



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 5, 2018 – 10:58 PM EST

PDB ID : 1OM3  
Title : FAB 2G12 unliganded  
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Deposited on : 2003-02-24  
Resolution : 2.20 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.

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

MolProbity : 4.02b-467  
Xtriage (Phenix) : **NOT EXECUTED**  
EDS : **NOT EXECUTED**  
Percentile statistics : 20161228.v01 (using entries in the PDB archive December 28th 2016)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : rb-20030736

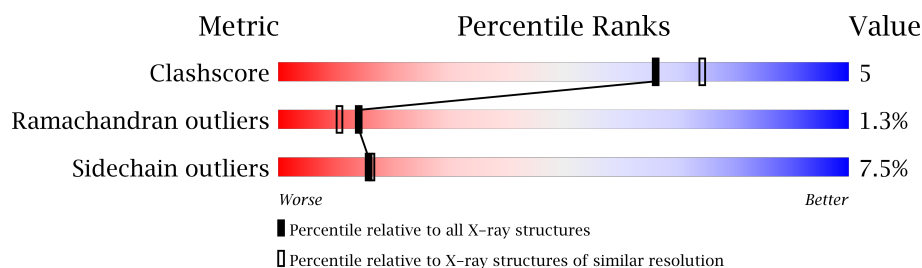
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.20 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	112137	4730 (2.20-2.20)
Ramachandran outliers	110173	4656 (2.20-2.20)
Sidechain outliers	110143	4657 (2.20-2.20)

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	L	212	
1	M	212	
2	H	225	
2	K	225	

## 2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 6855 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 FAB 2G12, light chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	L	212	Total	C	N	O	S	0	0	0
			1620	1016	273	326	5			
1	M	212	Total	C	N	O	S	0	0	0
			1620	1016	273	326	5			

- Molecule 2 is a protein called FAB 2G12, heavy chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	H	224	Total	C	N	O	S	42	0	0
			1670	1048	286	329	7			
2	K	225	Total	C	N	O	S	34	0	0
			1676	1051	287	331	7			

- Molecule 3 is water.

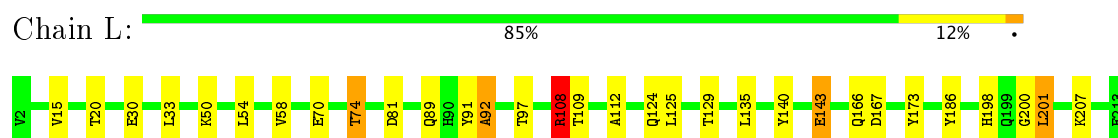
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	L	60	Total	O	0	0
			60	60		
3	H	48	Total	O	0	0
			48	48		
3	M	103	Total	O	0	0
			103	103		
3	K	58	Total	O	0	0
			58	58		

### 3 Residue-property plots [i](#)

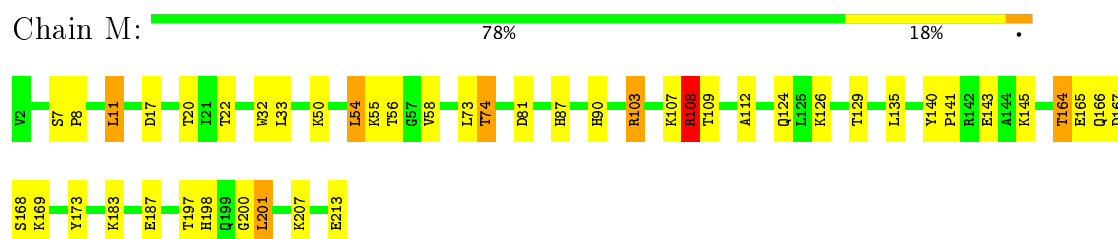
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are 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.

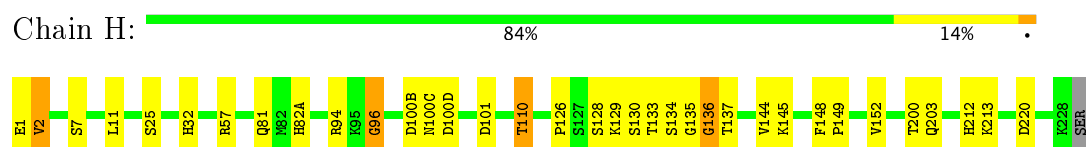
- Molecule 1: FAB 2G12, light chain



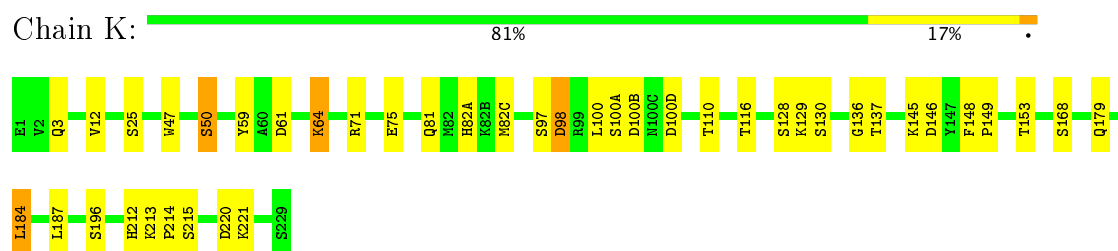
- Molecule 1: FAB 2G12, light chain



- Molecule 2: FAB 2G12, heavy chain



- Molecule 2: FAB 2G12, heavy chain



## 4 Data and refinement statistics

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

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	76.82Å 94.18Å 171.11Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	50.00 – 2.20	Depositor
% Data completeness (in resolution range)	93.6 (50.00-2.20)	Depositor
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	0.06	Depositor
Refinement program	REFMAC 5.1.24	Depositor
R, $R_{free}$	0.225 , 0.266	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	6855	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	22.0	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	L	0.56	0/1656	0.83	4/2251 (0.2%)
1	M	0.71	0/1656	0.90	6/2251 (0.3%)
2	H	0.85	2/1708 (0.1%)	1.01	7/2326 (0.3%)
2	K	0.68	1/1713 (0.1%)	0.88	5/2331 (0.2%)
All	All	0.71	3/6733 (0.0%)	0.91	22/9159 (0.2%)

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	H	0	6
2	K	0	1
All	All	0	7

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	H	136	GLY	C-N	-21.49	0.84	1.34
2	H	136	GLY	N-CA	-7.74	1.34	1.46
2	K	82(C)	MET	SD-CE	-5.31	1.48	1.77

All (22) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	H	136	GLY	O-C-N	-23.13	85.69	122.70
2	H	136	GLY	C-N-CA	15.32	160.00	121.70
1	L	108	ARG	NE-CZ-NH2	-9.32	115.64	120.30
1	M	108	ARG	NE-CZ-NH2	-8.82	115.89	120.30
2	H	136	GLY	CA-C-N	7.69	134.12	117.20
1	M	108	ARG	NE-CZ-NH1	7.55	124.08	120.30
2	K	220	ASP	CB-CG-OD2	7.52	125.07	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	K	61	ASP	CB-CG-OD2	6.47	124.12	118.30
2	K	100(D)	ASP	CB-CG-OD2	6.43	124.09	118.30
1	M	81	ASP	CB-CG-OD2	6.42	124.08	118.30
1	L	81	ASP	CB-CG-OD2	6.17	123.85	118.30
1	L	167	ASP	CB-CG-OD2	6.13	123.82	118.30
2	K	71	ARG	NE-CZ-NH2	-6.12	117.24	120.30
1	M	17	ASP	CB-CG-OD2	6.09	123.78	118.30
1	L	108	ARG	NE-CZ-NH1	6.01	123.30	120.30
2	K	98	ASP	CB-CG-OD2	5.86	123.57	118.30
2	H	100(D)	ASP	CB-CG-OD2	5.82	123.53	118.30
1	M	11	LEU	CA-CB-CG	5.52	127.99	115.30
2	H	100(B)	ASP	CB-CG-OD2	5.22	123.00	118.30
2	H	101	ASP	CB-CG-OD2	5.20	122.98	118.30
1	M	167	ASP	CB-CG-OD2	5.16	122.94	118.30
2	H	220	ASP	CB-CG-OD2	5.02	122.82	118.30

There are no chirality outliers.

All (7) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	H	126	PRO	Peptide
2	H	128	SER	Peptide
2	H	130	SER	Peptide
2	H	135	GLY	Peptide
2	H	136	GLY	Mainchain,Peptide
2	K	128	SER	Peptide

## 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	L	1620	0	1551	14	0
1	M	1620	0	1551	21	0
2	H	1670	0	1621	11	0
2	K	1676	0	1626	15	0
3	H	48	0	0	1	0
3	K	58	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	L	60	0	0	1	0
3	M	103	0	0	3	0
All	All	6855	0	6349	59	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 5.

All (59) 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:M:103:ARG:NH1	3:M:310:HOH:O	1.97	0.95
1:L:198:HIS:CD2	1:L:200:GLY:H	2.00	0.79
2:K:81:GLN:HE21	2:K:82(A):HIS:HE1	1.33	0.75
1:L:108:ARG:HD3	1:L:109:THR:O	1.88	0.72
1:M:54:LEU:HD22	1:M:58:VAL:HB	1.75	0.67
1:M:108:ARG:HD3	1:M:109:THR:O	1.94	0.66
1:L:54:LEU:HD21	1:L:58:VAL:O	1.95	0.66
2:H:149:PRO:O	2:H:212:HIS:HE1	1.79	0.65
1:M:145:LYS:HB3	1:M:197:THR:HG22	1.78	0.65
1:M:198:HIS:CD2	1:M:200:GLY:H	2.14	0.65
2:H:1:GLU:O	2:H:2:VAL:HB	1.95	0.65
1:M:198:HIS:HD2	1:M:200:GLY:H	1.42	0.65
1:L:198:HIS:HD2	1:L:200:GLY:H	1.44	0.65
1:M:20:THR:HG22	1:M:74:THR:HB	1.81	0.62
1:L:124:GLN:HG2	1:L:129:THR:O	2.03	0.58
2:H:110:THR:HG23	3:H:274:HOH:O	2.03	0.57
1:M:164:THR:HG23	1:M:165:GLU:O	2.05	0.56
1:M:112:ALA:HB1	1:M:201:LEU:HD13	1.87	0.56
2:K:149:PRO:O	2:K:212:HIS:HE1	1.89	0.55
2:K:3:GLN:HB2	2:K:25:SER:HB2	1.89	0.54
2:K:98:ASP:CB	2:K:100(A):SER:HB2	2.39	0.53
1:L:143:GLU:H	1:L:143:GLU:CD	2.11	0.53
1:L:166:GLN:HG3	1:L:173:TYR:CZ	2.43	0.53
1:M:54:LEU:CD2	1:M:58:VAL:HB	2.37	0.53
2:K:146:ASP:HB3	2:K:184:LEU:HD23	1.90	0.53
2:H:32:HIS:HA	2:H:96:GLY:O	2.09	0.53
2:K:212:HIS:HD2	2:K:215:SER:OG	1.92	0.53
1:M:183:LYS:O	1:M:187:GLU:HG3	2.08	0.52
2:K:145:LYS:HE2	2:K:179:GLN:OE1	2.09	0.52
1:M:108:ARG:HD2	1:M:140:TYR:CG	2.44	0.52
2:K:98:ASP:HB2	2:K:100(A):SER:HB2	1.92	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:M:141:PRO:O	1:M:198:HIS:HE1	1.93	0.52
2:H:81:GLN:HE21	2:H:82(A):HIS:HE1	1.58	0.51
2:K:47:TRP:HZ2	2:K:50:SER:HB2	1.75	0.51
2:K:81:GLN:NE2	2:K:82(A):HIS:HE1	2.05	0.50
1:L:112:ALA:HB1	1:L:201:LEU:HD13	1.94	0.49
1:L:20:THR:HG22	1:L:74:THR:HB	1.97	0.47
2:K:81:GLN:HE21	2:K:82(A):HIS:CE1	2.23	0.46
1:L:15:VAL:HG23	3:L:258:HOH:O	2.17	0.45
2:H:57:ARG:CZ	2:K:75:GLU:HG3	2.47	0.44
2:H:81:GLN:NE2	2:H:82(A):HIS:HE1	2.16	0.44
1:L:125:LEU:HD11	1:L:186:TYR:CD2	2.52	0.44
2:K:213:LYS:N	2:K:214:PRO:CD	2.81	0.44
1:M:124:GLN:HG2	1:M:129:THR:O	2.18	0.43
1:L:91:TYR:O	1:L:92:ALA:HB2	2.19	0.42
1:M:103:ARG:NH2	1:M:173:TYR:OH	2.53	0.42
2:H:145:LYS:HE3	3:M:291:HOH:O	2.18	0.42
2:H:148:PHE:HA	2:H:149:PRO:HA	1.90	0.42
1:L:92:ALA:HA	2:H:100(C):ASN:OD1	2.20	0.42
2:H:144:VAL:HG11	2:H:152:VAL:HG11	2.02	0.41
2:K:59:TYR:HB2	2:K:64:LYS:HG2	2.02	0.41
1:M:166:GLN:HG2	1:M:173:TYR:CZ	2.56	0.41
1:L:108:ARG:HD2	1:L:140:TYR:CB	2.50	0.41
1:M:108:ARG:HD2	1:M:140:TYR:CB	2.51	0.41
1:M:87:HIS:CD2	3:M:260:HOH:O	2.74	0.41
1:M:32:TRP:O	1:M:90:HIS:HD2	2.03	0.41
1:M:107:LYS:HG3	1:M:108:ARG:N	2.37	0.40
2:K:148:PHE:HA	2:K:149:PRO:HA	1.90	0.40
1:M:7:SER:HA	1:M:8:PRO:HA	1.93	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	L	210/212 (99%)	200 (95%)	8 (4%)	2 (1%)	18	16
1	M	210/212 (99%)	204 (97%)	6 (3%)	0	100	100
2	H	220/225 (98%)	207 (94%)	8 (4%)	5 (2%)	7	4
2	K	219/225 (97%)	207 (94%)	8 (4%)	4 (2%)	10	6
All	All	859/874 (98%)	818 (95%)	30 (4%)	11 (1%)	14	11

All (11) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	L	92	ALA
2	H	129	LYS
2	H	133	THR
2	H	134	SER
2	K	100(B)	ASP
2	H	96	GLY
2	K	129	LYS
2	K	130	SER
1	L	30	GLU
2	H	2	VAL
2	K	136	GLY

### 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	L	176/183 (96%)	165 (94%)	11 (6%)	21	23
1	M	176/183 (96%)	156 (89%)	20 (11%)	7	6
2	H	184/190 (97%)	175 (95%)	9 (5%)	29	35
2	K	185/190 (97%)	171 (92%)	14 (8%)	15	16
All	All	721/746 (97%)	667 (92%)	54 (8%)	16	16

All (54) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	L	33	LEU
1	L	50	LYS
1	L	70	GLU
1	L	74	THR
1	L	89	GLN
1	L	97	THR
1	L	108	ARG
1	L	135	LEU
1	L	143	GLU
1	L	201	LEU
1	L	207	LYS
2	H	7	SER
2	H	11	LEU
2	H	25	SER
2	H	94	ARG
2	H	110	THR
2	H	137	THR
2	H	200	THR
2	H	203	GLN
2	H	213	LYS
1	M	11	LEU
1	M	22	THR
1	M	33	LEU
1	M	50	LYS
1	M	54	LEU
1	M	55	LYS
1	M	56	THR
1	M	73	LEU
1	M	74	THR
1	M	103	ARG
1	M	108	ARG
1	M	126	LYS
1	M	135	LEU
1	M	143	GLU
1	M	164	THR
1	M	168	SER
1	M	169	LYS
1	M	201	LEU
1	M	207	LYS
1	M	213	GLU
2	K	12	VAL
2	K	50	SER
2	K	64	LYS

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Mol	Chain	Res	Type
2	K	97	SER
2	K	100	LEU
2	K	110	THR
2	K	116	THR
2	K	137	THR
2	K	153	THR
2	K	168	SER
2	K	184	LEU
2	K	187	LEU
2	K	196	SER
2	K	221	LYS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (18) such sidechains are listed below:

Mol	Chain	Res	Type
1	L	89	GLN
1	L	90	HIS
1	L	147	GLN
1	L	198	HIS
1	L	210	ASN
2	H	26	ASN
2	H	81	GLN
2	H	82(A)	HIS
2	H	212	HIS
1	M	87	HIS
1	M	89	GLN
1	M	90	HIS
1	M	198	HIS
1	M	210	ASN
2	K	32	HIS
2	K	81	GLN
2	K	82(A)	HIS
2	K	212	HIS

### 5.3.3 RNA ⓘ

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](#)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
2	H	2
2	K	2

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	K	134:SER	C	135:GLY	N	4.30
1	H	127:SER	C	128:SER	N	2.28
1	K	127:SER	C	128:SER	N	2.07
1	H	136:GLY	C	137:THR	N	0.84

## 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.