Full wwPDB X-ray Structure Validation Report (i)

Jan 31, 2016 – 10:14 PM GMT

PDB ID	:	1SRP
Title	:	STRUCTURAL ANALYSIS OF SERRATIA PROTEASE
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Deposited on	:	1994-11-02
Resolution	:	2.00 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 (i) symbol.

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

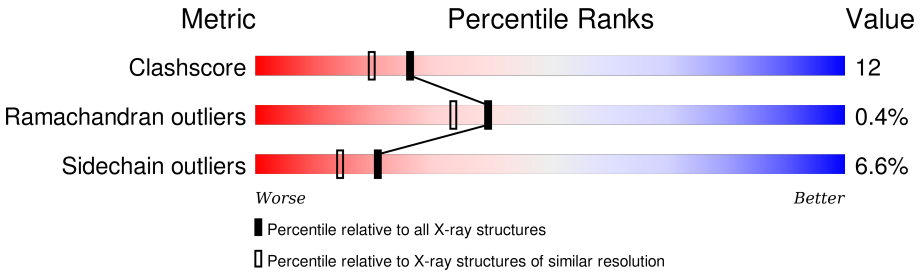
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	NOT EXECUTED
EDS	:	NOT EXECUTED
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)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

1 Overall quality at a glance

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

The reported resolution of this entry is 2.00 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	7340 (2.00-2.00)
Ramachandran outliers	100387	7248 (2.00-2.00)
Sidechain outliers	100360	7247 (2.00-2.00)

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	471	77% 17% 5% •

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 3780 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 SERRALYSIN.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	468	Total	C	N	O	S	0	0	0
			3560	2227	609	723	1			

There are 5 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	200	ARG	ASN	CONFLICT	UNP P07268
A	250	LEU	PRO	CONFLICT	UNP P07268
A	412	GLN	ASN	CONFLICT	UNP P07268
A	426	ALA	THR	CONFLICT	UNP P07268
A	438	ASN	SER	CONFLICT	UNP P07268

- Molecule 2 is CALCIUM ION (three-letter code: CA) (formula: Ca).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	7	Total	Ca	0	0
			7	7		

- Molecule 3 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	1	Total	Zn	0	0
			1	1		

- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	212	Total	O	0	0
			212	212		

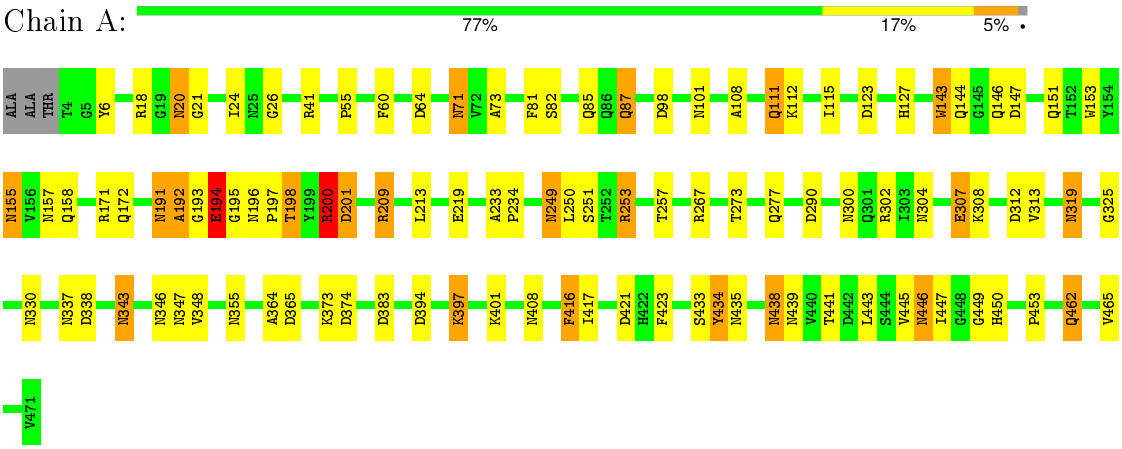
3 Residue-property plots (i)

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: SERRALYSIN

Chain A:



4 Data and refinement statistics (i)

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

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	109.14Å 150.89Å 42.64Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	8.00 – 2.00	Depositor
% Data completeness (in resolution range)	78.6 (8.00-2.00)	Depositor
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	GPRLSA	Depositor
R, R_{free}	0.193 , 0.184	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	3780	wwPDB-VP
Average B, all atoms (Å^2)	18.0	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: ZN, CA

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	0.85	1/3645 (0.0%)	1.60	41/4952 (0.8%)

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	1

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	307	GLU	CD-OE1	-5.05	1.20	1.25

All (41) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	374	ASP	CB-CG-OD2	10.96	128.16	118.30
1	A	302	ARG	NE-CZ-NH2	-10.06	115.27	120.30
1	A	18	ARG	NE-CZ-NH1	9.85	125.22	120.30
1	A	64	ASP	CB-CG-OD2	-9.73	109.54	118.30
1	A	41	ARG	NE-CZ-NH1	9.42	125.01	120.30
1	A	200	ARG	CD-NE-CZ	-8.61	111.54	123.60
1	A	365	ASP	CB-CG-OD2	8.24	125.72	118.30
1	A	312	ASP	CB-CG-OD2	8.20	125.68	118.30
1	A	374	ASP	CB-CG-OD1	-7.93	111.17	118.30
1	A	421	ASP	CB-CG-OD1	7.86	125.37	118.30
1	A	171	ARG	NE-CZ-NH1	7.23	123.91	120.30
1	A	307	GLU	CG-CD-OE2	-6.38	105.54	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	201	ASP	CB-CG-OD2	6.29	123.96	118.30
1	A	194	GLU	CA-CB-CG	6.26	127.17	113.40
1	A	98	ASP	CB-CG-OD1	6.10	123.79	118.30
1	A	6	TYR	CB-CG-CD1	-6.06	117.37	121.00
1	A	416	PHE	CB-CA-C	5.90	122.21	110.40
1	A	434	TYR	CB-CG-CD2	-5.84	117.49	121.00
1	A	433	SER	N-CA-CB	5.83	119.25	110.50
1	A	267	ARG	NE-CZ-NH2	-5.76	117.42	120.30
1	A	394	ASP	CB-CG-OD1	5.71	123.44	118.30
1	A	253	ARG	NE-CZ-NH1	5.66	123.13	120.30
1	A	383	ASP	CB-CG-OD2	-5.64	113.23	118.30
1	A	307	GLU	CB-CA-C	-5.61	99.19	110.40
1	A	365	ASP	CB-CG-OD1	-5.39	113.45	118.30
1	A	401	LYS	CB-CA-C	-5.36	99.67	110.40
1	A	6	TYR	CB-CG-CD2	5.36	124.21	121.00
1	A	462	GLN	CA-CB-CG	5.33	125.13	113.40
1	A	338	ASP	CB-CG-OD1	5.31	123.08	118.30
1	A	198	THR	CA-CB-CG2	5.28	119.80	112.40
1	A	219	GLU	OE1-CD-OE2	-5.19	117.07	123.30
1	A	308	LYS	CA-CB-CG	-5.16	102.06	113.40
1	A	98	ASP	CB-CG-OD2	-5.12	113.69	118.30
1	A	290	ASP	O-C-N	5.09	130.84	122.70
1	A	209	ARG	NE-CZ-NH2	5.09	122.84	120.30
1	A	201	ASP	CB-CG-OD1	-5.07	113.74	118.30
1	A	198	THR	N-CA-CB	-5.07	100.68	110.30
1	A	416	PHE	CB-CG-CD1	-5.07	117.25	120.80
1	A	147	ASP	CB-CG-OD1	5.05	122.84	118.30
1	A	441	THR	CA-CB-CG2	5.04	119.45	112.40
1	A	171	ARG	NE-CZ-NH2	-5.03	117.79	120.30

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	200	ARG	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	3560	0	3277	84	0
2	A	7	0	0	0	0
3	A	1	0	0	0	0
4	A	212	0	0	1	0
All	All	3780	0	3277	84	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 12.

All (84) 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:198:THR:HG22	1:A:200:ARG:HB2	1.30	1.12
1:A:408:ASN:HD21	1:A:417:ILE:H	1.11	0.95
1:A:198:THR:CG2	1:A:200:ARG:HB2	1.96	0.95
1:A:20:ASN:ND2	1:A:21:GLY:N	2.20	0.89
1:A:20:ASN:ND2	1:A:21:GLY:H	1.74	0.86
1:A:123:ASP:OD1	1:A:127:HIS:HD2	1.58	0.85
1:A:337:ASN:ND2	1:A:355:ASN:H	1.75	0.84
1:A:337:ASN:HD22	1:A:355:ASN:H	1.27	0.83
1:A:198:THR:HG22	1:A:200:ARG:H	1.46	0.80
1:A:198:THR:HG22	1:A:200:ARG:CB	2.12	0.79
1:A:313:VAL:H	1:A:319:ASN:HD21	1.27	0.79
1:A:20:ASN:HD22	1:A:21:GLY:N	1.80	0.79
1:A:151:GLN:HE21	1:A:153:TRP:HE1	1.31	0.78
1:A:82:SER:H	1:A:85:GLN:HE21	1.31	0.77
1:A:143:TRP:HA	1:A:143:TRP:CE3	2.20	0.76
1:A:330:ASN:HD22	1:A:348:VAL:H	1.37	0.71
1:A:108:ALA:HB3	1:A:111:GLN:CG	2.21	0.71
1:A:191:ASN:HD22	1:A:191:ASN:C	1.92	0.70
1:A:438:ASN:HD22	1:A:438:ASN:C	1.95	0.70
1:A:194:GLU:OE1	1:A:195:GLY:N	2.24	0.70
1:A:143:TRP:HA	1:A:143:TRP:HE3	1.53	0.70
1:A:172:GLN:HE22	1:A:209:ARG:HE	1.41	0.68
1:A:319:ASN:H	1:A:319:ASN:HD22	1.41	0.67
1:A:198:THR:HG22	1:A:200:ARG:N	2.09	0.66
1:A:108:ALA:HB3	1:A:111:GLN:CD	2.16	0.66
1:A:108:ALA:HB3	1:A:111:GLN:HG2	1.76	0.66
1:A:20:ASN:CG	1:A:21:GLY:H	1.97	0.65
1:A:197:PRO:HA	1:A:201:ASP:OD2	1.97	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:355:ASN:ND2	1:A:373:LYS:H	1.96	0.64
1:A:155:ASN:HD22	1:A:157:ASN:H	1.48	0.61
1:A:172:GLN:NE2	1:A:209:ARG:HE	1.98	0.61
1:A:194:GLU:CD	1:A:195:GLY:H	2.05	0.60
1:A:71:ASN:C	1:A:71:ASN:HD22	2.06	0.59
1:A:155:ASN:ND2	1:A:157:ASN:H	2.00	0.59
1:A:446:ASN:HD21	1:A:450:HIS:H	1.51	0.59
1:A:20:ASN:C	1:A:20:ASN:HD22	2.02	0.59
1:A:249:ASN:C	1:A:249:ASN:HD22	2.07	0.58
1:A:355:ASN:HD22	1:A:373:LYS:H	1.52	0.58
1:A:300:ASN:ND2	1:A:337:ASN:H	2.01	0.58
1:A:249:ASN:ND2	1:A:251:SER:H	2.02	0.57
1:A:155:ASN:C	1:A:155:ASN:HD22	2.09	0.56
1:A:319:ASN:H	1:A:319:ASN:ND2	2.03	0.56
1:A:346:ASN:ND2	1:A:364:ALA:H	2.03	0.56
1:A:435:ASN:HB3	1:A:438:ASN:HD21	1.71	0.56
1:A:446:ASN:ND2	1:A:449:GLY:H	2.04	0.56
1:A:198:THR:CG2	1:A:200:ARG:H	2.15	0.56
1:A:337:ASN:HD22	1:A:355:ASN:N	2.01	0.55
1:A:123:ASP:OD1	1:A:127:HIS:CD2	2.49	0.55
1:A:249:ASN:HD22	1:A:251:SER:H	1.56	0.54
1:A:434:TYR:CZ	1:A:462:GLN:HG2	2.43	0.54
1:A:172:GLN:NE2	4:A:625:HOH:O	2.40	0.53
1:A:307:GLU:CD	1:A:325:GLY:H	2.12	0.51
1:A:273:THR:H	1:A:277:GLN:NE2	2.08	0.51
1:A:249:ASN:HD21	1:A:251:SER:HB2	1.75	0.51
1:A:172:GLN:HE22	1:A:209:ARG:NE	2.07	0.50
1:A:82:SER:H	1:A:85:GLN:NE2	2.05	0.50
1:A:194:GLU:CG	1:A:195:GLY:H	2.23	0.50
1:A:60:PHE:HA	1:A:115:ILE:O	2.11	0.50
1:A:397:LYS:HB3	1:A:462:GLN:O	2.12	0.50
1:A:195:GLY:C	1:A:197:PRO:HD3	2.32	0.50
1:A:423:PHE:CE2	1:A:453:PRO:HG3	2.46	0.49
1:A:191:ASN:ND2	1:A:191:ASN:C	2.61	0.49
1:A:408:ASN:ND2	1:A:416:PHE:HB3	2.28	0.49
1:A:343:ASN:ND2	1:A:347:ASN:HD21	2.11	0.48
1:A:24:ILE:C	1:A:26:GLY:H	2.16	0.48
1:A:445:VAL:HG12	1:A:447:ILE:HG13	1.95	0.48
1:A:253:ARG:HD2	1:A:257:THR:HG21	1.96	0.47
1:A:191:ASN:HD22	1:A:192:ALA:N	2.13	0.47
1:A:158:GLN:HE21	1:A:158:GLN:HA	1.80	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:155:ASN:HD21	1:A:157:ASN:HB2	1.80	0.46
1:A:343:ASN:HD22	1:A:343:ASN:C	2.20	0.46
1:A:438:ASN:C	1:A:438:ASN:ND2	2.67	0.45
1:A:200:ARG:CZ	1:A:200:ARG:HB3	2.47	0.44
1:A:111:GLN:H	1:A:111:GLN:HG2	1.36	0.44
1:A:71:ASN:ND2	1:A:73:ALA:H	2.16	0.44
1:A:55:PRO:HB3	1:A:101:ASN:HB3	2.00	0.44
1:A:143:TRP:CA	1:A:143:TRP:CE3	2.98	0.44
1:A:343:ASN:HD21	1:A:347:ASN:HD21	1.67	0.42
1:A:233:ALA:HB1	1:A:234:PRO:HD2	2.01	0.42
1:A:435:ASN:HB3	1:A:438:ASN:ND2	2.36	0.41
1:A:191:ASN:O	1:A:192:ALA:O	2.37	0.41
1:A:438:ASN:HD22	1:A:439:ASN:N	2.19	0.41
1:A:87:GLN:HE21	1:A:87:GLN:HB3	1.41	0.41
1:A:191:ASN:ND2	1:A:192:ALA:N	2.69	0.40

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	466/471 (99%)	449 (96%)	15 (3%)	2 (0%)	39 33

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	193	GLY
1	A	192	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	365/366 (100%)	341 (93%)	24 (7%)	21 14

All (24) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	20	ASN
1	A	71	ASN
1	A	81	PHE
1	A	87	GLN
1	A	111	GLN
1	A	112	LYS
1	A	143	TRP
1	A	144	GLN
1	A	146	GLN
1	A	155	ASN
1	A	191	ASN
1	A	194	GLU
1	A	196	ASN
1	A	213	LEU
1	A	249	ASN
1	A	250	LEU
1	A	304	ASN
1	A	319	ASN
1	A	343	ASN
1	A	397	LYS
1	A	438	ASN
1	A	443	LEU
1	A	446	ASN
1	A	465	VAL

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (40) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	20	ASN

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Mol	Chain	Res	Type
1	A	23	GLN
1	A	34	GLN
1	A	54	GLN
1	A	71	ASN
1	A	85	GLN
1	A	86	GLN
1	A	87	GLN
1	A	101	ASN
1	A	119	ASN
1	A	122	GLN
1	A	127	HIS
1	A	140	ASN
1	A	144	GLN
1	A	151	GLN
1	A	155	ASN
1	A	157	ASN
1	A	158	GLN
1	A	172	GLN
1	A	191	ASN
1	A	196	ASN
1	A	210	GLN
1	A	226	ASN
1	A	249	ASN
1	A	277	GLN
1	A	300	ASN
1	A	304	ASN
1	A	306	ASN
1	A	319	ASN
1	A	330	ASN
1	A	337	ASN
1	A	343	ASN
1	A	346	ASN
1	A	355	ASN
1	A	408	ASN
1	A	412	GLN
1	A	422	HIS
1	A	438	ASN
1	A	439	ASN
1	A	446	ASN

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

Of 8 ligands modelled in this entry, 8 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

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.