



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 8, 2026 – 02:57 PM UTC

PDB ID : 1MDP / pdb_00001mdp
Title : REFINED STRUCTURES OF TWO INSERTION(SLASH)DELETION MUTANTS PROBE FUNCTION OF THE MALTODEXTRIN BINDING PROTEIN
Authors : Sharff, A.J.; Quiococho, F.A.
Deposited on : 1994-08-10
Resolution : 2.30 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	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	NOT EXECUTED
EDS	:	NOT EXECUTED
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

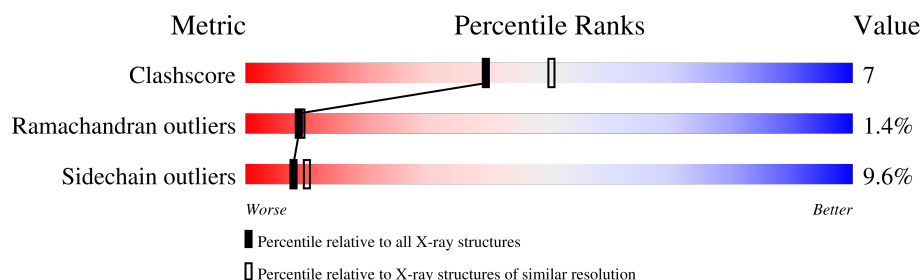
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.30 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	190562	6919 (2.30-2.30)
Ramachandran outliers	187476	6854 (2.30-2.30)
Sidechain outliers	187428	6854 (2.30-2.30)

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 $\leq 5\%$

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	1	363	66% 29% 5%
1	2	363	64% 30% 6%
2	A	2	50% 50%
2	B	2	50% 50%

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 5851 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 MALTODEXTRIN BINDING PROTEIN.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	1	363	Total	C	N	O	S	0	0	0
			2822	1817	459	540	6			
1	2	363	Total	C	N	O	S	0	0	0
			2822	1817	459	540	6			

There are 18 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
1	134	ASP	LYS	engineered mutation	UNP P02928
1	135	PRO	LYS	engineered mutation	UNP P02928
1	?	-	ALA	deletion	UNP P02928
1	?	-	LEU	deletion	UNP P02928
1	?	-	LYS	deletion	UNP P02928
1	?	-	GLU	deletion	UNP P02928
1	?	-	LEU	deletion	UNP P02928
1	?	-	LYS	deletion	UNP P02928
1	?	-	ALA	deletion	UNP P02928
2	134	ASP	LYS	engineered mutation	UNP P02928
2	135	PRO	LYS	engineered mutation	UNP P02928
2	?	-	ALA	deletion	UNP P02928
2	?	-	LEU	deletion	UNP P02928
2	?	-	LYS	deletion	UNP P02928
2	?	-	GLU	deletion	UNP P02928
2	?	-	LEU	deletion	UNP P02928
2	?	-	LYS	deletion	UNP P02928
2	?	-	ALA	deletion	UNP P02928

- Molecule 2 is an oligosaccharide called alpha-D-glucopyranose-(1-4)-alpha-D-glucopyranose.



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf	Trace
2	A	2	Total	C	O	0	0	0
			23	12	11			
2	B	2	Total	C	O	0	0	0
			23	12	11			

- Molecule 3 is water.

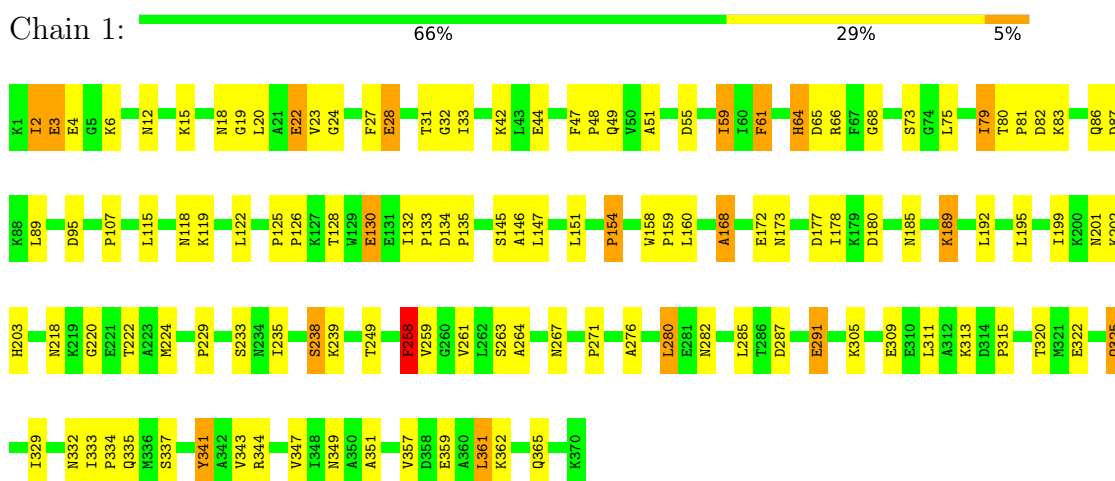
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	1	76	Total	O	0	0
			76	76		
3	2	85	Total	O	0	0
			85	85		

3 Residue-property plots

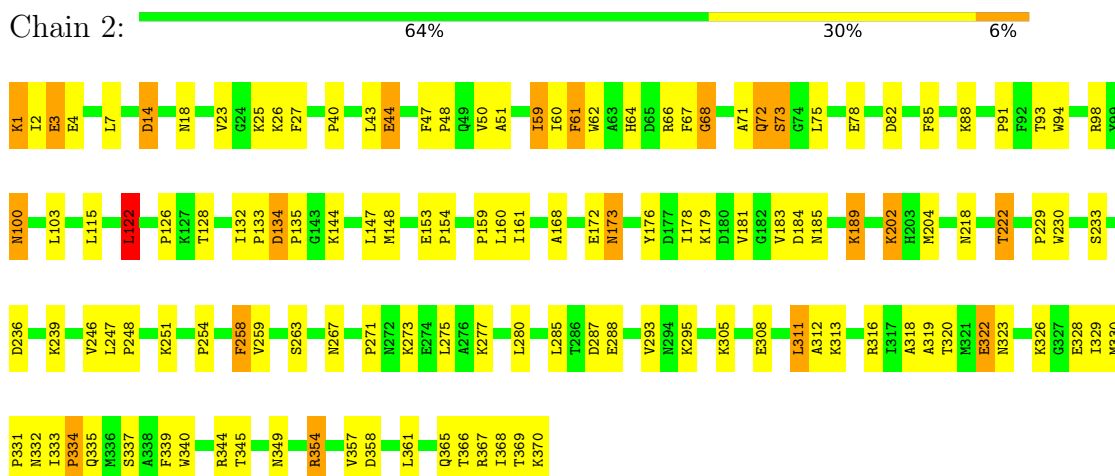
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry. Residues are color-coded 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: MALTODEXTRIN BINDING PROTEIN



• Molecule 1: MALTODEXTRIN BINDING PROTEIN



• Molecule 2: alpha-D-glucopyranose-(1-4)-alpha-D-glucopyranose





- Molecule 2: alpha-D-glucopyranose-(1-4)-alpha-D-glucopyranose

Chain B:  50% 50%



4 Data and refinement statistics

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

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	55.51Å 88.33Å 75.79Å 90.00° 95.00° 90.00°	Depositor
Resolution (Å)	10.00 – 2.30	Depositor
% Data completeness (in resolution range)	(Not available) (10.00-2.30)	Depositor
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	PROLSQ, X-PLOR	Depositor
R, R_{free}	0.187 , (Not available)	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	5851	wwPDB-VP
Average B, all atoms (Å ²)	17.0	wwPDB-VP

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: GLC

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	1	0.89	1/2891 (0.0%)	1.89	84/3925 (2.1%)
1	2	0.90	0/2891	1.92	94/3925 (2.4%)
All	All	0.89	1/5782 (0.0%)	1.91	178/7850 (2.3%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	1	80	THR	CA-CB	7.67	1.61	1.53

All (178) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	2	316	ARG	CD-NE-CZ	14.93	145.30	124.40
1	2	100	ASN	CA-CB-CG	11.99	124.59	112.60
1	1	154	PRO	CA-C-N	10.13	134.87	120.28
1	1	154	PRO	C-N-CA	10.13	134.87	120.28
1	1	201	ASN	CA-C-N	9.88	136.40	122.36
1	1	201	ASN	C-N-CA	9.88	136.40	122.36
1	1	61	PHE	CA-CB-CG	9.54	123.34	113.80
1	2	71	ALA	CA-C-N	9.20	132.61	120.28
1	2	71	ALA	C-N-CA	9.20	132.61	120.28
1	1	238	SER	CA-C-N	8.82	136.96	123.47
1	1	238	SER	C-N-CA	8.82	136.96	123.47
1	2	61	PHE	CA-CB-CG	8.73	122.53	113.80
1	1	12	ASN	CA-C-N	8.67	130.97	120.14
1	1	12	ASN	C-N-CA	8.67	130.97	120.14
1	1	27	PHE	CA-C-N	8.56	132.09	120.54
1	1	27	PHE	C-N-CA	8.56	132.09	120.54
1	2	267	ASN	CA-CB-CG	8.38	120.98	112.60
1	2	293	VAL	CA-C-N	8.36	131.48	120.28

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	2	293	VAL	C-N-CA	8.36	131.48	120.28
1	2	154	PRO	CA-C-N	8.33	131.78	120.54
1	2	154	PRO	C-N-CA	8.33	131.78	120.54
1	2	271	PRO	CA-C-N	8.06	135.19	122.86
1	2	271	PRO	C-N-CA	8.06	135.19	122.86
1	2	3	GLU	CB-CG-CD	8.03	126.25	112.60
1	2	285	LEU	CA-C-N	7.71	135.50	121.85
1	2	285	LEU	C-N-CA	7.71	135.50	121.85
1	2	312	ALA	CA-C-N	7.61	131.09	120.29
1	2	312	ALA	C-N-CA	7.61	131.09	120.29
1	1	173	ASN	CA-CB-CG	7.09	119.69	112.60
1	2	322	GLU	CB-CG-CD	7.03	124.55	112.60
1	2	23	VAL	CA-C-N	7.01	129.12	120.22
1	2	23	VAL	C-N-CA	7.01	129.12	120.22
1	1	341	TYR	CA-CB-CG	6.91	126.34	113.90
1	1	68	GLY	CA-C-N	6.88	129.01	120.34
1	1	68	GLY	C-N-CA	6.88	129.01	120.34
1	2	229	PRO	CA-C-N	6.87	131.59	120.60
1	2	229	PRO	C-N-CA	6.87	131.59	120.60
1	1	320	THR	CA-C-N	6.83	130.00	120.29
1	1	320	THR	C-N-CA	6.83	130.00	120.29
1	1	359	GLU	CB-CG-CD	6.83	124.22	112.60
1	2	320	THR	CA-C-N	6.82	129.41	120.28
1	2	320	THR	C-N-CA	6.82	129.41	120.28
1	2	287	ASP	CA-C-N	6.81	129.96	120.29
1	2	287	ASP	C-N-CA	6.81	129.96	120.29
1	1	95	ASP	CA-C-N	6.79	129.93	120.29
1	1	95	ASP	C-N-CA	6.79	129.93	120.29
1	1	24	GLY	CA-C-N	6.70	130.50	120.31
1	1	24	GLY	C-N-CA	6.70	130.50	120.31
1	2	44	GLU	CA-CB-CG	6.68	127.46	114.10
1	2	134	ASP	N-CA-C	6.67	120.31	110.10
1	2	44	GLU	CB-CG-CD	6.63	123.87	112.60
1	2	64	HIS	N-CA-C	6.61	119.32	111.71
1	2	308	GLU	CA-C-N	6.61	129.03	120.44
1	2	308	GLU	C-N-CA	6.61	129.03	120.44
1	1	20	LEU	CA-C-N	6.60	130.34	120.31
1	1	20	LEU	C-N-CA	6.60	130.34	120.31
1	1	172	GLU	CA-C-N	6.57	133.37	123.05
1	1	172	GLU	C-N-CA	6.57	133.37	123.05
1	2	258	PHE	CA-CB-CG	6.50	120.30	113.80
1	1	285	LEU	CA-C-N	6.48	132.72	122.36

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	1	285	LEU	C-N-CA	6.48	132.72	122.36
1	2	357	VAL	CA-C-N	6.46	129.26	120.54
1	2	357	VAL	C-N-CA	6.46	129.26	120.54
1	1	23	VAL	CA-C-N	6.41	127.09	119.98
1	1	23	VAL	C-N-CA	6.41	127.09	119.98
1	2	334	PRO	CA-C-N	6.30	133.66	121.18
1	2	334	PRO	C-N-CA	6.30	133.66	121.18
1	1	309	GLU	CB-CG-CD	6.29	123.30	112.60
1	2	308	GLU	CB-CG-CD	6.25	123.22	112.60
1	1	51	ALA	CA-C-N	6.17	128.83	120.38
1	1	51	ALA	C-N-CA	6.17	128.83	120.38
1	1	18	ASN	CA-C-N	6.13	126.74	120.00
1	1	18	ASN	C-N-CA	6.13	126.74	120.00
1	2	14	ASP	CA-CB-CG	6.08	118.68	112.60
1	1	66	ARG	CA-C-N	6.07	128.42	120.28
1	1	66	ARG	C-N-CA	6.07	128.42	120.28
1	2	94	TRP	CA-C-N	6.07	128.42	120.28
1	2	94	TRP	C-N-CA	6.07	128.42	120.28
1	1	349	ASN	CA-C-N	6.06	128.40	120.28
1	1	349	ASN	C-N-CA	6.06	128.40	120.28
1	1	80	THR	N-CA-C	6.03	119.43	109.79
1	2	91	PRO	CA-C-N	5.91	129.29	120.31
1	2	91	PRO	C-N-CA	5.91	129.29	120.31
1	2	173	ASN	CA-CB-CG	5.90	118.50	112.60
1	2	233	SER	CA-C-N	5.90	128.67	120.29
1	2	233	SER	C-N-CA	5.90	128.67	120.29
1	1	64	HIS	N-CA-C	5.89	118.49	111.71
1	1	32	GLY	CA-C-N	5.79	129.61	122.37
1	1	32	GLY	C-N-CA	5.79	129.61	122.37
1	2	305	LYS	CA-C-N	5.70	128.23	120.54
1	2	305	LYS	C-N-CA	5.70	128.23	120.54
1	1	202	LYS	N-CA-C	5.70	119.25	111.39
1	1	276	ALA	CA-C-N	5.69	127.90	120.28
1	1	276	ALA	C-N-CA	5.69	127.90	120.28
1	2	27	PHE	CA-C-N	5.69	127.90	120.28
1	2	27	PHE	C-N-CA	5.69	127.90	120.28
1	1	361	LEU	CA-C-N	5.64	127.84	120.28
1	1	361	LEU	C-N-CA	5.64	127.84	120.28
1	2	319	ALA	CA-C-N	5.63	127.76	120.44
1	2	319	ALA	C-N-CA	5.63	127.76	120.44
1	2	27	PHE	CA-CB-CG	5.62	119.42	113.80
1	1	325	GLN	CA-C-N	5.61	131.18	122.49

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	1	325	GLN	C-N-CA	5.61	131.18	122.49
1	2	251	LYS	CA-C-N	5.61	130.63	122.28
1	2	251	LYS	C-N-CA	5.61	130.63	122.28
1	2	344	ARG	CA-C-N	5.57	127.75	120.28
1	2	344	ARG	C-N-CA	5.57	127.75	120.28
1	1	258	PHE	CA-CB-CG	5.57	119.37	113.80
1	2	311	LEU	CA-C-N	5.55	128.48	120.38
1	2	311	LEU	C-N-CA	5.55	128.48	120.38
1	1	115	LEU	CB-CA-C	5.53	119.15	110.19
1	2	93	THR	CA-C-N	5.51	127.67	120.28
1	2	93	THR	C-N-CA	5.51	127.67	120.28
1	2	159	PRO	CA-C-N	5.47	128.06	120.29
1	2	159	PRO	C-N-CA	5.47	128.06	120.29
1	2	64	HIS	CA-C-N	5.46	127.86	120.38
1	2	64	HIS	C-N-CA	5.46	127.86	120.38
1	2	185	ASN	CA-CB-CG	5.46	118.06	112.60
1	2	349	ASN	CA-C-N	5.46	127.60	120.28
1	2	349	ASN	C-N-CA	5.46	127.60	120.28
1	1	125	PRO	O-C-N	5.45	123.71	121.15
1	2	18	ASN	CA-C-N	5.44	127.20	120.34
1	2	18	ASN	C-N-CA	5.44	127.20	120.34
1	1	185	ASN	CA-CB-CG	5.41	118.01	112.60
1	2	316	ARG	NE-CZ-NH1	5.39	126.89	121.50
1	2	275	LEU	CA-C-N	5.39	127.94	120.29
1	2	275	LEU	C-N-CA	5.39	127.94	120.29
1	1	362	LYS	CA-C-N	5.38	127.94	120.29
1	1	362	LYS	C-N-CA	5.38	127.94	120.29
1	1	87	ASP	CA-C-N	5.38	129.82	120.68
1	1	87	ASP	C-N-CA	5.38	129.82	120.68
1	2	51	ALA	CA-C-N	5.37	128.48	120.31
1	2	51	ALA	C-N-CA	5.37	128.48	120.31
1	2	1	LYS	CA-C-N	5.37	131.64	121.97
1	2	1	LYS	C-N-CA	5.37	131.64	121.97
1	1	44	GLU	CB-CG-CD	5.37	121.72	112.60
1	2	68	GLY	CA-C-N	5.35	125.92	119.98
1	2	68	GLY	C-N-CA	5.35	125.92	119.98
1	1	267	ASN	CA-CB-CG	5.32	117.92	112.60
1	2	189	LYS	CA-C-N	5.31	127.39	120.28
1	2	189	LYS	C-N-CA	5.31	127.39	120.28
1	1	19	GLY	CA-C-N	5.30	128.36	120.31
1	1	19	GLY	C-N-CA	5.30	128.36	120.31
1	1	365	GLN	CA-C-N	5.29	127.37	120.28

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	1	365	GLN	C-N-CA	5.29	127.37	120.28
1	2	122	LEU	N-CA-CB	-5.26	104.51	111.40
1	2	236	ASP	CA-CB-CG	5.26	117.86	112.60
1	1	280	LEU	N-CA-C	5.25	116.69	111.07
1	1	82	ASP	CA-CB-CG	5.24	117.84	112.60
1	1	203	HIS	CA-C-N	5.22	130.67	122.21
1	1	203	HIS	C-N-CA	5.22	130.67	122.21
1	1	341	TYR	N-CA-CB	5.22	117.88	110.16
1	1	118	ASN	CA-CB-CG	5.21	117.81	112.60
1	2	328	GLU	CB-CG-CD	5.19	121.42	112.60
1	1	28	GLU	CA-C-N	5.18	127.18	120.44
1	1	28	GLU	C-N-CA	5.18	127.18	120.44
1	2	337	SER	CA-C-N	5.17	127.47	120.44
1	2	337	SER	C-N-CA	5.17	127.47	120.44
1	1	305	LYS	CA-C-N	5.14	127.48	120.54
1	1	305	LYS	C-N-CA	5.14	127.48	120.54
1	1	22	GLU	N-CA-CB	5.13	117.75	110.16
1	1	178	ILE	CA-C-N	5.10	130.80	122.65
1	1	178	ILE	C-N-CA	5.10	130.80	122.65
1	2	72	GLN	CA-C-N	5.09	130.06	121.14
1	2	72	GLN	C-N-CA	5.09	130.06	121.14
1	2	277	LYS	CA-C-N	5.08	127.05	120.44
1	2	277	LYS	C-N-CA	5.08	127.05	120.44
1	2	153	GLU	CA-C-N	5.08	124.87	119.28
1	2	153	GLU	C-N-CA	5.08	124.87	119.28
1	1	315	PRO	CA-C-N	5.06	128.01	120.31
1	1	315	PRO	C-N-CA	5.06	128.01	120.31
1	2	82	ASP	CA-CB-CG	5.06	117.66	112.60
1	2	78	GLU	CB-CG-CD	5.05	121.19	112.60
1	1	229	PRO	CA-C-N	5.05	129.15	120.72
1	1	229	PRO	C-N-CA	5.05	129.15	120.72
1	1	282	ASN	CA-CB-CG	5.03	117.63	112.60
1	1	86	GLN	CA-C-N	5.03	128.64	120.60
1	1	86	GLN	C-N-CA	5.03	128.64	120.60

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	1	2822	0	2785	37	0
1	2	2822	0	2785	40	0
2	A	23	0	21	0	0
2	B	23	0	20	1	0
3	1	76	0	0	1	0
3	2	85	0	0	0	0
All	All	5851	0	5611	76	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 7.

All (76) 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)
1:2:122:LEU:HD21	1:2:126:PRO:HD3	1.70	0.73
1:1:333:ILE:HD12	1:1:335:GLN:HE21	1.54	0.73
1:2:333:ILE:HD12	1:2:335:GLN:HE21	1.56	0.70
1:2:189:LYS:HG2	1:2:361:LEU:HD12	1.73	0.70
1:2:1:LYS:HE2	1:2:4:GLU:HG2	1.76	0.67
1:2:40:PRO:HG2	1:2:43:LEU:HB3	1.76	0.66
1:1:31:THR:HG22	1:1:33:ILE:HD13	1.78	0.64
1:1:42:LYS:HG3	1:2:354:ARG:HD2	1.80	0.64
1:1:189:LYS:HG2	1:1:361:LEU:HD12	1.81	0.63
1:1:47:PHE:HB3	1:1:48:PRO:HD3	1.83	0.61
1:1:122:LEU:HD21	1:1:126:PRO:HD3	1.85	0.59
1:2:47:PHE:HB3	1:2:48:PRO:HD3	1.86	0.58
1:2:73:SER:HB3	1:2:75:LEU:HG	1.89	0.55
1:2:259:VAL:HB	1:2:329:ILE:HA	1.89	0.55
1:1:177:ASP:HB3	1:1:180:ASP:HB3	1.88	0.54
1:1:73:SER:HB2	1:1:75:LEU:HG	1.89	0.54
1:2:1:LYS:HB2	1:2:4:GLU:HB3	1.89	0.54
1:2:366:THR:HG23	1:2:370:LYS:HD2	1.90	0.54
1:1:134:ASP:HB2	1:1:135:PRO:HD2	1.91	0.53
1:2:181:VAL:HG12	1:2:183:VAL:HG22	1.90	0.53
1:1:333:ILE:HB	1:1:334:PRO:HD2	1.91	0.51
1:1:259:VAL:HG12	1:1:329:ILE:HD12	1.93	0.50
1:2:345:THR:HG21	1:2:367:ARG:HH12	1.78	0.49
1:2:333:ILE:HD12	1:2:335:GLN:NE2	2.26	0.48
1:1:218:ASN:HD21	1:1:235:ILE:HG12	1.77	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:2:318:ALA:O	1:2:322:GLU:HG3	2.15	0.47
1:1:192:LEU:HD23	1:1:357:VAL:HG13	1.95	0.47
1:1:64:HIS:HD2	1:1:261:VAL:H	1.63	0.47
1:1:59:ILE:CD1	1:1:280:LEU:HD21	2.45	0.47
1:1:65:ASP:HA	1:1:332:ASN:HA	1.98	0.46
1:1:220:GLY:HA2	3:1:419:HOH:O	2.16	0.46
1:2:144:LYS:NZ	1:2:202:LYS:HD3	2.31	0.45
1:2:247:LEU:HA	1:2:248:PRO:HD3	1.82	0.45
1:1:61:PHE:HA	1:1:263:SER:O	2.16	0.45
1:1:59:ILE:CD1	1:1:264:ALA:HB1	2.47	0.44
1:2:132:ILE:HB	1:2:133:PRO:HD3	1.98	0.44
1:1:168:ALA:HB2	1:1:258:PHE:HZ	1.81	0.44
1:2:62:TRP:HB3	1:2:67:PHE:HE1	1.82	0.44
1:2:59:ILE:HD11	1:2:61:PHE:CE1	2.53	0.44
1:2:148:MET:HB2	1:2:222:THR:HG21	2.00	0.43
1:2:72:GLN:HG3	1:2:334:PRO:HG3	2.00	0.43
1:2:176:TYR:CZ	1:2:331:PRO:HB3	2.54	0.43
1:2:254:PRO:HB3	1:2:326:LYS:NZ	2.34	0.43
1:2:134:ASP:HA	1:2:135:PRO:HD3	1.91	0.43
1:1:333:ILE:HD12	1:1:335:GLN:NE2	2.28	0.43
1:1:89:LEU:HD13	1:1:107:PRO:HG2	1.99	0.43
1:2:59:ILE:CD1	1:2:280:LEU:HD21	2.49	0.42
1:2:184:ASP:HB3	1:2:365:GLN:NE2	2.34	0.42
1:2:246:VAL:HA	1:2:323:ASN:HD21	1.83	0.42
1:1:154:PRO:HG3	1:1:344:ARG:HB2	2.01	0.42
1:2:339:PHE:HA	1:2:368:ILE:HG12	2.02	0.42
1:1:132:ILE:N	1:1:133:PRO:HD2	2.34	0.42
1:1:128:THR:HG22	1:1:249:THR:OG1	2.19	0.42
1:1:132:ILE:N	1:1:133:PRO:CD	2.82	0.42
1:1:199:ILE:HD13	1:1:351:ALA:HB1	2.02	0.42
1:1:343:VAL:O	1:1:347:VAL:HG22	2.19	0.42
1:2:68:GLY:HA3	1:2:332:ASN:O	2.19	0.42
1:2:259:VAL:O	1:2:330:MET:HG3	2.19	0.42
1:2:132:ILE:N	1:2:133:PRO:CD	2.83	0.42
1:2:340:TRP:CD1	2:B:2:GLC:H4	2.55	0.41
1:2:1:LYS:HD2	1:2:4:GLU:OE2	2.20	0.41
1:1:79:ILE:HD12	1:1:81:PRO:HD3	2.01	0.41
1:2:85:PHE:HA	1:2:88:LYS:HD3	2.02	0.41
1:2:98:ARG:HH11	1:2:103:LEU:HD21	1.85	0.41
1:2:14:ASP:O	1:2:230:TRP:HB2	2.21	0.41
1:1:287:ASP:O	1:1:291:GLU:HB2	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:1:128:THR:HB	1:1:130:GLU:OE2	2.20	0.41
1:2:178:ILE:HD11	1:2:179:LYS:HZ1	1.85	0.41
1:1:158:TRP:HB3	1:1:159:PRO:HD3	2.03	0.41
1:1:224:MET:HE3	1:1:224:MET:HB2	1.95	0.41
1:2:218:ASN:HD22	1:2:218:ASN:N	2.19	0.41
1:1:59:ILE:HD12	1:1:264:ALA:HB1	2.02	0.40
1:1:151:LEU:HD21	1:1:195:LEU:HD11	2.04	0.40
1:1:4:GLU:HG3	1:1:271:PRO:HB2	2.02	0.40
1:2:44:GLU:HB2	1:2:66:ARG:HD3	2.02	0.40
1:1:64:HIS:CD2	1:1:261:VAL:H	2.39	0.40

There are no symmetry-related clashes.

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

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	1	359/363 (99%)	338 (94%)	16 (4%)	5 (1%)	9	9
1	2	359/363 (99%)	335 (93%)	19 (5%)	5 (1%)	9	9
All	All	718/726 (99%)	673 (94%)	35 (5%)	10 (1%)	9	9

All (10) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	1	2	ILE
1	1	3	GLU
1	2	2	ILE
1	2	100	ASN
1	2	173	ASN
1	2	369	THR
1	1	145	SER
1	1	146	ALA

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Mol	Chain	Res	Type
1	1	168	ALA
1	2	168	ALA

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	1	291/292 (100%)	263 (90%)	28 (10%)	8	10
1	2	291/292 (100%)	263 (90%)	28 (10%)	8	10
All	All	582/584 (100%)	526 (90%)	56 (10%)	8	10

All (56) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	1	2	ILE
1	1	3	GLU
1	1	6	LYS
1	1	15	LYS
1	1	22	GLU
1	1	28	GLU
1	1	49	GLN
1	1	55	ASP
1	1	59	ILE
1	1	79	ILE
1	1	83	LYS
1	1	119	LYS
1	1	130	GLU
1	1	147	LEU
1	1	160	LEU
1	1	189	LYS
1	1	222	THR
1	1	233	SER
1	1	238	SER
1	1	239	LYS
1	1	258	PHE

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Mol	Chain	Res	Type
1	1	291	GLU
1	1	311	LEU
1	1	313	LYS
1	1	322	GLU
1	1	325	GLN
1	1	337	SER
1	1	341	TYR
1	2	3	GLU
1	2	7	LEU
1	2	25	LYS
1	2	26	LYS
1	2	50	VAL
1	2	59	ILE
1	2	60	ILE
1	2	73	SER
1	2	115	LEU
1	2	122	LEU
1	2	128	THR
1	2	147	LEU
1	2	160	LEU
1	2	161	ILE
1	2	172	GLU
1	2	202	LYS
1	2	204	MET
1	2	222	THR
1	2	239	LYS
1	2	258	PHE
1	2	263	SER
1	2	273	LYS
1	2	288	GLU
1	2	295	LYS
1	2	311	LEU
1	2	313	LYS
1	2	354	ARG
1	2	358	ASP

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (13) such sidechains are listed below:

Mol	Chain	Res	Type
1	1	18	ASN
1	1	49	GLN
1	1	64	HIS

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Mol	Chain	Res	Type
1	1	118	ASN
1	1	205	ASN
1	1	218	ASN
1	1	253	GLN
1	1	282	ASN
1	1	332	ASN
1	1	335	GLN
1	2	218	ASN
1	2	335	GLN
1	2	365	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	$\# Z > 2$
2	GLC	A	1	2	12,12,12	1.12	1 (8%)	17,17,17	1.98	3 (17%)
2	GLC	A	2	2	11,11,12	0.47	0	15,15,17	0.72	0
2	GLC	B	1	2	12,12,12	1.24	1 (8%)	17,17,17	2.81	3 (17%)
2	GLC	B	2	2	11,11,12	0.50	0	15,15,17	0.93	1 (6%)

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
2	GLC	A	1	2	-	2/2/22/22	0/1/1/1
2	GLC	A	2	2	-	1/2/19/22	0/1/1/1
2	GLC	B	1	2	-	1/2/22/22	0/1/1/1
2	GLC	B	2	2	-	0/2/19/22	0/1/1/1

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	1	GLC	O5-C1	-3.59	1.34	1.42
2	A	1	GLC	O5-C1	-3.53	1.34	1.42

All (7) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	1	GLC	O1-C1-O5	-7.13	89.23	110.41
2	B	1	GLC	C1-O5-C5	6.08	125.41	113.65
2	B	1	GLC	O5-C1-C2	5.73	120.37	110.30
2	A	1	GLC	C1-O5-C5	5.05	123.42	113.65
2	A	1	GLC	O1-C1-O5	-4.32	97.57	110.41
2	A	1	GLC	O5-C1-C2	3.63	116.69	110.30
2	B	2	GLC	C1-O5-C5	2.01	114.89	112.19

There are no chirality outliers.

All (4) torsion outliers are listed below:

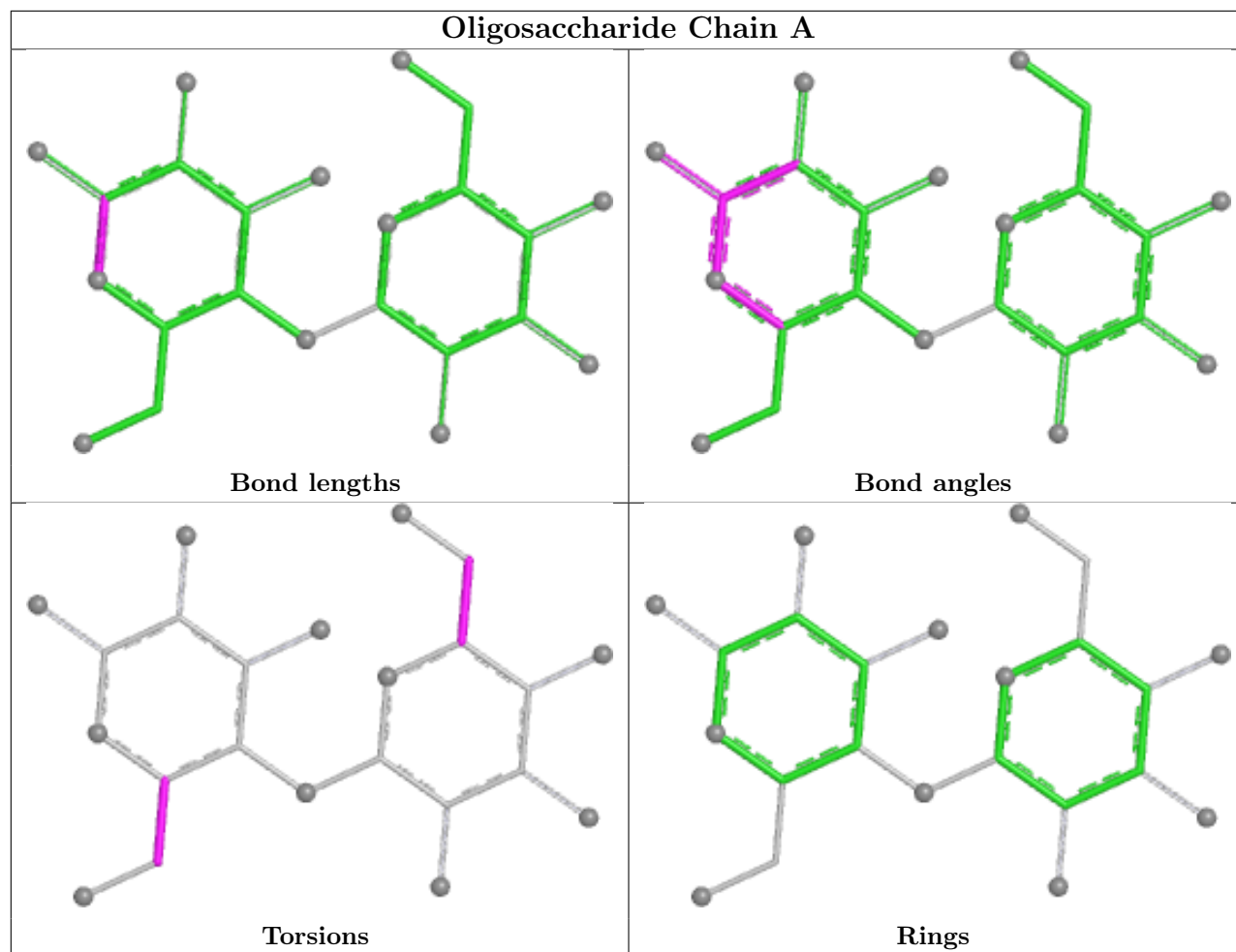
Mol	Chain	Res	Type	Atoms
2	A	1	GLC	C4-C5-C6-O6
2	A	1	GLC	O5-C5-C6-O6
2	B	1	GLC	O5-C5-C6-O6
2	A	2	GLC	C4-C5-C6-O6

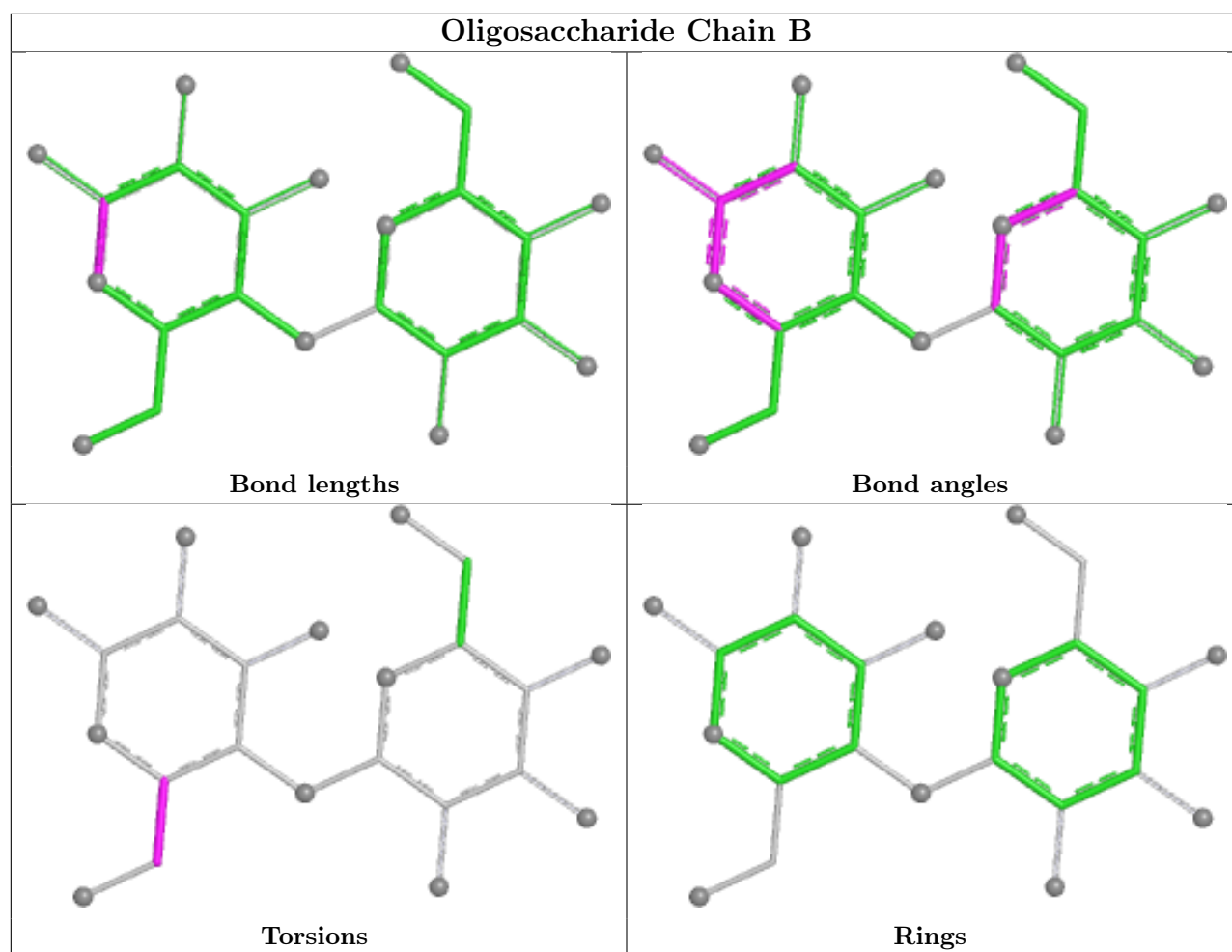
There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	2	GLC	1	0

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





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
1	1	1
1	2	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	1	135:PRO	C	143:GLY	N	3.54
1	2	135:PRO	C	143:GLY	N	3.48

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.