



wwPDB X-ray Structure Validation Summary Report ⓘ

Feb 14, 2017 – 06:34 am GMT

PDB ID : 1ZLW
Title : Fab 2G12 + Man8
Authors : Calarese, D.A.; Lee, H.-K.; Best, M.D.; Astronomo, R.D.; Stanfield, R.L.;
Burton, D.R.; Wong, C.H.; Wilson, I.A.
Deposited on : 2005-05-09
Resolution : 2.85 Å(reported)

This is a wwPDB X-ray Structure Validation Summary 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 ⓘ symbol.

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

MolProbity : 4.02b-467
Mogul : 1.7.2 (RC1), CSD as538be (2017)
Xtrriage (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) : recalc28949

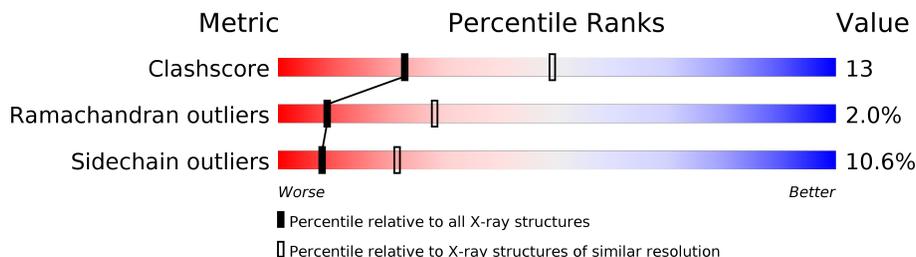
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.85 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	2749 (2.90-2.82)
Ramachandran outliers	110173	2687 (2.90-2.82)
Sidechain outliers	110143	2690 (2.90-2.82)

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 $\leq 5\%$. 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	K	211	 64% 30% . .
1	L	211	 70% 27% . .
2	H	224	 71% 25% .
2	M	224	 62% 27% . . 7%

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
3	BMA	M	235	X	-	-	-

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 6535 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
			Total	C	N	O	S			
1	L	209	Total	C	N	O	S	0	0	0
			1599	1007	266	321	5			
1	K	209	Total	C	N	O	S	0	0	0
			1602	1008	269	320	5			

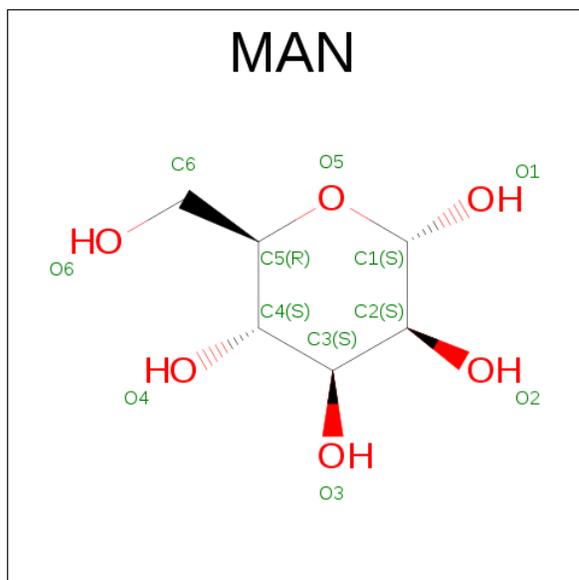
- Molecule 2 is a protein called FAB 2G12, heavy chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
2	H	224	Total	C	N	O	S	0	0	0
			1671	1050	285	329	7			
2	M	209	Total	C	N	O	S	0	0	0
			1575	994	269	305	7			

- Molecule 3 is a polymer of unknown type called SUGAR (7-MER).

Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	C	O		
3	M	7	Total	C	O	0	0
			77	42	35		

- Molecule 4 is SUGAR (ALPHA-D-MANNOSE) (three-letter code: MAN) (formula: C₆H₁₂O₆).



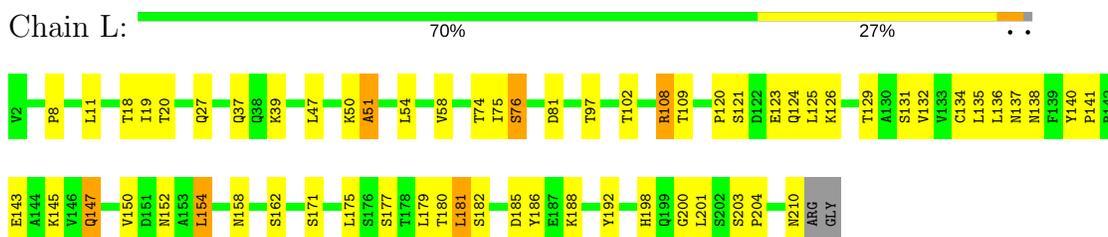
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	M	1	Total	C	O	0	0
			11	6	5		

3 Residue-property plots [i](#)

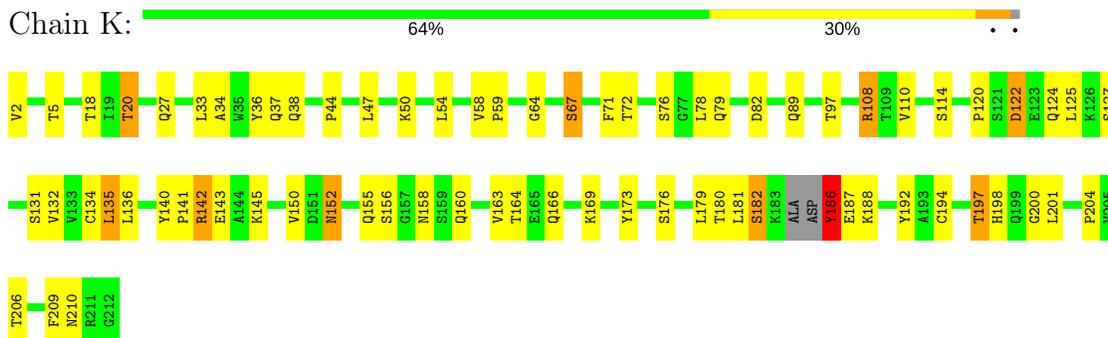
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are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

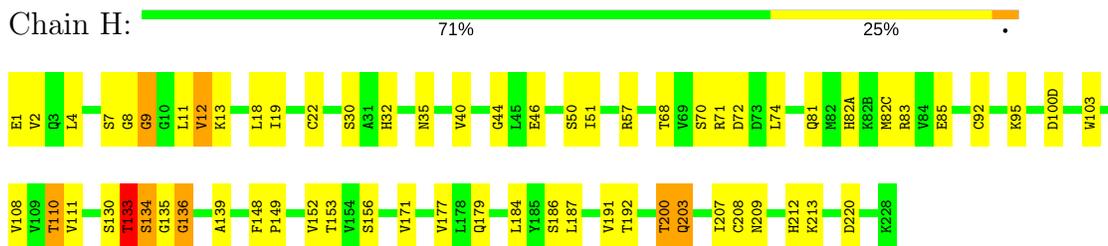
- Molecule 1: FAB 2G12, light chain



- Molecule 1: FAB 2G12, light chain

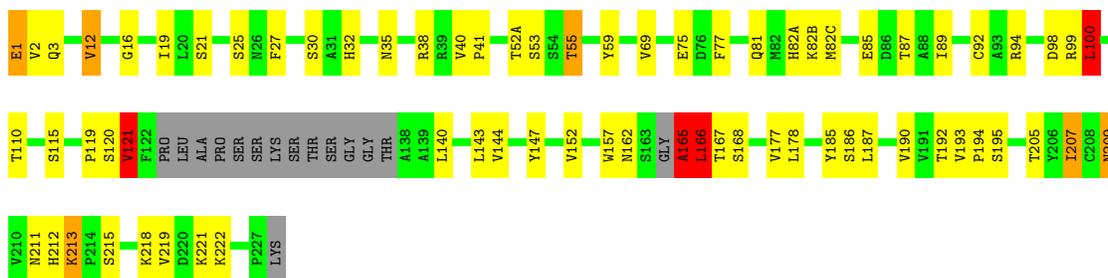


- Molecule 2: FAB 2G12, heavy chain



- Molecule 2: FAB 2G12, heavy chain





4 Data and refinement statistics

Xtrriage (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, α , β , γ	45.21Å 165.71Å 169.57Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	50.00 – 2.85	Depositor
% Data completeness (in resolution range)	99.5 (50.00-2.85)	Depositor
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	REFMAC 5.2	Depositor
R, R_{free}	0.221 , 0.279	Depositor
Estimated twinning fraction	No twinning to report.	Xtrriage
Total number of atoms	6535	wwPDB-VP
Average B, all atoms (Å ²)	59.0	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: BMA, MAN

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	K	0.87	0/1638	0.89	2/2224 (0.1%)
1	L	0.80	1/1635 (0.1%)	0.81	0/2223
2	H	0.89	1/1710 (0.1%)	0.92	0/2330
2	M	0.85	0/1611	0.89	1/2194 (0.0%)
All	All	0.85	2/6594 (0.0%)	0.88	3/8971 (0.0%)

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	1
2	M	0	1
3	M	1	0
All	All	1	2

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	L	210	ASN	C-O	9.23	1.40	1.23
2	H	46	GLU	CG-CD	5.32	1.59	1.51

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	M	166	LEU	N-CA-C	-5.31	96.67	111.00
1	K	186	TYR	CB-CG-CD2	5.12	124.08	121.00
1	K	2	VAL	CB-CA-C	-5.01	101.88	111.40

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
3	M	235	BMA	C1

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	H	133	THR	Peptide
2	M	165	ALA	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	K	1602	0	1560	45	0
1	L	1599	0	1553	42	0
2	H	1671	0	1637	40	0
2	M	1575	0	1541	48	0
3	M	77	0	64	2	0
4	M	11	0	10	2	0
All	All	6535	0	6365	167	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.

The worst 5 of 167 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:L:147:GLN:NE2	1:L:154:LEU:HD11	1.64	1.11
1:L:147:GLN:HE22	1:L:154:LEU:HD11	1.19	1.07
3:M:234:MAN:O2	4:M:236:MAN:C1	2.08	1.01
1:L:158:ASN:ND2	1:L:179:LEU:HD11	1.87	0.90
1:L:18:THR:HG23	1:L:76:SER:HA	1.54	0.88

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	K	207/211 (98%)	190 (92%)	15 (7%)	2 (1%)	18	46
1	L	207/211 (98%)	188 (91%)	15 (7%)	4 (2%)	9	29
2	H	222/224 (99%)	203 (91%)	13 (6%)	6 (3%)	6	20
2	M	205/224 (92%)	178 (87%)	22 (11%)	5 (2%)	7	23
All	All	841/870 (97%)	759 (90%)	65 (8%)	17 (2%)	9	28

5 of 17 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	H	133	THR
2	H	136	GLY
2	H	200	THR
1	K	188	LYS
2	M	121	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	K	180/182 (99%)	158 (88%)	22 (12%)	6	15
1	L	180/182 (99%)	163 (91%)	17 (9%)	10	27
2	H	188/189 (100%)	169 (90%)	19 (10%)	9	24
2	M	176/189 (93%)	157 (89%)	19 (11%)	7	20
All	All	724/742 (98%)	647 (89%)	77 (11%)	8	21

5 of 77 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	H	208	CYS
1	K	114	SER
2	M	195	SER
2	H	213	LYS
1	K	50	LYS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 24 such sidechains are listed below:

Mol	Chain	Res	Type
1	K	27	GLN
1	K	89	GLN
2	M	209	ASN
1	K	38	GLN
1	K	87	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](#)

7 carbohydrates are 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$
3	MAN	M	229	3	11,11,12	1.09	1 (9%)	13,15,17	2.46	5 (38%)
3	MAN	M	230	3	11,11,12	0.66	0	13,15,17	2.18	6 (46%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
3	MAN	M	231	3	11,11,12	1.15	2 (18%)	13,15,17	1.96	6 (46%)
3	MAN	M	232	3	11,11,12	0.63	0	13,15,17	1.40	1 (7%)
3	BMA	M	233	3	11,11,12	0.88	0	13,15,17	6.34	10 (76%)
3	MAN	M	234	3	11,11,12	1.03	1 (9%)	13,15,17	2.36	5 (38%)
3	BMA	M	235	3	11,11,12	1.28	1 (9%)	13,15,17	4.10	7 (53%)

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
3	MAN	M	229	3	-	0/2/19/22	0/1/1/1
3	MAN	M	230	3	-	0/2/19/22	0/1/1/1
3	MAN	M	231	3	-	0/2/19/22	0/1/1/1
3	MAN	M	232	3	-	0/2/19/22	0/1/1/1
3	BMA	M	233	3	-	0/2/19/22	0/1/1/1
3	MAN	M	234	3	-	0/2/19/22	0/1/1/1
3	BMA	M	235	3	1/1/4/5	0/2/19/22	0/1/1/1

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	M	229	MAN	O5-C1	-2.49	1.39	1.43
3	M	235	BMA	O5-C1	-2.28	1.40	1.43
3	M	234	MAN	O4-C4	-2.27	1.37	1.43
3	M	231	MAN	O5-C1	-2.24	1.40	1.43
3	M	231	MAN	O4-C4	-2.05	1.38	1.43

The worst 5 of 40 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	M	233	BMA	C2-C3-C4	-14.84	84.99	110.88
3	M	235	BMA	C1-O5-C5	-9.86	98.57	112.17
3	M	235	BMA	C1-C2-C3	-9.51	97.59	109.65
3	M	233	BMA	C3-C4-C5	-8.74	94.81	110.22
3	M	233	BMA	O2-C2-C1	-6.35	96.27	109.18

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
3	M	235	BMA	C1

There are no torsion outliers.

There are no ring outliers.

1 monomer is involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	M	234	MAN	2	0

5.6 Ligand geometry [i](#)

1 ligand 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$
4	MAN	M	236	-	11,11,12	1.00	1 (9%)	13,15,17	3.01	6 (46%)

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
4	MAN	M	236	-	-	0/2/19/22	0/1/1/1

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	M	236	MAN	O5-C5	-2.18	1.38	1.43

The worst 5 of 6 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	M	236	MAN	O2-C2-C3	-2.45	105.36	110.17

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	M	236	MAN	O3-C3-C2	-2.41	105.64	110.02
4	M	236	MAN	C6-C5-C4	-2.13	108.02	113.00
4	M	236	MAN	C1-C2-C3	3.43	113.99	109.65
4	M	236	MAN	C1-O5-C5	3.98	117.66	112.17

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

1 monomer is involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	M	236	MAN	2	0

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

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.