WORLDWIDE PDB PROTEIN DATA BANK

wwPDB X-ray Structure Validation Summary Report (i)

Aug 9, 2020 – 10:33 AM BST

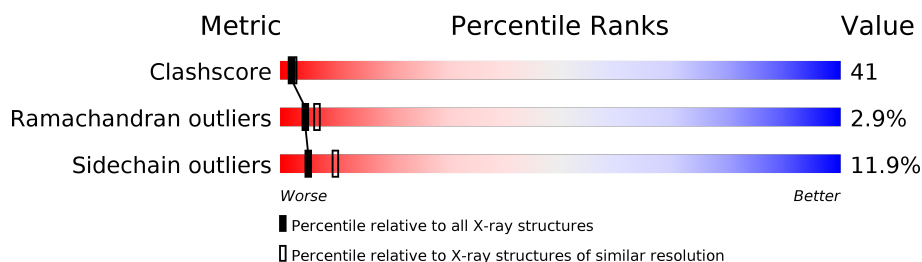|		
PDB ID	:	1FZG
Title	:	CRYSTAL STRUCTURE OF FRAGMENT D FROM HUMAN FIBRINO-GEN WITH THE PEPTIDE LIGAND GLY-HIS-ARG-PRO-AMIDE
Authors	:	Everse, S.J.; Spraggon, G.; Veerapandian, L.; Doolittle, R.F.
Deposited on	:	1999-01-01
Resolution	:	2.50 Å(reported)

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 2.50 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	Percentile Ranks	Value
Clashscore		41
Ramachandran outliers		2.9%
Sidechain outliers		11.9%

Worse   *Better*

■ Percentile relative to all X-ray structures
▯ Percentile relative to X-ray structures of similar resolution

Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
Clashscore	141614	5346 (2.50-2.50)
Ramachandran outliers	138981	5231 (2.50-2.50)
Sidechain outliers	138945	5233 (2.50-2.50)

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 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 <=5%

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	87	20% 34% 21% • 23%
1	D	87	20% 28% 10% 5% 38%
2	B	328	40% 36% 13% • 8%
2	E	328	43% 35% 10% • 10%
3	C	319	49% 33% 8% • 8%
3	F	319	41% 36% 9% • 11%
4	M	4	50% 25% 25%
4	N	4	25% 50% 25%

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Mol	Chain	Length	Quality of chain
4	S	4	<table showing 50% green, 25% yellow, 25% red>
4	T	4	<100% yellow>
5	G	2	<100% orange>
5	H	2	<100% orange>

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
5	NAG	G	1	-	-	X	-
5	NAG	H	1	-	-	X	-
5	NAG	H	2	-	-	X	-

2 Entry composition (i)

There are 7 unique types of molecules in this entry. The entry contains 10713 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 FIBRINOGEN.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	67	Total 546	C 337	N 103	O 103	S 3	0	0	0
1	D	54	Total 440	C 269	N 84	O 84	S 3	0	0	0

- Molecule 2 is a protein called FIBRINOGEN.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	303	Total 2427	C 1515	N 429	O 461	S 22	0	0	0
2	E	296	Total 2376	C 1484	N 420	O 450	S 22	0	0	0

- Molecule 3 is a protein called FIBRINOGEN.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	C	292	Total 2342	C 1485	N 396	O 450	S 11	0	0	0
3	F	285	Total 2287	C 1453	N 384	O 439	S 11	0	0	0

- Molecule 4 is a protein called FIBRINOGEN.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
4	S	4	Total 31	C 19	N 9	O 3	0	0	0
4	T	4	Total 31	C 19	N 9	O 3	0	0	0
4	M	4	Total 31	C 19	N 9	O 3	0	0	0
4	N	4	Total 31	C 19	N 9	O 3	0	0	0

- Molecule 5 is an oligosaccharide called 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-a
  cetamido-2-deoxy-beta-D-glucopyranose.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
5	G	2	Total 28	C 16	N 2	O 10	0	0	0
5	H	2	Total 28	C 16	N 2	O 10	0	0	0

- Molecule 6 is CALCIUM ION (three-letter code: CA) (formula: Ca).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	B	2	Total 2	Ca 2	0	0
6	C	2	Total 2	Ca 2	0	0
6	F	2	Total 2	Ca 2	0	0
6	E	2	Total 2	Ca 2	0	0

- Molecule 7 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	A	1	Total 1	O 1	0	0
7	B	31	Total 31	O 31	0	0
7	C	20	Total 20	O 20	0	0
7	D	3	Total 3	O 3	0	0
7	E	29	Total 29	O 29	0	0
7	F	23	Total 23	O 23	0	0

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: FIBRINOGEN

Chain A:

- Molecule 1: FIBRINOGEN

Chain D:

- Molecule 2: FIBRINOGEN

Chain B:

• Molecule 2: FIBRINOGEN

Chain E:

• Molecule 3: FIBRINOGEN

Chain C:

• Molecule 3: FIBRINOGEN

Chain F:

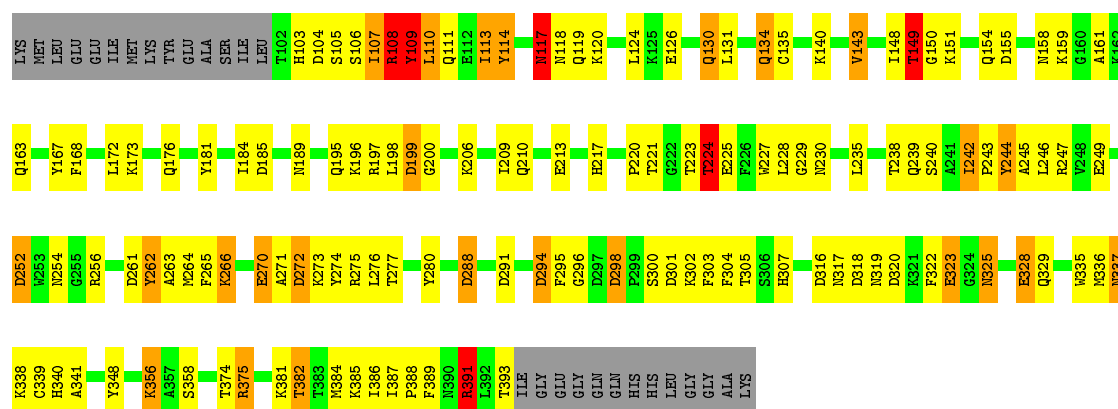M310 D316 N317 D318 E323 G324 N325 E328 Q329 D330 G333 W334 W335 M336 N337 K338 C339 H340 A341 G342 H343 L344 V347 K356 T359 P360 N361 G362 Y363 D364 I367 I368 W369 A370 K373 T374 R375 W376 Y377 T382 K385 F389 N390 R391 L392 T393 ILE GLY

GLU GLY GLN GLN HIS HIS LEU GLY GLY ALA LYS

• Molecule 4: FIBRINOGEN

Chain S:

50%	25%	25%

G1 H2 R3 P4

• Molecule 4: FIBRINOGEN

Chain T:

100%

G1 H2 R3 P4

• Molecule 4: FIBRINOGEN

Chain M:

50%	25%	25%

G1 H2 R3 P4

• Molecule 4: FIBRINOGEN

Chain N:

25%	50%	25%

G1 H2 R3 P4

• Molecule 5: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain G:

100%

NAG1 NAG2

• Molecule 5: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain H:

100%

NAG1 NAG2

4 Data and refinement statistics (i)

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, α, β, γ	54.80Å 149.40Å 234.70Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	30.00 – 2.50	Depositor
% Data completeness (in resolution range)	88.5 (30.00-2.50)	Depositor
R_{merge}	0.11	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	X-PLOR 3.843	Depositor
R, R_{free}	0.233 , 0.302	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	10713	wwPDB-VP
Average B, all atoms (Å^2)	53.0	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: CA, NAG

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	0.72	0/547	2.37	20/730 (2.7%)
1	D	0.73	0/440	2.68	21/586 (3.6%)
2	B	0.95	2/2489 (0.1%)	2.25	110/3363 (3.3%)
2	E	0.86	1/2437 (0.0%)	2.24	92/3290 (2.8%)
3	C	0.86	2/2407 (0.1%)	2.02	71/3256 (2.2%)
3	F	0.77	1/2351 (0.0%)	1.89	57/3180 (1.8%)
4	M	1.13	0/32	4.00	3/42 (7.1%)
4	N	0.84	0/32	4.64	2/42 (4.8%)
4	S	1.04	0/32	4.51	4/42 (9.5%)
4	T	0.83	0/32	1.68	0/42
All	All	0.85	6/10799 (0.1%)	2.18	380/14573 (2.6%)

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
2	B	0	1

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

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	C	200	GLY	N-CA	8.02	1.58	1.46
2	E	350	GLY	N-CA	7.45	1.57	1.46
3	C	229	GLY	N-CA	7.23	1.56	1.46
3	F	229	GLY	N-CA	6.59	1.55	1.46
2	B	395	SER	CB-OG	-5.82	1.34	1.42

The worst 5 of 380 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	E	448	ARG	CD-NE-CZ	35.69	173.56	123.60
1	D	162	ARG	CD-NE-CZ	34.21	171.49	123.60
4	N	3	ARG	CD-NE-CZ	27.48	162.08	123.60
2	E	455	ARG	NE-CZ-NH2	-23.33	108.63	120.30
1	A	159	ARG	NE-CZ-NH1	22.89	131.74	120.30

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	B	427	ALA	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	546	0	573	106	0
1	D	440	0	456	108	0
2	B	2427	0	2295	163	0
2	E	2376	0	2243	214	0
3	C	2342	0	2188	143	6
3	F	2287	0	2136	223	5
4	M	31	0	32	5	0
4	N	31	0	32	9	0
4	S	31	0	32	7	0
4	T	31	0	32	6	0
5	G	28	0	25	10	0
5	H	28	0	25	11	0
6	B	2	0	0	0	0
6	C	2	0	0	0	0
6	E	2	0	0	0	0
6	F	2	0	0	0	0
7	A	1	0	0	0	0
7	B	31	0	0	10	0
7	C	20	0	0	2	0
7	D	3	0	0	2	0
7	E	29	0	0	8	0
7	F	23	0	0	2	1

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
All	All	10713	0	10069	841	6

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 41.

The worst 5 of 841 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)
2:E:172:LEU:HD11	3:F:114:TYR:CD2	1.31	1.59
3:C:104:ASP:HA	3:C:107:ILE:CD1	1.33	1.53
2:E:171:ILE:CG2	2:E:172:LEU:CD2	1.86	1.50
2:E:171:ILE:CG2	2:E:172:LEU:HD23	1.08	1.49
3:F:109:TYR:N	3:F:112:GLU:CB	1.78	1.46

The worst 5 of 6 symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:374:THR:OG1	3:F:328:GLU:OE2[4_466]	1.16	1.04
3:C:375:ARG:NH2	3:F:361:ASN:OD1[4_466]	1.42	0.78
3:C:375:ARG:N	7:F:426:HOH:O[4_466]	1.52	0.68
3:C:374:THR:OG1	3:F:328:GLU:CD[4_466]	1.80	0.40
3:C:295:PHE:O	3:F:329:GLN:OE1[4_466]	2.01	0.19

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	65/87 (75%)	52 (80%)	6 (9%)	7 (11%)	0	0
1	D	52/87 (60%)	39 (75%)	8 (15%)	5 (10%)	0	0

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	B	301/328 (92%)	273 (91%)	19 (6%)	9 (3%)	4	6
2	E	294/328 (90%)	262 (89%)	23 (8%)	9 (3%)	4	5
3	C	290/319 (91%)	265 (91%)	24 (8%)	1 (0%)	41	61
3	F	283/319 (89%)	261 (92%)	16 (6%)	6 (2%)	7	11
4	M	2/4 (50%)	2 (100%)	0	0	100	100
4	N	2/4 (50%)	2 (100%)	0	0	100	100
4	S	2/4 (50%)	2 (100%)	0	0	100	100
4	T	2/4 (50%)	2 (100%)	0	0	100	100
All	All	1293/1484 (87%)	1160 (90%)	96 (7%)	37 (3%)	4	6

5 of 37 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	134	GLN
1	A	190	ALA
2	B	169	ARG
2	B	171	ILE
2	B	281	ASP

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	62/82 (76%)	46 (74%)	16 (26%)	0	1
1	D	50/82 (61%)	40 (80%)	10 (20%)	1	2
2	B	261/286 (91%)	226 (87%)	35 (13%)	4	7
2	E	254/286 (89%)	231 (91%)	23 (9%)	9	18
3	C	246/267 (92%)	223 (91%)	23 (9%)	9	17
3	F	239/267 (90%)	214 (90%)	25 (10%)	7	13
4	M	3/3 (100%)	3 (100%)	0	100	100
4	N	3/3 (100%)	2 (67%)	1 (33%)	0	0

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
4	S	3/3 (100%)	2 (67%)	1 (33%)	0	0
4	T	3/3 (100%)	3 (100%)	0	100	100
All	All	1124/1282 (88%)	990 (88%)	134 (12%)	5	10

5 of 134 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
3	C	163	GLN
1	D	138	LYS
3	F	323	GLU
3	C	242	ILE
3	C	328	GLU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 54 such sidechains are listed below:

Mol	Chain	Res	Type
3	C	325	ASN
2	E	271	GLN
3	F	307	HIS
3	C	329	GLN
2	E	189	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

There are no non-standard protein/DNA/RNA residues in this entry.

5.5 Carbohydrates ⓘ

4 monosaccharides 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	$\#|Z| > 2$
5	NAG	G	1	2,5	14,14,15	1.25	1 (7%)	17,19,21	4.23	7 (41%)
5	NAG	G	2	5	14,14,15	1.57	2 (14%)	17,19,21	4.73	6 (35%)
5	NAG	H	1	2,5	14,14,15	1.33	1 (7%)	17,19,21	2.09	7 (41%)
5	NAG	H	2	5	14,14,15	1.40	2 (14%)	17,19,21	2.27	5 (29%)

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
5	NAG	G	1	2,5	-	4/6/23/26	0/1/1/1
5	NAG	G	2	5	-	2/6/23/26	0/1/1/1
5	NAG	H	1	2,5	-	3/6/23/26	0/1/1/1
5	NAG	H	2	5	-	2/6/23/26	0/1/1/1

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

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	H	2	NAG	O7-C7	-3.87	1.14	1.23
5	H	1	NAG	O7-C7	-3.83	1.14	1.23
5	G	2	NAG	O5-C1	3.83	1.49	1.43
5	G	1	NAG	O7-C7	-3.36	1.15	1.23
5	G	2	NAG	O7-C7	-3.13	1.16	1.23

The worst 5 of 25 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
5	G	2	NAG	C1-O5-C5	-12.46	95.31	112.19
5	G	1	NAG	C3-C4-C5	9.50	127.19	110.24
5	G	2	NAG	O5-C1-C2	-9.04	97.01	111.29
5	G	1	NAG	C4-C3-C2	-8.74	98.21	111.02
5	G	2	NAG	C1-C2-N2	8.56	125.10	110.49

There are no chirality outliers.

5 of 11 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	G	2	NAG	C8-C7-N2-C2
5	G	2	NAG	O7-C7-N2-C2
5	H	1	NAG	O5-C5-C6-O6
5	G	1	NAG	C8-C7-N2-C2
5	H	2	NAG	O5-C5-C6-O6

There are no ring outliers.

4 monomers are involved in 21 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	G	2	NAG	4	0
5	H	2	NAG	10	0
5	H	1	NAG	11	0
5	G	1	NAG	10	0

5.6 Ligand geometry (i)

Of 8 ligands modelled in this entry, 8 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

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 is therefore empty.

6.2 Non-standard residues in protein, DNA, RNA chains (i)

EDS was not executed - this section is therefore empty.

6.3 Carbohydrates (i)

EDS was not executed - this section is therefore empty.

6.4 Ligands (i)

EDS was not executed - this section is therefore empty.

6.5 Other polymers (i)

EDS was not executed - this section is therefore empty.