#)) were used in the production of this report:

MolProbity	:	4.02b-467
Mogul	:	1.15 2013
Xtriage (Phenix)	:	NOT EXECUTED
EDS	:	NOT EXECUTED
Percentile statistics	:	21963
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et. al. (1996)
Validation Pipeline (wwPDB-VP)	:	stable22683

# 1 Overall quality at a glance

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	79885	1078 (3.26-3.14)
Ramachandran outliers	78287	1059 (3.26-3.14)
Sidechain outliers	78261	1058 (3.26-3.14)

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  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density.

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	545	
2	B	543	

## 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 deuterium.

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
1	A	503	Total	C	H	N	O	S	884	0	0
			4668	2356	884	662	752	14			

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

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

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

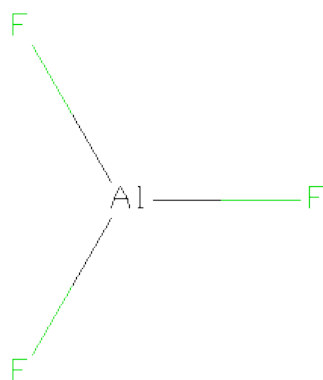
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	B	1	Total	Mg	0	0
			1	1		
3	A	1	Total	Mg	0	0
			1	1		

- Molecule 4 is ADENOSINE-5'-DIPHOSPHATE (three-letter code: ADP) (formula: C<sub>10</sub>H<sub>15</sub>N<sub>5</sub>O<sub>10</sub>P<sub>2</sub>).



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:  $\text{AlF}_3$ ).



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	0	0
			1	1		
6	B	1	Total	O	0	0
			1	1		

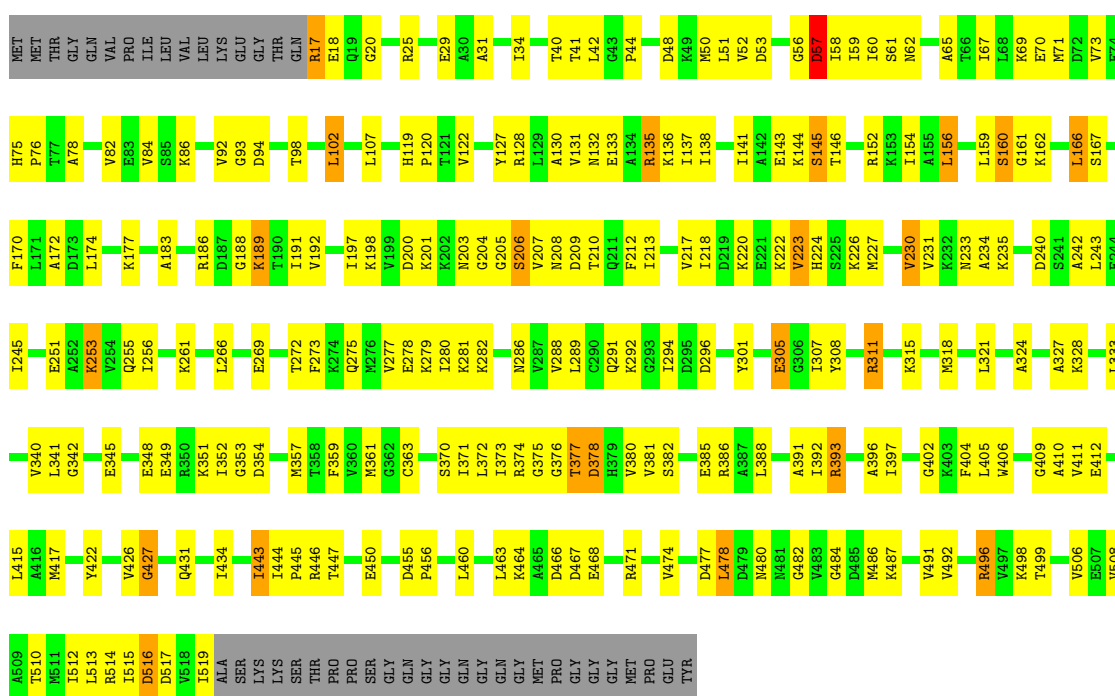
### 3 Residue-property plots

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.

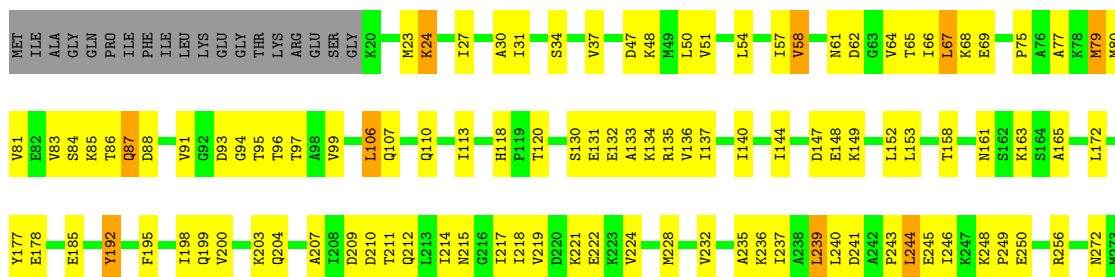
#### • Molecule 1: THERMOSOME (ALPHA SUBUNIT)

Chain A:



#### • Molecule 2: THERMOSOME (BETA SUBUNIT)

Chain B:



V519	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	N487	V488	K489	N490	G491	V492	P495	I496	R497	V498	G499	R500	Q501	A502	I503	T507	A510	I511	N512	I513	L514	R515	I516		
I520	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	N487	V488	K489	N490	G491	V492	P495	I496	R497	V498	G499	R500	Q501	A502	I503	T507	A510	I511	N512	I513	L514	R515	I516			
A521	V351	K352	V353	M354	E355	D356	Y357	M358	T359	F360	V361	T362	G363	N366	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		
THR	L274	R275	E276	M277	V278	I281	V284	I290	T291	Q292	K293	D296	D297	M298	A299	Q300	H301	Y302	I303	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
LYS	Q350	V351	K352	V353	M354	E355	D356	Y357	M358	T359	F360	V361	T362	G363	N366	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	
SER	L274	R275	E276	M277	V278	I281	V284	I290	T291	Q292	K293	D296	D297	M298	A299	Q300	H301	Y302	I303	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
SER	Q350	V351	K352	V353	M354	E355	D356	Y357	M358	T359	F360	V361	T362	G363	N366	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	
SER	L274	R275	E276	M277	V278	I281	V284	I290	T291	Q292	K293	D296	D297	M298	A299	Q300	H301	Y302	I303	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
ASN	Q350	V351	K352	V353	M354	E355	D356	Y357	M358	T359	F360	V361	T362	G363	N366	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	
PRO	L274	R275	E276	M277	V278	I281	V284	I290	T291	Q292	K293	D296	D297	M298	A299	Q300	H301	Y302	I303	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
PRO	Q350	V351	K352	V353	M354	E355	D356	Y357	M358	T359	F360	V361	T362	G363	N366	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	
LYS	L274	R275	E276	M277	V278	I281	V284	I290	T291	Q292	K293	D296	D297	M298	A299	Q300	H301	Y302	I303	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
SER	Q350	V351	K352	V353	M354	E355	D356	Y357	M358	T359	F360	V361	T362	G363	N366	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	
ASP	L274	R275	E276	M277	V278	I281	V284	I290	T291	Q292	K293	D296	D297	M298	A299	Q300	H301	Y302	I303	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

## 4 Data and refinement statistics

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, $\alpha$ , $\beta$ , $\gamma$	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 <sup>2</sup> )	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(°)	Ideal(°)
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 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 hydrogens added by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, and the number in parentheses is this value normalized per 1000 atoms of the molecule in the chain. The Symm-Clashes column gives symmetry related clashes, in the same way as for the Clashes column.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3784	884	3051	184	0
2	B	3798	858	3034	179	0
3	A	1	0	0	0	0
3	B	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	A	27	0	12	1	0
4	B	27	0	12	3	0
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	6109	353	0

Clashscore is defined as the number of clashes calculated for the entry per 1000 atoms (including hydrogens) of the entry. The overall clashscore for this entry is 26.

The worst 5 of 353 close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(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

### 5.3.1 Protein backbone ⓘ

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%)	11	56
2	B	500/543 (92%)	463 (93%)	36 (7%)	1 (0%)	56	93
All	All	1001/1088 (92%)	913 (91%)	77 (8%)	11 (1%)	21	72

5 of 11 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	57	ASP
1	A	145	SER

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Mol	Chain	Res	Type
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%)	14	50
2	B	410/446 (92%)	376 (92%)	34 (8%)	16	55
All	All	821/888 (92%)	751 (92%)	70 (8%)	15	53

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 13 such sidechains are listed below:

Mol	Chain	Res	Type
2	B	26	ASN
2	B	87	GLN
2	B	301	HIS
1	A	300	HIS
2	B	300	GLN

### 5.3.3 RNA ⓘ

There are no RNA chains 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 ⓘ

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	29,29,29	1.47	5 (17%)	45,45,45	2.33	7 (15%)
5	AF3	A	899	3,4,6	0,3,3	0.00	-	0,3,3	0.00	-
4	ADP	B	998	3,5	29,29,29	1.38	6 (20%)	45,45,45	2.23	8 (17%)
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	-	0/16/32/32	0/1/3/3
5	AF3	A	899	3,4,6	-	0/0/0/0	0/0/0/0
4	ADP	B	998	3,5	-	0/16/32/32	0/1/3/3
5	AF3	B	999	3,4,6	-	0/0/0/0	0/0/0/0

The worst 5 of 11 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	898	ADP	C4-N9	-4.16	1.31	1.37
4	B	998	ADP	C4-N9	-4.09	1.31	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	898	ADP	C2'-C1'	-3.01	1.49	1.53
4	A	898	ADP	PB-O2B	2.89	1.65	1.54
4	B	998	ADP	PB-O2B	2.75	1.64	1.54

The worst 5 of 15 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	B	998	ADP	N3-C2-N1	-11.12	119.41	128.71
4	A	898	ADP	N3-C2-N1	-10.67	119.79	128.71
4	A	898	ADP	O4'-C1'-N9	6.75	114.71	108.44
4	B	998	ADP	N3-C4-N9	4.66	133.85	125.43
4	A	898	ADP	N3-C4-N9	4.63	133.80	125.43

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

## 5.7 Other polymers ⓘ

There are no such residues in this entry.

## 5.8 Polymer linkage issues

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.