



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 10, 2026 – 08:45 AM UTC

PDB ID : 1GTA / pdb_00001gta
Title : CRYSTAL STRUCTURES OF A SCHISTOSOMAL DRUG AND VACCINE TARGET: GLUTATHIONE S-TRANSFERASE FROM SCHISTOSOMA JAPONICA AND ITS COMPLEX WITH THE LEADING ANTISCHISTOSOMAL DRUG PRAZIQUANTEL
Authors : Mctigue, M.A.; Tainer, J.A.
Deposited on : 1994-12-01
Resolution : 2.40 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 ⓘ 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 ⓘ](#)) were used in the production of this report:

MolProbity : 4-5-2 with Phenix2.0
Xtriage (Phenix) : **NOT EXECUTED**
EDS : **NOT EXECUTED**
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

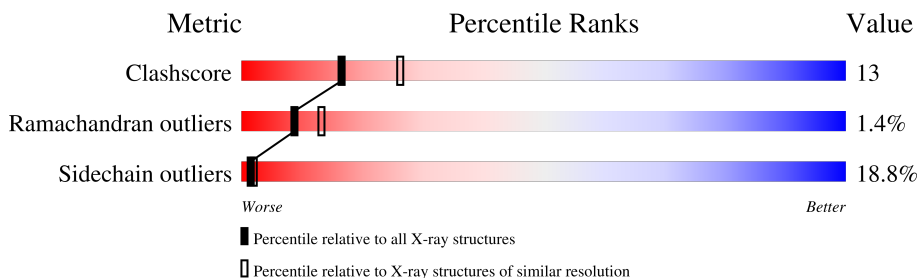
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.40 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	190562	5391 (2.40-2.40)
Ramachandran outliers	187476	5320 (2.40-2.40)
Sidechain outliers	187428	5321 (2.40-2.40)

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 $\leq 5\%$

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	218	

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 1900 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 GLUTATHIONE S-TRANSFERASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	218	Total	C	N	O	S	0	0	0
			1786	1163	288	322	13			

- Molecule 2 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	114	Total	O	0	0
			114	114		

3 Residue-property plots

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: GLUTATHIONE S-TRANSFERASE



4 Data and refinement statistics

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

Property	Value	Source
Space group	P 63 2 2	Depositor
Cell constants a, b, c, α , β , γ	125.20Å 125.20Å 70.20Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	7.00 – 2.40	Depositor
% Data completeness (in resolution range)	(Not available) (7.00-2.40)	Depositor
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	X-PLOR	Depositor
R, R_{free}	0.197 , (Not available)	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	1900	wwPDB-VP
Average B, all atoms (Å ²)	30.0	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	1.49	17/1834 (0.9%)	2.46	113/2475 (4.6%)

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
1	A	0	2

All (17) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	99	VAL	CA-CB	9.00	1.65	1.54
1	A	110	ALA	CA-CB	-7.58	1.42	1.53
1	A	117	THR	CA-CB	7.16	1.64	1.53
1	A	150	HIS	CD2-NE2	-6.74	1.30	1.37
1	A	120	VAL	CA-CB	6.48	1.63	1.54
1	A	51	GLU	CA-CB	-6.40	1.42	1.53
1	A	31	HIS	CD2-NE2	-6.29	1.30	1.37
1	A	147	HIS	CD2-NE2	-6.10	1.31	1.37
1	A	139	HIS	CD2-NE2	-5.95	1.31	1.37
1	A	73	ARG	NE-CZ	5.73	1.39	1.33
1	A	128	GLU	CA-CB	-5.69	1.43	1.53
1	A	151	PRO	CA-CB	-5.56	1.46	1.53
1	A	66	THR	C-O	5.56	1.30	1.24
1	A	150	HIS	CA-CB	5.43	1.62	1.54
1	A	111	TYR	CA-C	5.41	1.60	1.52
1	A	79	HIS	CD2-NE2	-5.19	1.32	1.37
1	A	26	GLU	CA-CB	-5.03	1.46	1.53

All (113) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	216	PRO	N-CA-C	24.63	140.75	110.70
1	A	215	HIS	CA-C-N	16.07	136.93	120.38
1	A	215	HIS	C-N-CA	16.07	136.93	120.38
1	A	94	MET	CG-SD-CE	-12.25	73.95	100.90
1	A	69	MET	CG-SD-CE	-12.01	74.48	100.90
1	A	66	THR	N-CA-C	11.60	131.21	114.39
1	A	18	ARG	NE-CZ-NH1	10.61	132.11	121.50
1	A	214	ASP	CA-CB-CG	10.16	122.76	112.60
1	A	150	HIS	CA-CB-CG	9.04	122.84	113.80
1	A	171	ASP	CA-C-O	-8.76	111.41	120.96
1	A	165	MET	CG-SD-CE	-8.60	81.98	100.90
1	A	150	HIS	CB-CG-CD2	-8.39	120.29	131.20
1	A	144	ASN	OD1-CG-ND2	-8.28	114.32	122.60
1	A	150	HIS	CB-CG-ND1	8.28	135.13	122.70
1	A	215	HIS	N-CA-C	8.25	128.04	109.81
1	A	54	ASN	CB-CG-ND2	8.19	128.68	116.40
1	A	116	GLU	N-CA-C	8.08	121.00	111.71
1	A	188	GLN	OE1-CD-NE2	-8.03	114.57	122.60
1	A	63	VAL	N-CA-CB	-8.02	96.93	111.92
1	A	54	ASN	OD1-CG-ND2	-7.97	114.63	122.60
1	A	186	ILE	N-CA-C	-7.66	102.04	108.63
1	A	204	GLN	OE1-CD-NE2	-7.65	114.95	122.60
1	A	36	ASP	CA-CB-CG	7.56	120.16	112.60
1	A	34	GLU	CA-CB-CG	-7.47	99.16	114.10
1	A	29	GLU	O-C-N	-7.44	113.79	123.16
1	A	104	TYR	N-CA-C	-7.36	103.76	112.89
1	A	148	VAL	CG1-CB-CG2	-7.15	95.07	110.80
1	A	161	VAL	CA-C-O	-7.08	112.53	120.96
1	A	121	ASP	CA-C-N	7.07	129.75	120.28
1	A	121	ASP	C-N-CA	7.07	129.75	120.28
1	A	85	CYS	CA-C-O	-7.04	114.58	120.71
1	A	158	ALA	O-C-N	-6.94	114.93	122.07
1	A	146	ASP	CA-CB-CG	6.90	119.50	112.60
1	A	201	TRP	O-C-N	-6.88	116.46	121.83
1	A	121	ASP	CA-C-O	-6.78	113.71	120.70
1	A	23	TYR	CA-C-O	6.78	127.74	120.55
1	A	79	HIS	CA-CB-CG	-6.78	107.02	113.80
1	A	149	THR	O-C-N	-6.74	113.31	122.94
1	A	37	GLU	N-CA-C	6.71	120.77	112.59
1	A	196	SER	N-CA-C	-6.61	104.15	111.82
1	A	204	GLN	CG-CD-NE2	6.59	126.29	116.40
1	A	78	LYS	CG-CD-CE	6.59	126.45	111.30
1	A	41	TRP	CG-CD2-CE3	6.56	140.46	133.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	117	THR	N-CA-C	-6.44	105.56	113.41
1	A	216	PRO	CA-C-N	6.42	127.87	119.84
1	A	216	PRO	C-N-CA	6.42	127.87	119.84
1	A	216	PRO	CA-N-CD	-6.39	103.05	112.00
1	A	87	LYS	CA-C-O	-6.33	113.71	120.42
1	A	32	LEU	O-C-N	-6.32	116.13	123.27
1	A	111	TYR	O-C-N	-6.28	114.23	122.59
1	A	164	TYR	CA-C-O	6.26	127.17	119.97
1	A	67	GLN	OE1-CD-NE2	-6.25	116.35	122.60
1	A	138	CYS	CA-CB-SG	-6.24	100.04	114.40
1	A	83	GLY	O-C-N	-6.24	114.59	122.70
1	A	26	GLU	CA-CB-CG	-6.23	101.64	114.10
1	A	148	VAL	O-C-N	-6.21	116.34	122.67
1	A	141	THR	CA-CB-OG1	-6.16	100.36	109.60
1	A	100	LEU	N-CA-C	-6.16	104.68	111.82
1	A	10	ILE	O-C-N	-6.14	116.47	122.92
1	A	171	ASP	N-CA-C	-6.14	101.22	110.24
1	A	15	GLN	OE1-CD-NE2	-6.13	116.47	122.60
1	A	106	VAL	N-CA-C	-6.09	104.80	110.53
1	A	83	GLY	CA-C-O	-6.08	109.98	120.57
1	A	59	ILE	CA-C-O	6.04	127.61	120.72
1	A	150	HIS	CA-C-N	5.90	125.77	119.28
1	A	150	HIS	C-N-CA	5.90	125.77	119.28
1	A	91	GLU	CA-CB-CG	5.86	125.83	114.10
1	A	65	LEU	N-CA-CB	-5.83	100.75	111.37
1	A	95	LEU	CA-C-O	5.81	126.67	120.10
1	A	150	HIS	O-C-N	-5.81	115.23	120.92
1	A	188	GLN	CA-CB-CG	5.80	125.70	114.10
1	A	79	HIS	CB-CG-CD2	-5.79	123.67	131.20
1	A	182	ARG	CA-C-O	-5.77	114.31	120.42
1	A	67	GLN	CG-CD-NE2	5.76	125.04	116.40
1	A	41	TRP	CB-CG-CD1	-5.71	118.34	126.90
1	A	58	TYR	O-C-N	-5.66	116.65	123.27
1	A	139	HIS	CB-CG-CD2	-5.66	123.84	131.20
1	A	43	ASN	OD1-CG-ND2	-5.66	116.94	122.60
1	A	62	ASP	N-CA-C	-5.62	105.54	112.90
1	A	8	TRP	CD1-CG-CD2	5.60	115.26	106.30
1	A	41	TRP	CE2-CD2-CG	-5.58	100.50	107.20
1	A	107	SER	CA-CB-OG	-5.57	99.96	111.10
1	A	66	THR	CA-C-O	5.56	125.09	118.69
1	A	109	ILE	CA-CB-CG2	-5.49	101.16	110.50
1	A	108	ARG	CB-CA-C	-5.49	102.02	110.81

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	183	ILE	N-CA-C	-5.48	105.19	110.72
1	A	18	ARG	NE-CZ-NH2	-5.48	114.27	119.20
1	A	52	PHE	CA-C-N	5.47	125.39	119.76
1	A	52	PHE	C-N-CA	5.47	125.39	119.76
1	A	35	ARG	N-CA-C	5.45	119.09	112.23
1	A	72	ILE	O-C-N	-5.42	115.67	121.80
1	A	172	ALA	N-CA-CB	5.42	119.66	110.49
1	A	103	ARG	N-CA-C	5.42	116.99	111.14
1	A	60	ASP	CA-C-N	-5.41	114.82	123.31
1	A	60	ASP	C-N-CA	-5.41	114.82	123.31
1	A	2	SER	O-C-N	-5.34	115.94	121.28
1	A	107	SER	CA-C-O	-5.34	114.89	120.55
1	A	210	PHE	O-C-N	-5.29	116.32	123.19
1	A	153	PHE	CA-CB-CG	-5.28	108.52	113.80
1	A	194	LYS	CA-C-N	5.28	129.80	120.87
1	A	194	LYS	C-N-CA	5.28	129.80	120.87
1	A	61	GLY	O-C-N	-5.28	117.16	122.65
1	A	21	LEU	CD1-CG-CD2	5.26	122.38	110.80
1	A	8	TRP	CG-CD1-NE1	-5.23	103.40	110.20
1	A	89	ARG	CB-CG-CD	5.21	123.27	111.30
1	A	172	ALA	CB-CA-C	-5.18	100.12	110.42
1	A	67	GLN	N-CA-CB	-5.16	101.64	110.16
1	A	41	TRP	CG-CD1-NE1	-5.14	103.51	110.20
1	A	72	ILE	N-CA-C	-5.12	104.68	111.09
1	A	41	TRP	CD1-CG-CD2	5.11	114.47	106.30
1	A	98	ALA	CA-C-O	-5.07	114.37	120.10
1	A	68	SER	CA-C-O	-5.07	115.16	120.63
1	A	61	GLY	CA-C-O	5.04	124.99	119.55

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	215	HIS	Mainchain,Peptide

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	1786	0	1780	46	0
2	A	114	0	0	14	0
All	All	1900	0	1780	46	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 13.

All (46) 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:83:GLY:HA3	1:A:89:ARG:HG3	1.54	0.89
1:A:66:THR:N	2:A:379:HOH:O	2.27	0.66
1:A:123:LEU:HD13	1:A:165:MET:HE2	1.77	0.66
1:A:75:ILE:O	1:A:79:HIS:HD2	1.80	0.64
1:A:210:PHE:HD1	1:A:218:LYS:HA	1.62	0.64
1:A:210:PHE:CD1	1:A:218:LYS:HA	2.32	0.64
1:A:138:CYS:HB3	2:A:339:HOH:O	1.99	0.62
1:A:123:LEU:CD1	1:A:165:MET:HE2	2.31	0.60
1:A:203:LEU:HB3	2:A:414:HOH:O	2.04	0.57
1:A:201:TRP:NE1	1:A:215:HIS:H	2.03	0.56
1:A:204:GLN:HG2	2:A:414:HOH:O	2.05	0.55
1:A:10:ILE:HG22	1:A:202:PRO:HG2	1.89	0.55
1:A:95:LEU:O	1:A:99:VAL:HG13	2.08	0.54
1:A:210:PHE:HD2	2:A:395:HOH:O	1.92	0.53
1:A:122:PHE:HA	2:A:324:HOH:O	2.09	0.52
1:A:114:ASP:C	1:A:118:LEU:HD22	2.35	0.52
1:A:60:ASP:HB2	1:A:63:VAL:HG12	1.90	0.52
1:A:44:LYS:HA	1:A:47:GLU:HG2	1.93	0.51
1:A:138:CYS:SG	1:A:175:LYS:HE3	2.51	0.50
1:A:114:ASP:O	1:A:118:LEU:HD22	2.13	0.49
1:A:188:GLN:N	1:A:188:GLN:NE2	2.61	0.48
1:A:188:GLN:NE2	1:A:188:GLN:H	2.11	0.48
1:A:54:ASN:HD22	1:A:55:LEU:H	1.62	0.47
1:A:118:LEU:HD21	2:A:418:HOH:O	2.15	0.47
1:A:34:GLU:HB3	2:A:365:HOH:O	2.13	0.47
1:A:69:MET:HE1	2:A:351:HOH:O	2.14	0.47
1:A:161:VAL:HG22	1:A:203:LEU:HG	1.97	0.47
1:A:35:ARG:HB3	1:A:206:TRP:CE2	2.51	0.46
1:A:122:PHE:HD2	1:A:165:MET:HE1	1.79	0.46
1:A:10:ILE:O	1:A:18:ARG:NH2	2.49	0.45
1:A:13:LEU:HD23	2:A:303:HOH:O	2.17	0.45
1:A:18:ARG:O	1:A:22:GLU:HG2	2.16	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:197:LYS:HD3	2:A:330:HOH:O	2.16	0.45
1:A:4:ILE:HD12	2:A:389:HOH:O	2.16	0.45
1:A:84:GLY:N	2:A:380:HOH:O	2.49	0.45
1:A:165:MET:HB2	1:A:210:PHE:CZ	2.52	0.44
1:A:20:LEU:O	1:A:24:LEU:HB2	2.18	0.43
1:A:123:LEU:HD13	1:A:165:MET:CE	2.45	0.43
1:A:4:ILE:HG21	1:A:31:HIS:CE1	2.54	0.42
1:A:63:VAL:HG13	1:A:65:LEU:HD22	2.01	0.42
1:A:171:ASP:O	1:A:172:ALA:CB	2.66	0.42
1:A:35:ARG:HB3	1:A:206:TRP:CD2	2.55	0.42
1:A:201:TRP:CD1	1:A:215:HIS:H	2.38	0.41
1:A:110:ALA:HB2	2:A:395:HOH:O	2.20	0.41
1:A:177:VAL:O	1:A:181:LYS:HG3	2.21	0.41
1:A:11:LYS:HE3	1:A:199:ILE:O	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	A	216/218 (99%)	202 (94%)	11 (5%)	3 (1%)	9 13

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	216	PRO
1	A	111	TYR
1	A	172	ALA

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	192/194 (99%)	156 (81%)	36 (19%)	1 2

All (36) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	1	MET
1	A	5	LEU
1	A	14	VAL
1	A	20	LEU
1	A	21	LEU
1	A	24	LEU
1	A	26	GLU
1	A	32	LEU
1	A	36	ASP
1	A	42	ARG
1	A	43	ASN
1	A	44	LYS
1	A	63	VAL
1	A	65	LEU
1	A	86	PRO
1	A	89	ARG
1	A	94	MET
1	A	99	VAL
1	A	100	LEU
1	A	113	LYS
1	A	118	LEU
1	A	120	VAL
1	A	123	LEU
1	A	126	LEU
1	A	130	LEU
1	A	131	LYS
1	A	138	CYS
1	A	143	LEU
1	A	155	LEU
1	A	163	LEU

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Mol	Chain	Res	Type
1	A	175	LYS
1	A	176	LEU
1	A	188	GLN
1	A	203	LEU
1	A	214	ASP
1	A	216	PRO

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	15	GLN
1	A	43	ASN
1	A	54	ASN
1	A	79	HIS
1	A	188	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 oligosaccharides 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 ⓘ

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 is therefore empty.

6.2 Non-standard residues in protein, DNA, RNA chains

EDS was not executed - this section is therefore empty.

6.3 Carbohydrates

EDS was not executed - this section is therefore empty.

6.4 Ligands

EDS was not executed - this section is therefore empty.

6.5 Other polymers

EDS was not executed - this section is therefore empty.