Full wwPDB X-ray Structure Validation Report (i)

Jun 12, 2024 – 02:09 PM EDT

PDB ID	:	1APV
Title	:	CRYSTALLOGRAPHIC ANALYSIS OF TRANSITION STATE MIMICS BOUND TO PENICILLOPEPSIN: DIFLUOROSTATINE-AND DIFLUOR OSTATONE-CONTAINING PEPTIDES
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Deposited on	:	1991-12-16
Resolution	:	1.80 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
https://www.wwpdb.org/validation/2017/XrayValidationReportHelp
with specific help available everywhere you see the (i) symbol.

The types of validation reports are described at
http://www.wwpdb.org/validation/2017/FAQs#types.

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

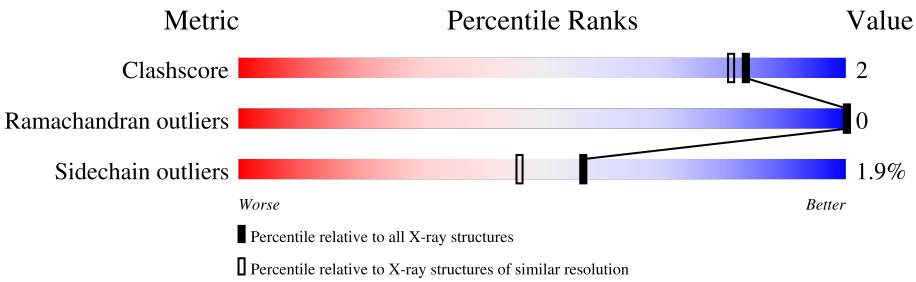
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	NOT EXECUTED
EDS	:	NOT EXECUTED
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36.2

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 1.80 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	141614	6793 (1.80-1.80)
Ramachandran outliers	138981	6697 (1.80-1.80)
Sidechain outliers	138945	6696 (1.80-1.80)

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 >=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 <=5%

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	E	323	89% 11% •
2	I	5	80% 20%

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
4	XYS	E	399	X	-	-	-
5	SO4	E	365	-	-	X	-

2 Entry composition (i)

There are 7 unique types of molecules in this entry. The entry contains 2709 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.

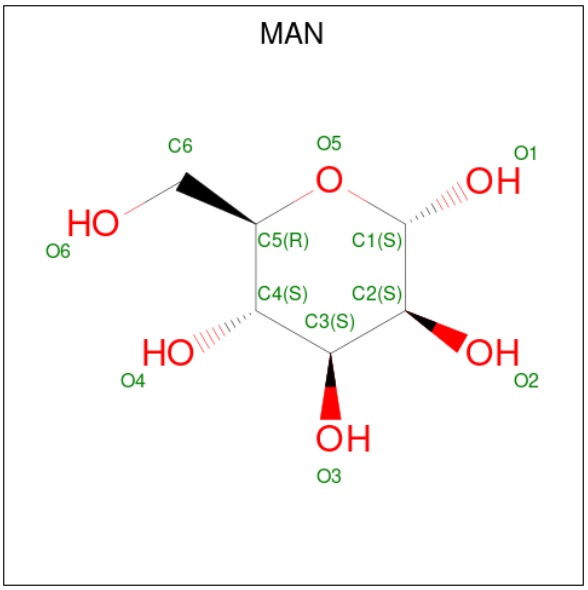
- Molecule 1 is a protein called PENICILLOPEPSIN.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	E	323	2366	1479	377	508	2	0	0	0

- Molecule 2 is a protein called INHIBITOR ISOVALERYL (IVA)-VAL-VAL-HYDRATED DIFLUOROSTATONE-N-METHYLAMINE.

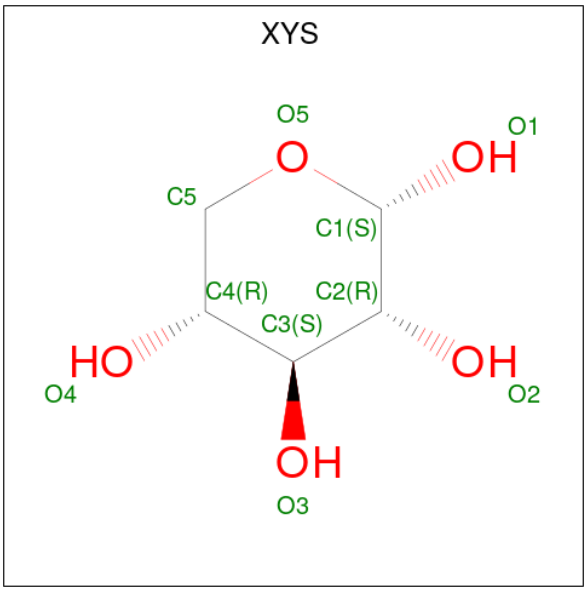
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	F	N	O			
2	I	5	36	24	2	4	6	0	0	1

- Molecule 3 is alpha-D-mannopyranose (three-letter code: MAN) (formula: $C_6H_{12}O_6$).



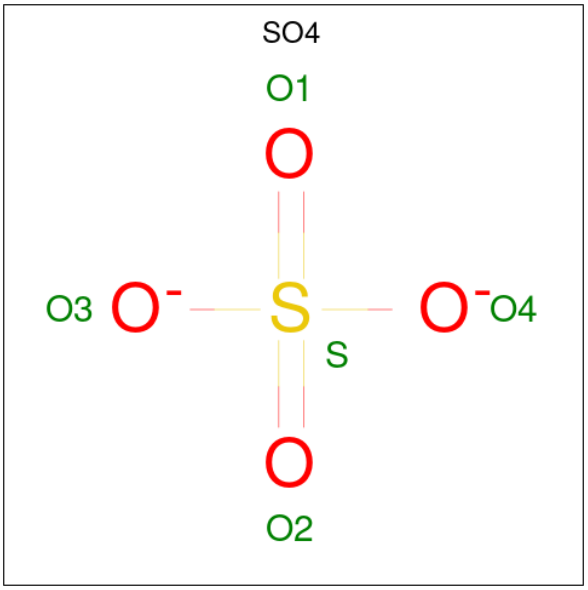
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	C	O		
3	E	1	11	6	5	0	0

- Molecule 4 is alpha-D-xylopyranose (three-letter code: XYS) (formula: $C_5H_{10}O_5$).



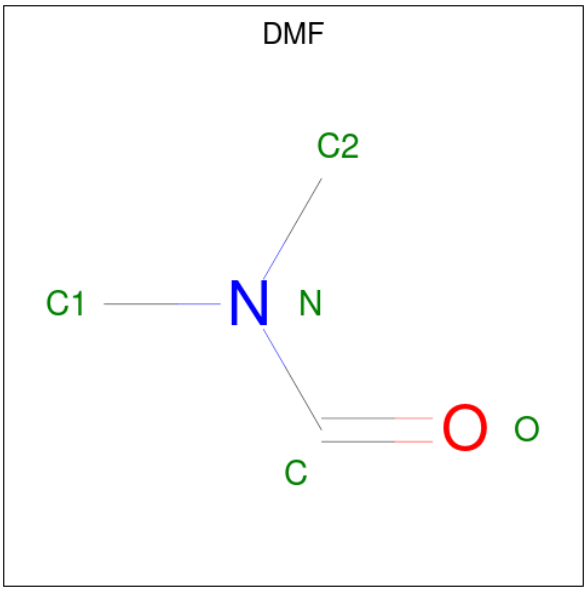
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	E	1	Total C O 9 5 4	0	0

- Molecule 5 is SULFATE ION (three-letter code: SO4) (formula: O_4S).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	E	1	Total O S 5 4 1	0	0

- Molecule 6 is DIMETHYLFORMAMIDE (three-letter code: DMF) (formula: C_3H_7NO).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	C	N	O		
6	I	1	5	3	1	1	0	0

- Molecule 7 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
7	E	274	274	274	0	0
			Total	O		
7	I	3	3	3	0	0

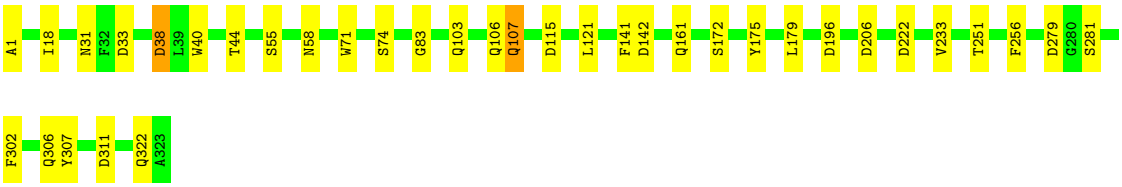
3 Residue-property plots (i)

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: PENICILLOPEPSIN

Chain E:



• Molecule 2: INHIBITOR ISOVALERYL (IVA)-VAL-VAL-HYDRATED DIFLUOROSTATON E-N-METHYLAMINE

Chain I:

4 Data and refinement statistics (i)

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

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α, β, γ	97.52Å 46.57Å 66.23Å 90.00° 116.03° 90.00°	Depositor
Resolution (Å)	8.00 – 1.80	Depositor
% Data completeness (in resolution range)	(Not available) (8.00-1.80)	Depositor
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	PROLSQ	Depositor
R, R_{free}	0.131 , (Not available)	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	2709	wwPDB-VP
Average B, all atoms ($Å^2$)	13.0	wwPDB-VP

5 Model quality (i)

5.1 Standard geometry (i)

Bond lengths and bond angles in the following residue types are not validated in this section: XYS, SO4, IVA, NME, DFO, DMF, MAN

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	E	1.07	0/2420	1.62	21/3304 (0.6%)
2	I	1.27	0/13	2.09	0/17
All	All	1.07	0/2433	1.63	21/3321 (0.6%)

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
2	I	0	1

There are no bond length outliers.

All (21) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	E	33	ASP	CB-CG-OD2	7.92	125.43	118.30
1	E	307	TYR	CB-CG-CD2	-7.89	116.27	121.00
1	E	196	ASP	CB-CG-OD1	-7.56	111.50	118.30
1	E	115	ASP	CB-CG-OD1	7.06	124.66	118.30
1	E	222	ASP	CB-CG-OD2	-7.00	112.00	118.30
1	E	142	ASP	CB-CG-OD1	6.89	124.50	118.30
1	E	222	ASP	CB-CG-OD1	6.83	124.45	118.30
1	E	141	PHE	CB-CG-CD1	-6.77	116.06	120.80
1	E	256	PHE	CB-CG-CD1	-6.59	116.19	120.80
1	E	206	ASP	CB-CG-OD1	6.25	123.92	118.30
1	E	33	ASP	N-CA-CB	-6.00	99.81	110.60
1	E	38	ASP	CB-CG-OD1	5.96	123.66	118.30
1	E	311	ASP	CB-CG-OD2	-5.57	113.28	118.30
1	E	55	SER	N-CA-C	-5.52	96.09	111.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	E	1	ALA	CB-CA-C	5.51	118.36	110.10
1	E	161	GLN	N-CA-CB	5.40	120.32	110.60
1	E	83	GLY	O-C-N	5.35	131.26	122.70
1	E	281	SER	N-CA-C	5.28	125.26	111.00
1	E	307	TYR	N-CA-C	-5.26	96.79	111.00
1	E	279	ASP	CB-CG-OD1	5.21	122.99	118.30
1	E	302	PHE	CB-CG-CD2	-5.17	117.18	120.80

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	I	1	DFO	Mainchain

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	E	2366	0	2181	11	0
2	I	36	0	39	1	0
3	E	11	0	10	0	0
4	E	9	0	8	0	0
5	E	5	0	0	2	0
6	I	5	0	7	0	0
7	E	274	0	0	0	0
7	I	3	0	0	0	0
All	All	2709	0	2245	11	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 2.

All (11) 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:E:106:GLN:C	1:E:107:GLN:HG2	2.06	0.76

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:233:VAL:HG13	1:E:251:THR:HG21	1.89	0.55
1:E:121:LEU:HD21	2:I:1:DFO:HD12	1.90	0.54
1:E:179:LEU:N	5:E:365:SO4:O2	2.35	0.54
1:E:107:GLN:HE21	1:E:107:GLN:HB3	1.54	0.44
1:E:306:GLN:C	1:E:322:GLN:HG3	2.39	0.43
1:E:172:SER:HA	1:E:175:TYR:CE1	2.54	0.43
1:E:40:TRP:HA	1:E:103:GLN:O	2.19	0.43
1:E:71:TRP:CE2	1:E:103:GLN:HB3	2.54	0.42
1:E:44:THR:HG21	1:E:58:ASN:HB2	2.04	0.40
1:E:175:TYR:OH	5:E:365:SO4:O4	2.22	0.40

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	E	321/323 (99%)	319 (99%)	2 (1%)	0	100	100
2	I	2/5 (40%)	1 (50%)	1 (50%)	0	100	100
All	All	323/328 (98%)	320 (99%)	3 (1%)	0	100	100

There are no Ramachandran outliers to report.

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	E	259/259 (100%)	254 (98%)	5 (2%)	57	46
2	I	2/2 (100%)	2 (100%)	0	100	100
All	All	261/261 (100%)	256 (98%)	5 (2%)	57	46

All (5) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	E	18	ILE
1	E	31	ASN
1	E	38	ASP
1	E	74	SER
1	E	107	GLN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (6) such sidechains are listed below:

Mol	Chain	Res	Type
1	E	31	ASN
1	E	50	GLN
1	E	107	GLN
1	E	150	GLN
1	E	194	ASN
1	E	228	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)

1 non-standard protein/DNA/RNA residue is modelled in this entry.

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	$\#\|Z\| > 2$
2	DFO	I	1	2	10,13,14	2.41	1 (10%)	7,20,22	0.59	0

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
2	DFO	I	1	2	-	0/8/22/25	-

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	I	1	DFO	OH2-CH	7.01	1.47	1.40

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	I	1	DFO	1	0

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

4 ligands are modelled in this entry.

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	$\#\|Z\| > 2$
5	SO4	E	365	-	4,4,4	0.54	0	6,6,6	0.32	0
3	MAN	E	328	1	11,11,12	0.98	0	15,15,17	1.24	2 (13%)
4	XYS	E	399	1	9,9,10	1.17	0	10,12,14	3.59	4 (40%)
6	DMF	I	587	-	4,4,4	0.34	0	4,4,4	0.63	0

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
3	MAN	E	328	1	-	0/2/19/22	0/1/1/1
4	XYS	E	399	1	4/4/3/4	-	0/1/1/1
6	DMF	I	587	-	-	1/2/2/2	-

There are no bond length outliers.

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	E	399	XYS	C5-O5-C1	7.10	122.44	111.52
4	E	399	XYS	C5-C4-C3	6.89	118.14	109.67
4	E	399	XYS	O4-C4-C5	4.20	117.74	109.15
3	E	328	MAN	O2-C2-C1	-3.08	102.86	109.15
4	E	399	XYS	O2-C2-C3	2.70	115.55	110.14
3	E	328	MAN	C3-C4-C5	-2.13	106.44	110.24

All (4) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
4	E	399	XYS	C2
4	E	399	XYS	C4
4	E	399	XYS	C3
4	E	399	XYS	C1

All (1) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
6	I	587	DMF	O-C-N-C1

There are no ring outliers.

1 monomer is involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	E	365	SO4	2	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 (i)

6.1 Protein, DNA and RNA chains (i)

EDS was not executed - this section is therefore empty.

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

EDS was not executed - this section is therefore empty.

6.3 Carbohydrates (i)

EDS was not executed - this section is therefore empty.

6.4 Ligands (i)

EDS was not executed - this section is therefore empty.

6.5 Other polymers (i)

EDS was not executed - this section is therefore empty.