Full wwPDB X-ray Structure Validation Report (i)

Dec 17, 2023 – 10:47 AM EST

PDB ID	:	1B7H
Title	:	OLIGO-PEPTIDE BINDING PROTEIN COMPLEXED WITH LYSYL-NORLEUCYL-LYSINE
Authors	:	Davies, T.G.; Tame, J.R.H.
Deposited on	:	1998-11-16
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
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:

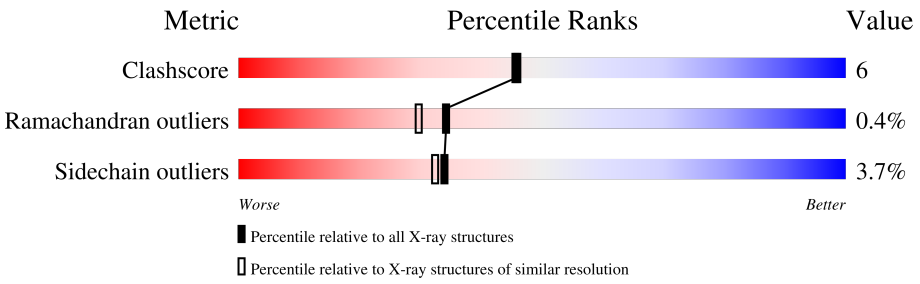
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	NOT EXECUTED
EDS	:	NOT EXECUTED
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

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 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	141614	9178 (2.00-2.00)
Ramachandran outliers	138981	9054 (2.00-2.00)
Sidechain outliers	138945	9053 (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 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	A	517	78% 18% •
2	B	3	67% 33%

2 Entry composition (i)

There are 4 unique types of molecules in this entry. The entry contains 4467 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 Periplasmic oligopeptide-binding protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	517	4165	2666	700	794	5	9	0	0

- Molecule 2 is a protein called LYS-NLE-LYS PEPTIDE.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
			Total	C	N	O			
2	B	3	27	18	5	4	0	0	0

- Molecule 3 is URANIUM ATOM (three-letter code: U1) (formula: U).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	U		
3	A	2	2	2	0	0

- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
4	A	270	270	270	0	0
4	B	3	3	3	0	0

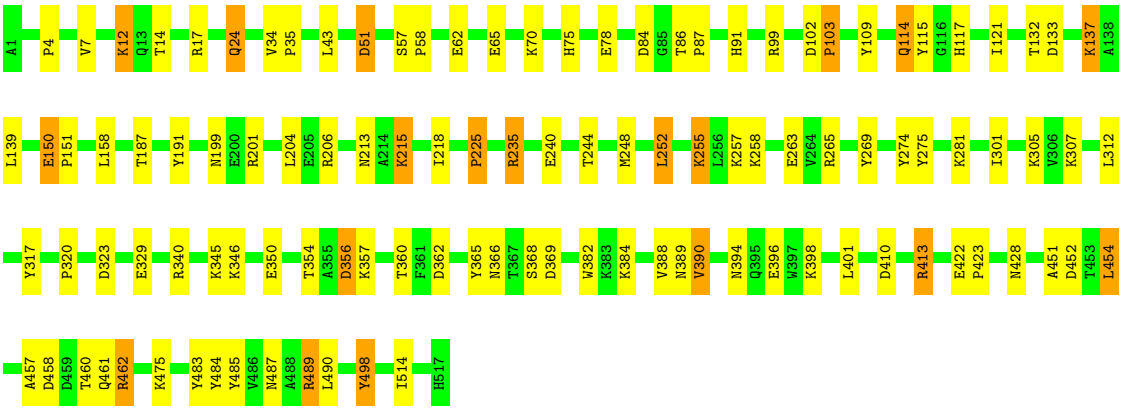
3 Residue-property plots (i)

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: Periplasmic oligopeptide-binding protein

Chain A: 78% 18% •



• Molecule 2: LYS-NLE-LYS PEPTIDE

Chain B: 67% 33%

4 Data and refinement statistics (i)

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

Property	Value	Source
Space group	P 21 21 2 A	Depositor
Cell constants a, b, c, α, β, γ	104.01Å 74.08Å 69.61Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	20.00 – 2.00	Depositor
% Data completeness (in resolution range)	99.0 (20.00-2.00)	Depositor
R_{merge}	0.09	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	REFMAC	Depositor
R, R_{free}	0.210 , 0.260	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	4467	wwPDB-VP
Average B, all atoms (Å^2)	38.0	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: NLE, U1

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	0.83	4/4276 (0.1%)	1.78	63/5830 (1.1%)
2	B	1.12	0/17	1.73	0/16
All	All	0.83	4/4293 (0.1%)	1.78	63/5846 (1.1%)

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 (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	329	GLU	CD-OE1	-7.33	1.17	1.25
1	A	150	GLU	CG-CD	6.48	1.61	1.51
1	A	329	GLU	CG-CD	6.37	1.61	1.51
1	A	384	LYS	CD-CE	-5.70	1.37	1.51

All (63) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	413	ARG	NE-CZ-NH1	30.58	135.59	120.30
1	A	413	ARG	NE-CZ-NH2	-28.36	106.12	120.30
1	A	201	ARG	CD-NE-CZ	26.06	160.09	123.60
1	A	356	ASP	CB-CG-OD1	-23.11	97.50	118.30
1	A	356	ASP	CB-CG-OD2	22.51	138.56	118.30
1	A	489	ARG	NE-CZ-NH1	19.86	130.23	120.30
1	A	235	ARG	CD-NE-CZ	11.90	140.26	123.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	114	GLN	CA-CB-CG	11.12	137.87	113.40
1	A	51	ASP	CB-CG-OD2	10.62	127.86	118.30
1	A	410	ASP	CB-CG-OD2	10.60	127.84	118.30
1	A	410	ASP	CB-CG-OD1	-9.91	109.39	118.30
1	A	102	ASP	CB-CG-OD2	8.37	125.83	118.30
1	A	12	LYS	CA-CB-CG	8.28	131.61	113.40
1	A	452	ASP	CB-CG-OD1	8.13	125.62	118.30
1	A	340	ARG	NE-CZ-NH1	-8.06	116.27	120.30
1	A	489	ARG	CD-NE-CZ	7.70	134.37	123.60
1	A	484	TYR	CB-CG-CD1	-7.62	116.43	121.00
1	A	265	ARG	NE-CZ-NH1	7.58	124.09	120.30
1	A	99	ARG	NE-CZ-NH1	-7.47	116.57	120.30
1	A	329	GLU	OE1-CD-OE2	7.46	132.25	123.30
1	A	457	ALA	N-CA-CB	-7.05	100.24	110.10
1	A	317	TYR	CB-CG-CD2	-6.99	116.81	121.00
1	A	102	ASP	CB-CG-OD1	-6.90	112.09	118.30
1	A	235	ARG	NE-CZ-NH2	6.82	123.71	120.30
1	A	201	ARG	NE-CZ-NH1	-6.82	116.89	120.30
1	A	17	ARG	NE-CZ-NH1	-6.63	116.98	120.30
1	A	369	ASP	CB-CG-OD1	6.54	124.18	118.30
1	A	133	ASP	CB-CG-OD1	6.50	124.15	118.30
1	A	489	ARG	NE-CZ-NH2	-6.47	117.06	120.30
1	A	51	ASP	CB-CG-OD1	-6.35	112.59	118.30
1	A	99	ARG	NE-CZ-NH2	6.31	123.45	120.30
1	A	84	ASP	CB-CG-OD2	6.28	123.95	118.30
1	A	422	GLU	OE1-CD-OE2	-6.26	115.79	123.30
1	A	485	TYR	CA-CB-CG	6.15	125.09	113.40
1	A	489	ARG	NH1-CZ-NH2	-6.14	112.65	119.40
1	A	275	TYR	CA-CB-CG	-6.07	101.86	113.40
1	A	345	LYS	CD-CE-NZ	6.07	125.67	111.70
1	A	362	ASP	CB-CG-OD1	6.04	123.74	118.30
1	A	62	GLU	OE1-CD-OE2	5.89	130.37	123.30
1	A	109	TYR	CB-CG-CD1	5.87	124.52	121.00
1	A	498	TYR	CB-CG-CD1	5.83	124.50	121.00
1	A	366	ASN	N-CA-CB	5.80	121.03	110.60
1	A	281	LYS	CA-CB-CG	5.79	126.15	113.40
1	A	103	PRO	N-CA-CB	5.79	110.25	103.30
1	A	475	LYS	CD-CE-NZ	5.76	124.94	111.70
1	A	329	GLU	CG-CD-OE1	-5.70	106.91	118.30
1	A	133	ASP	CB-CG-OD2	-5.66	113.21	118.30
1	A	274	TYR	CZ-CE2-CD2	-5.63	114.74	119.80
1	A	452	ASP	CB-CG-OD2	-5.62	113.24	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	484	TYR	CB-CG-CD2	5.59	124.36	121.00
1	A	320	PRO	N-CA-CB	5.47	109.87	103.30
1	A	91	HIS	CA-CB-CG	-5.44	104.35	113.60
1	A	201	ARG	NE-CZ-NH2	5.44	123.02	120.30
1	A	462	ARG	NE-CZ-NH2	-5.41	117.59	120.30
1	A	158	LEU	CB-CA-C	-5.25	100.22	110.20
1	A	390	VAL	N-CA-CB	-5.25	99.96	111.50
1	A	485	TYR	CB-CG-CD2	-5.23	117.86	121.00
1	A	461	GLN	CG-CD-OE1	-5.11	111.39	121.60
1	A	109	TYR	CB-CG-CD2	-5.08	117.95	121.00
1	A	317	TYR	CB-CG-CD1	5.07	124.04	121.00
1	A	396	GLU	OE1-CD-OE2	-5.05	117.24	123.30
1	A	191	TYR	CB-CG-CD1	5.04	124.03	121.00
1	A	12	LYS	CB-CA-C	5.02	120.45	110.40

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	24	GLN	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	A	4165	0	4076	53	0
2	B	27	0	38	2	0
3	A	2	0	0	0	0
4	A	270	0	0	11	0
4	B	3	0	0	0	0
All	All	4467	0	4114	53	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 6.

All (53) 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:199:ASN:CB	4:A:779:HOH:O	1.87	1.19
1:A:451:ALA:CA	4:A:754:HOH:O	1.78	1.16
1:A:451:ALA:HA	4:A:754:HOH:O	1.29	1.15
1:A:199:ASN:CA	4:A:779:HOH:O	1.93	1.14
1:A:215:LYS:HE3	4:A:777:HOH:O	0.82	1.00
1:A:451:ALA:O	4:A:754:HOH:O	1.80	0.99
1:A:199:ASN:HA	4:A:779:HOH:O	1.62	0.89
1:A:199:ASN:HB3	4:A:779:HOH:O	1.58	0.87
1:A:252:LEU:HA	1:A:255:LYS:HE2	1.58	0.84
1:A:401:LEU:HD22	2:B:2:NLE:HD2	1.67	0.76
1:A:451:ALA:C	4:A:754:HOH:O	1.96	0.74
1:A:215:LYS:CE	4:A:777:HOH:O	1.66	0.65
1:A:255:LYS:H	1:A:255:LYS:NZ	1.95	0.64
1:A:150:GLU:HB3	1:A:151:PRO:HD2	1.82	0.61
1:A:255:LYS:H	1:A:255:LYS:HZ3	1.49	0.60
1:A:218:ILE:HD11	1:A:514:ILE:HG12	1.84	0.59
1:A:137:LYS:HG3	1:A:139:LEU:HD23	1.87	0.56
1:A:252:LEU:HA	1:A:255:LYS:CE	2.35	0.55
1:A:24:GLN:O	1:A:398:LYS:HE3	2.09	0.53
1:A:199:ASN:ND2	4:A:779:HOH:O	2.41	0.52
1:A:218:ILE:CD1	1:A:514:ILE:HG12	2.39	0.52
1:A:307:LYS:HE3	1:A:483:TYR:OH	2.09	0.51
1:A:382:TRP:HB3	1:A:388:VAL:HG22	1.92	0.51
1:A:115:TYR:CE1	1:A:428:ASN:HB3	2.48	0.49
1:A:365:TYR:O	1:A:394:ASN:HA	2.13	0.49
1:A:458:ASP:OD2	1:A:460:THR:HB	2.12	0.49
1:A:117:HIS:ND1	1:A:454:LEU:HD11	2.27	0.49
1:A:244:THR:HG23	1:A:490:LEU:HB2	1.95	0.49
1:A:401:LEU:HD22	2:B:2:NLE:CD	2.40	0.49
1:A:4:PRO:O	1:A:7:VAL:HG13	2.13	0.49
1:A:360:THR:HA	1:A:389:ASN:O	2.13	0.48
1:A:43:LEU:O	1:A:187:THR:HB	2.14	0.47
1:A:323:ASP:O	1:A:423:PRO:HD3	2.15	0.47
1:A:235:ARG:HD3	1:A:240:GLU:OE1	2.14	0.47
1:A:248:MET:HA	1:A:248:MET:CE	2.44	0.47
1:A:354:THR:OG1	1:A:357:LYS:N	2.48	0.47
1:A:114:GLN:HA	1:A:121:ILE:HG21	1.97	0.46
1:A:263:GLU:O	1:A:490:LEU:HA	2.15	0.46
1:A:346:LYS:HE2	1:A:350:GLU:OE2	2.15	0.46
1:A:301:ILE:HA	1:A:305:LYS:HG3	1.97	0.45
1:A:137:LYS:HB3	1:A:137:LYS:HE2	1.57	0.45
1:A:269:TYR:HB2	1:A:487:ASN:HB2	1.99	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:489:ARG:HD2	1:A:498:TYR:CZ	2.53	0.43
1:A:43:LEU:HD21	1:A:204:LEU:HD22	2.01	0.42
1:A:206:ARG:HD3	1:A:213:ASN:OD1	2.19	0.42
1:A:57:SER:HB3	1:A:58:PRO:HD2	2.00	0.42
1:A:34:VAL:HB	1:A:35:PRO:HD3	2.02	0.42
1:A:51:ASP:HB3	1:A:57:SER:OG	2.20	0.42
1:A:269:TYR:CG	1:A:487:ASN:HB2	2.55	0.41
1:A:240:GLU:HG2	1:A:240:GLU:O	2.19	0.41
1:A:12:LYS:HD2	1:A:14:THR:HG23	2.03	0.41
1:A:65:GLU:OE2	1:A:75:HIS:NE2	2.48	0.41
1:A:86:THR:HA	1:A:87:PRO:HD3	1.85	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	A	515/517 (100%)	492 (96%)	21 (4%)	2 (0%)	34 30

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	225	PRO
1	A	368	SER

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	455/455 (100%)	438 (96%)	17 (4%)	34 32
2	B	2/2 (100%)	2 (100%)	0	100 100
All	All	457/457 (100%)	440 (96%)	17 (4%)	34 32

All (17) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	70	LYS
1	A	78	GLU
1	A	103	PRO
1	A	132	THR
1	A	137	LYS
1	A	215	LYS
1	A	225	PRO
1	A	252	LEU
1	A	255	LYS
1	A	257	LYS
1	A	258	LYS
1	A	312	LEU
1	A	356	ASP
1	A	390	VAL
1	A	413	ARG
1	A	454	LEU
1	A	462	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	199	ASN
1	A	279	ASN
1	A	280	GLN
1	A	304	ASN
1	A	338	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	NLE	B	2	2	6,7,8	1.04	1 (16%)	2,7,9	0.92	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	NLE	B	2	2	-	1/5/6/8	-

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	2	NLE	CB-CA	-2.04	1.50	1.53

There are no bond angle outliers.

There are no chirality outliers.

All (1) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	B	2	NLE	CE-CD-CG-CB

There are no ring outliers.

1 monomer is involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	2	NLE	2	0

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

Of 2 ligands modelled in this entry, 2 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 (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.