



# Full wwPDB X-ray Structure Validation Report ⓘ

Jan 31, 2016 – 06:40 PM GMT

PDB ID : 1BXT  
Title : STREPTOCOCCAL SUPERANTIGEN (SSA) FROM STREPTOCOCCUS  
PYOGENES  
Authors : Sundberg, E.; Jardetzky, T.  
Deposited on : 1998-10-08  
Resolution : 1.85 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  
<http://wwpdb.org/validation/2016/XrayValidationReportHelp>  
with specific help available everywhere you see the ⓘ symbol.

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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 : 1.7 (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

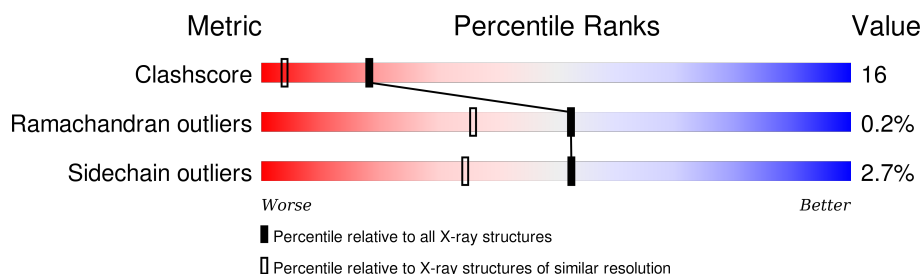
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 1.85 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	1898 (1.86-1.86)
Ramachandran outliers	100387	1875 (1.86-1.86)
Sidechain outliers	100360	1875 (1.86-1.86)

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. 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	234	 71% 22% • 5%
1	B	234	 68% 24% • •

## 2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 3970 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 (STREPTOCOCCAL SUPERANTIGEN).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	222	Total	C	N	O	S	0	0	0
			1786	1130	297	350	9			
1	B	224	Total	C	N	O	S	0	0	0
			1810	1150	297	354	9			

- Molecule 2 is water.

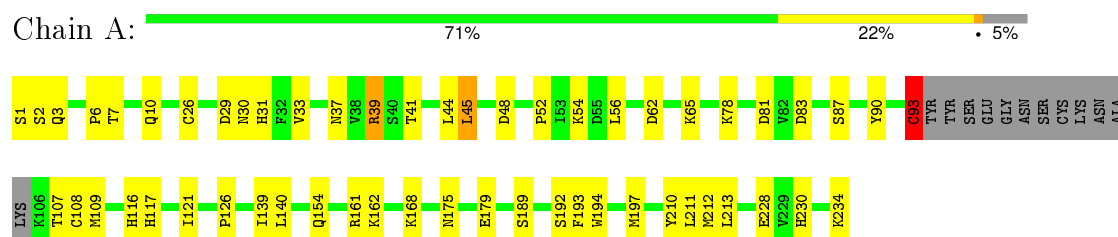
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	190	Total	O	0	0
			190	190		
2	B	184	Total	O	0	0
			184	184		

### 3 Residue-property plots [i](#)

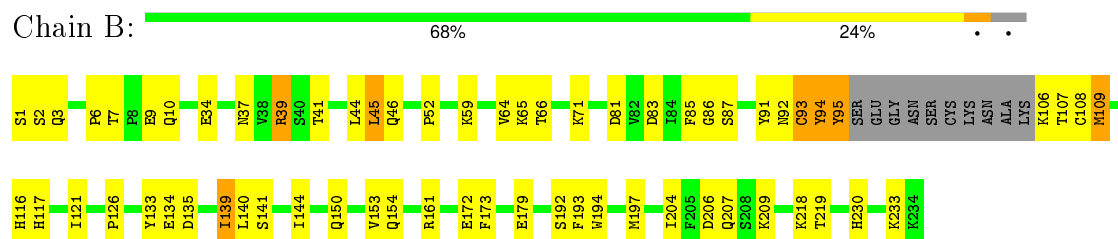
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according 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: PROTEIN (STREPTOCOCCAL SUPERANTIGEN)



#### • Molecule 1: PROTEIN (STREPTOCOCCAL SUPERANTIGEN)



## 4 Data and refinement statistics

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

Property	Value	Source
Space group	C 2 2 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	81.90 Å 84.55 Å 144.01 Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	10.00 – 1.85	Depositor
% Data completeness (in resolution range)	82.9 (10.00-1.85)	Depositor
$R_{merge}$	0.08	Depositor
$R_{sym}$	(Not available)	Depositor
Refinement program	X-PLOR 3.1	Depositor
R, $R_{free}$	0.237 , 0.263	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	3970	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	17.0	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	0.48	0/1823	0.78	3/2461 (0.1%)
1	B	0.54	1/1850 (0.1%)	0.84	3/2500 (0.1%)
All	All	0.51	1/3673 (0.0%)	0.81	6/4961 (0.1%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	95	TYR	C-O	10.27	1.42	1.23

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	95	TYR	CA-C-O	-21.07	75.84	120.10
1	A	93	CYS	CA-C-O	-14.98	88.63	120.10
1	A	109	MET	CG-SD-CE	6.12	109.99	100.20
1	B	109	MET	CG-SD-CE	5.88	109.60	100.20
1	A	212	MET	CG-SD-CE	5.77	109.43	100.20
1	B	94	TYR	O-C-N	5.63	131.71	122.70

There are no chirality outliers.

There are no planarity outliers.

### 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	1786	0	1734	55	2

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	B	1810	0	1744	54	14
2	A	190	0	0	15	4
2	B	184	0	0	15	4
All	All	3970	0	3478	108	18

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 (108) 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:140:LEU:HD23	2:A:423:HOH:O	1.25	1.34
1:A:189:SER:HB3	2:A:414:HOH:O	1.42	1.20
1:B:144:ILE:HD12	2:B:397:HOH:O	1.44	1.14
1:A:93:CYS:CB	1:A:108:CYS:SG	2.39	1.09
1:A:93:CYS:HB2	1:A:108:CYS:SG	1.94	1.07
1:A:1:SER:HB3	2:A:323:HOH:O	1.54	1.06
1:A:1:SER:HA	2:A:249:HOH:O	1.56	1.03
1:A:93:CYS:CB	1:A:108:CYS:HG	1.72	1.00
1:B:95:TYR:CE1	1:B:106:LYS:HD2	1.99	0.96
1:A:30:ASN:OD1	2:A:380:HOH:O	1.84	0.96
1:B:93:CYS:HG	1:B:108:CYS:HG	0.94	0.93
1:A:54:LYS:HE2	2:A:417:HOH:O	1.72	0.90
1:B:134:GLU:HB3	1:B:233:LYS:HE2	1.57	0.85
1:B:135:ASP:OD2	1:B:233:LYS:HE3	1.76	0.85
1:B:93:CYS:CB	1:B:108:CYS:SG	2.65	0.83
1:B:204:ILE:HG22	2:B:349:HOH:O	1.77	0.83
1:A:140:LEU:CD2	2:A:423:HOH:O	1.93	0.82
1:A:44:LEU:HG	1:A:45:LEU:HD13	1.65	0.79
1:B:219:THR:HG21	2:B:400:HOH:O	1.81	0.78
1:A:93:CYS:HG	1:A:108:CYS:HG	1.34	0.76
1:B:93:CYS:HB2	1:B:108:CYS:SG	2.25	0.76
1:A:210:TYR:O	1:A:213:LEU:HD22	1.88	0.73
1:A:7:THR:HG22	1:A:10:GLN:CG	2.19	0.73
1:B:95:TYR:CD1	1:B:106:LYS:HD2	2.24	0.72
1:B:39:ARG:HH11	1:B:39:ARG:HG3	1.54	0.71
1:B:207:GLN:HB3	2:B:402:HOH:O	1.91	0.69
1:A:26:CYS:SG	2:A:397:HOH:O	2.24	0.68
1:A:230:HIS:HD2	2:A:308:HOH:O	1.76	0.68
1:B:1:SER:CA	2:B:301:HOH:O	2.40	0.68
1:B:134:GLU:HB2	1:B:139:ILE:HD12	1.77	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:64:VAL:HG13	1:B:107:THR:HG23	1.78	0.65
1:A:7:THR:HG22	1:A:10:GLN:HB2	1.79	0.64
1:B:87:SER:H	1:B:154:GLN:HE21	1.46	0.62
1:B:134:GLU:HB2	1:B:139:ILE:CD1	2.30	0.61
1:A:7:THR:HG22	1:A:10:GLN:CB	2.30	0.61
1:A:48:ASP:OD1	1:A:48:ASP:C	2.39	0.61
1:A:39:ARG:HD2	1:A:81:ASP:OD1	2.01	0.61
1:A:2:SER:HB2	1:A:192:SER:H	1.65	0.60
1:B:2:SER:HB2	1:B:192:SER:H	1.66	0.59
1:A:87:SER:H	1:A:154:GLN:HE21	1.49	0.59
1:B:39:ARG:HG3	1:B:39:ARG:NH1	2.19	0.57
1:A:90:TYR:CE1	1:A:107:THR:HB	2.39	0.57
1:A:37:ASN:CG	2:A:406:HOH:O	2.43	0.57
1:A:29:ASP:OD1	1:A:30:ASN:HB2	2.05	0.56
1:A:121:ILE:HD13	1:A:126:PRO:HD3	1.87	0.56
1:B:161:ARG:HD3	1:B:197:MET:HE2	1.89	0.55
1:B:121:ILE:HD13	1:B:126:PRO:HD3	1.88	0.55
1:A:78:LYS:NZ	2:A:353:HOH:O	2.39	0.55
1:A:161:ARG:HD3	1:A:197:MET:HE2	1.90	0.54
1:A:30:ASN:O	1:A:162:LYS:HE3	2.08	0.54
1:B:81:ASP:OD2	1:B:117:HIS:HE1	1.91	0.53
1:A:37:ASN:OD1	2:A:406:HOH:O	2.19	0.53
1:A:81:ASP:OD2	1:A:117:HIS:HE1	1.92	0.53
1:A:29:ASP:OD2	2:A:407:HOH:O	2.18	0.52
1:A:87:SER:H	1:A:154:GLN:NE2	2.08	0.52
1:A:168:LYS:HG3	2:A:423:HOH:O	2.11	0.51
1:B:37:ASN:OD1	1:B:81:ASP:HB3	2.10	0.51
1:B:86:GLY:HA3	2:B:258:HOH:O	2.09	0.51
1:A:117:HIS:HD2	1:B:172:GLU:OE1	1.95	0.50
1:A:30:ASN:CG	1:A:31:HIS:H	2.14	0.50
1:A:83:ASP:OD1	1:A:116:HIS:HD2	1.95	0.50
1:A:210:TYR:O	1:A:213:LEU:CD2	2.59	0.49
1:A:48:ASP:OD2	1:A:65:LYS:HD2	2.12	0.49
1:B:87:SER:H	1:B:154:GLN:NE2	2.08	0.49
1:B:1:SER:N	2:B:301:HOH:O	2.09	0.49
1:B:133:TYR:CD1	1:B:230:HIS:CE1	3.01	0.49
1:A:7:THR:HG22	1:A:10:GLN:HG3	1.94	0.49
1:A:37:ASN:OD1	1:A:81:ASP:HB3	2.12	0.48
1:B:140:LEU:HG	1:B:141:SER:N	2.28	0.48
1:B:3:GLN:NE2	1:B:194:TRP:H	2.11	0.48
1:B:41:THR:HB	2:B:407:HOH:O	2.12	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:83:ASP:OD1	1:B:116:HIS:HD2	1.96	0.48
1:A:3:GLN:NE2	1:A:194:TRP:H	2.11	0.48
1:B:66:THR:HA	1:B:109:MET:O	2.14	0.47
1:B:153:VAL:HG22	1:B:218:LYS:O	2.14	0.46
1:A:175:ASN:OD1	1:A:234:LYS:NZ	2.47	0.46
1:A:39:ARG:HB3	1:A:39:ARG:HE	1.56	0.46
1:B:6:PRO:HB3	1:B:194:TRP:CZ2	2.49	0.46
1:B:65:LYS:HB2	1:B:95:TYR:CE2	2.50	0.46
1:A:54:LYS:HD3	1:A:62:ASP:O	2.15	0.45
1:B:34:GLU:OE2	1:B:85:PHE:CE2	2.69	0.45
1:A:6:PRO:HA	1:A:10:GLN:OE1	2.16	0.45
1:A:230:HIS:CD2	2:A:308:HOH:O	2.60	0.45
1:A:41:THR:HG23	1:A:52:PRO:HD3	1.98	0.44
1:B:46:GLN:HB3	1:B:71:LYS:HG2	1.99	0.44
1:A:211:LEU:C	1:A:213:LEU:HD23	2.38	0.44
1:B:207:GLN:CB	2:B:402:HOH:O	2.60	0.43
1:B:95:TYR:H	1:B:106:LYS:HZ1	1.67	0.43
1:A:211:LEU:HA	1:A:213:LEU:CD2	2.47	0.43
1:A:7:THR:HG22	1:A:10:GLN:CD	2.39	0.43
1:B:39:ARG:HD3	2:B:264:HOH:O	2.19	0.43
1:B:9:GLU:HG3	2:B:416:HOH:O	2.18	0.43
1:B:150:GLN:OE1	2:B:336:HOH:O	2.21	0.43
1:B:133:TYR:HB2	1:B:230:HIS:ND1	2.34	0.42
1:B:204:ILE:CG2	2:B:349:HOH:O	2.51	0.42
1:B:3:GLN:HE21	1:B:193:PHE:HA	1.85	0.42
1:A:179:GLU:OE1	1:A:179:GLU:HA	2.20	0.42
1:A:3:GLN:HE21	1:A:193:PHE:HA	1.85	0.42
1:B:207:GLN:CA	2:B:402:HOH:O	2.68	0.41
1:B:41:THR:HG23	1:B:52:PRO:HD3	2.00	0.41
1:A:228:GLU:OE1	1:A:230:HIS:HE1	2.03	0.41
1:A:93:CYS:HB3	1:A:108:CYS:SG	2.47	0.41
1:B:1:SER:HA	2:B:301:HOH:O	2.15	0.41
1:B:44:LEU:HG	1:B:45:LEU:HD13	2.03	0.41
1:B:7:THR:HG22	1:B:10:GLN:CG	2.51	0.41
1:B:179:GLU:OE1	1:B:179:GLU:HA	2.20	0.40
1:B:2:SER:CB	1:B:192:SER:H	2.31	0.40
1:B:206:ASP:HB3	1:B:209:LYS:HB3	2.03	0.40

All (18) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:91:TYR:CD2	1:B:91:TYR:CD2[3_555]	1.37	0.83
1:B:91:TYR:CG	1:B:91:TYR:CE2[3_555]	1.38	0.82
1:B:91:TYR:CD1	1:B:91:TYR:CZ[3_555]	1.41	0.79
1:B:91:TYR:CE1	1:B:91:TYR:CE1[3_555]	1.43	0.77
1:B:91:TYR:CE1	1:B:91:TYR:CZ[3_555]	1.67	0.53
1:B:91:TYR:CD1	1:B:91:TYR:OH[3_555]	1.76	0.44
1:B:91:TYR:CD2	1:B:91:TYR:CE2[3_555]	1.83	0.37
2:A:261:HOH:O	2:B:409:HOH:O[3_655]	1.85	0.35
1:A:1:SER:OG	2:B:276:HOH:O[3_655]	1.88	0.32
1:B:91:TYR:CD1	1:B:91:TYR:CE2[3_555]	1.89	0.31
1:B:1:SER:N	2:A:271:HOH:O[7_555]	1.91	0.29
1:B:91:TYR:OH	2:B:383:HOH:O[3_555]	2.01	0.19
1:B:94:TYR:OH	1:B:173:PHE:CZ[3_555]	2.01	0.19
1:B:91:TYR:CG	1:B:91:TYR:CZ[3_555]	2.06	0.14
1:B:91:TYR:CG	1:B:91:TYR:CD2[3_555]	2.08	0.12
2:A:253:HOH:O	2:A:414:HOH:O[3_655]	2.13	0.07
1:B:1:SER:OG	2:A:290:HOH:O[7_555]	2.16	0.04
1:A:1:SER:N	2:B:276:HOH:O[3_655]	2.19	0.01

## 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	218/234 (93%)	209 (96%)	9 (4%)	0	100	100
1	B	220/234 (94%)	211 (96%)	8 (4%)	1 (0%)	34	17
All	All	438/468 (94%)	420 (96%)	17 (4%)	1 (0%)	52	36

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	92	ASN

### 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	203/216 (94%)	197 (97%)	6 (3%)	48	29
1	B	204/216 (94%)	199 (98%)	5 (2%)	55	37
All	All	407/432 (94%)	396 (97%)	11 (3%)	52	34

All (11) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	33	VAL
1	A	39	ARG
1	A	45	LEU
1	A	56	LEU
1	A	93	CYS
1	A	139	ILE
1	B	39	ARG
1	B	45	LEU
1	B	59	LYS
1	B	93	CYS
1	B	139	ILE

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (19) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	3	GLN
1	A	60	ASN
1	A	116	HIS
1	A	117	HIS
1	A	120	GLN
1	A	127	ASN
1	A	154	GLN
1	A	169	ASN
1	A	230	HIS
1	B	3	GLN
1	B	30	ASN

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Mol	Chain	Res	Type
1	B	43	GLN
1	B	60	ASN
1	B	116	HIS
1	B	117	HIS
1	B	120	GLN
1	B	127	ASN
1	B	150	GLN
1	B	154	GLN

### 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 carbohydrates 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 [i](#)

There are no chain breaks in this entry.

## 6 Fit of model and data [i](#)

### 6.1 Protein, DNA and RNA chains [i](#)

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

### 6.2 Non-standard residues in protein, DNA, RNA chains [i](#)

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

### 6.3 Carbohydrates [i](#)

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

### 6.4 Ligands [i](#)

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

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

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