Full wwPDB X-ray Structure Validation Report (i)

Jan 31, 2016 – 07:33 PM GMT

PDB ID	:	1G3J
Title	:	CRYSTAL STRUCTURE OF THE XTCF3-CBD/BETA-CATENIN ARMADILLO REPEAT COMPLEX
Authors	:	Graham, T.A.; Weaver, C.; Mao, F.; Kimelman, D.; Xu, W.
Deposited on	:	2000-10-24
Resolution	:	2.10 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:

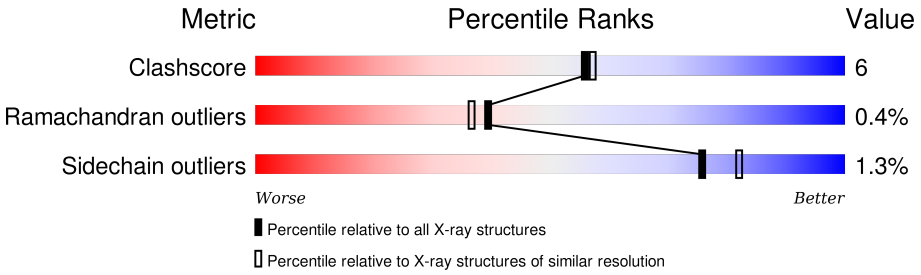
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	NOT EXECUTED
EDS	:	NOT EXECUTED
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)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

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 2.10 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	4460 (2.10-2.10)
Ramachandran outliers	100387	4413 (2.10-2.10)
Sidechain outliers	100360	4414 (2.10-2.10)

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	532	87% 11% • •
1	C	532	71% 10% • 17%
2	B	61	46% 18% • 33%
2	D	61	48% 8% 44%

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 7794 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 BETA-CATENIN ARMADILLO REPEAT REGION.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	522	Total	C	N	O	S	0	0	0
			3864	2435	694	709	26			
1	C	439	Total	C	N	O	S	0	0	0
			3148	1988	560	582	18			

- Molecule 2 is a protein called TCF3-CBD (CATENIN BINDING DOMAIN).

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
2	B	41	Total	C	N	O	0	0	0
			286	172	47	67			
2	D	34	Total	C	N	O	0	0	0
			233	143	39	51			

- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	180	Total	O	0	0
			180	180		
3	B	12	Total	O	0	0
			12	12		
3	C	67	Total	O	0	0
			67	67		
3	D	4	Total	O	0	0
			4	4		

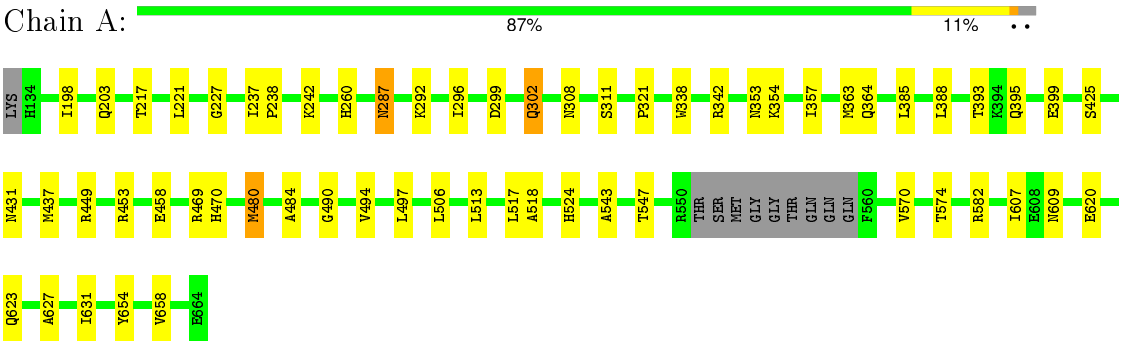
3 Residue-property plots (i)

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.

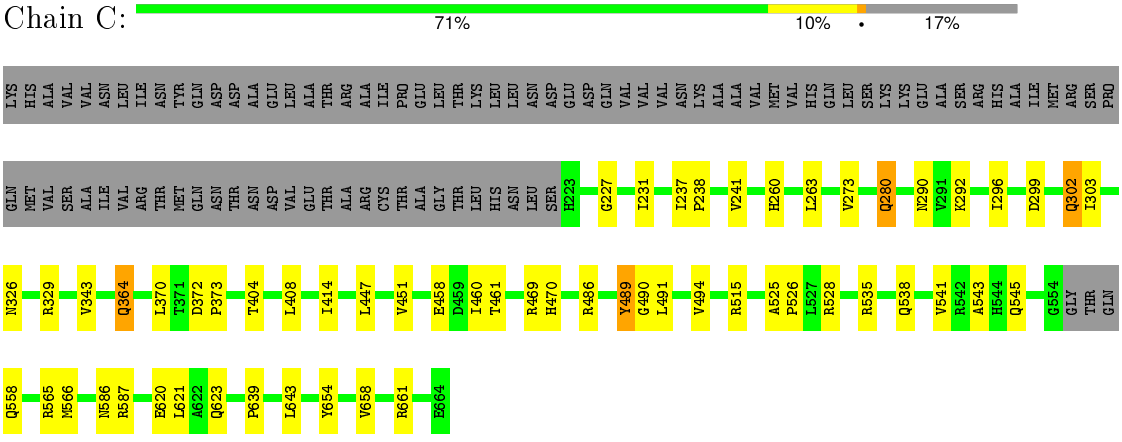
- Molecule 1: BETA-CATENIN ARMADILLO REPEAT REGION

Chain A:



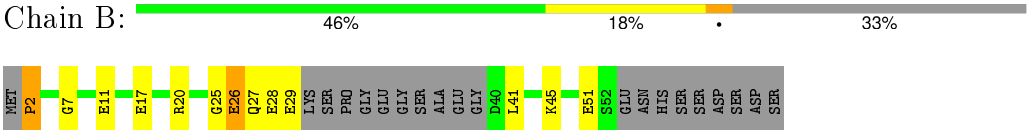
- Molecule 1: BETA-CATENIN ARMADILLO REPEAT REGION

Chain C:



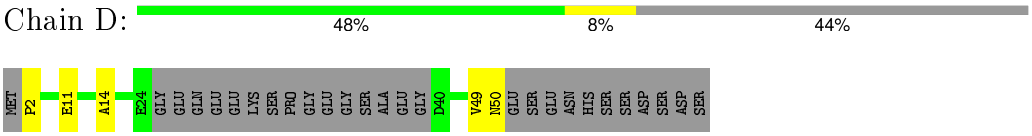
- Molecule 2: TCF3-CBD (CATENIN BINDING DOMAIN)

Chain B:



- Molecule 2: TCF3-CBD (CATENIN BINDING DOMAIN)

Chain D:


48%
8%
44%
MET
P2
E11
A14
P24
GLY
GLU
GLN
GLU
GLU
LYS
SER
PRO
GLY
GLU
GLY
SER
ALA
GLU
GLY
P40
V49
N50
GLU
SER
GLU
ASN
HIS
SER
SER
ASP
SER
ASP
SER

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	52.13Å 153.25Å 188.12Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	25.00 – 2.10	Depositor
% Data completeness (in resolution range)	(Not available) (25.00-2.10)	Depositor
R_{merge}	0.05	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	CNS	Depositor
R, R_{free}	0.229 , 0.255	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	7794	wwPDB-VP
Average B, all atoms (Å^2)	38.0	wwPDB-VP

5 Model quality

5.1 Standard geometry

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	0.29	0/3918	0.50	0/5335
1	C	0.27	0/3190	0.48	0/4356
2	B	0.34	0/285	0.73	1/382 (0.3%)
2	D	0.32	0/232	0.64	1/311 (0.3%)
All	All	0.28	0/7625	0.51	2/10384 (0.0%)

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	B	2	PRO	N-CA-CB	5.64	110.06	103.30
2	D	2	PRO	N-CA-CB	5.58	109.99	103.30

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

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	3864	0	3918	48	0
1	C	3148	0	3116	39	0
2	B	286	0	238	9	0
2	D	233	0	203	4	0
3	A	180	0	0	4	0
3	B	12	0	0	1	0
3	C	67	0	0	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	D	4	0	0	0	0
All	All	7794	0	7475	93	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 (93) 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:C:280:GLN:HE21	1:C:280:GLN:N	1.72	0.87
1:C:280:GLN:HE21	1:C:280:GLN:H	0.89	0.87
1:A:399:GLU:HG3	1:A:437:MET:SD	2.15	0.87
1:C:280:GLN:H	1:C:280:GLN:NE2	1.75	0.83
1:A:363:MET:HA	1:A:363:MET:HE2	1.66	0.78
1:C:364:GLN:HE21	1:C:364:GLN:H	1.33	0.77
1:C:364:GLN:NE2	1:C:364:GLN:H	1.84	0.75
1:A:364:GLN:HE22	1:A:395:GLN:HE21	1.33	0.75
1:C:587:ARG:HG3	1:C:621:LEU:HD23	1.70	0.74
1:A:469:ARG:HH21	1:A:470:HIS:CE1	2.07	0.72
1:A:363:MET:HE2	1:A:385:LEU:HD23	1.72	0.71
1:C:543:ALA:HA	1:C:566:MET:HE3	1.71	0.71
1:C:469:ARG:HH21	1:C:470:HIS:CE1	2.13	0.67
1:C:326:ASN:HD22	1:C:329:ARG:HH21	1.44	0.65
1:A:308:ASN:HD22	1:A:311:SER:H	1.43	0.65
1:A:287:ASN:H	1:A:287:ASN:HD22	1.45	0.64
1:A:469:ARG:HH21	1:A:470:HIS:HE1	1.46	0.63
1:C:326:ASN:ND2	1:C:329:ARG:HH21	1.98	0.62
1:C:491:LEU:HD23	1:C:526:PRO:HB2	1.81	0.61
1:A:321:PRO:HB3	1:A:357:ILE:HD13	1.82	0.60
1:C:525:ALA:HB3	1:C:526:PRO:HD3	1.83	0.59
1:C:302:GLN:HB2	1:C:343:VAL:HG22	1.86	0.57
1:A:354:LYS:HG3	1:A:388:LEU:HD23	1.87	0.57
1:C:458:GLU:HA	1:C:461:THR:OG1	2.05	0.56
1:C:620:GLU:O	1:C:623:GLN:HG2	2.06	0.56
1:A:260:HIS:HD2	2:B:45:LYS:NZ	2.05	0.55
1:A:260:HIS:HE1	1:A:299:ASP:OD1	1.92	0.53
1:A:364:GLN:HE22	1:A:395:GLN:NE2	2.02	0.52
1:A:203:GLN:HG3	1:A:242:LYS:HD3	1.91	0.52
1:A:287:ASN:N	1:A:287:ASN:HD22	2.05	0.52
1:A:237:ILE:HB	1:A:238:PRO:HD3	1.92	0.52
1:A:353:ASN:O	1:A:357:ILE:HG12	2.10	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:480:MET:HE2	1:A:484:ALA:HB2	1.92	0.51
1:C:237:ILE:O	1:C:241:VAL:HG23	2.10	0.50
1:A:518:ALA:O	1:A:524:HIS:HE1	1.94	0.50
1:A:221:LEU:O	1:A:227:GLY:HA3	2.11	0.50
1:C:299:ASP:O	1:C:303:ILE:HG13	2.12	0.49
1:A:302:GLN:OE1	2:B:27:GLN:HG2	2.11	0.49
1:C:292:LYS:O	1:C:296:ILE:HG12	2.13	0.49
1:A:363:MET:CE	1:A:385:LEU:HD23	2.40	0.49
1:A:620:GLU:O	1:A:623:GLN:HG2	2.13	0.49
1:C:654:TYR:O	1:C:658:VAL:HG23	2.12	0.49
1:C:558:GLN:HA	1:C:565:ARG:HH22	1.78	0.48
1:A:607:ILE:HA	2:B:2:PRO:O	2.13	0.48
1:C:414:ILE:HG13	1:C:460:ILE:HD11	1.95	0.48
2:B:20:ARG:HG2	3:B:351:HOH:O	2.13	0.48
1:C:469:ARG:HH21	1:C:470:HIS:HE1	1.61	0.47
1:A:543:ALA:O	1:A:547:THR:HG23	2.15	0.47
1:A:480:MET:CE	1:A:484:ALA:HB2	2.45	0.46
2:D:11:GLU:H	2:D:11:GLU:CD	2.18	0.46
1:A:198:ILE:HD13	1:A:217:THR:HG21	1.97	0.46
2:D:49:VAL:HG23	2:D:50:ASN:H	1.80	0.46
2:B:27:GLN:O	2:B:29:GLU:N	2.48	0.46
1:C:541:VAL:O	1:C:545:GLN:HG3	2.15	0.45
1:C:260:HIS:HE1	1:C:299:ASP:OD2	1.99	0.45
1:A:570:VAL:O	1:A:574:THR:HG23	2.17	0.44
1:C:237:ILE:N	1:C:238:PRO:HD2	2.32	0.44
1:C:486:ARG:HG3	1:C:491:LEU:HD22	1.98	0.44
2:D:49:VAL:HG23	2:D:50:ASN:N	2.32	0.44
1:A:524:HIS:HD2	3:A:749:HOH:O	2.01	0.44
1:A:292:LYS:HG3	3:A:830:HOH:O	2.17	0.44
1:C:447:LEU:O	1:C:451:VAL:HG23	2.18	0.44
1:A:449:ARG:HG3	1:A:449:ARG:HH11	1.82	0.44
1:C:404:THR:O	1:C:408:LEU:HG	2.17	0.44
1:A:582:ARG:NH2	2:B:11:GLU:HG3	2.32	0.44
1:A:296:ILE:HD13	2:B:41:LEU:HD13	2.00	0.44
1:C:489:TYR:HB3	3:C:668:HOH:O	2.18	0.44
1:A:393:THR:O	1:A:431:ASN:ND2	2.45	0.43
1:A:363:MET:HA	1:A:363:MET:CE	2.43	0.43
1:C:535:ARG:HA	1:C:538:GLN:HG2	2.00	0.43
1:C:227:GLY:O	1:C:231:ILE:HG13	2.19	0.43
1:A:513:LEU:O	1:A:517:LEU:HG	2.19	0.42
1:A:453:ARG:HD2	3:A:843:HOH:O	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:363:MET:HE3	1:A:388:LEU:HD13	2.01	0.42
1:C:370:LEU:HB2	1:C:404:THR:HG21	2.02	0.42
1:A:654:TYR:O	1:A:658:VAL:HG23	2.20	0.42
1:A:480:MET:HE2	3:A:791:HOH:O	2.19	0.41
1:C:490:GLY:O	1:C:494:VAL:HG23	2.20	0.41
1:A:627:ALA:O	1:A:631:ILE:HG13	2.20	0.41
1:A:260:HIS:HD2	2:B:45:LYS:HZ2	1.69	0.41
2:B:7:GLY:HA2	2:B:17:GLU:OE2	2.21	0.41
1:A:490:GLY:O	1:A:494:VAL:HG23	2.20	0.41
1:A:425:SER:O	1:A:470:HIS:HD2	2.04	0.41
1:A:497:LEU:HD22	1:A:506:LEU:HD21	2.03	0.41
1:A:338:TRP:O	1:A:342:ARG:HG3	2.21	0.41
1:C:372:ASP:HA	1:C:373:PRO:HD3	1.92	0.41
1:C:515:ARG:HD3	2:D:14:ALA:HB2	2.03	0.40
1:C:263:LEU:HD21	1:C:273:VAL:HG21	2.03	0.40
1:A:458:GLU:HG2	1:A:506:LEU:HD22	2.03	0.40
1:C:528:ARG:HD3	1:C:586:ASN:OD1	2.20	0.40
1:C:326:ASN:ND2	1:C:329:ARG:NH2	2.66	0.40
1:C:639:PRO:O	1:C:643:LEU:HG	2.21	0.40
1:A:609:ASN:HA	1:A:609:ASN:HD22	1.67	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	518/532 (97%)	514 (99%)	4 (1%)	0	100 100
1	C	435/532 (82%)	428 (98%)	7 (2%)	0	100 100
2	B	37/61 (61%)	31 (84%)	2 (5%)	4 (11%)	0 0
2	D	30/61 (49%)	29 (97%)	1 (3%)	0	100 100
All	All	1020/1186 (86%)	1002 (98%)	14 (1%)	4 (0%)	39 37

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	B	25	GLY
2	B	51	GLU
2	B	28	GLU
2	B	26	GLU

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	403/441 (91%)	400 (99%)	3 (1%)	88	92
1	C	312/441 (71%)	306 (98%)	6 (2%)	65	70
2	B	26/50 (52%)	25 (96%)	1 (4%)	40	40
2	D	21/50 (42%)	21 (100%)	0	100	100
All	All	762/982 (78%)	752 (99%)	10 (1%)	76	82

All (10) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	287	ASN
1	A	302	GLN
1	A	480	MET
2	B	26	GLU
1	C	280	GLN
1	C	290	ASN
1	C	302	GLN
1	C	364	GLN
1	C	489	TYR
1	C	661	ARG

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (34) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	138	ASN

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Mol	Chain	Res	Type
1	A	165	GLN
1	A	204	ASN
1	A	220	ASN
1	A	260	HIS
1	A	287	ASN
1	A	308	ASN
1	A	322	GLN
1	A	395	GLN
1	A	470	HIS
1	A	482	GLN
1	A	524	HIS
1	A	548	GLN
1	A	611	GLN
1	C	260	HIS
1	C	261	ASN
1	C	280	GLN
1	C	290	ASN
1	C	302	GLN
1	C	326	ASN
1	C	353	ASN
1	C	364	GLN
1	C	369	HIS
1	C	395	GLN
1	C	434	ASN
1	C	440	GLN
1	C	470	HIS
1	C	482	GLN
1	C	499	HIS
1	C	503	HIS
1	C	538	GLN
1	C	545	GLN
1	C	611	GLN
1	C	623	GLN

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

There are no ligands in this entry.

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.