



wwPDB X-ray Structure Validation Summary Report ⓘ

Feb 18, 2018 – 09:34 am GMT

PDB ID : 1A6T
Title : FAB FRAGMENT OF MAB1-IA MONOCLONAL ANTIBODY TO HUMAN RHINOVIRUS 14 NIM-IA SITE
Authors : Che, Z.; Smith, T.J.
Deposited on : 1998-03-03
Resolution : 2.70 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

<https://www.wwpdb.org/validation/2017/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
Xtriage (Phenix) : **NOT EXECUTED**
EDS : **NOT EXECUTED**
Percentile statistics : 20171227.v01 (using entries in the PDB archive December 27th 2017)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : trunk30686

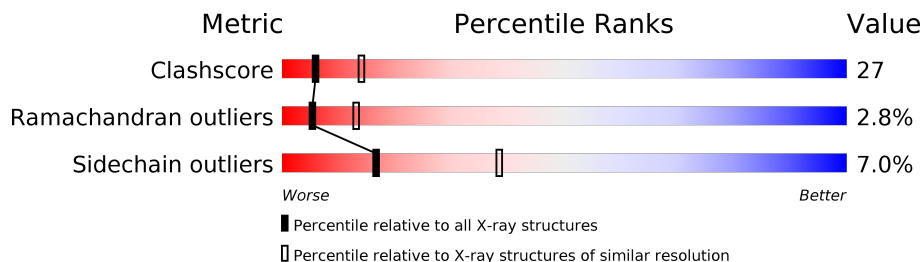
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.70 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	122078	2755 (2.70-2.70)
Ramachandran outliers	120005	2715 (2.70-2.70)
Sidechain outliers	119972	2715 (2.70-2.70)

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	A	210	
1	C	210	
2	B	217	
2	D	217	

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 6468 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 IGG1 FAB1-IA FAB (LIGHT CHAIN).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	210	Total	C	N	O	S	0	0	0
			1595	994	265	329	7			
1	C	210	Total	C	N	O	S	0	0	0
			1595	994	265	329	7			

There are 36 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	2	SER	ILE	CONFLICT	PIR S25058
A	5	SER	THR	CONFLICT	PIR S25058
A	11	LEU	MET	CONFLICT	PIR S25058
A	20	ILE	THR	CONFLICT	PIR S25058
A	25	PRO	ALA	CONFLICT	PIR S25058
A	32	TYR	LYS	CONFLICT	PIR S25058
A	40	PRO	SER	CONFLICT	PIR S25058
A	42	SER	THR	CONFLICT	PIR S25058
A	46	PRO	ARG	CONFLICT	PIR S25058
A	50	SER	ASP	CONFLICT	PIR S25058
A	53	ASN	LYS	CONFLICT	PIR S25058
A	65	GLY	SER	CONFLICT	PIR S25058
A	71	PHE	TYR	CONFLICT	PIR S25058
A	77	GLY	SER	CONFLICT	PIR S25058
A	78	VAL	MET	CONFLICT	PIR S25058
A	91	TYR	TRP	CONFLICT	PIR S25058
A	94	HIS	ASN	CONFLICT	PIR S25058
A	100	GLY	ALA	CONFLICT	PIR S25058
C	2	SER	ILE	CONFLICT	PIR S25058
C	5	SER	THR	CONFLICT	PIR S25058
C	11	LEU	MET	CONFLICT	PIR S25058
C	20	ILE	THR	CONFLICT	PIR S25058
C	25	PRO	ALA	CONFLICT	PIR S25058
C	32	TYR	LYS	CONFLICT	PIR S25058
C	40	PRO	SER	CONFLICT	PIR S25058

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Chain	Residue	Modelled	Actual	Comment	Reference
C	42	SER	THR	CONFLICT	PIR S25058
C	46	PRO	ARG	CONFLICT	PIR S25058
C	50	SER	ASP	CONFLICT	PIR S25058
C	53	ASN	LYS	CONFLICT	PIR S25058
C	65	GLY	SER	CONFLICT	PIR S25058
C	71	PHE	TYR	CONFLICT	PIR S25058
C	77	GLY	SER	CONFLICT	PIR S25058
C	78	VAL	MET	CONFLICT	PIR S25058
C	91	TYR	TRP	CONFLICT	PIR S25058
C	94	HIS	ASN	CONFLICT	PIR S25058
C	100	GLY	ALA	CONFLICT	PIR S25058

- Molecule 2 is a protein called IGG1 FAB1-IA FAB (HEAVY CHAIN).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	217	Total	C	N	O	S	0	0	0
			1639	1037	268	327	7			
2	D	217	Total	C	N	O	S	0	0	0
			1639	1037	268	327	7			

There are 72 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	10	ASP	GLU	CONFLICT	PIR S38950
B	13	LYS	ARG	CONFLICT	PIR S38950
B	28	SER	THR	CONFLICT	PIR S38950
B	30	SER	THR	CONFLICT	PIR S38950
B	31	THR	ASP	CONFLICT	PIR S38950
B	34	MET	ILE	CONFLICT	PIR S38950
B	40	SER	ARG	CONFLICT	PIR S38950
B	41	HIS	PRO	CONFLICT	PIR S38950
B	43	LYS	GLU	CONFLICT	PIR S38950
B	44	SER	GLY	CONFLICT	PIR S38950
B	50	ARG	TRP	CONFLICT	PIR S38950
B	51	VAL	ILE	CONFLICT	PIR S38950
B	52	ASP	TYR	CONFLICT	PIR S38950
B	53	ASP	GLY	CONFLICT	PIR S38950
B	54	ASN	SER	CONFLICT	PIR S38950
B	56	GLY	ASN	CONFLICT	PIR S38950
B	58	SER	LYS	CONFLICT	PIR S38950
B	59	PHE	TYR	CONFLICT	PIR S38950
B	61	GLN	GLU	CONFLICT	PIR S38950

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Chain	Residue	Modelled	Actual	Comment	Reference
B	68	ILE	THR	CONFLICT	PIR S38950
B	73	LYS	THR	CONFLICT	PIR S38950
B	81	GLU	GLN	CONFLICT	PIR S38950
B	82A	GLY	SER	CONFLICT	PIR S38950
B	91	TYR	PHE	CONFLICT	PIR S38950
B	95	ARG	GLY	CONFLICT	PIR S38950
B	96	ASP	GLY	CONFLICT	PIR S38950
B	97	ASP	LYS	CONFLICT	PIR S38950
B	98	TYR	PHE	CONFLICT	PIR S38950
B	99	TYR	ALA	CONFLICT	PIR S38950
B	100	PHE	MET	CONFLICT	PIR S38950
B	102	PHE	TYR	CONFLICT	PIR S38950
B	109	LEU	VAL	CONFLICT	PIR S38950
B	118	PRO	ALA	CONFLICT	PIR S38950
B	130	GLY	ASP	CONFLICT	PIR S38950
B	173	GLY	ASP	CONFLICT	PIR S38950
B	192	THR	SER	CONFLICT	PIR S38950
D	10	ASP	GLU	CONFLICT	PIR S38950
D	13	LYS	ARG	CONFLICT	PIR S38950
D	28	SER	THR	CONFLICT	PIR S38950
D	30	SER	THR	CONFLICT	PIR S38950
D	31	THR	ASP	CONFLICT	PIR S38950
D	34	MET	ILE	CONFLICT	PIR S38950
D	40	SER	ARG	CONFLICT	PIR S38950
D	41	HIS	PRO	CONFLICT	PIR S38950
D	43	LYS	GLU	CONFLICT	PIR S38950
D	44	SER	GLY	CONFLICT	PIR S38950
D	50	ARG	TRP	CONFLICT	PIR S38950
D	51	VAL	ILE	CONFLICT	PIR S38950
D	52	ASP	TYR	CONFLICT	PIR S38950
D	53	ASP	GLY	CONFLICT	PIR S38950
D	54	ASN	SER	CONFLICT	PIR S38950
D	56	GLY	ASN	CONFLICT	PIR S38950
D	58	SER	LYS	CONFLICT	PIR S38950
D	59	PHE	TYR	CONFLICT	PIR S38950
D	61	GLN	GLU	CONFLICT	PIR S38950
D	68	ILE	THR	CONFLICT	PIR S38950
D	73	LYS	THR	CONFLICT	PIR S38950
D	81	GLU	GLN	CONFLICT	PIR S38950
D	82A	GLY	SER	CONFLICT	PIR S38950
D	91	TYR	PHE	CONFLICT	PIR S38950
D	95	ARG	GLY	CONFLICT	PIR S38950

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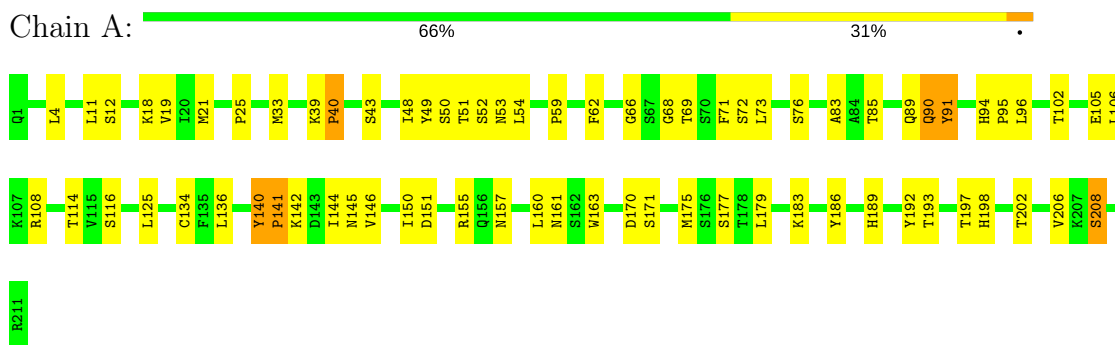
Chain	Residue	Modelled	Actual	Comment	Reference
D	96	ASP	GLY	CONFLICT	PIR S38950
D	97	ASP	LYS	CONFLICT	PIR S38950
D	98	TYR	PHE	CONFLICT	PIR S38950
D	99	TYR	ALA	CONFLICT	PIR S38950
D	100	PHE	MET	CONFLICT	PIR S38950
D	102	PHE	TYR	CONFLICT	PIR S38950
D	109	LEU	VAL	CONFLICT	PIR S38950
D	118	PRO	ALA	CONFLICT	PIR S38950
D	130	GLY	ASP	CONFLICT	PIR S38950
D	173	GLY	ASP	CONFLICT	PIR S38950
D	192	THR	SER	CONFLICT	PIR S38950

3 Residue-property plots

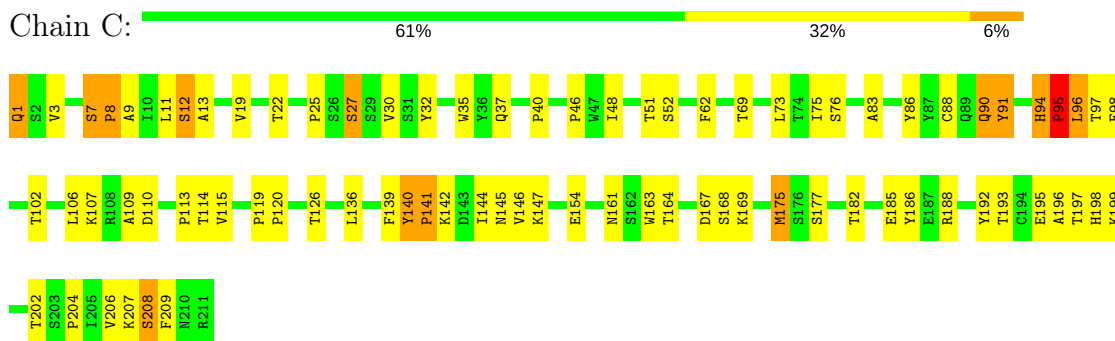
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are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

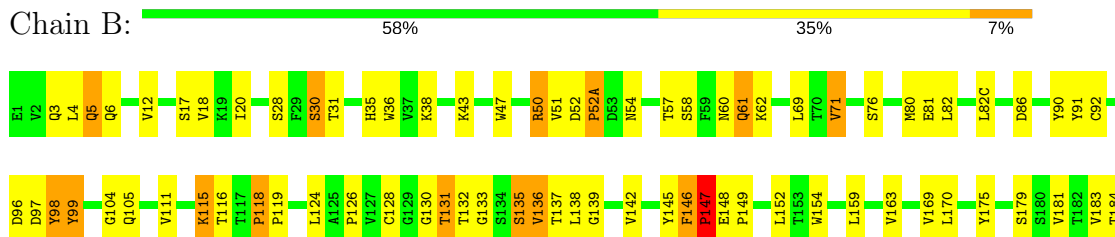
• Molecule 1: IGG1 FAB1-IA FAB (LIGHT CHAIN)

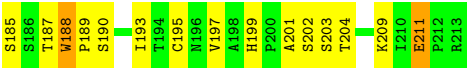


• Molecule 1: IGG1 FAB1-IA FAB (LIGHT CHAIN)

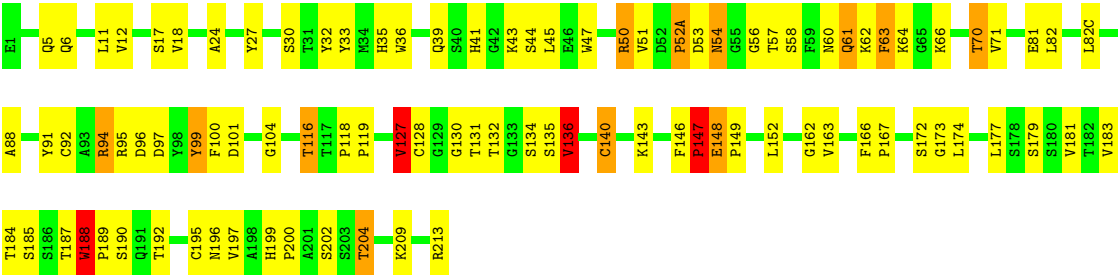


• Molecule 2: IGG1 FAB1-IA FAB (HEAVY CHAIN)





● Molecule 2: IGG1 FAB1-IA FAB (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 2	Depositor
Cell constants a, b, c, α , β , γ	92.17Å 135.95Å 81.08Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	6.00 – 2.70	Depositor
% Data completeness (in resolution range)	93.3 (6.00-2.70)	Depositor
R_{merge}	0.04	Depositor
R_{sym}	0.04	Depositor
Refinement program	X-PLOR	Depositor
R, R_{free}	0.169 , 0.266	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	6468	wwPDB-VP
Average B, all atoms (Å ²)	28.0	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	0.65	2/1635 (0.1%)	0.87	2/2221 (0.1%)
1	C	0.62	6/1635 (0.4%)	0.87	5/2221 (0.2%)
2	B	0.74	5/1683 (0.3%)	0.91	2/2293 (0.1%)
2	D	1.07	4/1683 (0.2%)	1.06	7/2293 (0.3%)
All	All	0.80	17/6636 (0.3%)	0.93	16/9028 (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	D	0	1

The worst 5 of 17 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	63	PHE	CB-CG	33.87	2.08	1.51
2	D	200	PRO	N-CD	5.36	1.55	1.47
2	D	147	PRO	N-CD	5.35	1.55	1.47
1	C	204	PRO	N-CD	5.34	1.55	1.47
2	B	118	PRO	N-CD	5.34	1.55	1.47

The worst 5 of 16 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	63	PHE	CB-CG-CD2	-14.76	110.47	120.80
2	D	63	PHE	CB-CG-CD1	14.43	130.90	120.80
2	D	63	PHE	CA-CB-CG	-9.70	90.62	113.90
2	D	136	VAL	CB-CA-C	-8.31	95.60	111.40
1	C	35	TRP	CA-CB-CG	8.10	129.10	113.70

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	D	188	TRP	Mainchain

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	A	1595	0	1523	74	0
1	C	1595	0	1523	83	0
2	B	1639	0	1593	97	0
2	D	1639	0	1595	113	0
All	All	6468	0	6234	337	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 27.

The worst 5 of 337 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:96:LEU:HD21	2:D:47:TRP:CD1	1.57	1.39
2:D:63:PHE:CG	2:D:63:PHE:CB	2.08	1.36
2:D:152:LEU:CD1	2:D:197:VAL:HG22	1.66	1.25
1:A:95:PRO:HG3	2:B:60:ASN:OD1	1.37	1.19
2:B:170:LEU:HD13	2:B:175:TYR:CZ	1.80	1.15

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	208/210 (99%)	188 (90%)	18 (9%)	2 (1%)	17	41
1	C	208/210 (99%)	190 (91%)	12 (6%)	6 (3%)	5	12
2	B	215/217 (99%)	199 (93%)	8 (4%)	8 (4%)	4	8
2	D	215/217 (99%)	189 (88%)	18 (8%)	8 (4%)	4	8
All	All	846/854 (99%)	766 (90%)	56 (7%)	24 (3%)	5	13

5 of 24 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	B	61	GLN
2	B	131	THR
1	C	7	SER
1	C	76	SER
2	D	188	TRP

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	183/183 (100%)	176 (96%)	7 (4%)	36	66
1	C	183/183 (100%)	166 (91%)	17 (9%)	10	23
2	B	187/187 (100%)	174 (93%)	13 (7%)	16	38
2	D	187/187 (100%)	172 (92%)	15 (8%)	13	30
All	All	740/740 (100%)	688 (93%)	52 (7%)	16	38

5 of 52 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	C	22	THR
1	C	91	TYR
2	D	143	LYS
1	C	27	SER

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Mol	Chain	Res	Type
1	C	48	ILE

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 19 such sidechains are listed below:

Mol	Chain	Res	Type
2	B	5	GLN
2	B	35	HIS
2	D	35	HIS
1	A	189	HIS
2	D	54	ASN

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

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.