



# Full wwPDB X-ray Structure Validation Report ⓘ

Jan 31, 2016 – 08:55 PM GMT

PDB ID : 1MR5  
Title : Orthorhombic form of Trypanosoma cruzi trans-sialidase  
Authors : Buschiazzo, A.; Amaya, M.F.; Cremona, M.L.; Frasch, A.C.; Alzari, P.M.  
Deposited on : 2002-09-18  
Resolution : 2.25 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.

---

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

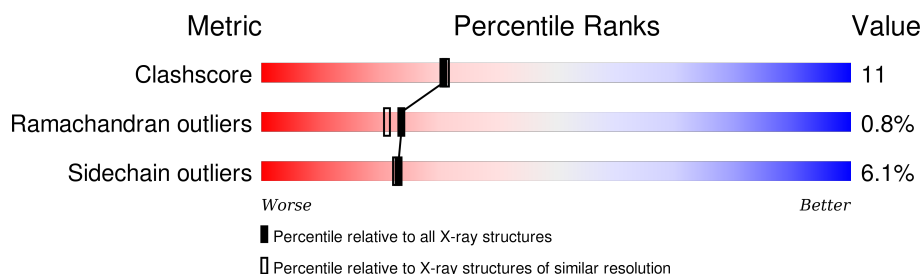
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.25 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	1095 (2.26-2.26)
Ramachandran outliers	100387	1063 (2.26-2.26)
Sidechain outliers	100360	1063 (2.26-2.26)

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	648	 73% 19% • •

## 2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 4974 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 trans-sialidase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	621	Total	C	N	O	S	0	2	0
			4842	3063	847	916	16			

There are 25 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-13	MET	-	EXPRESSION TAG	UNP Q26966
A	-12	GLY	-	EXPRESSION TAG	UNP Q26966
A	-11	GLY	-	EXPRESSION TAG	UNP Q26966
A	-10	SER	-	EXPRESSION TAG	UNP Q26966
A	-9	HIS	-	EXPRESSION TAG	UNP Q26966
A	-8	HIS	-	EXPRESSION TAG	UNP Q26966
A	-7	HIS	-	EXPRESSION TAG	UNP Q26966
A	-6	HIS	-	EXPRESSION TAG	UNP Q26966
A	-5	HIS	-	EXPRESSION TAG	UNP Q26966
A	-4	HIS	-	EXPRESSION TAG	UNP Q26966
A	-3	GLY	-	EXPRESSION TAG	UNP Q26966
A	-2	MET	-	EXPRESSION TAG	UNP Q26966
A	-1	ALA	-	EXPRESSION TAG	UNP Q26966
A	0	SER	-	EXPRESSION TAG	UNP Q26966
A	58	PHE	ASN	ENGINEERED	UNP Q26966
A	262	THR	SER	SEE REMARK 999	UNP Q26966
A	476	HIS	ARG	SEE REMARK 999	UNP Q26966
A	484	LEU	VAL	SEE REMARK 999	UNP Q26966
A	495	LYS	SER	ENGINEERED	UNP Q26966
A	496	GLY	VAL	ENGINEERED	UNP Q26966
A	520	LYS	GLU	ENGINEERED	UNP Q26966
A	558	VAL	GLU	SEE REMARK 999	UNP Q26966
A	593	GLY	ASP	ENGINEERED	UNP Q26966
A	597	ASP	ILE	ENGINEERED	UNP Q26966
A	599	ARG	HIS	ENGINEERED	UNP Q26966

- Molecule 2 is water.

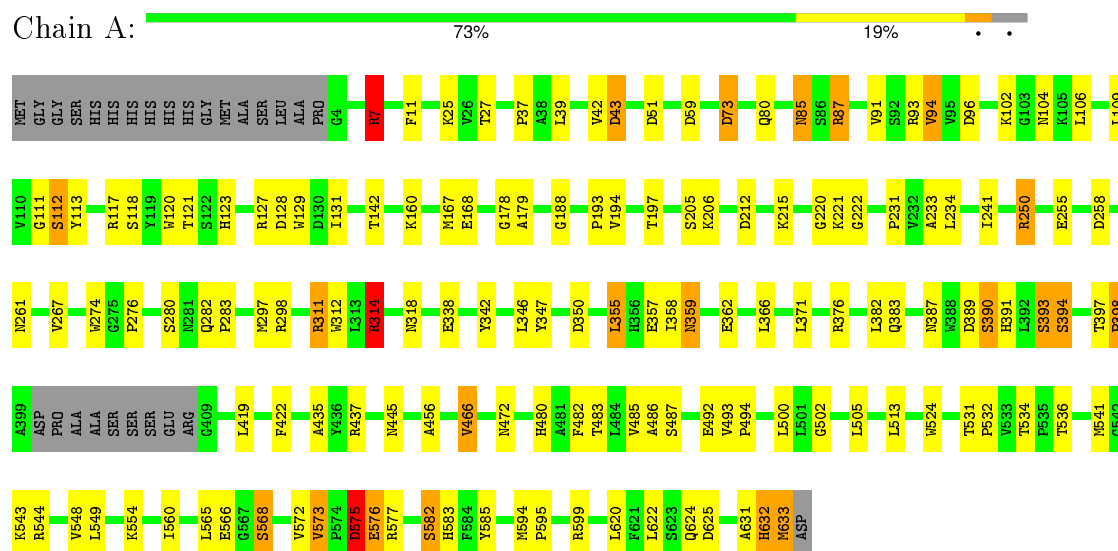
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	132	Total 132	O 132	0	0

### 3 Residue-property plots

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: trans-sialidase



## 4 Data and refinement statistics

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

Property	Value	Source
Space group	P 21 21 2	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	87.03 Å 88.02 Å 89.56 Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	27.84 – 2.25	Depositor
% Data completeness (in resolution range)	99.5 (27.84-2.25)	Depositor
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	0.06	Depositor
Refinement program	REFMAC 5	Depositor
R, $R_{free}$	0.218 , 0.274	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	4974	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	21.0	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	0.99	0/4954	1.09	20/6722 (0.3%)

There are no bond length outliers.

All (20) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	96	ASP	CB-CG-OD2	9.93	127.24	118.30
1	A	258	ASP	CB-CG-OD2	8.83	126.25	118.30
1	A	212	ASP	CB-CG-OD2	8.76	126.18	118.30
1	A	250	ARG	NE-CZ-NH2	-8.44	116.08	120.30
1	A	43	ASP	CB-CG-OD2	8.43	125.89	118.30
1	A	314	ARG	NE-CZ-NH2	-8.11	116.24	120.30
1	A	376	ARG	NE-CZ-NH1	-8.01	116.29	120.30
1	A	437	ARG	NE-CZ-NH1	-7.97	116.31	120.30
1	A	73	ASP	CB-CG-OD1	-7.86	111.22	118.30
1	A	73	ASP	CB-CG-OD2	7.69	125.22	118.30
1	A	7	ARG	NE-CZ-NH1	7.27	123.94	120.30
1	A	625	ASP	CB-CG-OD2	6.39	124.05	118.30
1	A	59	ASP	CB-CG-OD2	6.37	124.04	118.30
1	A	376	ARG	NE-CZ-NH2	6.26	123.43	120.30
1	A	51	ASP	CB-CA-C	-6.01	98.38	110.40
1	A	620	LEU	CB-CG-CD1	6.00	121.21	111.00
1	A	7	ARG	NE-CZ-NH2	-5.75	117.43	120.30
1	A	437	ARG	NE-CZ-NH2	5.63	123.12	120.30
1	A	575	ASP	CB-CG-OD2	5.50	123.25	118.30
1	A	87	ARG	NE-CZ-NH1	-5.05	117.77	120.30

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	4842	0	4764	105	0
2	A	132	0	0	5	0
All	All	4974	0	4764	105	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 11.

All (105) 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:505:LEU:HD11	1:A:513:LEU:HB2	1.46	0.97
1:A:383:GLN:HE21	1:A:387:ASN:ND2	1.71	0.89
1:A:312:TRP:O	1:A:314:ARG:HD2	1.80	0.81
1:A:312:TRP:O	1:A:314:ARG:CD	2.34	0.76
1:A:359:ASN:HD21	1:A:362:GLU:H	1.35	0.75
1:A:560:ILE:HD12	1:A:565:LEU:HD21	1.70	0.72
1:A:524:TRP:CE2	1:A:560:ILE:HD13	2.25	0.71
1:A:85:ASN:HD22	1:A:87:ARG:H	1.39	0.71
1:A:544:ARG:HD2	2:A:735:HOH:O	1.91	0.70
1:A:206:LYS:NZ	1:A:222:GLY:O	2.20	0.69
1:A:234:LEU:HD12	1:A:234:LEU:C	2.13	0.68
1:A:492:GLU:OE2	1:A:599:ARG:HD2	1.95	0.67
1:A:267:VAL:HB	1:A:480:HIS:CD2	2.32	0.64
1:A:631:ALA:C	1:A:633:MET:H	2.01	0.64
1:A:390:SER:O	1:A:394:SER:OG	2.15	0.63
1:A:312:TRP:C	1:A:314:ARG:HD2	2.22	0.60
1:A:383:GLN:NE2	1:A:387:ASN:ND2	2.46	0.59
1:A:397:THR:HG23	1:A:398:PRO:HD2	1.84	0.59
1:A:118:SER:O	1:A:123:HIS:HE1	1.85	0.59
1:A:383:GLN:HE21	1:A:387:ASN:CG	2.06	0.59
1:A:466:VAL:HG23	1:A:583:HIS:HA	1.84	0.58
1:A:524:TRP:NE1	1:A:560:ILE:HD13	2.19	0.57
1:A:39:LEU:HG	1:A:346:LEU:HD22	1.87	0.56
1:A:347:TYR:OH	1:A:350:ASP:OD2	2.16	0.56
1:A:383:GLN:NE2	1:A:387:ASN:HD21	2.04	0.55

*Continued on next page...*



*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:104:ASN:ND2	2:A:642:HOH:O	2.32	0.55
1:A:544:ARG:CD	2:A:735:HOH:O	2.51	0.55
1:A:91:VAL:HG11	1:A:117:ARG:HD3	1.88	0.55
1:A:342:TYR:HB2	1:A:357:GLU:CD	2.28	0.54
1:A:572:VAL:HG23	1:A:573:VAL:HG12	1.89	0.54
1:A:274:TRP:HA	1:A:472:ASN:HD22	1.72	0.53
1:A:43:ASP:CG	2:A:696:HOH:O	2.48	0.52
1:A:109:LEU:HD11	1:A:131:ILE:HD11	1.91	0.52
1:A:505:LEU:HD13	1:A:513:LEU:N	2.25	0.51
1:A:42:VAL:HG21	1:A:106:LEU:HD21	1.93	0.51
1:A:505:LEU:N	1:A:505:LEU:CD1	2.72	0.51
1:A:531:THR:CG2	1:A:532:PRO:HD2	2.40	0.51
1:A:193:PRO:HB2	1:A:231:PRO:HG2	1.92	0.51
1:A:11:PHE:HB2	1:A:366:LEU:HB2	1.93	0.50
1:A:297[B]:MET:SD	1:A:382:LEU:HD22	2.52	0.49
1:A:312:TRP:O	1:A:314:ARG:HD3	2.10	0.49
1:A:37:PRO:CB	1:A:355:LEU:HD13	2.43	0.49
1:A:193:PRO:HG3	1:A:233:ALA:HB3	1.93	0.49
1:A:398:PRO:HG2	1:A:622:LEU:HB3	1.95	0.49
1:A:241:ILE:CD1	1:A:255:GLU:HG2	2.42	0.49
1:A:311:ARG:HG3	1:A:311:ARG:HH11	1.78	0.48
1:A:276:PRO:HD2	1:A:280:SER:HA	1.94	0.48
1:A:505:LEU:HD11	1:A:513:LEU:CB	2.32	0.48
1:A:631:ALA:C	1:A:633:MET:N	2.65	0.48
1:A:565:LEU:O	1:A:568:SER:HB2	2.14	0.47
1:A:206:LYS:NZ	1:A:220:GLY:O	2.37	0.47
1:A:492:GLU:HA	1:A:541:MET:HE1	1.96	0.47
1:A:487:SER:CB	1:A:624:GLN:OE1	2.63	0.47
1:A:543:LYS:NZ	2:A:678:HOH:O	2.44	0.47
1:A:389:ASP:O	1:A:393:SER:HB2	2.14	0.47
1:A:524:TRP:CD1	1:A:560:ILE:CD1	2.98	0.47
1:A:129:TRP:O	1:A:160:LYS:NZ	2.48	0.47
1:A:359:ASN:HD21	1:A:362:GLU:N	2.08	0.46
1:A:37:PRO:HD2	1:A:342:TYR:HB3	1.96	0.46
1:A:485:VAL:HG12	1:A:486:ALA:N	2.30	0.46
1:A:487:SER:OG	1:A:624:GLN:OE1	2.33	0.46
1:A:178:GLY:O	1:A:179:ALA:HB3	2.16	0.46
1:A:391:HIS:HE1	1:A:632:HIS:CD2	2.34	0.46
1:A:94:VAL:HA	1:A:111:GLY:O	2.15	0.46
1:A:282:GLN:HB3	1:A:283:PRO:HD2	1.97	0.46
1:A:85:ASN:ND2	1:A:87:ARG:HH21	2.14	0.46

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:120:TRP:CZ3	1:A:197:THR:HG23	2.51	0.45
1:A:505:LEU:HD13	1:A:513:LEU:H	1.82	0.45
1:A:359:ASN:ND2	1:A:359:ASN:C	2.69	0.45
1:A:502:GLY:HA3	1:A:585:TYR:CZ	2.52	0.45
1:A:505:LEU:HD12	1:A:505:LEU:HA	1.79	0.45
1:A:554:LYS:NZ	1:A:573:VAL:HG22	2.32	0.45
1:A:85:ASN:ND2	1:A:87:ARG:H	2.10	0.44
1:A:575:ASP:O	1:A:576:GLU:C	2.55	0.44
1:A:234:LEU:CD1	1:A:234:LEU:C	2.83	0.44
1:A:206:LYS:NZ	1:A:221:LYS:C	2.71	0.44
1:A:422:PHE:HB3	1:A:435:ALA:HB3	1.99	0.44
1:A:234:LEU:HD12	1:A:234:LEU:O	2.16	0.44
1:A:102:LYS:NZ	1:A:188:GLY:O	2.45	0.44
1:A:594:MET:HA	1:A:595:PRO:HD3	1.75	0.44
1:A:483:THR:HA	1:A:549:LEU:O	2.18	0.44
1:A:312:TRP:HA	1:A:314:ARG:HD2	1.98	0.44
1:A:93:ARG:O	1:A:112:SER:HA	2.17	0.44
1:A:531:THR:HG23	1:A:532:PRO:HD2	2.00	0.44
1:A:342:TYR:HB2	1:A:357:GLU:CG	2.49	0.43
1:A:493:VAL:HG22	1:A:494:PRO:HD2	2.00	0.43
1:A:194:VAL:O	1:A:205:SER:HA	2.18	0.43
1:A:536:THR:HG21	1:A:566:GLU:HB3	2.00	0.43
1:A:312:TRP:CA	1:A:314:ARG:HD2	2.50	0.42
1:A:485:VAL:HG22	1:A:548:VAL:HG22	2.01	0.42
1:A:391:HIS:CE1	1:A:632:HIS:CD2	3.07	0.42
1:A:167:MET:O	1:A:168:GLU:C	2.57	0.42
1:A:282:GLN:HB3	1:A:283:PRO:CD	2.49	0.42
1:A:358:ILE:O	1:A:358:ILE:HG13	2.19	0.41
1:A:85:ASN:C	1:A:85:ASN:HD22	2.24	0.41
1:A:37:PRO:HB2	1:A:355:LEU:HD13	2.03	0.41
1:A:355:LEU:HD22	1:A:366:LEU:HB3	2.02	0.41
1:A:445:ASN:HB3	1:A:456:ALA:O	2.20	0.41
1:A:482:PHE:CD1	1:A:482:PHE:C	2.93	0.41
1:A:7:ARG:NH2	1:A:338:GLU:OE1	2.50	0.41
1:A:94:VAL:HG12	1:A:112:SER:HB2	2.02	0.41
1:A:113:TYR:HA	1:A:128:ASP:O	2.20	0.41
1:A:359:ASN:ND2	1:A:362:GLU:H	2.12	0.40
1:A:342:TYR:CD1	1:A:342:TYR:N	2.90	0.40
1:A:582:SER:OG	1:A:583:HIS:ND1	2.40	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	619/648 (96%)	586 (95%)	28 (4%)	5 (1%)	24	21

All (5) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	632	HIS
1	A	575	ASP
1	A	576	GLU
1	A	398	PRO
1	A	466	VAL

### 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	527/547 (96%)	495 (94%)	32 (6%)	23	23

All (32) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	7	ARG
1	A	25	LYS
1	A	27	THR
1	A	73	ASP
1	A	80	GLN
1	A	85	ASN

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
1	A	94	VAL
1	A	112	SER
1	A	121	THR
1	A	127	ARG
1	A	142	THR
1	A	215	LYS
1	A	250	ARG
1	A	261	ASN
1	A	298	ARG
1	A	311	ARG
1	A	314	ARG
1	A	318	ASN
1	A	355	LEU
1	A	359	ASN
1	A	371	LEU
1	A	390	SER
1	A	393	SER
1	A	394	SER
1	A	419	LEU
1	A	500	LEU
1	A	534	THR
1	A	568	SER
1	A	573	VAL
1	A	577	ARG
1	A	582	SER
1	A	633	MET

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (9) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	85	ASN
1	A	123	HIS
1	A	174	GLN
1	A	359	ASN
1	A	383	GLN
1	A	472	ASN
1	A	480	HIS
1	A	604	ASN
1	A	632	HIS

### 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.