Full wwPDB X-ray Structure Validation Report ⓘ

Dec 13, 2022 – 12:08 pm GMT

PDB ID	:	7ZIO
Title	:	JC Polyomavirus VP1 in complex with 6'-Sialyllactose glycomacromolecules (aromatic linker)
Authors	:	Freytag, J.; Mueller, J.C.; Stehle, T.
Deposited on	:	2022-04-08
Resolution	:	1.75 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:

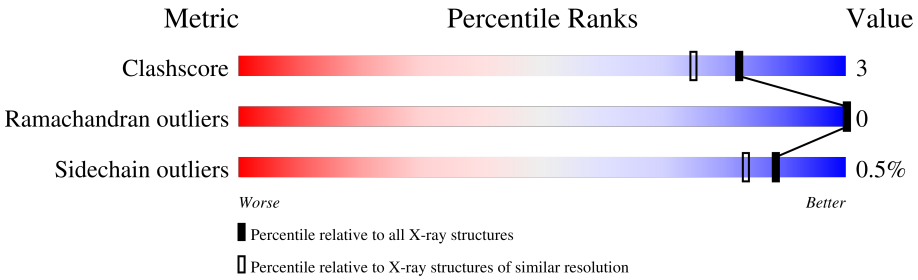
MolProbity	:	4.02b-467
Mogul	:	1.8.4, CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	FAILED
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.31.3

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 1.75 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	141614	2466 (1.76-1.76)
Ramachandran outliers	138981	2437 (1.76-1.76)
Sidechain outliers	138945	2437 (1.76-1.76)

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 <=5%

Note EDS failed to run properly.

Mol	Chain	Length	Quality of chain
1	AAA	272	90% · 6%
1	BBB	272	88% 7% 6%
1	CCC	272	92% · ·
1	DDD	272	93% · ·
1	EEE	272	91% · 5%
2	BaB	3	100%
2	CaC	3	33% 67%
3	A	2	50% 50%

2 Entry composition (i)

There are 8 unique types of molecules in this entry. The entry contains 11899 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 Major capsid protein VP1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	AAA	257	Total	C	N	O	S	0	6	0
			2026	1276	346	393	11			
1	BBB	256	Total	C	N	O	S	0	5	0
			2025	1278	348	388	11			
1	CCC	263	Total	C	N	O	S	0	8	0
			2091	1314	358	406	13			
1	DDD	263	Total	C	N	O	S	0	6	0
			2068	1298	354	403	13			
1	EEE	258	Total	C	N	O	S	0	3	0
			2018	1271	347	389	11			

There are 20 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
AAA	18	GLY	-	expression tag	UNP P03089
AAA	19	SER	-	expression tag	UNP P03089
AAA	20	HIS	-	expression tag	UNP P03089
AAA	21	MET	-	expression tag	UNP P03089
BBB	18	GLY	-	expression tag	UNP P03089
BBB	19	SER	-	expression tag	UNP P03089
BBB	20	HIS	-	expression tag	UNP P03089
BBB	21	MET	-	expression tag	UNP P03089
CCC	18	GLY	-	expression tag	UNP P03089
CCC	19	SER	-	expression tag	UNP P03089
CCC	20	HIS	-	expression tag	UNP P03089
CCC	21	MET	-	expression tag	UNP P03089
DDD	18	GLY	-	expression tag	UNP P03089
DDD	19	SER	-	expression tag	UNP P03089
DDD	20	HIS	-	expression tag	UNP P03089
DDD	21	MET	-	expression tag	UNP P03089
EEE	18	GLY	-	expression tag	UNP P03089
EEE	19	SER	-	expression tag	UNP P03089
EEE	20	HIS	-	expression tag	UNP P03089

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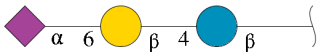
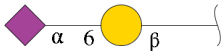
Chain	Residue	Modelled	Actual	Comment	Reference
EEE	21	MET	-	expression tag	UNP P03089

- Molecule 2 is an oligosaccharide called N-acetyl-alpha-neuraminic acid-(2-6)-beta-D-galacto pyranose-(1-4)-beta-D-glucopyranose.



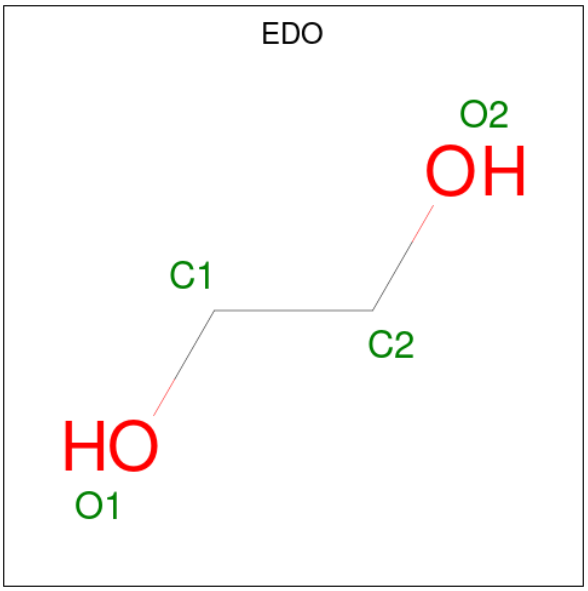
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
2	BaB	3	Total	C	N	O	0	0	0
			43	23	1	19			
2	CaC	3	Total	C	N	O	0	0	1
			32	17	1	14			

- Molecule 3 is an oligosaccharide called N-acetyl-alpha-neuraminic acid-(2-6)-beta-D-galacto pyranose.



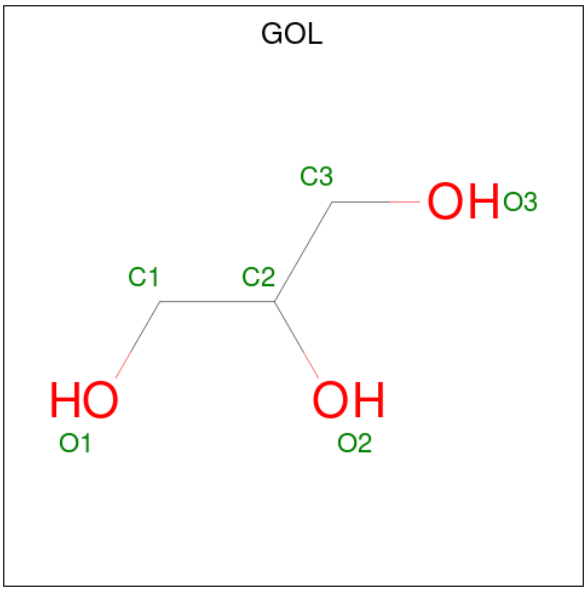
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
3	A	2	Total	C	N	O	0	0	1
			21	11	1	9			

- Molecule 4 is 1,2-ETHANEDIOL (three-letter code: EDO) (formula: $C_2H_6O_2$).



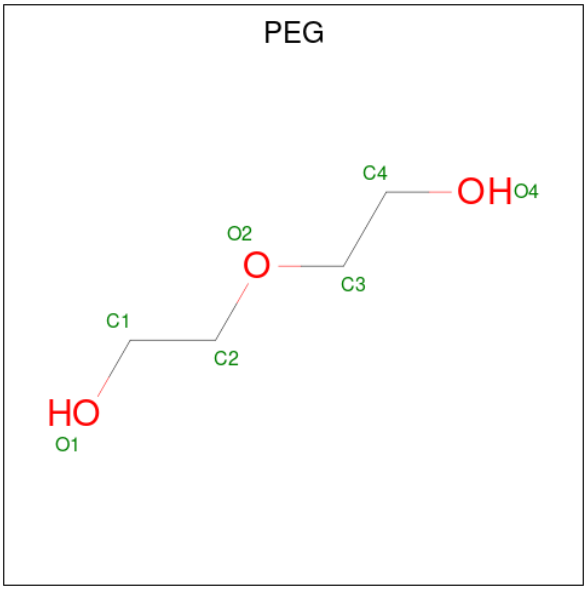
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	AAA	1	Total	C	O	0	0
			4	2	2		
4	AAA	1	Total	C	O	0	0
			4	2	2		
4	BBB	1	Total	C	O	0	0
			4	2	2		
4	BBB	1	Total	C	O	0	0
			4	2	2		
4	CCC	1	Total	C	O	0	0
			4	2	2		
4	DDD	1	Total	C	O	0	0
			4	2	2		
4	DDD	1	Total	C	O	0	0
			4	2	2		
4	DDD	1	Total	C	O	0	0
			4	2	2		
4	EEE	1	Total	C	O	0	0
			4	2	2		

- Molecule 5 is GLYCEROL (three-letter code: GOL) (formula: $C_3H_8O_3$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	C	O		
5	DDD	1	6	3	3	0	0

- Molecule 6 is DI(HYDROXYETHYL)ETHER (three-letter code: PEG) (formula: $C_4H_{10}O_3$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	C	O		
6	EEE	1	7	4	3	0	0

- Molecule 7 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
7	EEE	1	Total Cl 1 1	0	0

- Molecule 8 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
8	AAA	318	Total O 318 318	0	0
8	BBB	284	Total O 284 284	0	0
8	CCC	310	Total O 310 310	0	0
8	DDD	301	Total O 301 301	0	0
8	EEE	312	Total O 312 312	0	0

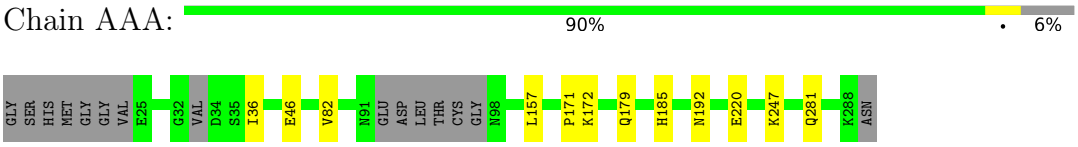
3 Residue-property plots (i)

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 failed to run properly.

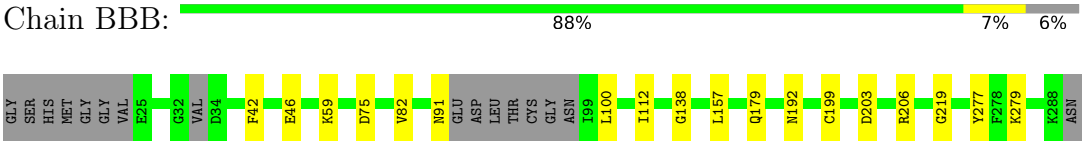
• Molecule 1: Major capsid protein VP1

Chain AAA:



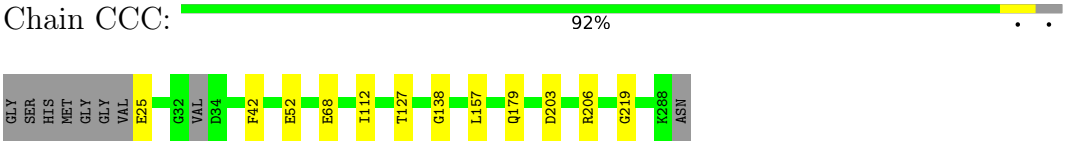
• Molecule 1: Major capsid protein VP1

Chain BBB:



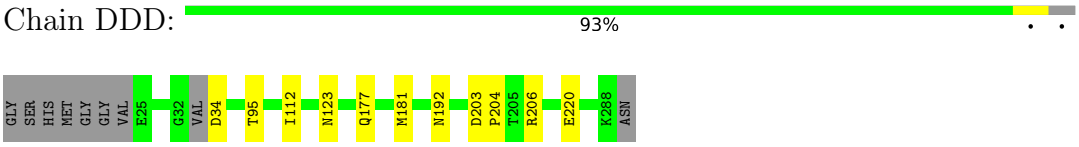
• Molecule 1: Major capsid protein VP1

Chain CCC:



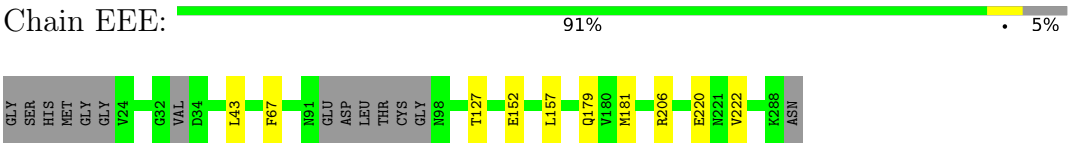
• Molecule 1: Major capsid protein VP1

Chain DDD:



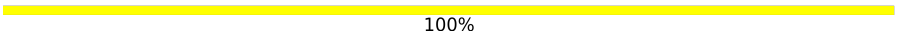
• Molecule 1: Major capsid protein VP1

Chain EEE:



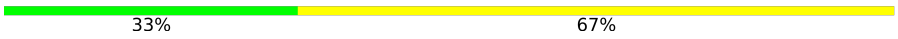
• Molecule 2: N-acetyl-alpha-neuraminic acid-(2-6)-beta-D-galactopyranose-(1-4)-beta-D-glucopyranose

Chain BaB:



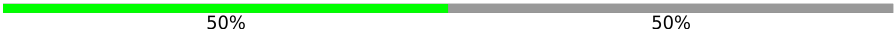
• Molecule 2: N-acetyl-alpha-neuraminic acid-(2-6)-beta-D-galactopyranose-(1-4)-beta-D-glucopyranose

Chain CaC:



• Molecule 3: N-acetyl-alpha-neuraminic acid-(2-6)-beta-D-galactopyranose

Chain A:



4 Data and refinement statistics (i)

EDS failed to run properly - this section is therefore incomplete.

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α, β, γ	150.02Å 97.26Å 129.07Å 90.00° 110.30° 90.00°	Depositor
Resolution (Å)	45.16 – 1.75	Depositor
% Data completeness (in resolution range)	99.3 (45.16-1.75)	Depositor
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	0.98 (at 1.75Å)	Xtriage
Refinement program	REFMAC 5.8.0258	Depositor
R, R_{free}	0.183 , 0.217	Depositor
Wilson B-factor (Å^2)	19.5	Xtriage
Anisotropy	0.072	Xtriage
L-test for twinning[2]	$< \|L\| > = 0.51$, $< L^2 > = 0.35$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	11899	wwPDB-VP
Average B, all atoms (Å^2)	21.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.70% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: CL, EDO, PEG, BGC, SIA, GAL, GOL

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	AAA	0.83	0/2079	0.82	0/2826
1	BBB	0.78	0/2079	0.82	0/2823
1	CCC	0.80	1/2148 (0.0%)	0.80	0/2919
1	DDD	0.83	0/2125	0.81	0/2889
1	EEE	0.84	0/2068	0.81	0/2810
All	All	0.82	1/10499 (0.0%)	0.81	0/14267

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	CCC	52	GLU	CD-OE1	5.03	1.31	1.25

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

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	AAA	2026	0	1964	11	0
1	BBB	2025	0	1971	18	0
1	CCC	2091	0	2026	9	0
1	DDD	2068	0	1994	13	0
1	EEE	2018	0	1951	7	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	BaB	43	0	37	0	0
2	CaC	32	0	26	0	0
3	A	21	0	17	0	0
4	AAA	8	0	12	1	0
4	BBB	8	0	12	0	0
4	CCC	4	0	6	0	0
4	DDD	12	0	18	0	0
4	EEE	4	0	6	0	0
5	DDD	6	0	8	0	0
6	EEE	7	0	10	1	0
7	EEE	1	0	0	0	0
8	AAA	318	0	0	8	0
8	BBB	284	0	0	2	0
8	CCC	310	0	0	0	0
8	DDD	301	0	0	5	0
8	EEE	312	0	0	0	0
All	All	11899	0	10058	52	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 3.

All (52) 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:DDD:112:ILE:HG21	1:EEE:181:MET:HE1	1.44	0.99
1:AAA:36:ILE:HB	8:AAA:688:HOH:O	1.74	0.88
1:BBB:91:ASN:HD21	1:BBB:100:LEU:H	1.36	0.73
1:DDD:203:ASP:OD2	1:DDD:206[B]:ARG:HD3	1.91	0.70
1:DDD:112:ILE:CG2	1:EEE:181:MET:HE1	2.19	0.70
1:BBB:82:VAL:O	1:BBB:192[B]:ASN:ND2	2.26	0.69
1:DDD:95:THR:CB	8:DDD:501:HOH:O	2.41	0.67
1:BBB:42[A]:PHE:CD2	1:BBB:112:ILE:CD1	2.78	0.66
1:AAA:172:LYS:HE3	8:AAA:607:HOH:O	1.98	0.64
1:AAA:192[A]:ASN:ND2	8:AAA:401:HOH:O	2.31	0.62
1:BBB:42[A]:PHE:CD2	1:BBB:112:ILE:HD13	2.35	0.61
1:CCC:127:THR:HG21	8:DDD:420:HOH:O	2.04	0.57
1:AAA:281:GLN:HG3	8:AAA:441:HOH:O	2.04	0.57
1:BBB:206[B]:ARG:NH2	8:BBB:502:HOH:O	2.30	0.56
1:BBB:203:ASP:OD2	1:BBB:206[B]:ARG:CD	2.55	0.55
1:CCC:203:ASP:OD2	1:CCC:206[B]:ARG:HD3	2.08	0.53
1:DDD:192[B]:ASN:ND2	8:DDD:406:HOH:O	2.41	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:BBB:42[A]:PHE:HD2	1:BBB:112:ILE:HD11	1.74	0.53
1:CCC:42:PHE:CD1	1:DDD:181[B]:MET:HG2	2.44	0.53
1:BBB:203:ASP:OD2	1:BBB:206[B]:ARG:HD3	2.09	0.53
1:BBB:42[A]:PHE:CD2	1:BBB:112:ILE:HD11	2.45	0.52
1:BBB:42[A]:PHE:HD2	1:BBB:112:ILE:CD1	2.24	0.51
1:EEE:157:LEU:O	1:EEE:179:GLN:HA	2.10	0.51
1:DDD:34:ASP:N	1:DDD:34:ASP:OD1	2.43	0.50
1:EEE:152:GLU:OE2	1:EEE:206[B]:ARG:HD2	2.13	0.49
1:DDD:123:ASN:ND2	8:DDD:403:HOH:O	2.28	0.49
1:AAA:36:ILE:CG2	8:AAA:688:HOH:O	2.61	0.48
1:CCC:25:GLU:OE2	1:CCC:25:GLU:HA	2.14	0.48
1:AAA:36:ILE:CB	8:AAA:688:HOH:O	2.45	0.48
1:DDD:123:ASN:HD22	1:EEE:67:PHE:H	1.61	0.48
1:CCC:42:PHE:CE1	1:DDD:181[B]:MET:HG2	2.51	0.46
1:DDD:203:ASP:OD2	1:DDD:206[B]:ARG:CD	2.60	0.46
1:AAA:46:GLU:HG3	8:AAA:401:HOH:O	2.15	0.46
1:BBB:203:ASP:OD2	1:BBB:206[B]:ARG:HD2	2.15	0.45
1:EEE:43:LEU:HA	6:EEE:302:PEG:H21	1.98	0.45
1:DDD:177:GLN:OE1	8:DDD:401:HOH:O	2.21	0.44
1:AAA:157:LEU:O	1:AAA:179:GLN:HA	2.17	0.44
1:CCC:203:ASP:OD2	1:CCC:206[B]:ARG:CD	2.66	0.43
1:BBB:46:GLU:HG3	8:BBB:504:HOH:O	2.19	0.43
1:BBB:42[A]:PHE:CE2	1:BBB:112:ILE:HD13	2.54	0.42
1:CCC:157:LEU:O	1:CCC:179:GLN:HA	2.19	0.42
1:BBB:138:GLY:HA2	1:BBB:219:GLY:O	2.19	0.42
1:CCC:112[B]:ILE:CD1	1:DDD:204:PRO:HG3	2.50	0.42
1:CCC:138:GLY:HA2	1:CCC:219:GLY:O	2.19	0.42
1:AAA:171:PRO:HB3	1:AAA:185:HIS:CG	2.55	0.41
1:BBB:59:LYS:HD2	1:BBB:75:ASP:OD2	2.20	0.41
1:AAA:82:VAL:O	1:AAA:192[B]:ASN:ND2	2.43	0.41
1:BBB:157:LEU:O	1:BBB:179:GLN:HA	2.20	0.41
8:AAA:457:HOH:O	1:EEE:127:THR:HG21	2.21	0.41
1:BBB:112:ILE:HD11	1:BBB:277:TYR:HB2	2.03	0.41
1:AAA:247:LYS:CE	4:AAA:302:EDO:H21	2.52	0.40
1:BBB:277:TYR:OH	1:BBB:279:LYS:HE2	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	AAA	257/272 (94%)	250 (97%)	7 (3%)	0	100	100
1	BBB	255/272 (94%)	245 (96%)	10 (4%)	0	100	100
1	CCC	267/272 (98%)	257 (96%)	10 (4%)	0	100	100
1	DDD	265/272 (97%)	256 (97%)	9 (3%)	0	100	100
1	EEE	255/272 (94%)	248 (97%)	7 (3%)	0	100	100
All	All	1299/1360 (96%)	1256 (97%)	43 (3%)	0	100	100

There are no Ramachandran outliers to report.

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	AAA	228/237 (96%)	227 (100%)	1 (0%)	91	87
1	BBB	227/237 (96%)	226 (100%)	1 (0%)	91	87
1	CCC	235/237 (99%)	234 (100%)	1 (0%)	91	87
1	DDD	232/237 (98%)	231 (100%)	1 (0%)	91	87
1	EEE	224/237 (94%)	222 (99%)	2 (1%)	78	67
All	All	1146/1185 (97%)	1140 (100%)	6 (0%)	88	83

All (6) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	AAA	220	GLU
1	BBB	199	CYS
1	CCC	68	GLU
1	DDD	220	GLU
1	EEE	220	GLU
1	EEE	222	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

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)

Of 8 monosaccharides modelled in this entry, 6 were used for Mogul analysis.

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	SIA	A	3	3	20,20,21	1.05	1 (5%)	24,28,31	1.08	2 (8%)
2	BGC	BaB	1	2	12,12,12	0.77	0	17,17,17	1.34	4 (23%)
2	GAL	BaB	2	2	11,11,12	0.98	1 (9%)	15,15,17	1.29	2 (13%)
2	SIA	BaB	3	2	20,20,21	1.42	2 (10%)	24,28,31	1.18	2 (8%)
2	GAL	CaC	2	2	11,11,12	0.88	1 (9%)	15,15,17	0.90	1 (6%)
2	SIA	CaC	3	2	20,20,21	1.55	1 (5%)	24,28,31	0.98	1 (4%)

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	SIA	A	3	3	-	0/18/34/38	0/1/1/1
2	BGC	BaB	1	2	-	2/2/22/22	0/1/1/1
2	GAL	BaB	2	2	-	0/2/19/22	0/1/1/1
2	SIA	BaB	3	2	-	0/18/34/38	0/1/1/1
2	GAL	CaC	2	2	-	0/2/19/22	0/1/1/1
2	SIA	CaC	3	2	-	2/18/34/38	0/1/1/1

All (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	CaC	3	SIA	C2-C1	5.16	1.57	1.52
2	BaB	3	SIA	C2-C1	3.90	1.55	1.52
2	BaB	3	SIA	C4-C5	3.21	1.56	1.53
2	BaB	2	GAL	C2-C3	2.37	1.56	1.52
2	CaC	2	GAL	C2-C3	2.36	1.56	1.52
3	A	3	SIA	C2-C1	2.14	1.54	1.52

All (12) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	BaB	2	GAL	O6-C6-C5	-3.05	100.82	111.29
2	BaB	1	BGC	O5-C1-C2	-2.92	105.08	110.28
2	BaB	1	BGC	C6-C5-C4	-2.58	106.95	113.00
2	BaB	3	SIA	O1B-C1-C2	2.58	120.39	113.03
2	BaB	2	GAL	O2-C2-C1	2.38	114.02	109.15
2	BaB	3	SIA	O6-C2-C1	2.33	112.27	107.70
2	BaB	1	BGC	O5-C5-C4	2.19	113.67	109.69
2	BaB	1	BGC	O6-C6-C5	-2.17	103.83	111.29
3	A	3	SIA	C6-C5-N5	-2.17	107.31	110.91
2	CaC	3	SIA	C3-C4-C5	-2.16	108.85	111.46
2	CaC	2	GAL	O5-C1-C2	-2.12	107.50	110.77
3	A	3	SIA	O9-C9-C8	-2.03	106.64	111.07

There are no chirality outliers.

All (4) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	BaB	1	BGC	C4-C5-C6-O6
2	BaB	1	BGC	O5-C5-C6-O6

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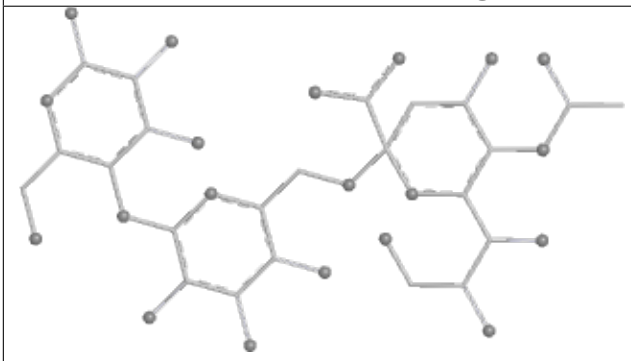
Mol	Chain	Res	Type	Atoms
2	CaC	3	SIA	O8-C8-C9-O9
2	CaC	3	SIA	O1A-C1-C2-O6

There are no ring outliers.

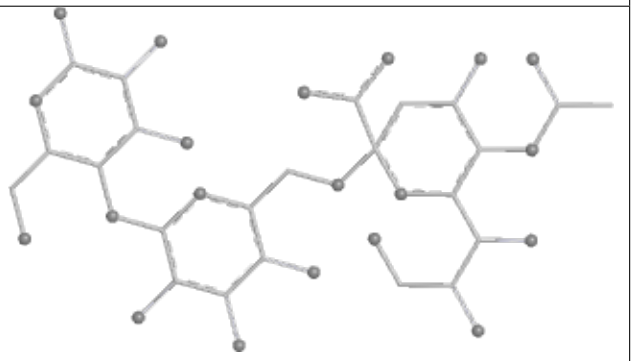
No monomer is involved in short contacts.

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for oligosaccharide.

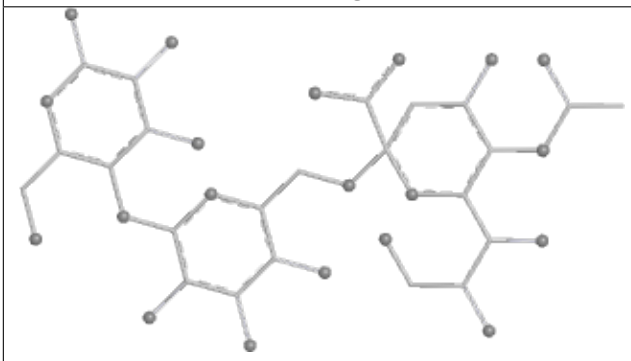
Oligosaccharide Chain BaB



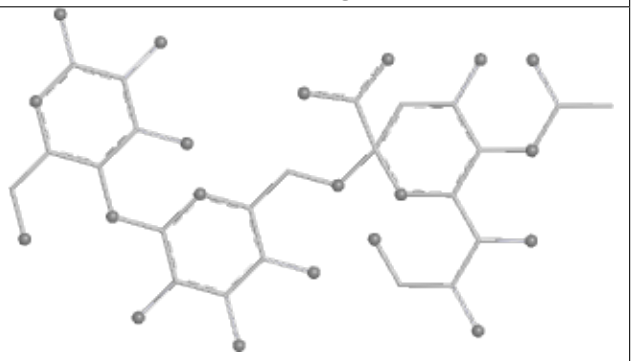
Bond lengths



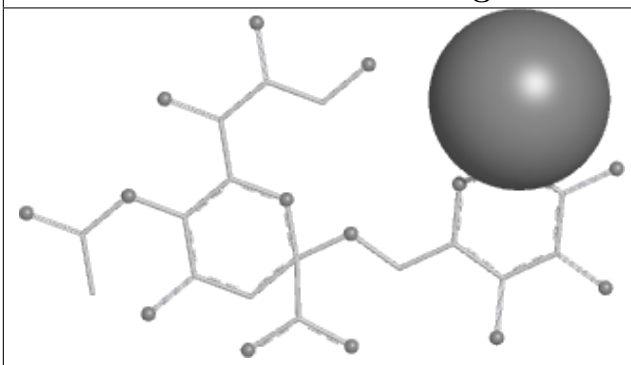
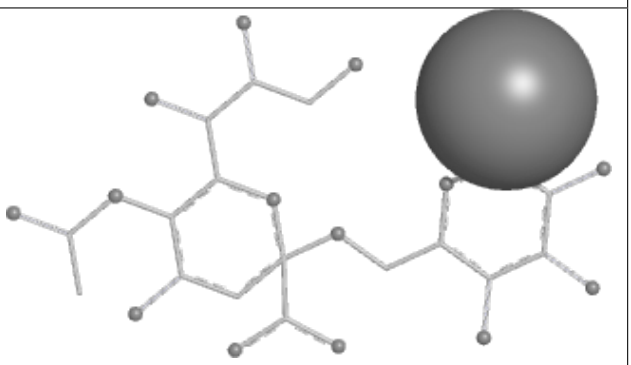
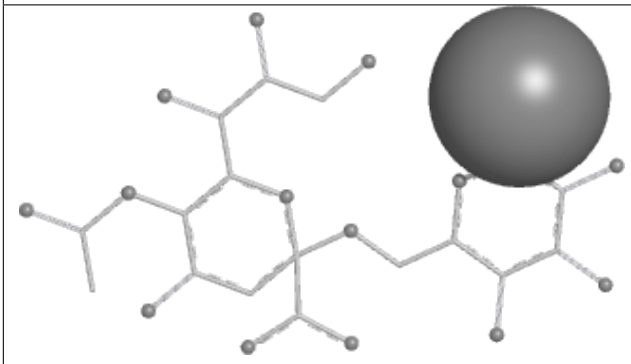
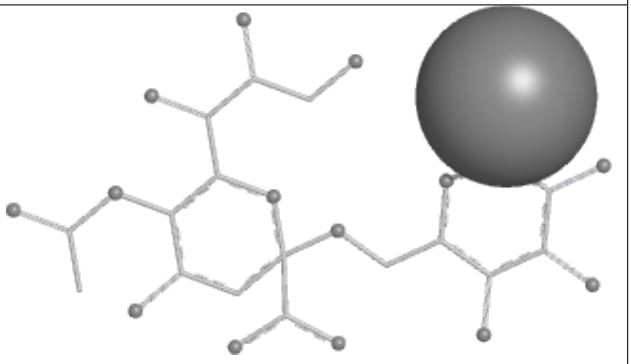
Bond angles

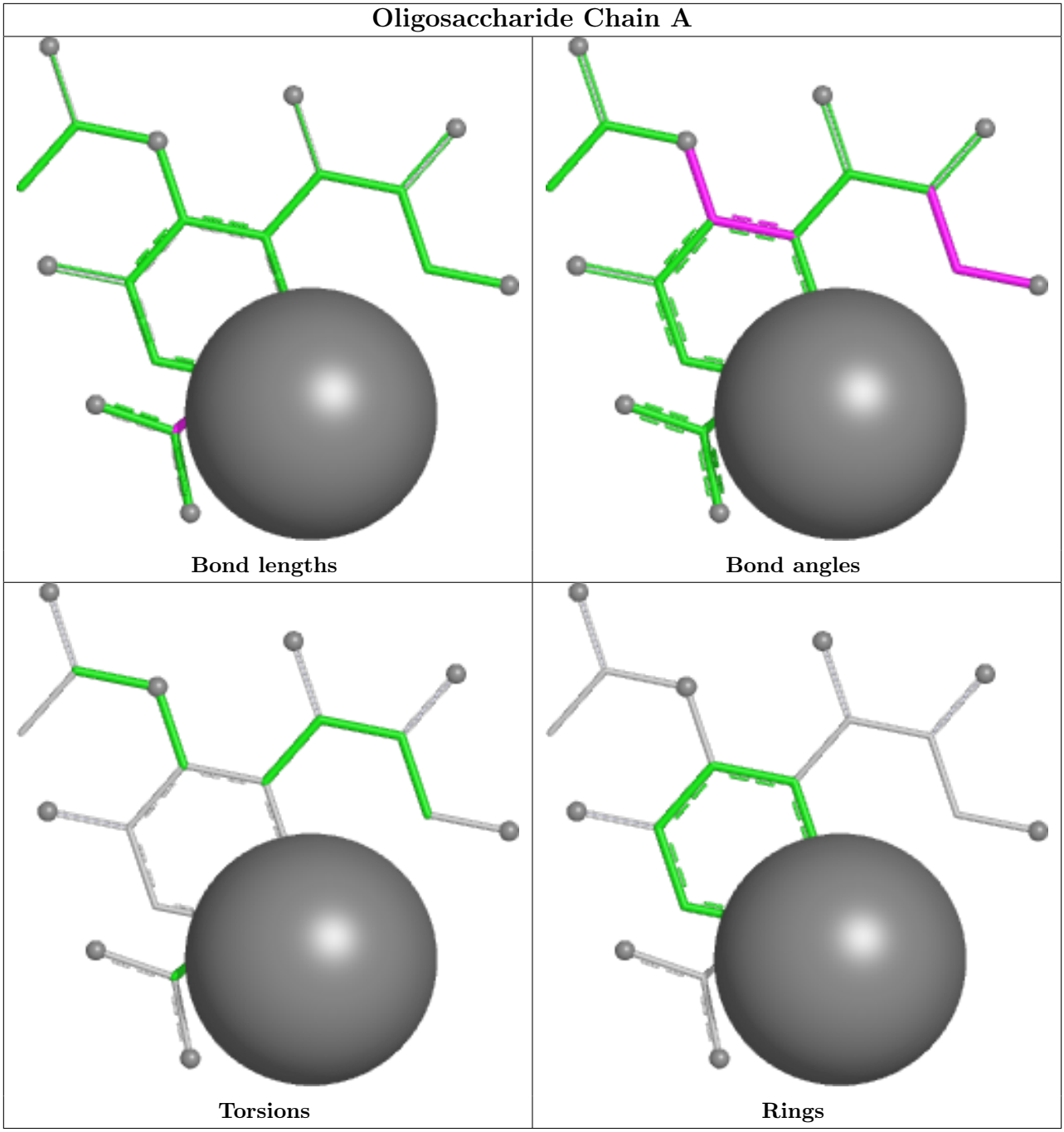


Torsions



Rings

Oligosaccharide Chain CaC	
	
Bond lengths	**Bond angles**
	
Torsions	**Rings**



5.6 Ligand geometry (i)

Of 12 ligands modelled in this entry, 1 is monoatomic - leaving 11 for Mogul analysis.

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	EDO	BBB	402	-	3,3,3	0.32	0	2,2,2	0.29	0
4	EDO	EEE	301	-	3,3,3	0.09	0	2,2,2	0.22	0
4	EDO	AAA	301	-	3,3,3	0.15	0	2,2,2	0.26	0
4	EDO	BBB	401	-	3,3,3	0.13	0	2,2,2	0.33	0
4	EDO	DDD	301	-	3,3,3	0.07	0	2,2,2	0.21	0
4	EDO	AAA	302	-	3,3,3	0.31	0	2,2,2	0.36	0
4	EDO	DDD	304	-	3,3,3	0.33	0	2,2,2	0.35	0
5	GOL	DDD	302	-	5,5,5	0.09	0	5,5,5	0.24	0
6	PEG	EEE	302	-	6,6,6	0.29	0	5,5,5	0.23	0
4	EDO	DDD	303	-	3,3,3	0.50	0	2,2,2	0.59	0
4	EDO	CCC	401	-	3,3,3	0.18	0	2,2,2	0.26	0

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	EDO	BBB	402	-	-	0/1/1/1	-
4	EDO	EEE	301	-	-	1/1/1/1	-
4	EDO	AAA	301	-	-	1/1/1/1	-
4	EDO	BBB	401	-	-	1/1/1/1	-
4	EDO	DDD	301	-	-	1/1/1/1	-
4	EDO	AAA	302	-	-	1/1/1/1	-
4	EDO	DDD	304	-	-	1/1/1/1	-
5	GOL	DDD	302	-	-	2/4/4/4	-
6	PEG	EEE	302	-	-	2/4/4/4	-
4	EDO	DDD	303	-	-	1/1/1/1	-
4	EDO	CCC	401	-	-	1/1/1/1	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (12) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	DDD	302	GOL	O1-C1-C2-C3
4	BBB	401	EDO	O1-C1-C2-O2
4	CCC	401	EDO	O1-C1-C2-O2

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Mol	Chain	Res	Type	Atoms
4	DDD	301	EDO	O1-C1-C2-O2
4	DDD	303	EDO	O1-C1-C2-O2
6	EEE	302	PEG	O2-C3-C4-O4
4	AAA	301	EDO	O1-C1-C2-O2
4	DDD	304	EDO	O1-C1-C2-O2
4	AAA	302	EDO	O1-C1-C2-O2
4	EEE	301	EDO	O1-C1-C2-O2
6	EEE	302	PEG	C4-C3-O2-C2
5	DDD	302	GOL	O1-C1-C2-O2

There are no ring outliers.

2 monomers are involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	AAA	302	EDO	1	0
6	EEE	302	PEG	1	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 failed to run properly - this section is therefore empty.

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

EDS failed to run properly - this section is therefore empty.

6.3 Carbohydrates

EDS failed to run properly - this section is therefore empty.

6.4 Ligands

EDS failed to run properly - this section is therefore empty.

6.5 Other polymers

EDS failed to run properly - this section is therefore empty.