wwPDB X-ray Structure Validation Summary Report (i)

Jun 15, 2024 – 10:57 PM EDT

PDB ID	:	1SID
Title	:	MURINE POLYOMAVIRUS COMPLEXED WITH 3'SIALYL LACTOSE
Authors	:	Stehle, T.; Harrison, S.C.
Deposited on	:	1995-12-12
Resolution	:	3.65 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 (i) 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 (i)) were used in the production of this report:

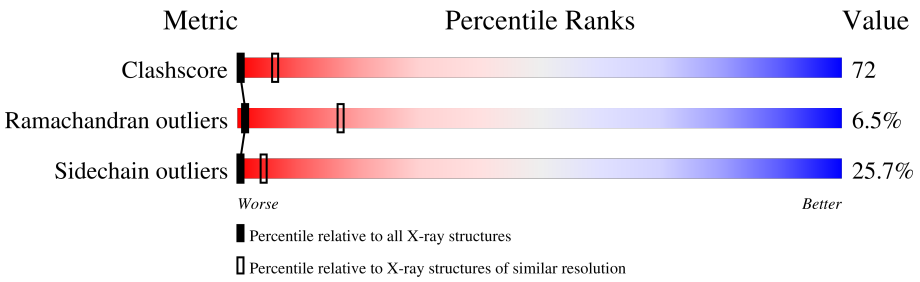
MolProbity	:	4.02b-467
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	NOT EXECUTED
EDS	:	NOT EXECUTED
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.37.1

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 3.65 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	1037 (3.80-3.52)
Ramachandran outliers	138981	1004 (3.80-3.52)
Sidechain outliers	138945	1002 (3.80-3.52)

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 was not executed.

Mol	Chain	Length	Quality of chain
1	A	383	23% 50% 20% • •
1	B	383	25% 46% 22% • •
1	C	383	22% 48% 21% • 7%
1	D	383	20% 44% 22% • 11%
1	E	383	20% 52% 21% • •
1	F	383	20% 46% 23% • 8%
2	G	3	67% 33%
2	H	3	33% 67%

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Mol	Chain	Length	Quality of chain
2	I	3	33% 67%
2	J	3	33% 67%
2	K	3	33% 67%
2	L	3	33% 67%

2 Entry composition (i)

There are 2 unique types of molecules in this entry. The entry contains 17003 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.

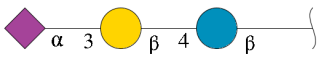
- Molecule 1 is a protein called POLYOMAVIRUS COAT PROTEIN VP1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	366	2849	1804	479	550	16	0	0	0
1	B	367	2857	1808	481	552	16	0	0	0
1	C	357	2784	1761	468	539	16	0	0	0
1	D	340	2645	1674	445	511	15	0	0	0
1	E	367	2857	1808	481	552	16	0	0	0
1	F	354	2753	1740	461	536	16	0	0	0

There are 6 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	6	ALA	SER	conflict	UNP P49302
B	6	ALA	SER	conflict	UNP P49302
C	6	ALA	SER	conflict	UNP P49302
D	6	ALA	SER	conflict	UNP P49302
E	6	ALA	SER	conflict	UNP P49302
F	6	ALA	SER	conflict	UNP P49302

- Molecule 2 is an oligosaccharide called N-acetyl-alpha-neuraminic acid-(2-3)-beta-D-galacto pyranose-(1-4)-beta-D-glucopyranose.



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
			Total	C	N	O			
2	G	3	43	23	1	19	0	0	0
2	H	3	43	23	1	19	0	0	0
2	I	3	43	23	1	19	0	0	0
2	J	3	43	23	1	19	0	0	0
2	K	3	43	23	1	19	0	0	0
2	L	3	43	23	1	19	0	0	0

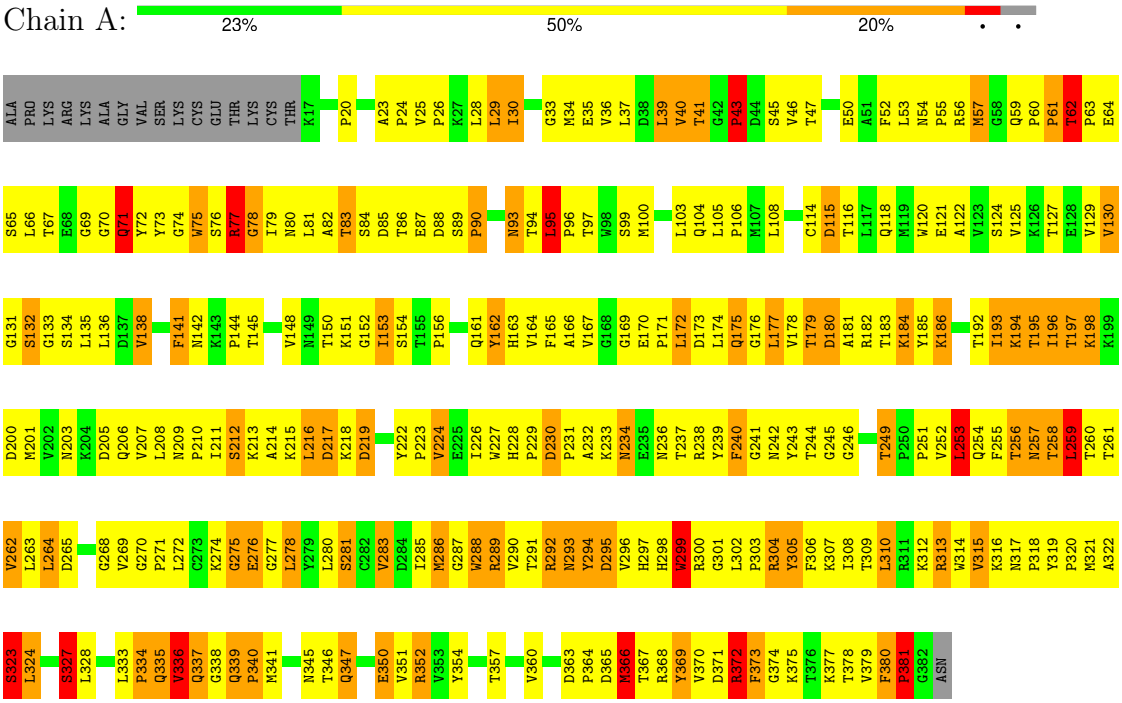
3 Residue-property plots (i)

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 was not executed.

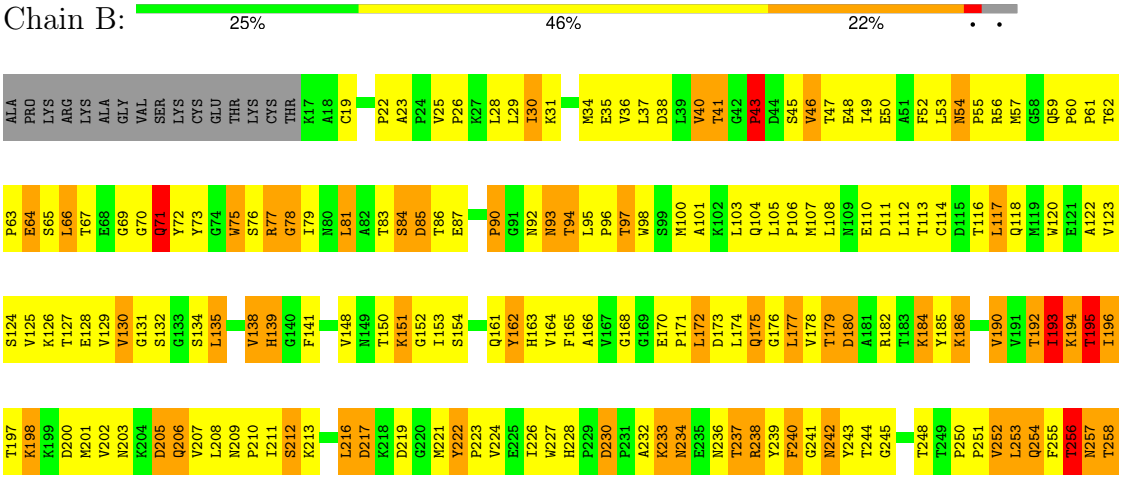
• Molecule 1: POLYOMAVIRUS COAT PROTEIN VP1

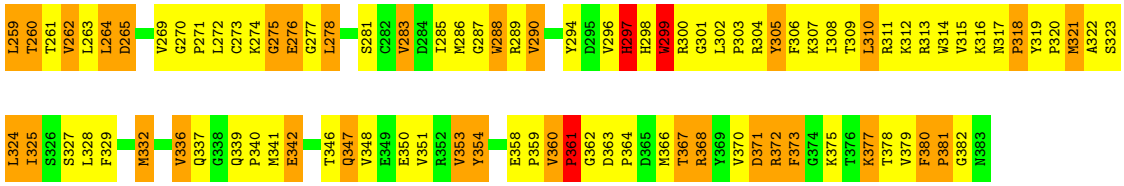
Chain A:



• Molecule 1: POLYOMAVIRUS COAT PROTEIN VP1

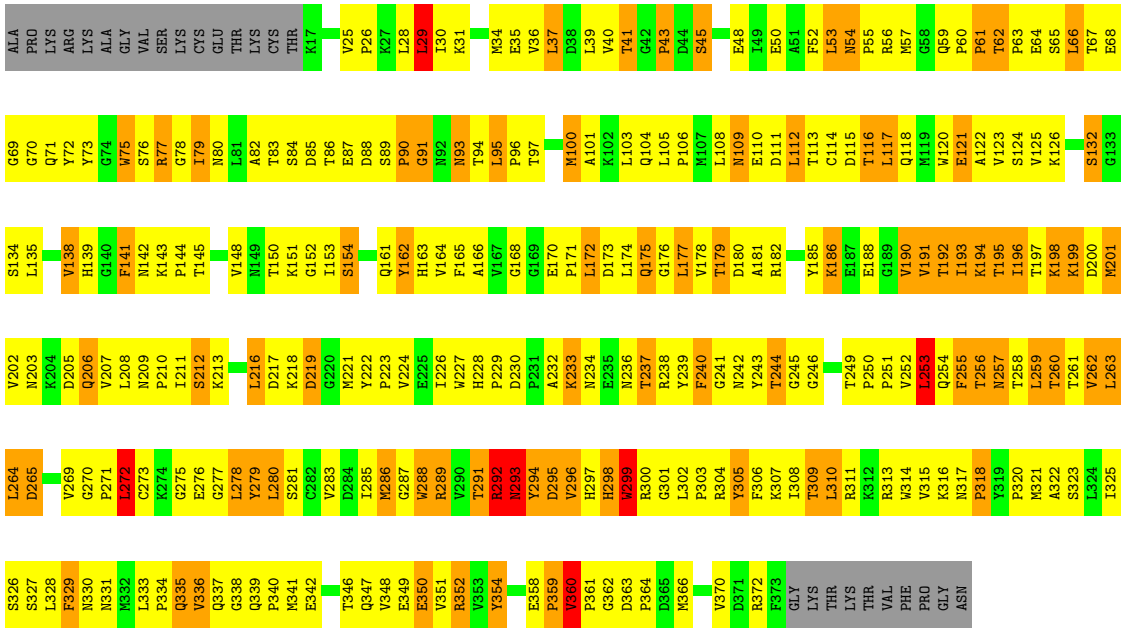
Chain B:





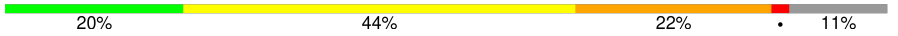
• Molecule 1: POLYOMAVIRUS COAT PROTEIN VP1

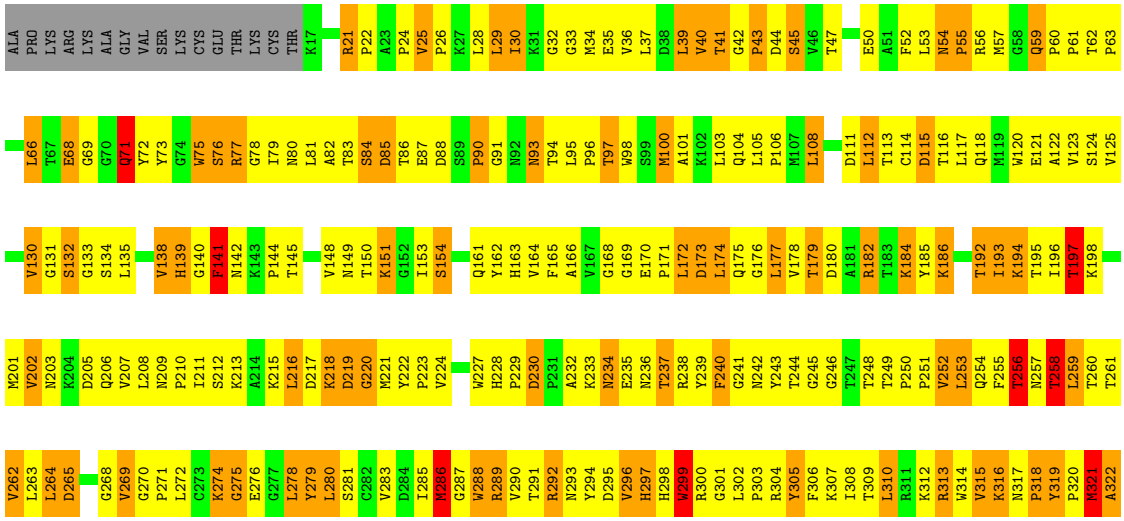
Chain C:

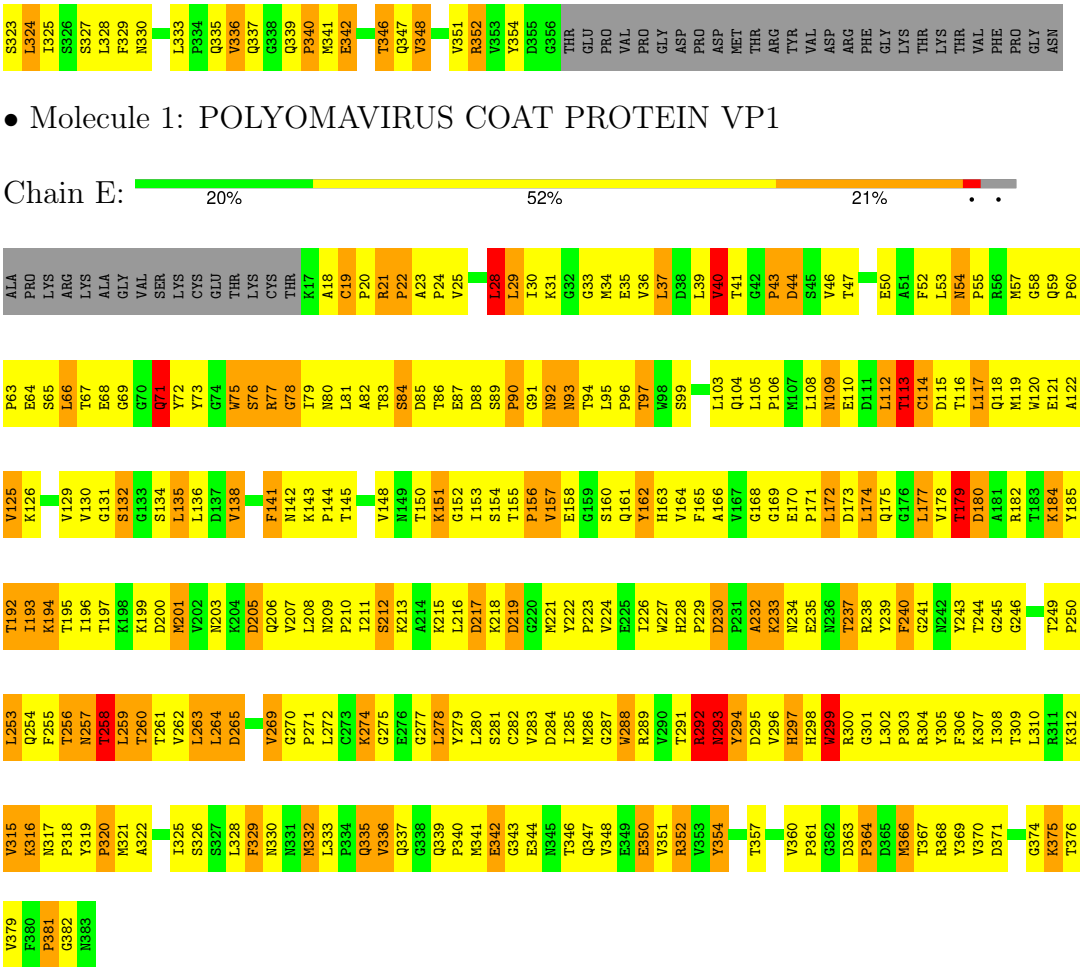


• Molecule 1: POLYOMAVIRUS COAT PROTEIN VP1

Chain D:






S323 L324 I325 S326 S327 L328 F329 N330 L333 P334 Q335 V336 Q337 G338 Q339 P340 M341 E342 T346 Q347 V348 V351 R352 V353 Y354 D355 G356 THR GLU PRO VAL PRO GLY ASP PRO ASP MET THR ARG TYR VAL ASP ARG PHE GLY LYS THR LYS THR VAL PHE PRO GLY ASN
• Molecule 1: POLYOMAVIRUS COAT PROTEIN VP1
Chain E:
20%
52%
21%
ALA PRO LYS ARG LYS ALA GLY VAL SER LYS CYS GLU THR LYS CYS THR K17 A18 C19 P20 R21 P22 A23 P24 V25 L28 L29 I30 K31 G32 G33 M34 E35 V36 L37 D38 L39 V40 T41 G42 P43 D44 S45 V46 T47 E50 A51 F52 L53 N54 P55 R56 M57 G58 Q59 P60 P61 T62
P63 E64 S65 L66 T67 E68 G69 G70 Q71 Y72 Y73 G74 W75 S76 R77 G78 I79 N80 L81 A82 T83 S84 D85 T86 E87 D88 S89 P90 G91 N92 N93 T94 L95 P96 T97 W98 S99 L103 Q104 L105 P106 M107 L108 N109 E110 D111 L112 T113 C114 D115 T116 L117 Q118 M119 W120 E121 A122 V123 S124
V125 K126 V129 V130 G131 S132 G133 S134 L135 L136 D137 V138 F141 N142 K143 P144 T145 V148 N149 T150 K151 G152 I153 S154 T155 P156 V157 E158 G159 S160 Q161 Y162 H163 V164 F165 A166 V167 G168 G169 E170 P171 L172 D173 L174 Q175 G176 L177 V178 T179 D180 A181 R182 T183 K184 Y185 K186
T192 I193 K194 T195 I196 T197 K198 K199 D200 M201 V202 N203 K204 D205 Q206 V207 L208 N209 P210 I211 S212 K213 A214 K215 L216 D217 K218 D219 G220 M221 Y222 P223 V224 E225 I226 W227 H228 P229 D230 P231 A232 K233 N234 E235 N236 T237 R238 Y239 F240 G241 N242 Y243 T244 G245 G246 T249 P250 P251 V252
L253 Q254 F255 T256 N257 T258 L259 T260 T261 V262 L263 L264 D265 V269 G270 P271 L272 C273 K274 G275 E276 G277 L278 Y279 L280 S281 C282 V283 D284 I285 M286 G287 W288 R289 V290 T291 R292 N293 Y294 D295 V296 H297 H298 W299 R300 G301 L302 P303 R304 Y305 F306 K307 I308 T309 L310 R311 K312 R313 W314
V315 K316 N317 P318 Y319 P320 M321 A322 I325 S326 S327 L328 F329 N330 N331 M332 L333 P334 Q335 V336 Q337 G338 Q339 P340 M341 E342 G343 E344 N345 T346 Q347 V348 E349 E350 V351 R352 V353 Y354 T357 V360 P361 G362 D363 P364 D365 M366 T367 R368 Y369 V370 D371 G374 K375 T376 K377 T378
V379 F380 P381 G382 N383
• Molecule 1: POLYOMAVIRUS COAT PROTEIN VP1
Chain F:
20%
46%
23%
8%
ALA PRO LYS ARG LYS ALA GLY VAL SER LYS CYS GLU THR LYS CYS THR LYS A18 C19 P20 R21 P22 A23 P24 V25 P26 L29 I30 K31 G32 G33 M34 E35 V36 L37 D38 L39 V40 T41 G42 P43 D44 S45 V46 E50 A51 F52 L53 N54 P55 R56 M57 G58 Q59 P60 P61 T62 P63
E64 S65 L66 T67 E68 G69 G70 Q71 Y72 Y73 G74 W75 S76 R77 G78 I79 N80 L81 A82 T83 S84 D85 T86 E87 P90 G91 N92 N93 T94 L95 P96 T97 M100 A101 K102 L103 Q104 L105 P106 M107 L108 D111 L112 T113 C114 D115 T116 L117 Q118 M119 W120 E121 A122 V123 S124 V125
V130 G131 S132 G133 S134 L135 L136 D137 V138 H139 G140 F141 N142 K143 P144 V148 N149 T150 K151 G152 I153 S154 T155 P156 Q161 Y162 H163 V164 F165 A166 V167 G168 G169 E170 P171 L172 D173 L174 Q175 G176 L177 V178 T179 D180 A181 R182 T183 K184 Y185 K186 V190 V191 T192 I193 K194 T195 I196
T197 W201 V202 N203 K204 D205 Q206 V207 L208 N209 P210 I211 S212 K213 L216 D217 K218 D219 G220 M221 Y222 P223 V224 E225 I226 W227 H228 P229 D230 P231 A232 K233 N234 E235 N236 T237 R238 Y239 F240 G241 N242 Y243 T244 G245 P250 P251 V252 L253 Q254 F255 T256 N257 T258 L259 T260 T261 V262
L263 L264 D265 G268 V269 G270 P271 L272 C273 K274 G275 E276 G277 L278 Y279 L280 S281 C282 V283 D284 I285 M286 G287 W288 R289 V290 T291 R292 N293 Y294 D295 V296 H297 H298 W299 R300 G301 L302 P303 R304 Y305 F306 K307 I308 T309 L310 R311 K312 R313 K314 V315 K316 N317 P318 Y319 P320 M321 A322 S323
L324 I325 S326 S327 L328 F329 N330 N331 M332 L333 P334 Q335 V336 Q337 G338 Q339 P340 M341 E342 G343 E344 N345 T346 Q347 E350 V351 R352 V353 Y354 T357 E358 P359 V360 P361 G362 D363 P364 T367 R368 D371 ARG PHE GLY LYS THR LYS THR VAL PHE PRO GLY ASN

• Molecule 2: N-acetyl-alpha-neuraminic acid-(2-3)-beta-D-galactopyranose-(1-4)-beta-D-glucopyranose

Chain G: 67% 33%

• Molecule 2: N-acetyl-alpha-neuraminic acid-(2-3)-beta-D-galactopyranose-(1-4)-beta-D-glucopyranose

Chain H: 33% 67%

• Molecule 2: N-acetyl-alpha-neuraminic acid-(2-3)-beta-D-galactopyranose-(1-4)-beta-D-glucopyranose

Chain I: 33% 67%

• Molecule 2: N-acetyl-alpha-neuraminic acid-(2-3)-beta-D-galactopyranose-(1-4)-beta-D-glucopyranose

Chain J: 33% 67%

• Molecule 2: N-acetyl-alpha-neuraminic acid-(2-3)-beta-D-galactopyranose-(1-4)-beta-D-glucopyranose

Chain K: 33% 67%

• Molecule 2: N-acetyl-alpha-neuraminic acid-(2-3)-beta-D-galactopyranose-(1-4)-beta-D-glucopyranose

Chain L: 33% 67%

4 Data and refinement statistics (i)

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

Property	Value	Source
Space group	I 2 3	Depositor
Cell constants a, b, c, α, β, γ	570.00Å 570.00Å 570.00Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	12.00 – 3.65	Depositor
% Data completeness (in resolution range)	73.0 (12.00-3.65)	Depositor
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	X-PLOR	Depositor
R, R_{free}	0.236 , 0.253	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	17003	wwPDB-VP
Average B, all atoms (Å^2)	77.0	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: SIA, GAL, BGC

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	0.96	2/2920 (0.1%)	1.26	22/3981 (0.6%)
1	B	0.95	0/2927	1.25	19/3989 (0.5%)
1	C	0.97	0/2852	1.26	21/3888 (0.5%)
1	D	1.01	2/2708 (0.1%)	1.27	23/3690 (0.6%)
1	E	1.00	1/2928 (0.0%)	1.34	23/3992 (0.6%)
1	F	0.96	2/2820 (0.1%)	1.25	21/3847 (0.5%)
All	All	0.98	7/17155 (0.0%)	1.27	129/23387 (0.6%)

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
1	A	0	5
1	B	0	3
1	C	0	4
1	D	0	5
1	E	0	2
1	F	0	3
All	All	0	22

The worst 5 of 7 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	E	336	VAL	C-N	13.07	1.64	1.34
1	D	342	GLU	CD-OE2	6.37	1.32	1.25
1	A	336	VAL	C-N	-5.83	1.20	1.34
1	D	299	TRP	CB-CG	5.46	1.60	1.50
1	F	234	ASN	CB-CG	5.37	1.63	1.51

The worst 5 of 129 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	E	336	VAL	O-C-N	21.97	157.85	122.70
1	A	336	VAL	O-C-N	-17.79	94.24	122.70
1	E	336	VAL	CA-C-N	-16.45	81.00	117.20
1	C	29	LEU	CA-CB-CG	-11.50	88.85	115.30
1	F	264	LEU	CA-CB-CG	-11.09	89.80	115.30

There are no chirality outliers.

5 of 22 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	162	TYR	Sidechain
1	A	305	TYR	Sidechain
1	A	336	VAL	Peptide,Mainchain
1	A	71	GLN	Mainchain
1	B	71	GLN	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	2849	0	2814	457	2
1	B	2857	0	2820	454	0
1	C	2784	0	2743	441	0
1	D	2645	0	2616	404	0
1	E	2857	0	2821	472	0
1	F	2753	0	2710	420	0
2	G	43	0	37	1	0
2	H	43	0	37	5	0
2	I	43	0	37	3	0
2	J	43	0	37	1	0
2	K	43	0	37	3	0
2	L	43	0	37	5	0
All	All	17003	0	16746	2434	2

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 72.

The worst 5 of 2434 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:A:328:LEU:CD2	1:A:333:LEU:HD21	1.37	1.52
1:A:328:LEU:HD21	1:A:333:LEU:CD2	1.40	1.50
1:A:175:GLN:HB2	1:A:230:ASP:HB2	1.26	1.11
1:F:175:GLN:HB2	1:F:230:ASP:HB2	1.33	1.10
1:B:336:VAL:HA	1:B:337:GLN:N	1.68	1.09

All (2) 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)
1:A:274:LYS:CD	1:A:328:LEU:O[2_555]	1.75	0.45
1:A:217:ASP:O	1:A:336:VAL:O[2_555]	2.05	0.15

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	364/383 (95%)	270 (74%)	67 (18%)	27 (7%)	1 13
1	B	363/383 (95%)	280 (77%)	62 (17%)	21 (6%)	1 19
1	C	353/383 (92%)	275 (78%)	60 (17%)	18 (5%)	2 21
1	D	336/383 (88%)	264 (79%)	58 (17%)	14 (4%)	3 25
1	E	365/383 (95%)	278 (76%)	62 (17%)	25 (7%)	1 15
1	F	350/383 (91%)	271 (77%)	45 (13%)	34 (10%)	0 8
All	All	2131/2298 (93%)	1638 (77%)	354 (17%)	139 (6%)	1 17

5 of 139 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	43	PRO
1	A	62	THR
1	A	148	VAL
1	A	183	THR
1	A	276	GLU

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	321/335 (96%)	244 (76%)	77 (24%)	0 5
1	B	322/335 (96%)	237 (74%)	85 (26%)	0 3
1	C	314/335 (94%)	238 (76%)	76 (24%)	0 5
1	D	298/335 (89%)	214 (72%)	84 (28%)	0 2
1	E	322/335 (96%)	241 (75%)	81 (25%)	0 4
1	F	311/335 (93%)	228 (73%)	83 (27%)	0 3
All	All	1888/2010 (94%)	1402 (74%)	486 (26%)	0 4

5 of 486 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	C	335	GLN
1	F	192	THR
1	D	234	ASN
1	F	179	THR
1	F	328	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 79 such sidechains are listed below:

Mol	Chain	Res	Type
1	E	59	GLN
1	F	59	GLN
1	E	104	GLN
1	E	297	HIS

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Mol	Chain	Res	Type
1	F	317	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)

18 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	BGC	G	1	2	12,12,12	0.66	0	17,17,17	0.87	1 (5%)
2	GAL	G	2	2	11,11,12	0.33	0	15,15,17	1.08	1 (6%)
2	SIA	G	3	2	20,20,21	0.81	0	21,28,31	1.07	2 (9%)
2	BGC	H	1	2	12,12,12	0.69	0	17,17,17	0.75	1 (5%)
2	GAL	H	2	2	11,11,12	0.50	0	15,15,17	1.45	1 (6%)
2	SIA	H	3	2	20,20,21	0.81	0	21,28,31	1.06	1 (4%)
2	BGC	I	1	2	12,12,12	0.70	0	17,17,17	0.81	1 (5%)
2	GAL	I	2	2	11,11,12	0.40	0	15,15,17	1.59	1 (6%)
2	SIA	I	3	2	20,20,21	0.79	0	21,28,31	0.94	1 (4%)
2	BGC	J	1	2	12,12,12	0.68	0	17,17,17	0.84	1 (5%)
2	GAL	J	2	2	11,11,12	0.24	0	15,15,17	1.33	1 (6%)
2	SIA	J	3	2	20,20,21	1.09	1 (5%)	21,28,31	1.36	2 (9%)
2	BGC	K	1	2	12,12,12	0.79	0	17,17,17	1.06	1 (5%)
2	GAL	K	2	2	11,11,12	0.25	0	15,15,17	1.36	1 (6%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
2	SIA	K	3	2	20,20,21	0.84	0	21,28,31	1.10	2 (9%)
2	BGC	L	1	2	12,12,12	0.82	0	17,17,17	0.87	1 (5%)
2	GAL	L	2	2	11,11,12	0.35	0	15,15,17	1.06	1 (6%)
2	SIA	L	3	2	20,20,21	1.09	1 (5%)	21,28,31	1.23	2 (9%)

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	BGC	G	1	2	-	0/2/22/22	0/1/1/1
2	GAL	G	2	2	-	0/2/19/22	0/1/1/1
2	SIA	G	3	2	-	2/18/34/38	0/1/1/1
2	BGC	H	1	2	-	0/2/22/22	0/1/1/1
2	GAL	H	2	2	-	0/2/19/22	0/1/1/1
2	SIA	H	3	2	-	1/18/34/38	0/1/1/1
2	BGC	I	1	2	-	0/2/22/22	0/1/1/1
2	GAL	I	2	2	-	0/2/19/22	0/1/1/1
2	SIA	I	3	2	-	7/18/34/38	0/1/1/1
2	BGC	J	1	2	-	1/2/22/22	0/1/1/1
2	GAL	J	2	2	-	0/2/19/22	0/1/1/1
2	SIA	J	3	2	-	3/18/34/38	0/1/1/1
2	BGC	K	1	2	-	0/2/22/22	0/1/1/1
2	GAL	K	2	2	-	1/2/19/22	0/1/1/1
2	SIA	K	3	2	-	4/18/34/38	0/1/1/1
2	BGC	L	1	2	-	1/2/22/22	0/1/1/1
2	GAL	L	2	2	-	0/2/19/22	0/1/1/1
2	SIA	L	3	2	-	7/18/34/38	0/1/1/1

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	L	3	SIA	C2-C1	3.07	1.56	1.52
2	J	3	SIA	C2-C1	2.83	1.55	1.52

The worst 5 of 22 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	I	2	GAL	C1-C2-C3	-5.32	101.90	109.64

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	H	2	GAL	C1-C2-C3	-4.85	102.59	109.64
2	J	2	GAL	C1-C2-C3	-4.83	102.62	109.64
2	K	2	GAL	C1-C2-C3	-4.67	102.84	109.64
2	J	3	SIA	C8-C7-C6	-4.48	104.64	113.05

There are no chirality outliers.

5 of 27 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	I	3	SIA	C6-C7-C8-C9
2	I	3	SIA	C6-C7-C8-O8
2	I	3	SIA	O7-C7-C8-C9
2	I	3	SIA	O7-C7-C8-O8
2	J	3	SIA	C5-C6-C7-O7

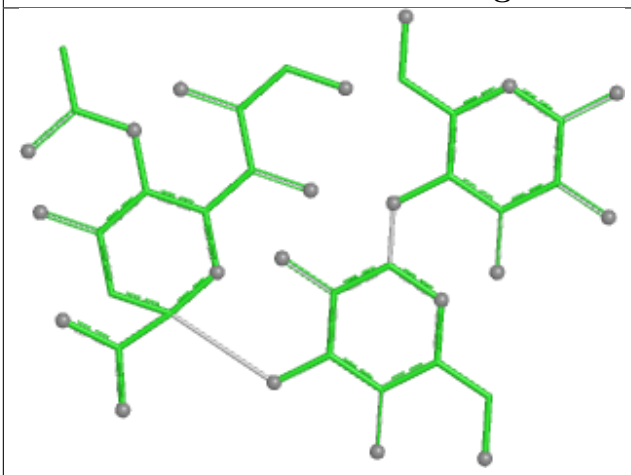
There are no ring outliers.

11 monomers are involved in 18 short contacts:

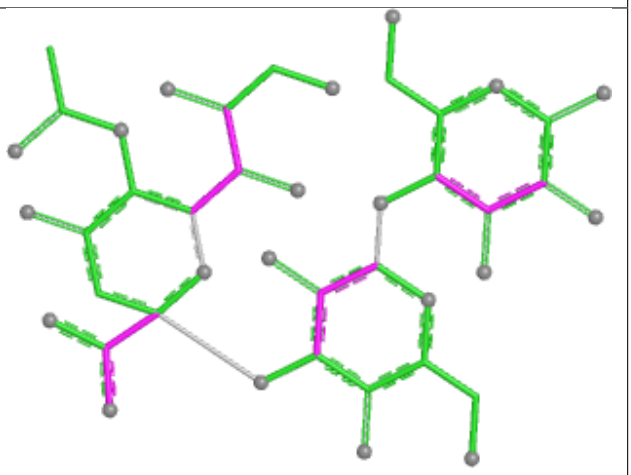
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	J	3	SIA	1	0
2	I	3	SIA	1	0
2	H	2	GAL	4	0
2	L	2	GAL	4	0
2	L	3	SIA	2	0
2	H	3	SIA	2	0
2	G	3	SIA	1	0
2	K	3	SIA	2	0
2	K	2	GAL	2	0
2	J	2	GAL	1	0
2	I	2	GAL	3	0

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

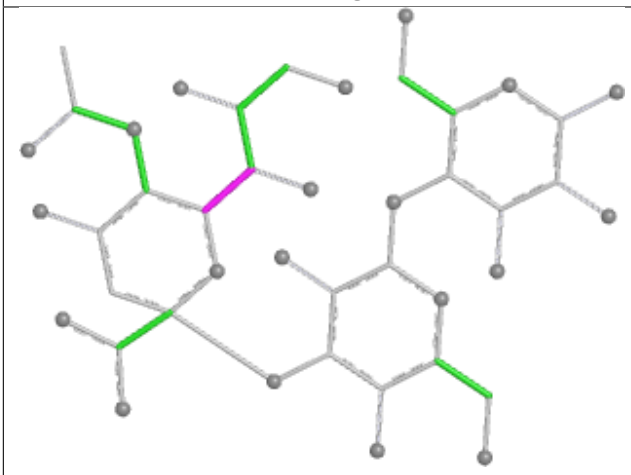
Oligosaccharide Chain G



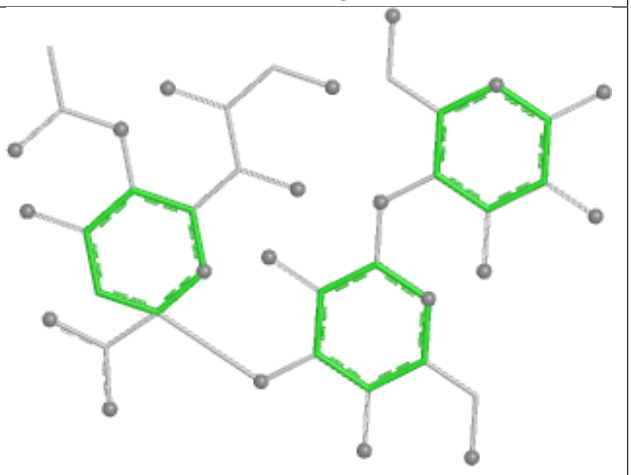
Bond lengths



Bond angles

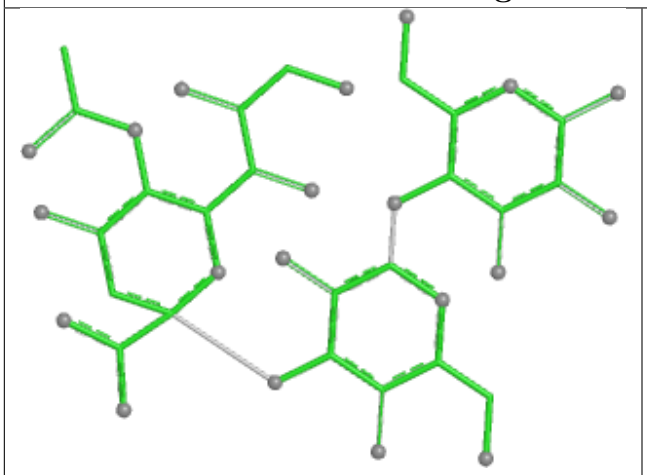


Torsions

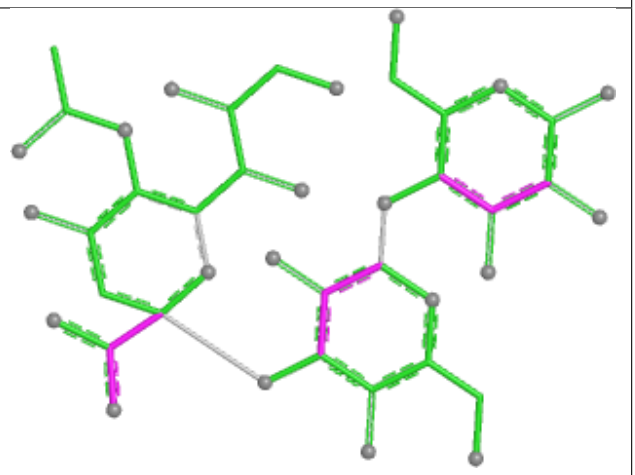


Rings

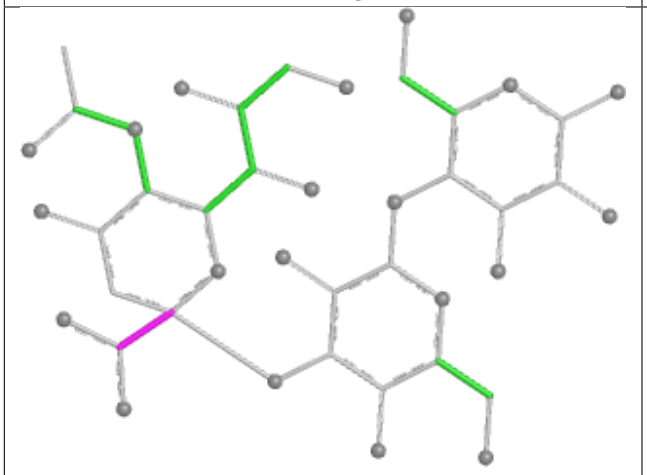
Oligosaccharide Chain H



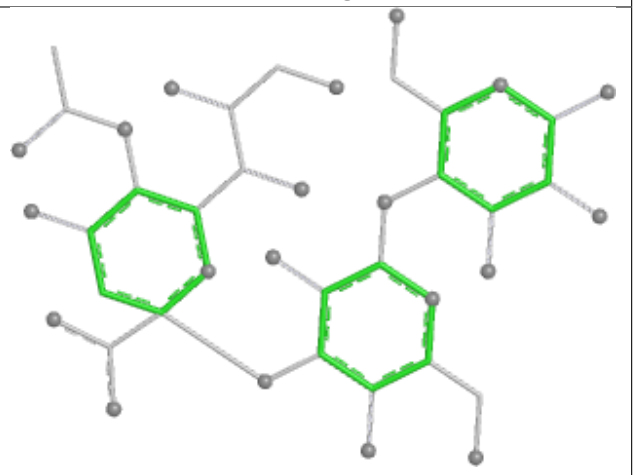
Bond lengths



Bond angles

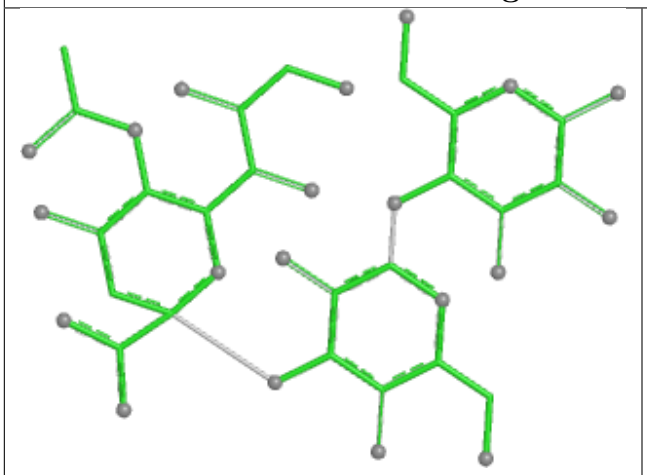


Torsions

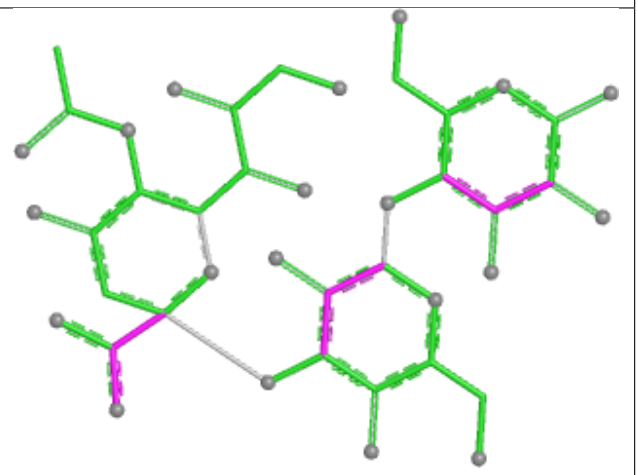


Rings

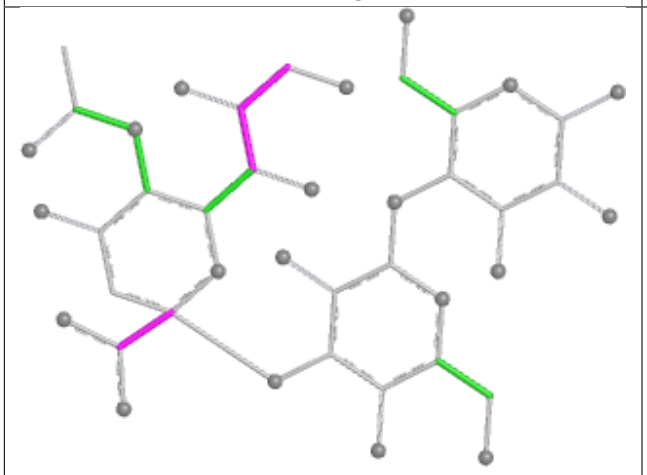
Oligosaccharide Chain I



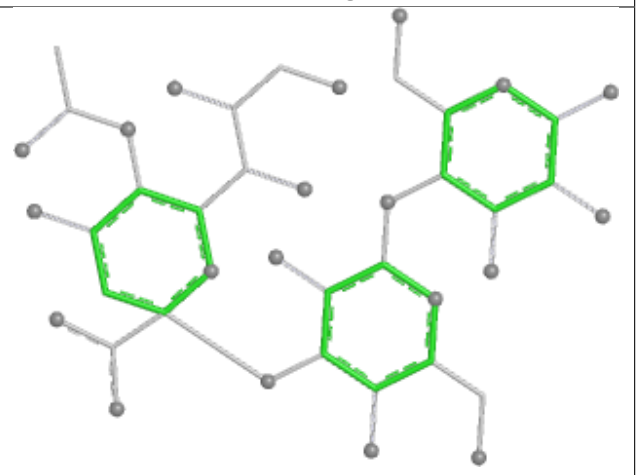
Bond lengths



Bond angles

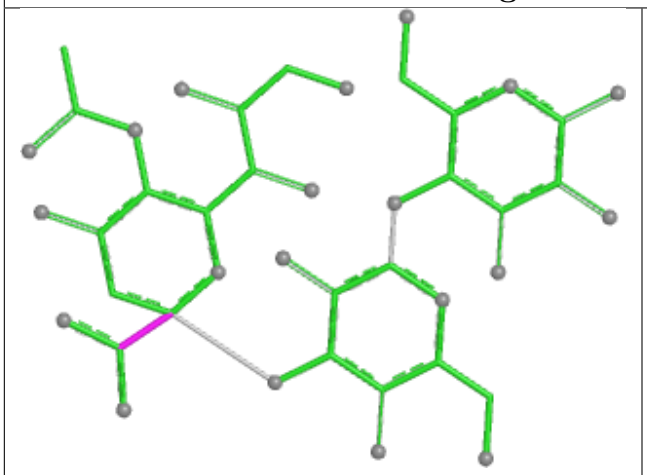


Torsions

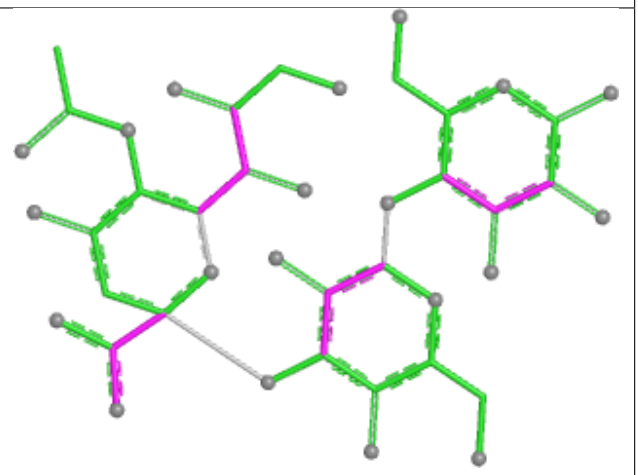


Rings

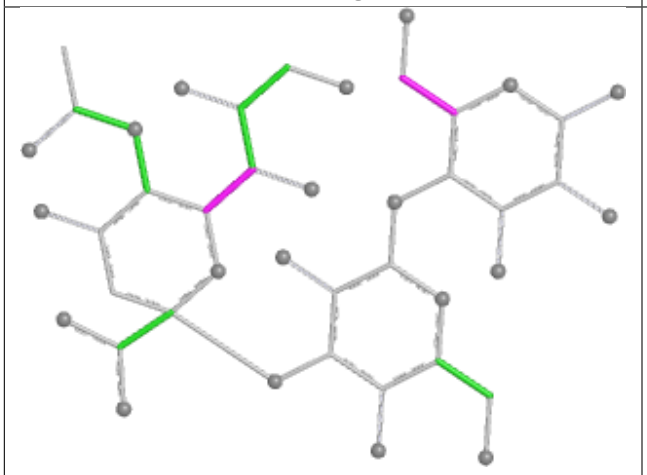
Oligosaccharide Chain J



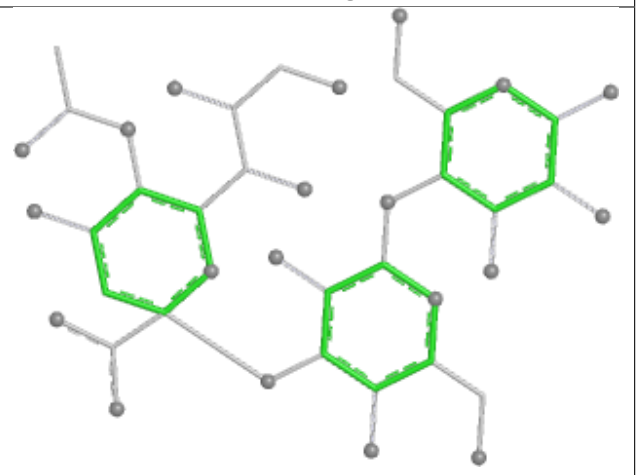
Bond lengths



Bond angles

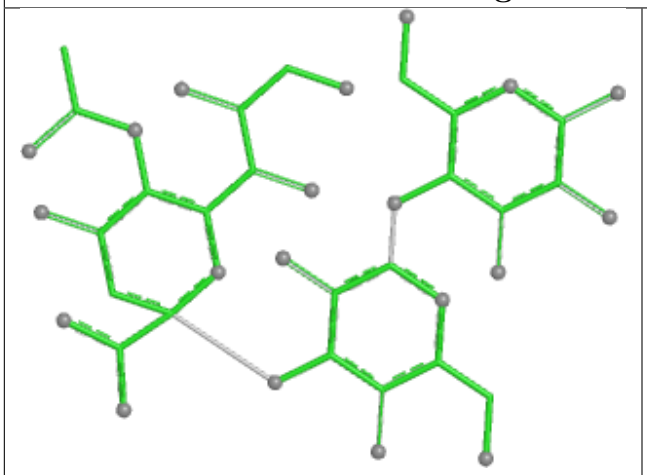


Torsions

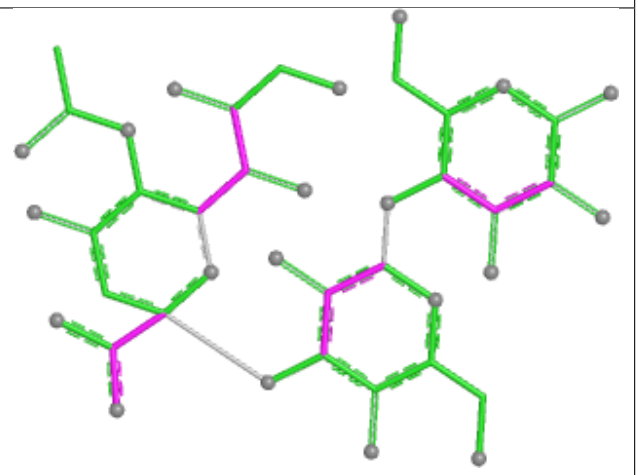


Rings

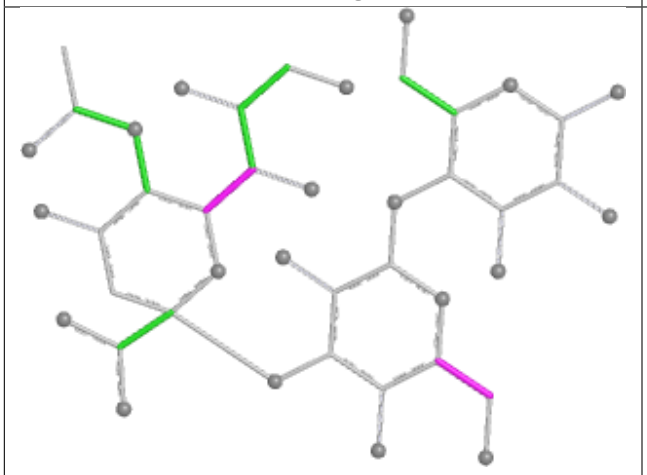
Oligosaccharide Chain K



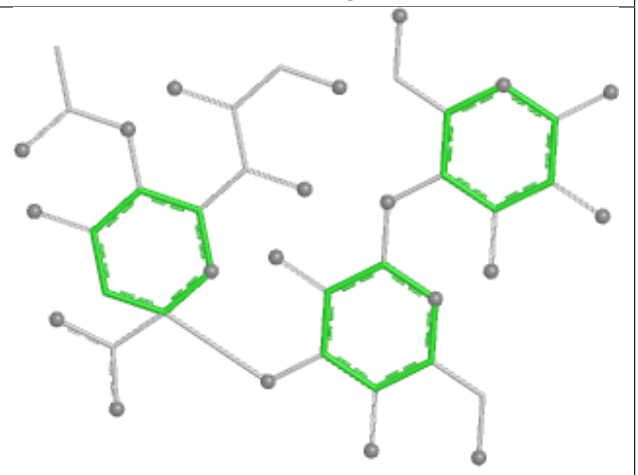
Bond lengths



Bond angles

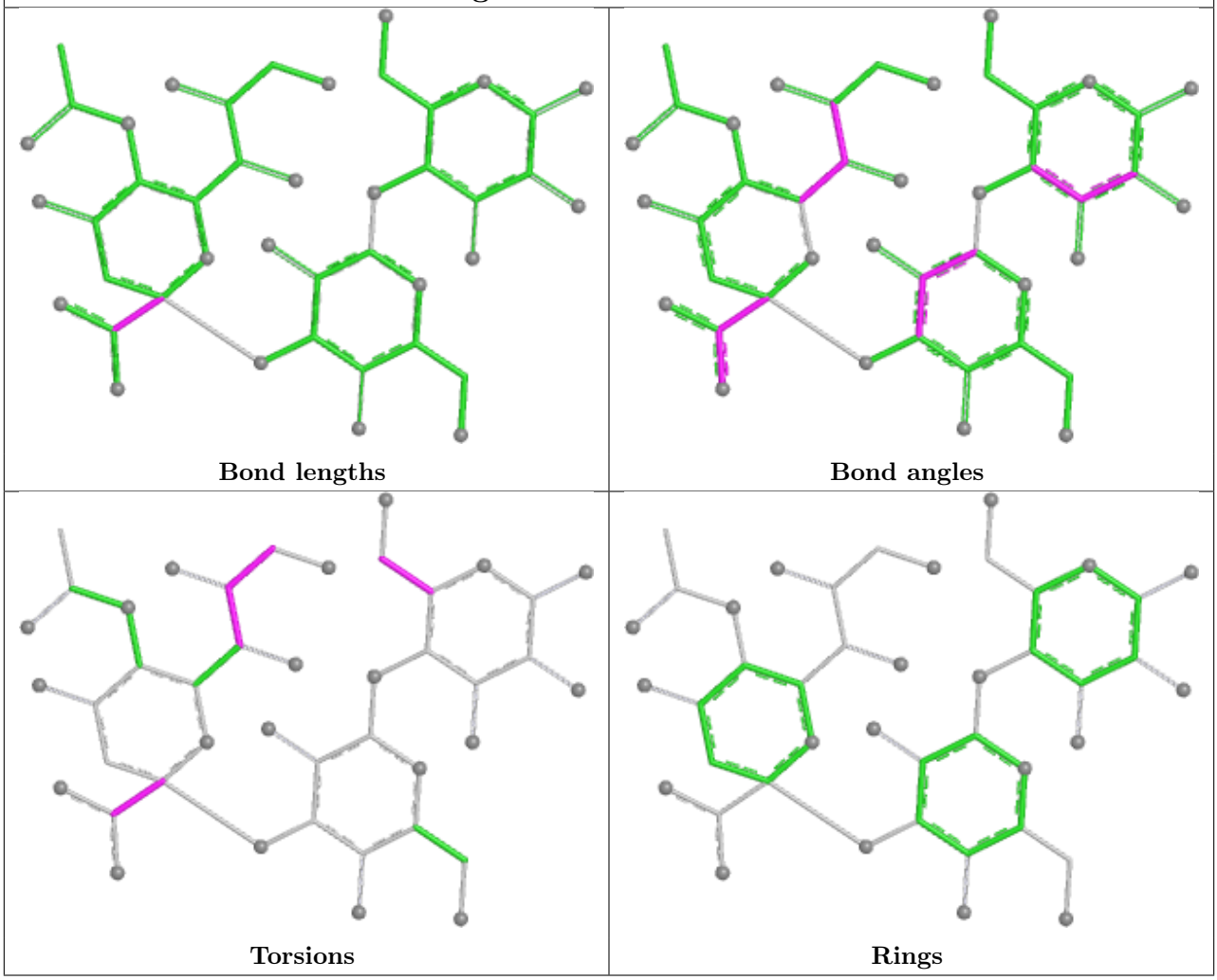


Torsions



Rings

Oligosaccharide Chain L



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	D	1
1	B	1

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Mol	Chain	Number of breaks
1	F	1
1	C	1
1	E	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	D	336:VAL	C	337:GLN	N	4.77
1	B	336:VAL	C	337:GLN	N	3.16
1	F	336:VAL	C	337:GLN	N	2.96
1	C	336:VAL	C	337:GLN	N	2.91
1	E	336:VAL	C	337:GLN	N	1.64

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.