



# Full wwPDB X-ray Structure Validation Report ⓘ

Mar 7, 2026 – 01:07 AM UTC

PDB ID : 3CAA / pdb\_00003caa  
Title : CLEAVED ANTICHYMOTRYPSIN A347R  
Authors : Lukacs, C.M.; Christianson, D.W.  
Deposited on : 1997-08-18  
Resolution : 2.40 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](mailto: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>.

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

MolProbity : 4-5-2 with Phenix2.0  
Xtrriage (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

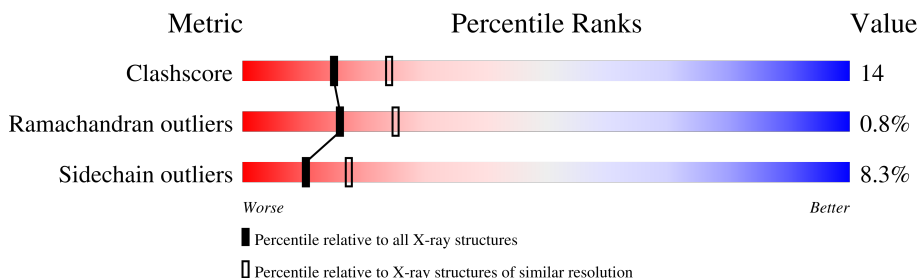
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.40 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	5391 (2.40-2.40)
Ramachandran outliers	187476	5320 (2.40-2.40)
Sidechain outliers	187428	5321 (2.40-2.40)

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  $\geq 3$ , 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	341	
2	B	37	

## 2 Entry composition [i](#)

There are 3 unique types of molecules in this entry. The entry contains 2978 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 ANTICHYMOTRYPSIN.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	334	2663	1707	437	508	11	0	0	0

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	347	ARG	ALA	engineered mutation	UNP P01011

- Molecule 2 is a protein called ANTICHYMOTRYPSIN.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
2	B	32	268	176	47	43	2	0	0	0

- Molecule 3 is water.

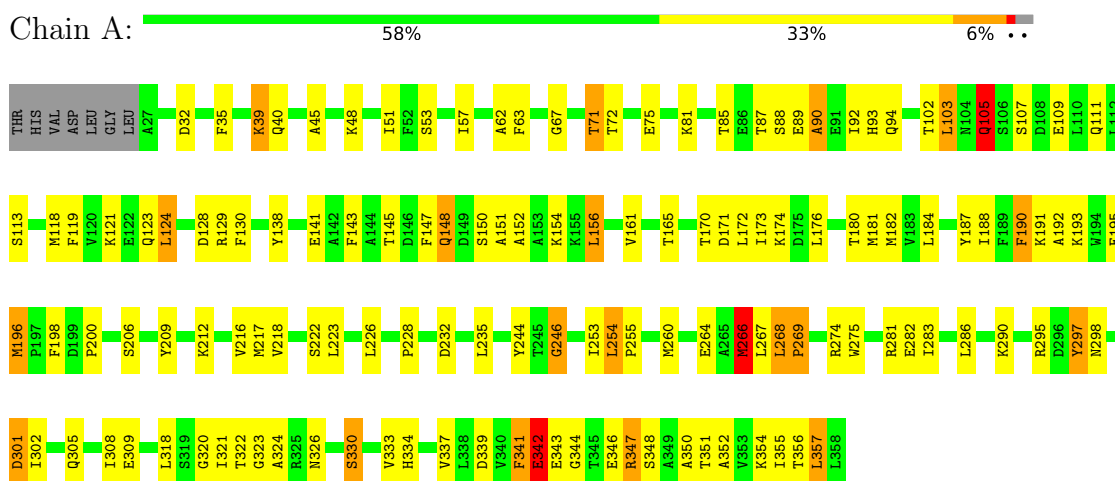
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	39	Total 39	O 39	0	0
3	B	8	Total 8	O 8	0	0

### 3 Residue-property plots

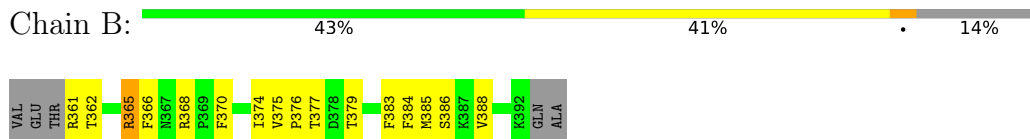
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry. Residues are color-coded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



#### • Molecule 2: ANTICHYMOTRYPSIN



## 4 Data and refinement statistics

Xtrriage (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, $\alpha$ , $\beta$ , $\gamma$	74.12Å 77.73Å 79.49Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	20.00 – 2.40	Depositor
% Data completeness (in resolution range)	78.5 (20.00-2.40)	Depositor
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	0.10	Depositor
Refinement program	X-PLOR	Depositor
R, $R_{free}$	0.190 , 0.280	Depositor
Estimated twinning fraction	No twinning to report.	Xtrriage
Total number of atoms	2978	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	35.0	wwPDB-VP

## 5 Model quality i

### 5.1 Standard geometry i

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	1.23	11/2713 (0.4%)	1.36	32/3666 (0.9%)
2	B	1.27	2/274 (0.7%)	1.38	4/370 (1.1%)
All	All	1.23	13/2987 (0.4%)	1.36	36/4036 (0.9%)

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	3

All (13) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	196	MET	SD-CE	8.71	2.01	1.79
1	A	283	ILE	CA-CB	6.22	1.61	1.54
2	B	388	VAL	CA-CB	6.21	1.61	1.53
1	A	57	ILE	CA-CB	5.69	1.61	1.54
1	A	218	VAL	CA-C	5.60	1.58	1.52
1	A	308	ILE	CA-CB	5.44	1.59	1.53
1	A	228	PRO	CA-C	5.43	1.58	1.52
1	A	218	VAL	CA-CB	5.36	1.63	1.54
2	B	368	ARG	CA-C	5.30	1.57	1.52
1	A	62	ALA	CA-CB	-5.29	1.44	1.53
1	A	266	MET	SD-CE	5.21	1.92	1.79
1	A	330	SER	CA-C	5.11	1.59	1.52
1	A	63	PHE	CA-C	5.05	1.59	1.52

All (36) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	103	LEU	N-CA-C	-9.84	100.12	113.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	124	LEU	N-CA-C	-8.17	95.59	109.24
2	B	386	SER	N-CA-C	7.79	120.36	108.52
1	A	290	LYS	N-CA-C	-7.59	96.86	109.24
1	A	53	SER	CA-C-N	7.08	126.91	119.05
1	A	53	SER	C-N-CA	7.08	126.91	119.05
1	A	342	GLU	N-CA-C	6.82	120.86	112.54
1	A	320	GLY	N-CA-C	-6.63	106.44	114.66
1	A	128	ASP	N-CA-C	-6.18	103.85	111.33
1	A	209	TYR	N-CA-C	6.09	118.12	108.67
1	A	171	ASP	N-CA-C	6.01	120.26	108.18
1	A	298	ASN	N-CA-C	-5.95	97.46	107.99
2	B	365	ARG	N-CA-C	5.78	118.31	108.02
1	A	85	THR	N-CA-C	-5.77	104.91	111.14
1	A	152	ALA	N-CA-C	5.76	118.67	111.24
1	A	105	GLN	N-CA-C	5.73	123.01	110.80
1	A	151	ALA	N-CA-C	-5.72	104.96	111.14
1	A	323	GLY	N-CA-C	-5.63	106.76	114.64
1	A	130	PHE	N-CA-C	-5.55	104.87	111.03
1	A	309	GLU	N-CA-C	5.49	119.65	112.13
1	A	72	THR	N-CA-C	-5.46	105.01	110.97
1	A	254	LEU	CA-C-N	5.43	125.33	119.85
1	A	254	LEU	C-N-CA	5.43	125.33	119.85
2	B	377	THR	N-CA-C	5.37	118.05	111.82
1	A	180	THR	N-CA-C	-5.33	101.09	109.25
1	A	195	GLU	N-CA-C	-5.30	105.59	111.36
1	A	161	VAL	N-CA-C	5.29	116.01	110.62
1	A	51	ILE	CB-CA-C	-5.25	102.68	111.29
1	A	246	GLY	CA-C-N	-5.21	115.40	123.17
1	A	246	GLY	C-N-CA	-5.21	115.40	123.17
1	A	102	THR	CB-CA-C	5.18	118.18	111.50
1	A	244	TYR	N-CA-C	-5.18	102.11	110.14
1	A	297	TYR	N-CA-C	5.09	117.12	109.23
1	A	90	ALA	CA-C-N	5.08	127.53	120.63
1	A	90	ALA	C-N-CA	5.08	127.53	120.63
2	B	370	PHE	N-CA-C	5.02	116.44	108.96

There are no chirality outliers.

All (3) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	138	TYR	Sidechain
1	A	187	TYR	Sidechain

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Mol	Chain	Res	Type	Group
1	A	297	TYR	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	2663	0	2679	75	0
2	B	268	0	284	12	0
3	A	39	0	0	0	0
3	B	8	0	0	1	0
All	All	2978	0	2963	81	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 14.

All (81) 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:191:LYS:HG3	1:A:346:GLU:HG2	1.52	0.90
1:A:281:ARG:NH1	2:B:362:THR:HG21	1.89	0.86
1:A:330:SER:HB2	1:A:356:THR:HG23	1.69	0.74
1:A:141:GLU:HG2	1:A:143:PHE:CE1	2.24	0.73
1:A:216:VAL:HG12	1:A:217:MET:H	1.58	0.69
1:A:40:GLN:HB3	1:A:302:ILE:CD1	2.24	0.67
1:A:40:GLN:HB3	1:A:302:ILE:HD12	1.76	0.66
1:A:71:THR:O	1:A:75:GLU:HG3	1.96	0.66
1:A:141:GLU:HG2	1:A:143:PHE:CZ	2.31	0.66
1:A:103:LEU:HD21	1:A:113:SER:HA	1.79	0.63
1:A:121:LYS:HD3	1:A:181:MET:HE1	1.80	0.63
1:A:121:LYS:HD3	1:A:181:MET:CE	2.28	0.63
1:A:281:ARG:HH11	2:B:362:THR:HG21	1.63	0.61
1:A:223:LEU:HD13	1:A:226:LEU:HD13	1.83	0.59
1:A:226:LEU:HD23	1:A:226:LEU:H	1.68	0.59
1:A:67:GLY:HA3	1:A:321:ILE:HG13	1.86	0.58
1:A:198:PHE:HB2	1:A:342:GLU:CB	2.35	0.56
2:B:376:PRO:HG3	2:B:383:PHE:CZ	2.41	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:267:LEU:O	1:A:268:LEU:HD23	2.05	0.55
1:A:281:ARG:HH12	2:B:362:THR:HG21	1.66	0.55
1:A:232:ASP:CG	1:A:274:ARG:HH12	2.14	0.55
1:A:318:LEU:HB3	1:A:321:ILE:HD12	1.89	0.54
1:A:35:PHE:HD2	1:A:269:PRO:HD3	1.73	0.54
1:A:154:LYS:HE3	1:A:174:LYS:O	2.08	0.53
1:A:196:MET:HE1	1:A:226:LEU:HB2	1.90	0.53
1:A:191:LYS:HG3	1:A:346:GLU:CG	2.34	0.53
1:A:193:LYS:HD2	1:A:343:GLU:O	2.09	0.52
1:A:45:ALA:HB1	1:A:48:LYS:HD3	1.91	0.52
1:A:109:GLU:OE2	1:A:193:LYS:HG3	2.09	0.52
1:A:301:ASP:O	1:A:305:GLN:HG2	2.09	0.52
1:A:281:ARG:HG2	1:A:282:GLU:N	2.25	0.52
1:A:216:VAL:HG12	1:A:217:MET:N	2.25	0.51
2:B:376:PRO:HB2	2:B:379:THR:HB	1.92	0.51
1:A:330:SER:HB2	1:A:356:THR:CG2	2.41	0.51
1:A:150:SER:O	1:A:154:LYS:HB2	2.13	0.48
1:A:103:LEU:CD2	1:A:113:SER:HA	2.43	0.48
1:A:223:LEU:HD13	1:A:226:LEU:CD1	2.44	0.48
1:A:337:VAL:O	1:A:347:ARG:HA	2.13	0.48
1:A:334:HIS:HA	1:A:350:ALA:O	2.14	0.48
1:A:182:MET:HE3	1:A:355:ILE:HG13	1.96	0.47
1:A:176:LEU:HD13	1:A:354:LYS:HE2	1.96	0.47
1:A:39:LYS:NZ	1:A:268:LEU:HD23	2.30	0.46
2:B:376:PRO:HG3	2:B:383:PHE:CE1	2.51	0.46
1:A:87:THR:HG21	1:A:92:ILE:HG13	1.97	0.46
1:A:87:THR:HG22	1:A:88:SER:O	2.15	0.46
1:A:254:LEU:HB2	2:B:366:PHE:CE2	2.50	0.46
1:A:121:LYS:NZ	1:A:148:GLN:HE22	2.14	0.46
1:A:35:PHE:HE1	2:B:385:MET:HE1	1.81	0.46
1:A:341:PHE:N	1:A:341:PHE:CD1	2.83	0.46
1:A:198:PHE:HB2	1:A:342:GLU:HB3	1.97	0.45
1:A:32:ASP:OD2	1:A:81:LYS:HD2	2.17	0.45
1:A:165:THR:HG22	1:A:348:SER:HB2	1.99	0.45
1:A:121:LYS:HD3	1:A:181:MET:HE3	1.98	0.45
1:A:119:PHE:HE2	1:A:156:LEU:HD13	1.82	0.44
2:B:365:ARG:NH1	3:B:547:HOH:O	2.49	0.44
1:A:40:GLN:HB3	1:A:302:ILE:HD13	1.96	0.44
1:A:111:GLN:O	1:A:190:PHE:HA	2.18	0.44
1:A:266:MET:HE2	1:A:266:MET:HB3	1.58	0.44
1:A:190:PHE:CD1	1:A:190:PHE:C	2.96	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:347:ARG:HD2	2:B:374:ILE:HD12	1.99	0.43
1:A:90:ALA:O	1:A:94:GLN:HG3	2.17	0.43
1:A:260:MET:O	1:A:264:GLU:HG3	2.18	0.43
1:A:333:VAL:O	1:A:351:THR:HA	2.19	0.43
1:A:89:GLU:O	1:A:93:HIS:HD2	2.02	0.43
1:A:192:ALA:O	1:A:344:GLY:HA3	2.18	0.43
2:B:374:ILE:HB	2:B:384:PHE:HB3	2.00	0.43
1:A:188:ILE:HD13	1:A:188:ILE:HG21	1.82	0.42
1:A:253:ILE:HG12	1:A:275:TRP:CZ3	2.53	0.42
2:B:375:VAL:HB	2:B:376:PRO:CD	2.49	0.42
1:A:103:LEU:C	1:A:105:GLN:N	2.77	0.42
1:A:200:PRO:HG3	1:A:342:GLU:HG3	2.01	0.42
1:A:184:LEU:O	1:A:352:ALA:HA	2.19	0.42
1:A:254:LEU:HA	1:A:255:PRO:HD3	1.83	0.42
1:A:301:ASP:OD1	1:A:301:ASP:N	2.53	0.42
1:A:222:SER:HA	1:A:286:LEU:O	2.19	0.42
1:A:357:LEU:HD12	1:A:357:LEU:H	1.85	0.42
1:A:295:ARG:HD2	1:A:295:ARG:HA	1.83	0.42
1:A:267:LEU:HA	1:A:267:LEU:HD23	1.85	0.41
1:A:129:ARG:HD2	1:A:129:ARG:O	2.19	0.41
1:A:324:ALA:HB3	1:A:326:ASN:OD1	2.20	0.41
1:A:147:PHE:HE1	1:A:176:LEU:HD21	1.85	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	332/341 (97%)	309 (93%)	20 (6%)	3 (1%)	14	22
2	B	30/37 (81%)	30 (100%)	0	0	100	100
All	All	362/378 (96%)	339 (94%)	20 (6%)	3 (1%)	16	25

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	105	GLN
1	A	246	GLY
1	A	123	GLN

### 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	295/301 (98%)	269 (91%)	26 (9%)	9 15
2	B	32/36 (89%)	31 (97%)	1 (3%)	35 57
All	All	327/337 (97%)	300 (92%)	27 (8%)	10 17

All (27) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	39	LYS
1	A	71	THR
1	A	105	GLN
1	A	107	SER
1	A	118	MET
1	A	124	LEU
1	A	145	THR
1	A	148	GLN
1	A	156	LEU
1	A	170	THR
1	A	172	LEU
1	A	173	ILE
1	A	190	PHE
1	A	206	SER
1	A	212	LYS
1	A	235	LEU
1	A	266	MET
1	A	268	LEU
1	A	269	PRO
1	A	301	ASP

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Mol	Chain	Res	Type
1	A	322	THR
1	A	339	ASP
1	A	341	PHE
1	A	342	GLU
1	A	347	ARG
1	A	357	LEU
2	B	361	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (5) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	93	HIS
1	A	94	GLN
1	A	148	GLN
1	A	204	HIS
1	A	247	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](#)

There are no ligands in this entry.

### 5.7 Other polymers [i](#)

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 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.