wwPDB EM Validation Summary Report (i)

Nov 20, 2022 – 05:27 am GMT

PDB ID	:	6H04
EMDB ID	:	EMD-0107
Title	:	Closed conformation of the Membrane Attack Complex
Authors	:	Menny, A.; Serna, M.; Boyd, C.M.; Gardner, S.; Joseph, A.P.; Topf, M.; Bubeck, D.
Deposited on	:	2018-07-06
Resolution	:	5.60 Å(reported)

This is a wwPDB EM 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/EMValidationReportHelp
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:

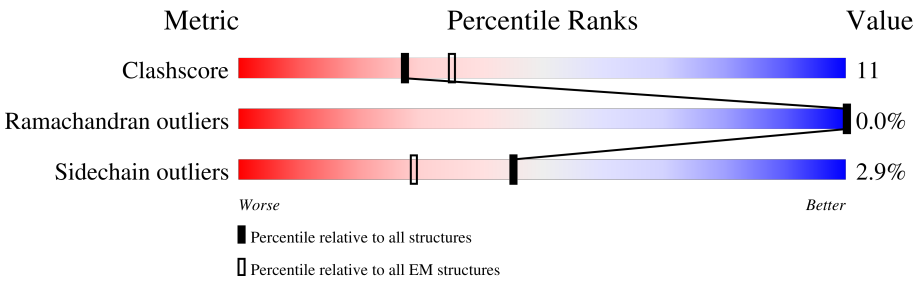
EMDB validation analysis	:	0.0.1.dev43
Mogul	:	1.8.4, CSD as541be (2020)
MolProbity	:	4.02b-467
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ	:	1.9.9
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.31.2

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
ELECTRON MICROSCOPY

The reported resolution of this entry is 5.60 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)	EM structures (#Entries)
Clashscore	158937	4297
Ramachandran outliers	154571	4023
Sidechain outliers	154315	3826

The table below summarises the geometric issues observed across the polymeric chains and their fit to the map. The red, orange, yellow and green segments of the 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% The upper red bar (where present) indicates the fraction of residues that have poor fit to the EM map (all-atom inclusion < 40%). The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	G	538	11% 61% 31% • 7%
1	H	538	• 68% 24% • 7%
1	I	538	• 67% 25% • 7%
1	J	538	• 67% 25% • 7%
1	K	538	• 66% 27% • 7%
1	L	538	• 64% 28% • 7%
1	M	538	• 64% 29% • 7%
1	N	538	• 62% 30% • 7%

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Mol	Chain	Length	Quality of chain
1	O	538	63% 30% 7%
1	P	538	7% 63% 30% 7%
1	Q	538	61% 32% 7%
1	R	538	62% 31% 7%
1	S	538	5% 63% 29% 7%
1	T	538	6% 65% 27% 7%
1	U	538	8% 66% 27% 7%
1	V	538	9% 66% 26% 7%
1	W	538	15% 67% 25% 7%
1	X	538	29% 70% 22% 7%
2	A	1580	52% 61% 16% 23%
3	C	537	13% 83% 12%
4	D	821	24% 69% 11% 20%
5	E	182	75% 76% 14% 9%
6	F	554	10% 71% 20% 8%
7	B	913	26% 63% 13% 25%
8	Y	2	50% 50% 50%
8	Z	2	50% 50% 50%
8	a	2	50% 50% 50%
8	b	2	50% 50% 50%
8	c	2	50% 50% 50%
8	d	2	50% 50% 50%
8	e	2	50% 50% 50%
8	f	2	50% 50% 50%
8	g	2	50% 50% 50%

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Mol	Chain	Length	Quality of chain
8	h	2	50% 50% 50%
8	i	2	50% 50% 50%
8	j	2	50% 50% 50%
8	k	2	50% 50% 50%
8	l	2	50% 50% 50%
8	m	2	50% 50% 50%
8	n	2	50% 50% 50%
8	o	2	50% 50% 50%
8	p	2	50% 50% 50%
8	q	2	50% 50% 50%

2 Entry composition (i)

There are 9 unique types of molecules in this entry. The entry contains 97178 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, 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 Complement component C9.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
1	L	501	3785	2363	670	721	31	0	0
1	M	501	3785	2363	670	721	31	0	0
1	N	501	3785	2363	670	721	31	0	0
1	O	501	3785	2363	670	721	31	0	0
1	Q	501	3785	2363	670	721	31	0	0
1	R	501	3785	2363	670	721	31	0	0
1	S	501	3785	2363	670	721	31	0	0
1	T	501	3785	2363	670	721	31	0	0
1	U	501	3785	2363	670	721	31	0	0
1	V	501	3785	2363	670	721	31	0	0
1	W	501	3785	2363	670	721	31	0	0
1	X	501	3785	2363	670	721	31	0	0
1	P	501	3785	2363	670	721	31	0	0
1	H	501	3785	2363	670	721	31	0	0
1	I	501	3785	2363	670	721	31	0	0
1	J	501	3785	2363	670	721	31	0	0
1	K	501	3785	2363	670	721	31	0	0

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Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
1	G	501	3770	2352	668	720	30	0	0

- Molecule 2 is a protein called Complement C5,Complement C5.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
2	A	1219	9497	6097	1572	1801	27	0	0

- Molecule 3 is a protein called Complement component C8 beta chain.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
3	C	513	3752	2345	664	713	30	0	0

- Molecule 4 is a protein called Complement component C7.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
4	D	660	4578	2844	825	867	42	0	0

- Molecule 5 is a protein called Complement component C8 gamma chain.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
5	E	165	1286	823	223	236	4	0	0

- Molecule 6 is a protein called Complement component C8 alpha chain.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
6	F	510	3758	2331	660	730	37	0	0

- Molecule 7 is a protein called Complement component C6.

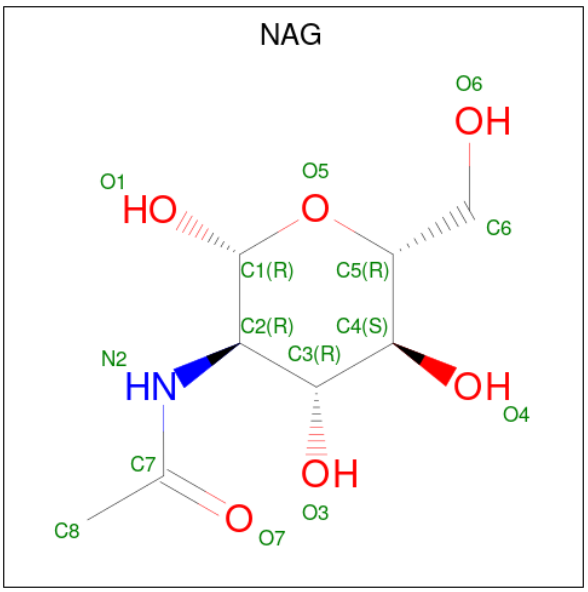
Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
7	B	688	5128	3174	918	990	46	0	0

- Molecule 8 is an oligosaccharide called 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose.

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
8	Y	2	28	16	2	10	0	0
8	Z	2	28	16	2	10	0	0
8	a	2	28	16	2	10	0	0
8	b	2	28	16	2	10	0	0
8	c	2	28	16	2	10	0	0
8	d	2	28	16	2	10	0	0
8	e	2	28	16	2	10	0	0
8	f	2	28	16	2	10	0	0
8	g	2	28	16	2	10	0	0
8	h	2	28	16	2	10	0	0
8	i	2	28	16	2	10	0	0
8	j	2	28	16	2	10	0	0
8	k	2	28	16	2	10	0	0
8	l	2	28	16	2	10	0	0
8	m	2	28	16	2	10	0	0
8	n	2	28	16	2	10	0	0
8	o	2	28	16	2	10	0	0
8	p	2	28	16	2	10	0	0
8	q	2	28	16	2	10	0	0

- Molecule 9 is 2-acetamido-2-deoxy-beta-D-glucopyranose (three-letter code: NAG) (formula:

$C_8H_{15}NO_6$).



Mol	Chain	Residues	Atoms				AltConf
			Total	C	N	O	
9	L	1	28	16	2	10	0
			Total	C	N	O	
9	L	1	28	16	2	10	0
			Total	C	N	O	
9	M	1	28	16	2	10	0
			Total	C	N	O	
9	M	1	28	16	2	10	0
			Total	C	N	O	
9	N	1	28	16	2	10	0
			Total	C	N	O	
9	N	1	28	16	2	10	0
			Total	C	N	O	
9	O	1	28	16	2	10	0
			Total	C	N	O	
9	O	1	28	16	2	10	0
			Total	C	N	O	
9	Q	1	28	16	2	10	0
			Total	C	N	O	
9	Q	1	28	16	2	10	0
			Total	C	N	O	
9	R	1	28	16	2	10	0
			Total	C	N	O	
9	R	1	28	16	2	10	0
			Total	C	N	O	
9	S	1	28	16	2	10	0

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Mol	Chain	Residues	Atoms				AltConf
			Total	C	N	O	
9	S	1	28	16	2	10	0
9	T	1	28	16	2	10	0
9	T	1	28	16	2	10	0
9	U	1	28	16	2	10	0
9	U	1	28	16	2	10	0
9	V	1	28	16	2	10	0
9	V	1	28	16	2	10	0
9	W	1	28	16	2	10	0
9	W	1	28	16	2	10	0
9	X	1	28	16	2	10	0
9	X	1	28	16	2	10	0
9	P	1	28	16	2	10	0
9	P	1	28	16	2	10	0
9	H	1	28	16	2	10	0
9	H	1	28	16	2	10	0
9	I	1	28	16	2	10	0
9	I	1	28	16	2	10	0
9	J	1	28	16	2	10	0
9	J	1	28	16	2	10	0
9	K	1	28	16	2	10	0
9	K	1	28	16	2	10	0

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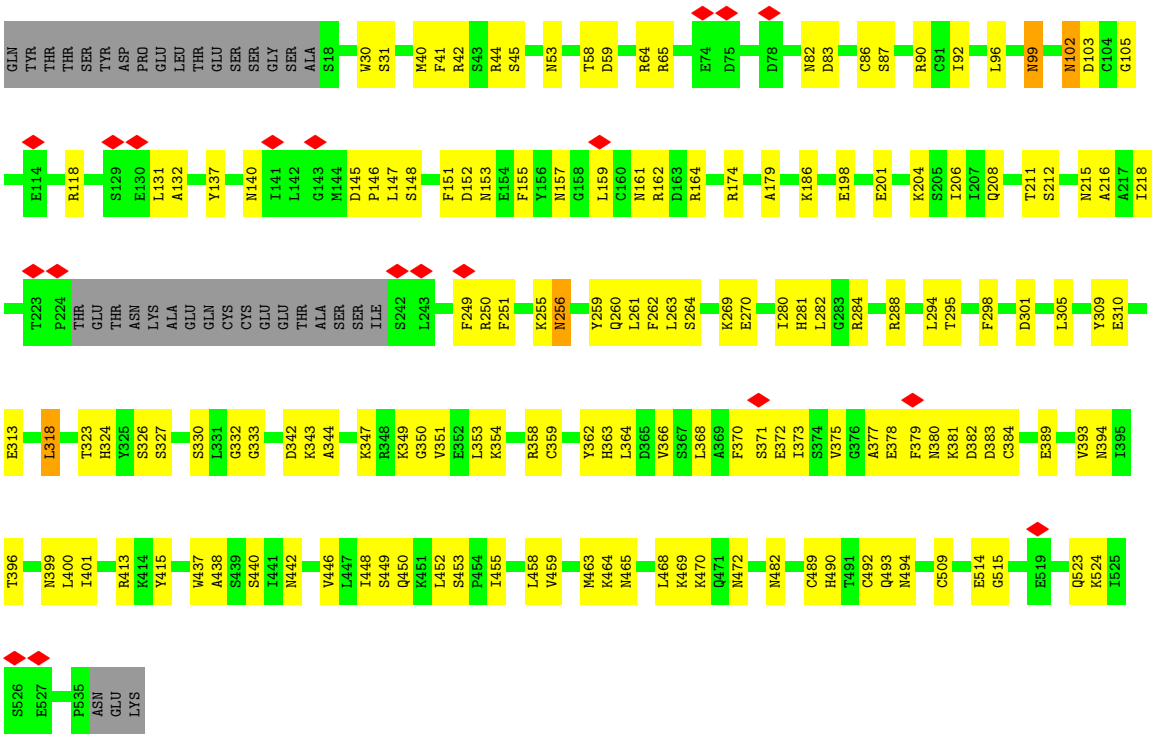
Mol	Chain	Residues	Atoms				AltConf
			Total	C	N	O	
9	G	1	28	16	2	10	0
			Total	C	N	O	
9	G	1	28	16	2	10	0
			Total	C	N	O	
9	D	1	14	8	1	5	0
			Total	C	N	O	
9	B	1	14	8	1	5	0

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 and atom inclusion in map density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red diamond above a residue indicates a poor fit to the EM map for this residue (all-atom inclusion < 40%). 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.

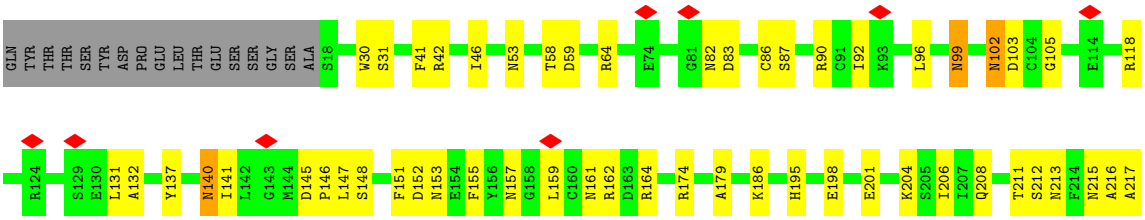
- Molecule 1: Complement component C9

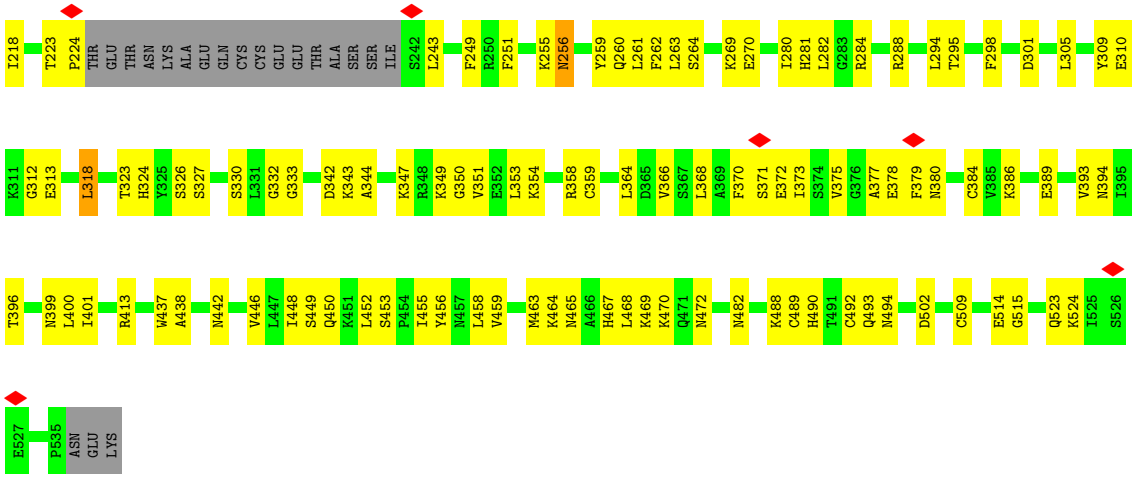
Chain L:



- Molecule 1: Complement component C9

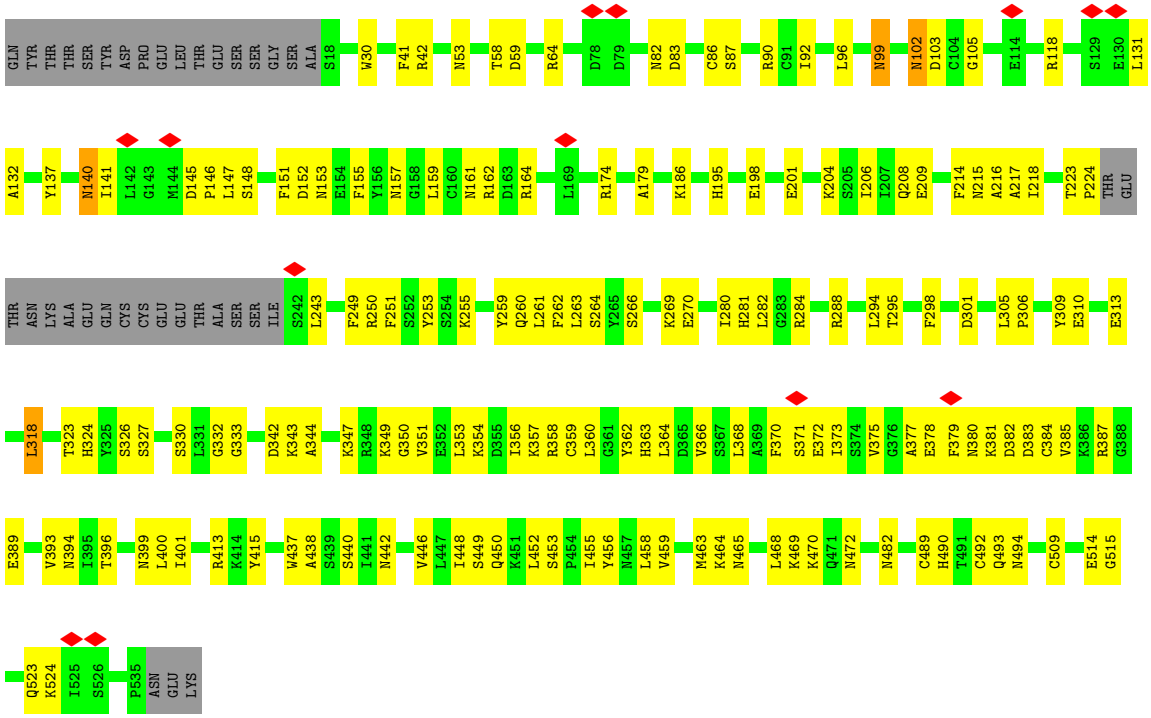
Chain M:





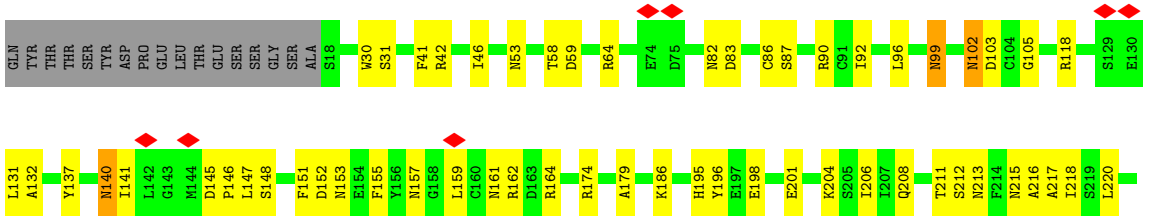
- Molecule 1: Complement component C9

Chain N:



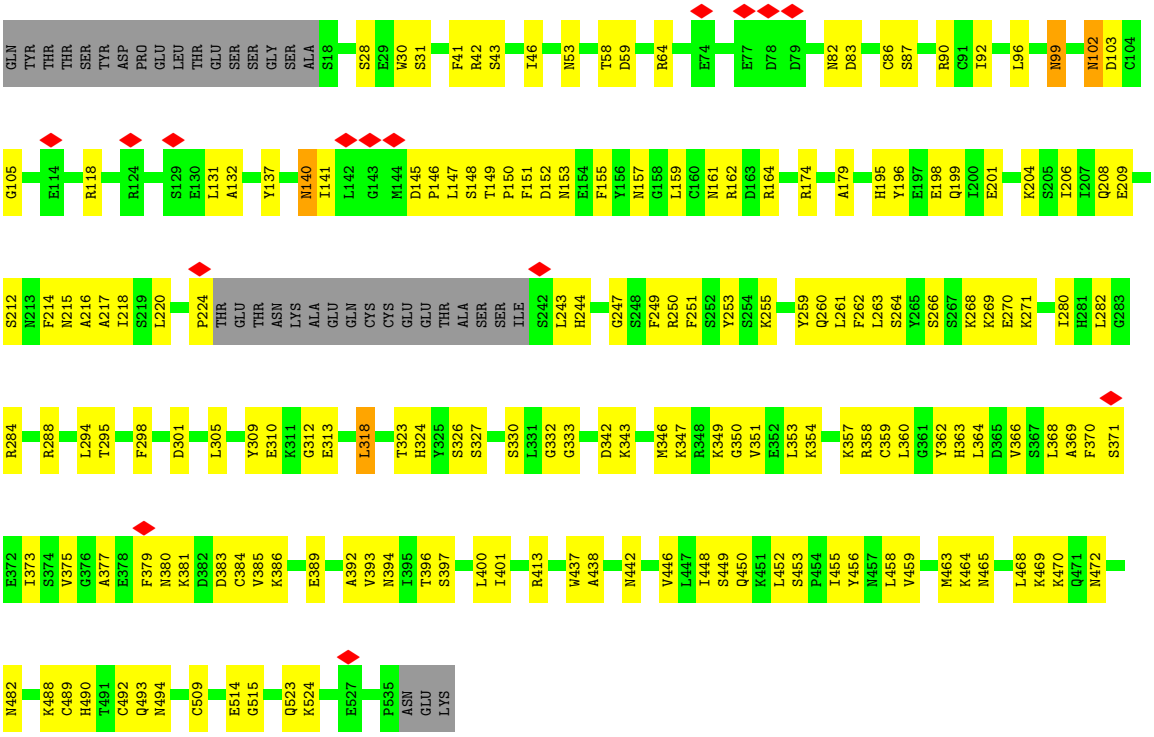
- Molecule 1: Complement component C9

Chain O:



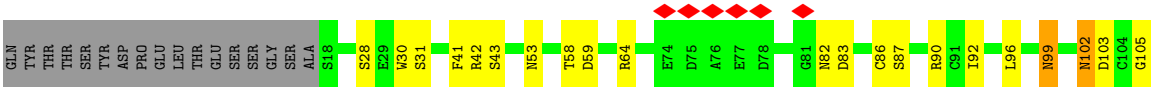
• Molecule 1: Complement component C9

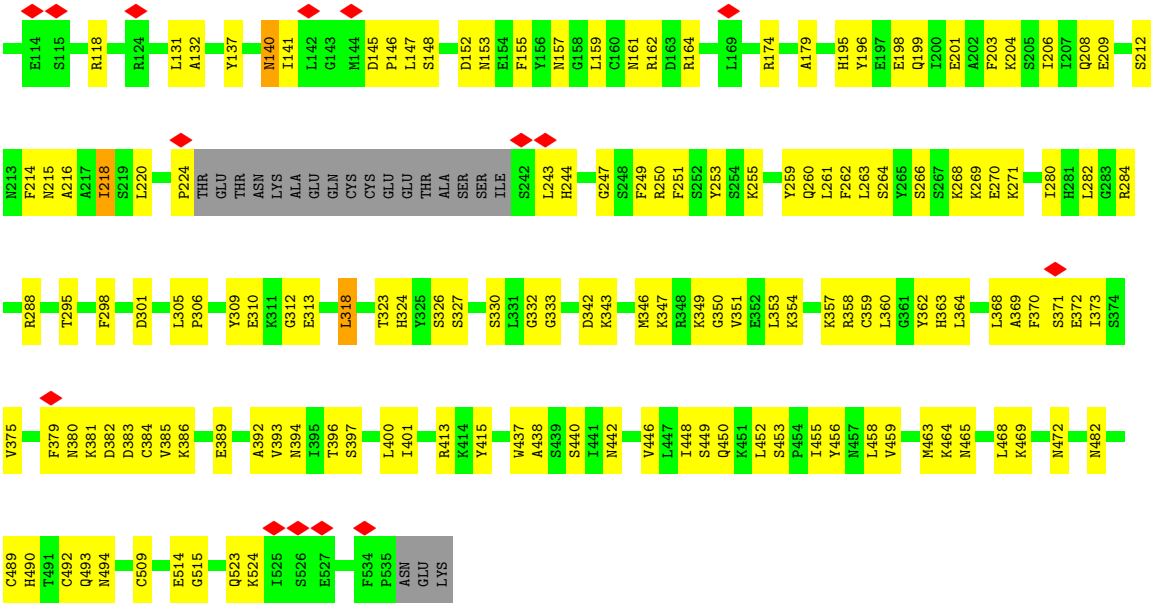
Chain Q: 61% 32% • 7%



• Molecule 1: Complement component C9

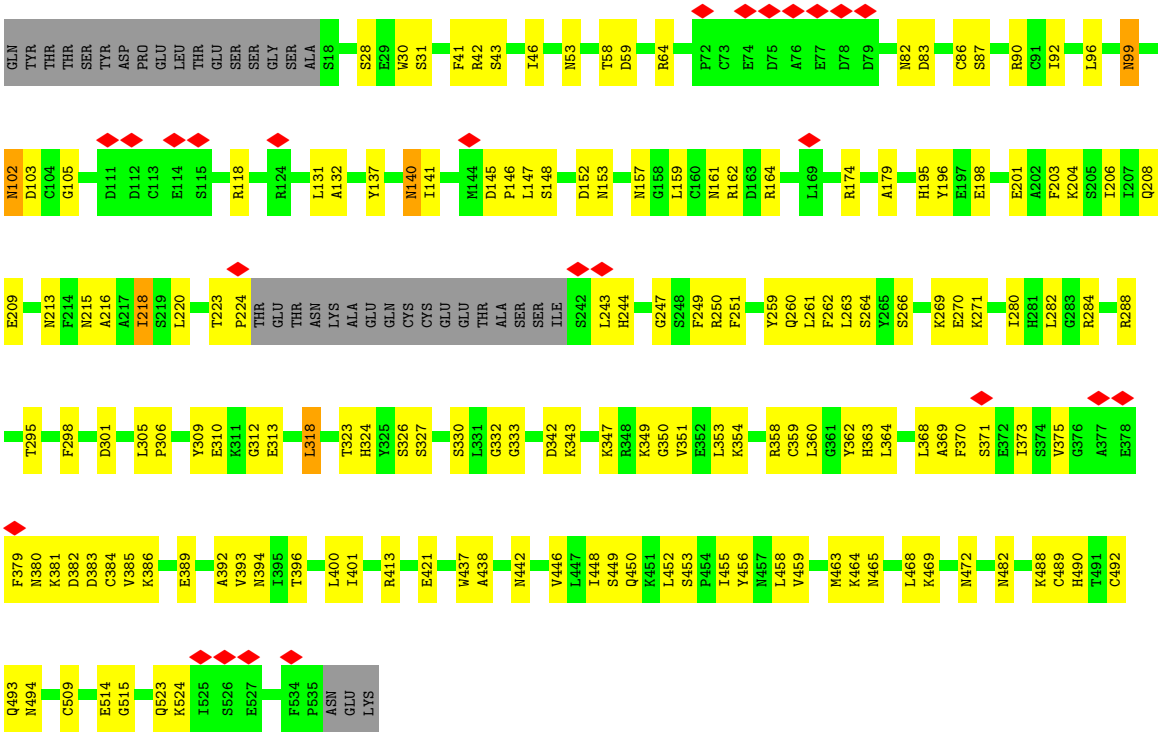
Chain R: 62% 31% • 7%





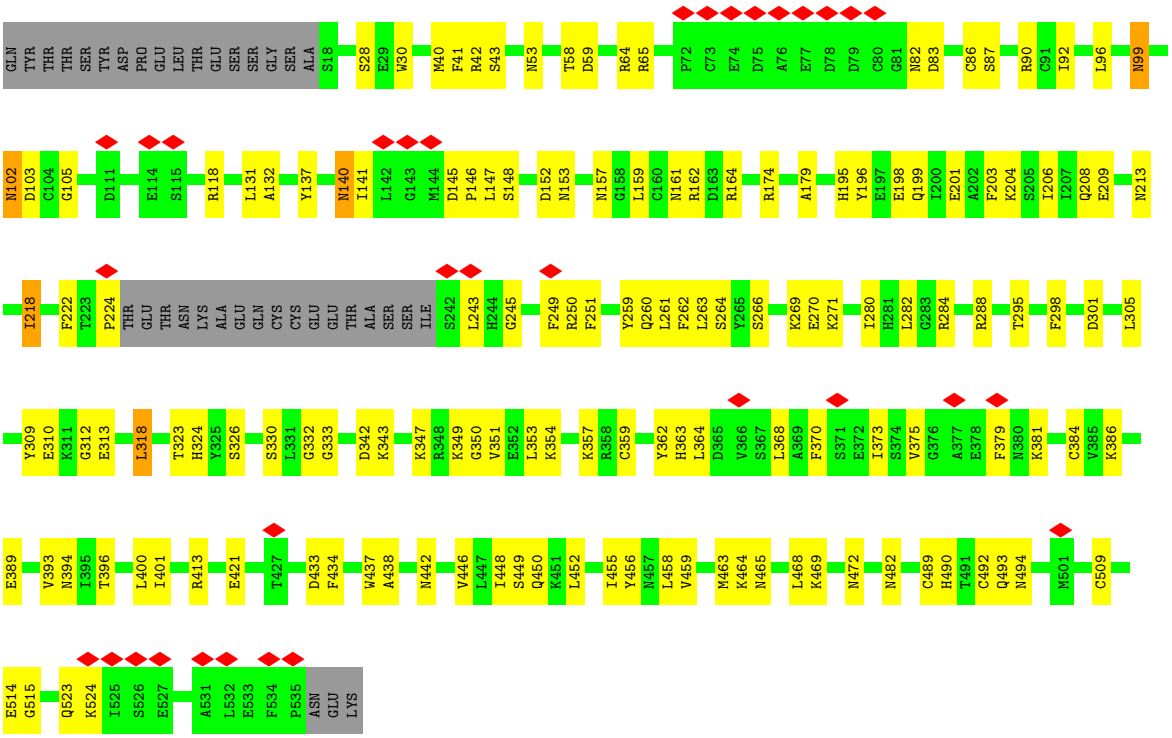
• Molecule 1: Complement component C9

Chain S:



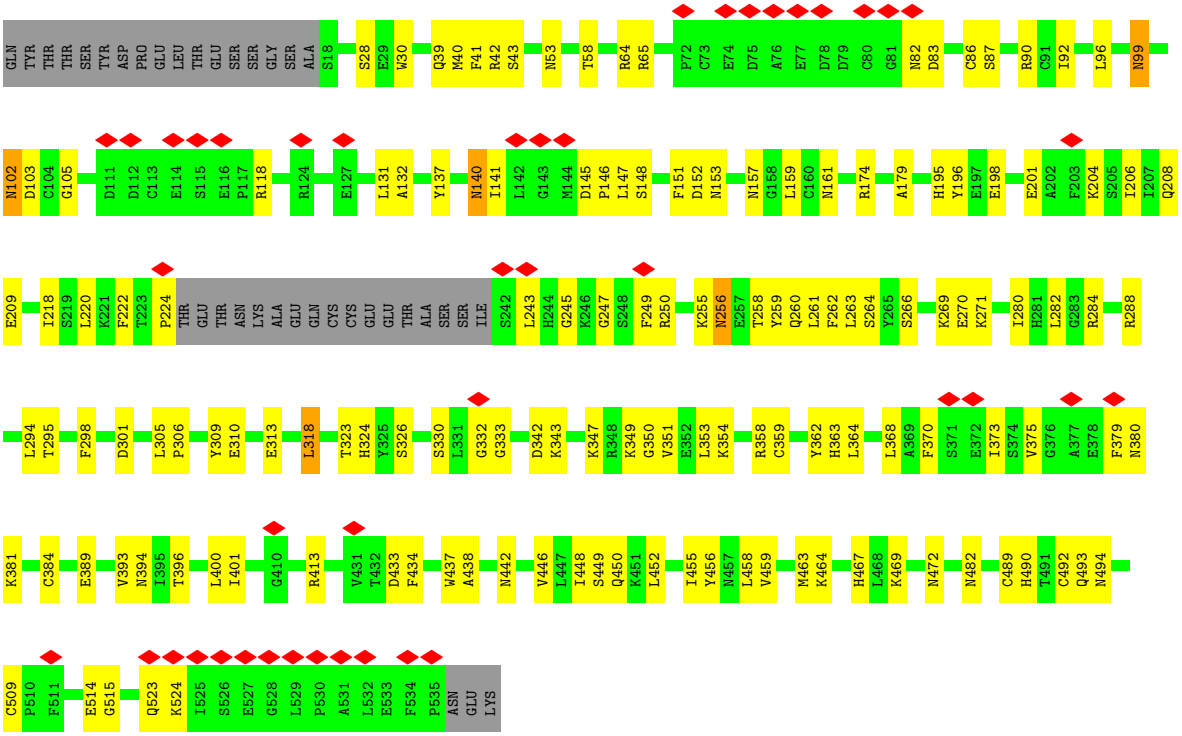
• Molecule 1: Complement component C9

Chain T:



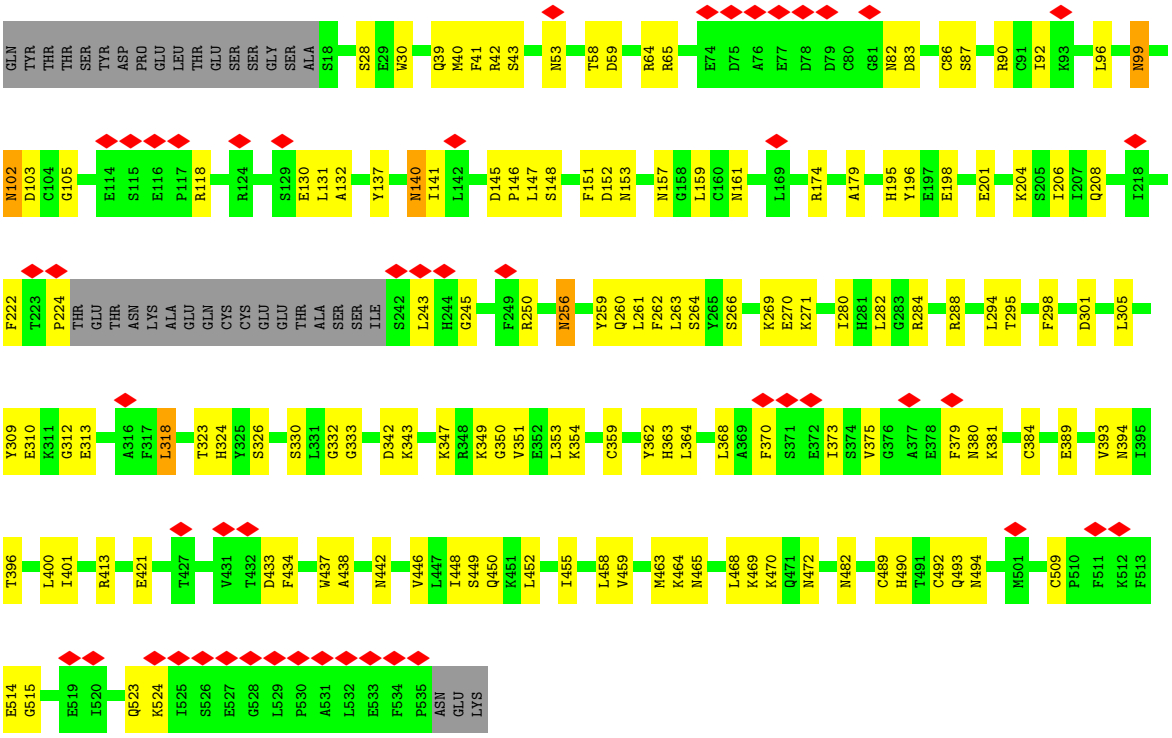
• Molecule 1: Complement component C9

Chain U:



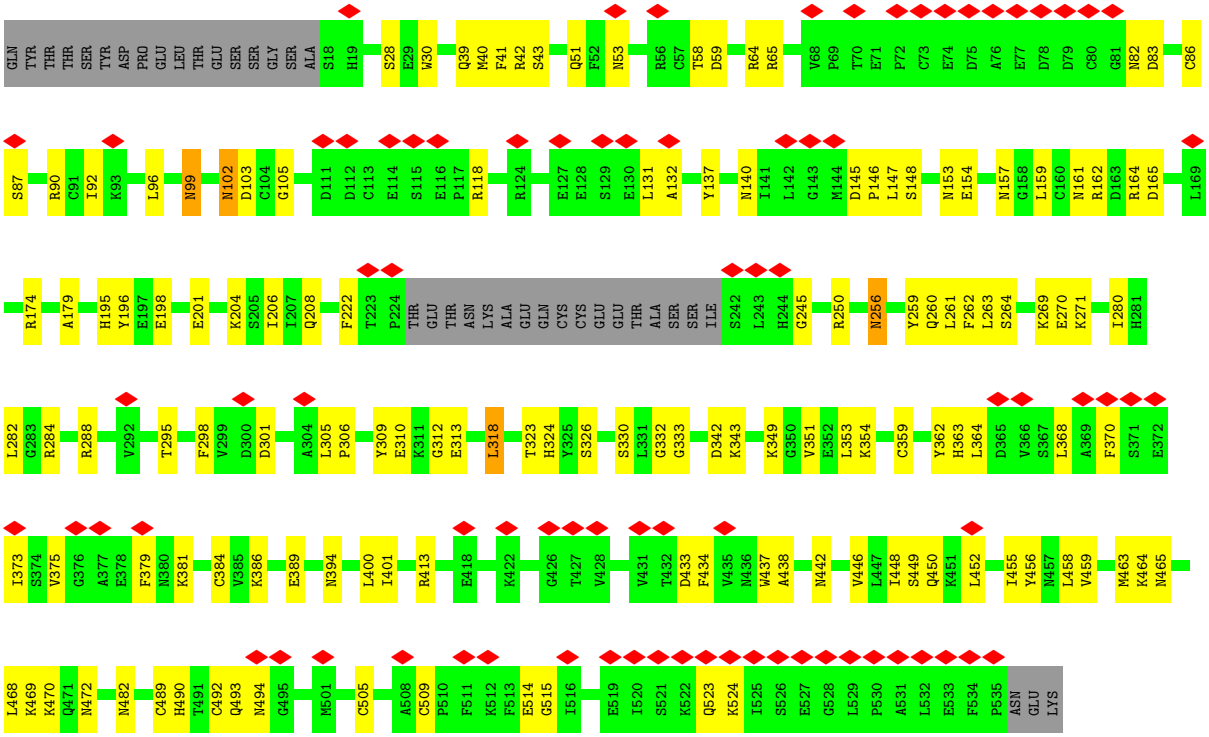
• Molecule 1: Complement component C9

Chain V: 9% 66% 26% • 7%



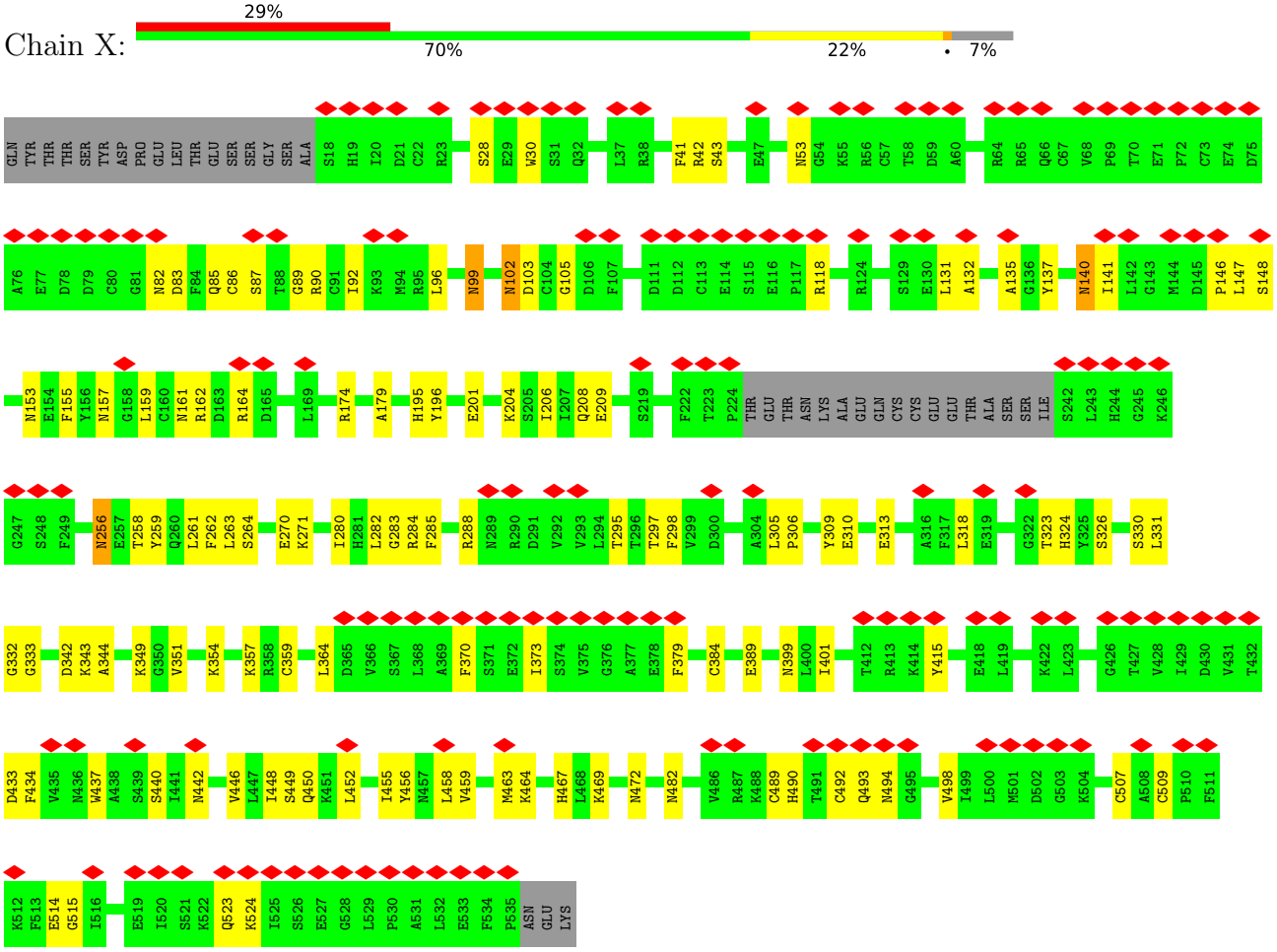
• Molecule 1: Complement component C9

Chain W: 15% 67% 25% • 7%



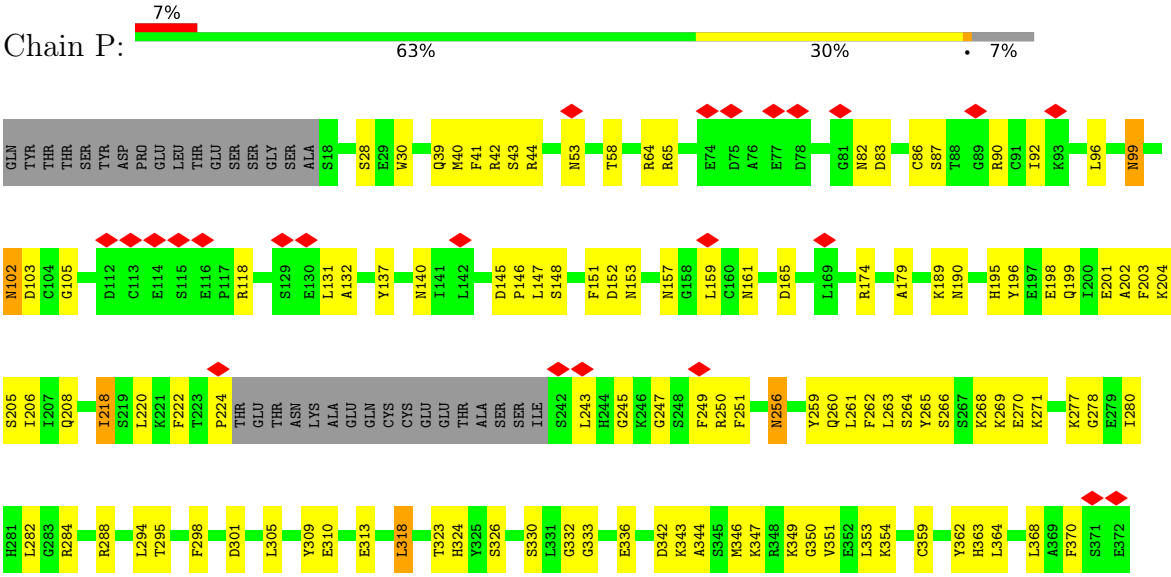
- Molecule 1: Complement component C9

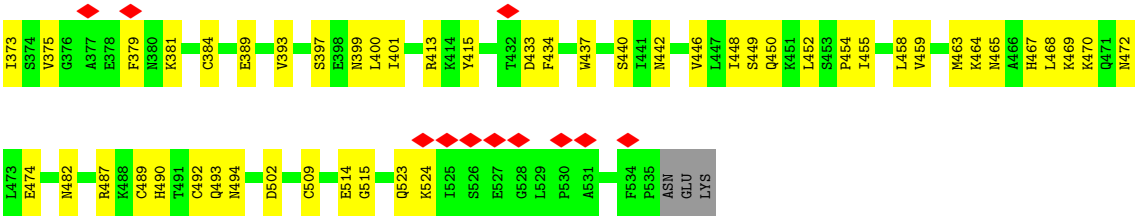
Chain X:



- Molecule 1: Complement component C9

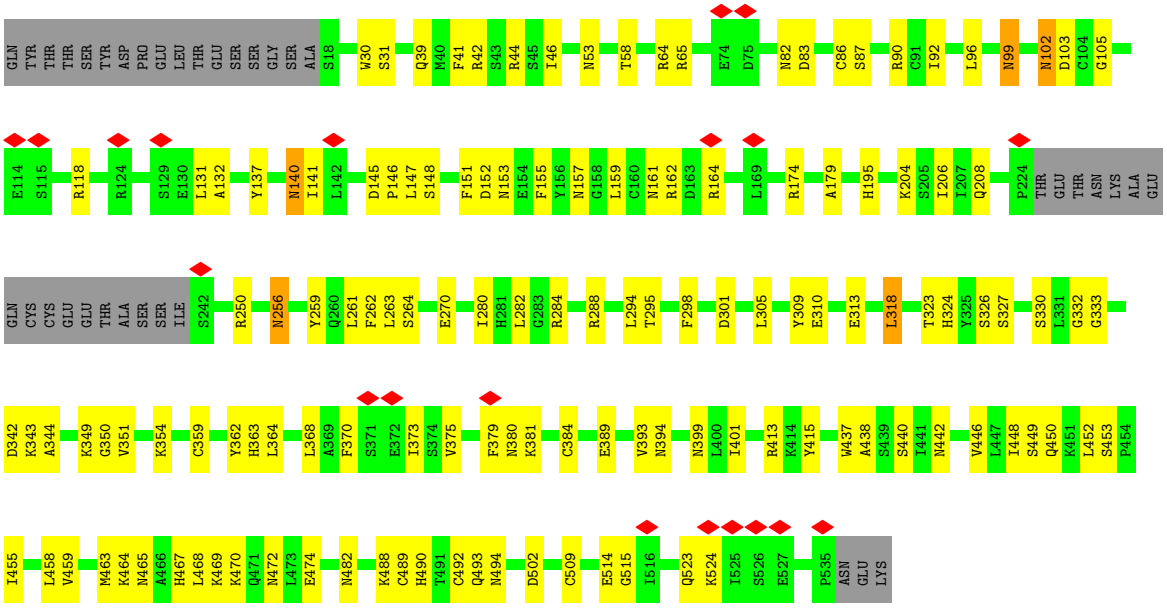
Chain P:





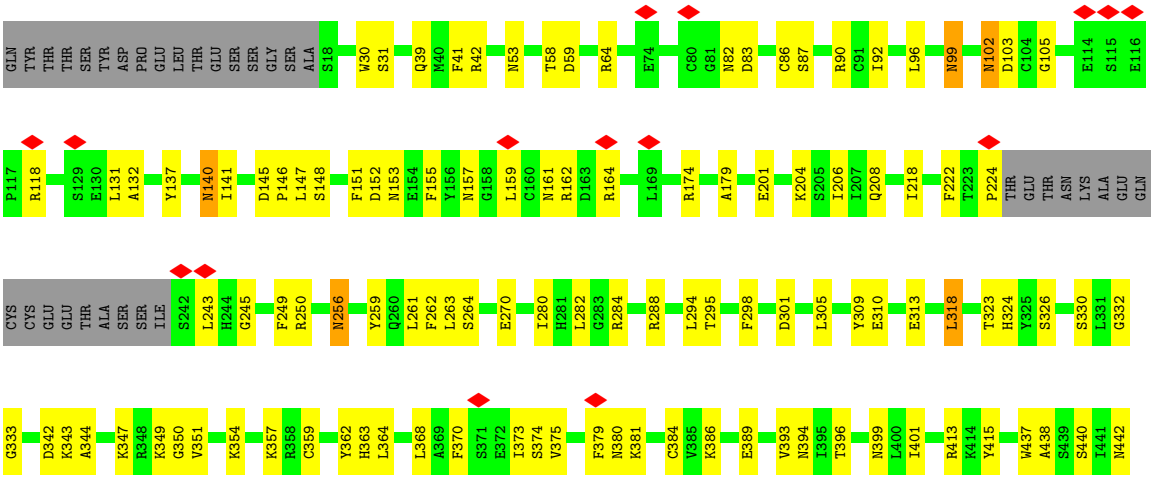
• Molecule 1: Complement component C9

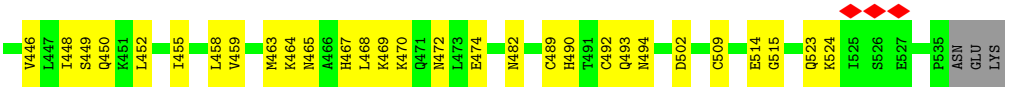
Chain H:



• Molecule 1: Complement component C9

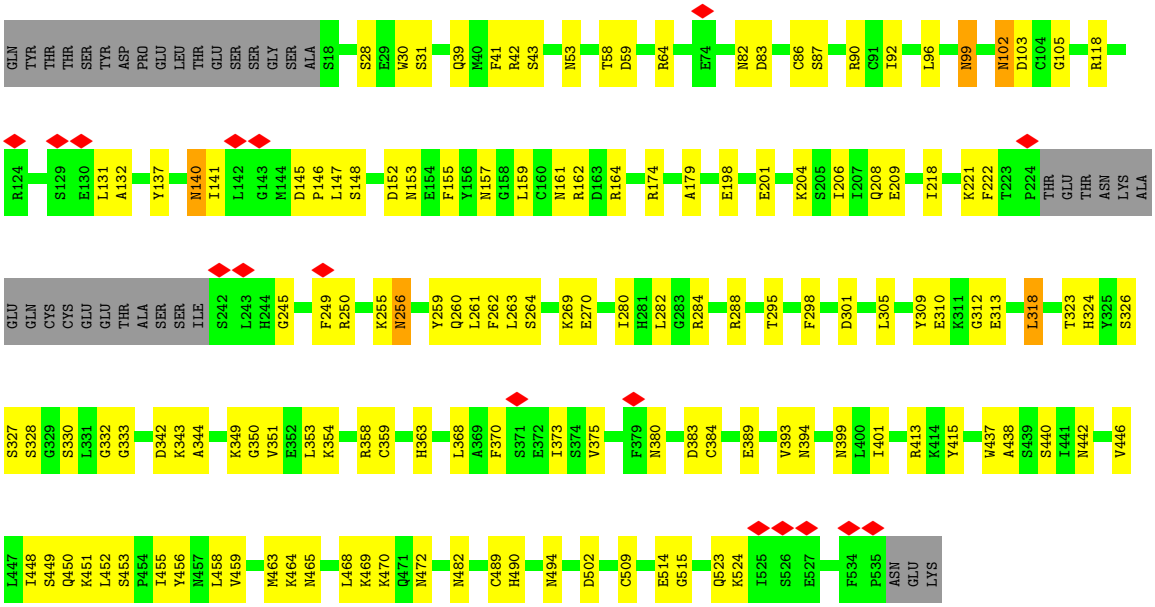
Chain I:





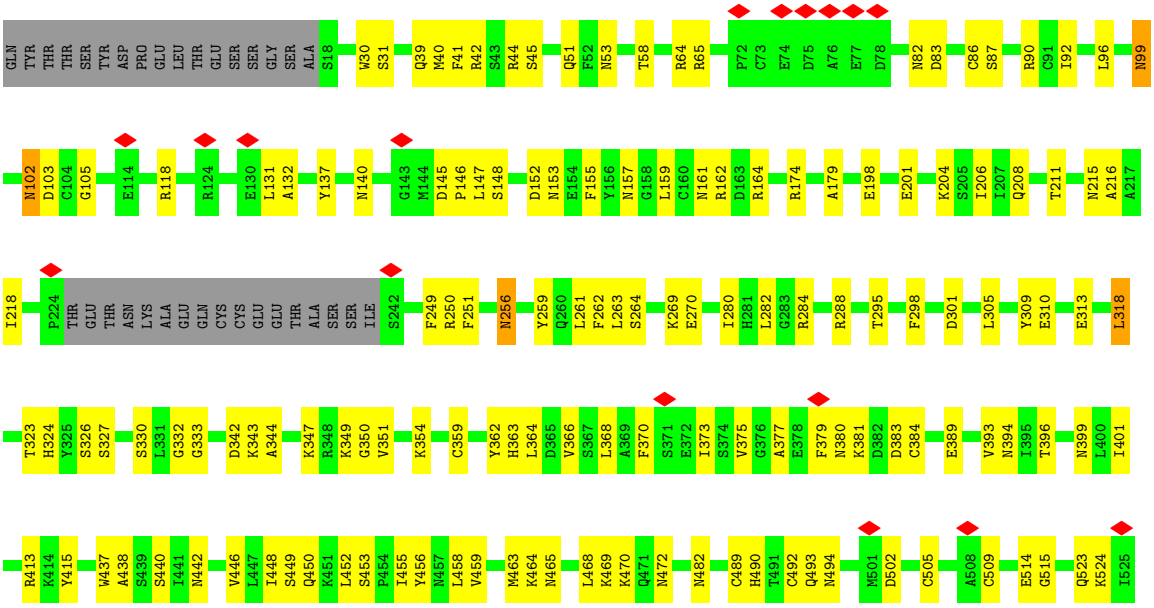
• Molecule 1: Complement component C9

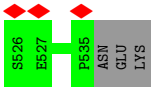
Chain J:



• Molecule 1: Complement component C9

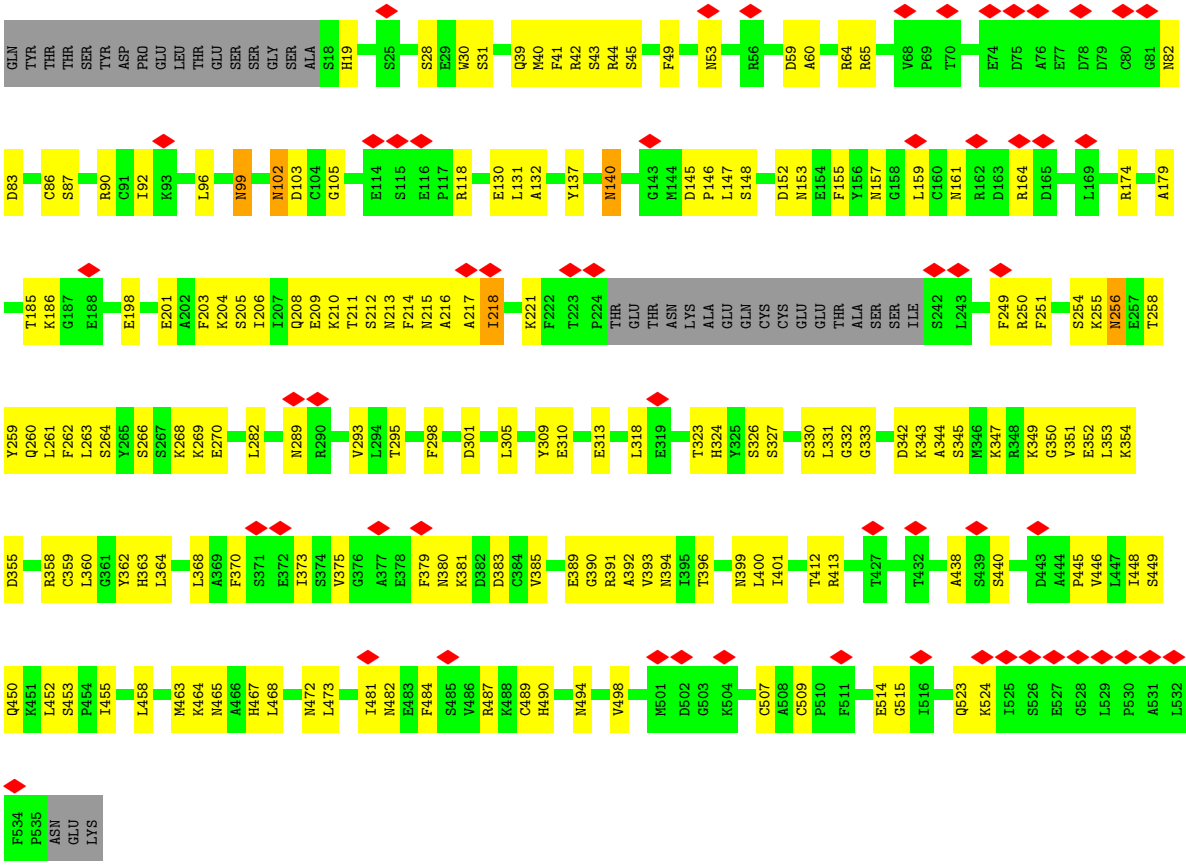
Chain K:





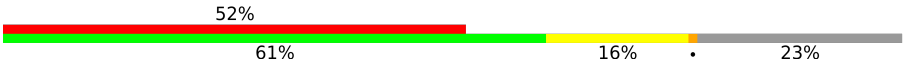
- Molecule 1: Complement component C9

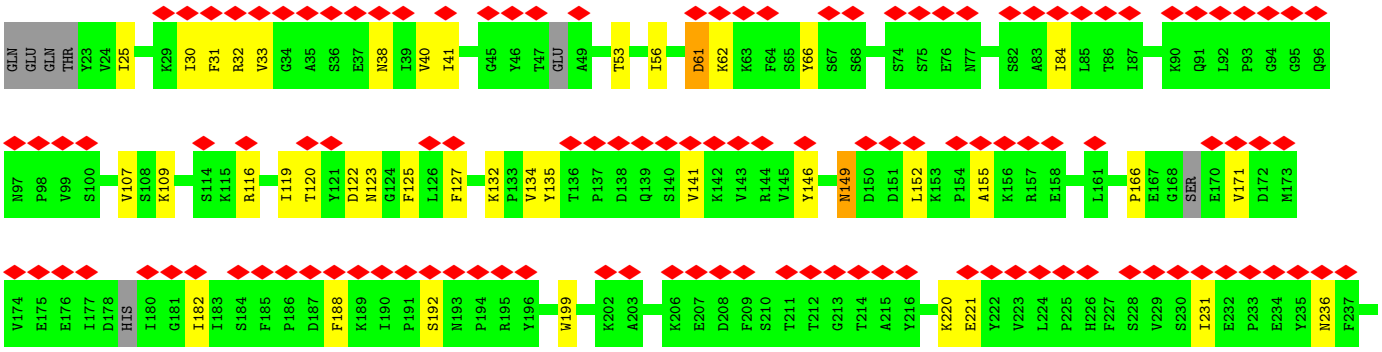
Chain G:



- Molecule 2: Complement C5,Complement C5

Chain A:





Y240 K241 N242 F243 K244 N245 F246 E247 I248 T249 I250 K251 A252 R253 N257 K258 V259 V260 T261 E262 A263 D264 V265 Y266 I267 T268 F269 G270 I271 R272 E273 D274 L275 K276 D277 D278 Q279 K280 E281 M282 M283 Q284 T285 A286 M287 Q288 N289 I293 N294 G295 I296 A297 Q298 V299 T300 F301 D302

T305 K308 E309 L310 S311 Y312 Y313 S314 L315 E316 D317 L318 N319 N320 K321 Y322 L323 A326 V327 T328 V329 I330 E331 S332 T333 F336 S337 E338 E339 A340 E341 I342 P343 G344 I345 V348 L349 S350 P351 Y352 K353 L354 N355 L356 V357 A358 T359 P360 L361 F362 L363 K364 P365 G366 I367 P368

Y369 P370 I371 Q374 V375 K376 D377 S378 L379 D380 Q381 L382 G385 L390 N391 A392 Q393 T394 V397 N398 Q399 E400 T401 S402 D403 L404 D405 P406 S407 K408 S409 V410 T411 R412 V413 D414 D415 G416 V417 A418 S419 F420 V421 L422 N423 L424 P425 S426 G427 V428 T429 V430 L431 E432 F433 N434

V435 A439 P440 D441 L442 P443 E444 E445 N446 Q447 A448 R449 E450 G451 Y452 R453 A454 I455 A456 Y457 SER S459 L460 S463 Y464 L465 Y466 I467 D468 W469 T470 D471 N472 H473 K474 L477 V478 G479 E480 H481 Y492 I493 D494 T497 H498 Y501 L502 I503 L504 S505 K506 G507 K508 I509

I510 H511 F512 G513 T514 R515 E516 K517 F518 S519 D520 A521 S522 Y523 I526 N527 I528 P529 V530 T531 Q532 N533 M534 V535 P536 R539 L540 L541 V542 Y543 Y544 T547 G548 D557 L561 E564 E565 K566 C567 G568 N569 Q570 L571 H574 L575 S576 P577 D578 A579 D580 A581 Y582 S583

P584 G585 Q586 T587 V588 S589 L590 N591 M592 A593 T594 G595 M596 D597 S598 W599 V600 A601 A604 Y610 G611 V612 Q613 R614 G615 A616 K617 K618 P619 L620 E621 R622 V623 F624 Q625 F626 L627 E628 K629 S630 D631 L632 G633 C634 G635 A636 G637 G638 G639 L640 N641 M642 A643 H647 F653 L654

N658 A659 D660 D661 S662 Q663 GLU ASN ASP GLU PRO CYS LYS GLU ILE LEU LEU HIS MET LYS THR LEU LEU PRO VAL SER LYS PRO GLU ILE R766 S767 Y768 F769 P770 E771 S772 W773 L774 W775 E776 V777 H778 L779 V780 P781 R782 R783 K784 Q785 L786 Q787 F788 A789 L790 P791 D792 E798

I799 Q800 G801 V802 G803 I804 S805 N806 T807 G808 I809 C810 V811 A812 D813 T814 V815 K816 A817 F820 K821 D822 V823 F824 L825 E826 M827 N828 I829 P830 Y831 S832 V833 V834 R835 G836 E837 Q838 I839 Q840 L841 K842 G843 T844 V845 Y846 N847 Y848 R849 T850 S851 G852 M853 Q854 F855 C856 V857 K858 M859

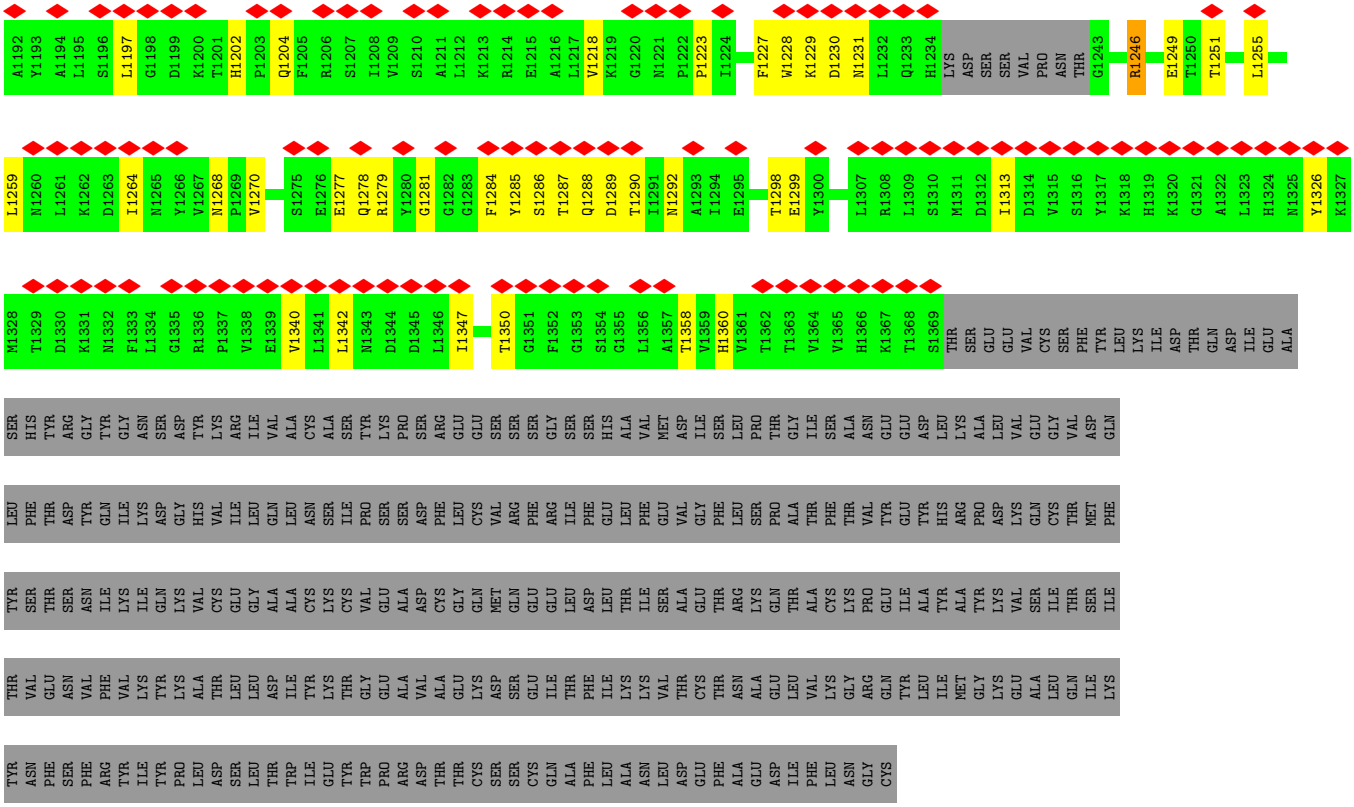
S860 A861 V862 E863 G864 I865 C866 T867 S868 E869 S870 P871 V872 I873 D874 H875 Q876 G877 T878 K879 S880 S881 K882 C883 V884 R885 Q886 K887 V888 E889 G890 S891 S892 S893 H894 L895 V896 T897 F898 T899 V900 L901 P902 L903 E904 I905 G906 L907 H908 N909 I910 N911 F912 S913 L914 E915 T916 W917 F918 G919

K920 E921 I922 L923 V924 K925 T926 L927 R928 V929 V930 P931 E932 G933 V934 K935 R936 E937 S938 Y939 V942 T943 L944 D945 F946 R947 G948 I949 Y950 G951 T952 I953 S954 R955 R956 K957 E958 F959 P960 Y961 R962 I963 P964 L965 D966 L967 V968 P969 K970 T971 E972 I973 K974 R975 I976 V979 K980 G981

L982 L983 V984 G985 E986 I987 L988 S989 A990 V991 L992 E995 G996 I997 N998 I999 L1000 T1001 H1002 LEU PRO LYS GLY SER A1008 E1009 A1010 E1011 L1012 M1013 V1016 P1017 V1018 F1019 Y1020 V1021 F1022 H1023 E1026 N1029 H1030 W1031 N1032 I1033 F1034 H1035 S1036 D1037 P1038 L1039 I1040 E1041 K1042 Q1043 K1044 L1045

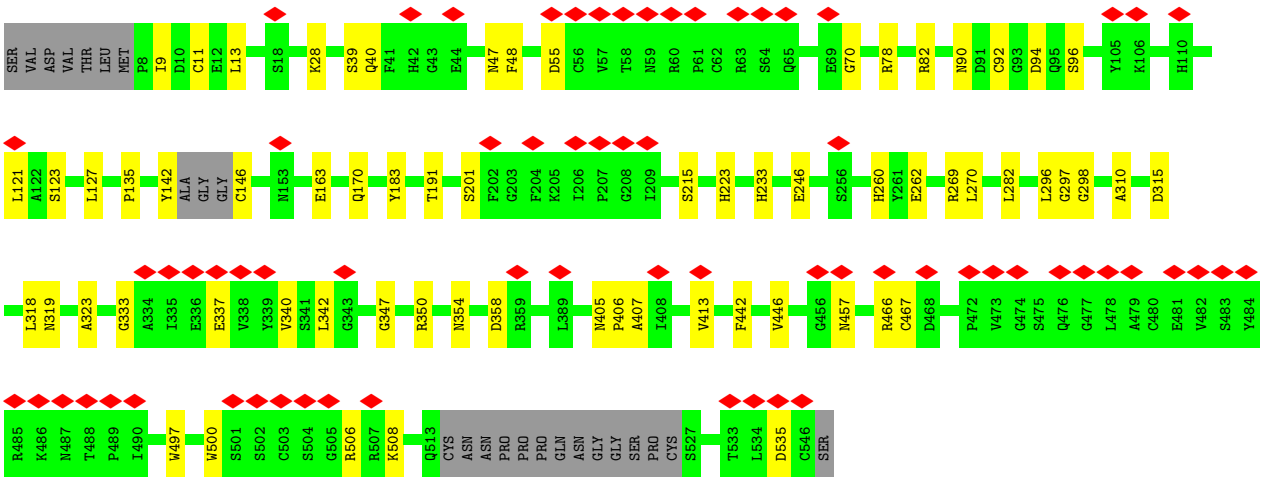
K1046 K1047 K1048 L1049 N1061 A1062 D1063 Y1064 S1067 V1068 W1069 K1070 G1071 G1072 S1073 A1074 W1077 L1078 T1079 A1080 F1081 L1086 G1087 N1090 K1091 Y1092 V1093 E1094 Q1095 N1096 Q1097 N1098 L1107 V1108 E1109 N1110 Y1111 Q1112 L1113 D1114 N1115 G1116 S1117 F1118 K1119 E1120 N1121 S1122 Q1123 TYR GLN PRO ILE LYS

LEU GLN GLY THR L1133 P1134 V1135 E1136 A1137 R1138 E1139 N1140 S1141 L1142 Y1143 A1146 V1149 I1150 G1151 I1152 R1153 K1154 A1155 F1156 D1157 I1158 C1159 P1160 L1161 V1162 K1163 T1166 A1167 L1168 I1169 K1170 A1171 D1172 N1173 F1174 L1175 L1176 E1177 N1178 T1179 L1180 P1181 A1182 Q1183 S1184 T1185 F1186 T1187 L1188 A1189 I1190 S1191



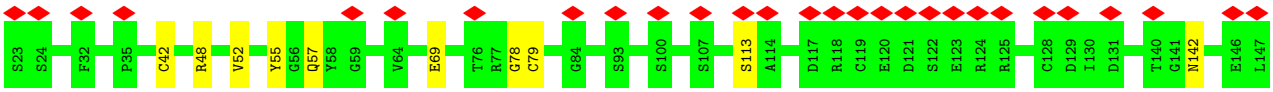
• Molecule 3: Complement component C8 beta chain

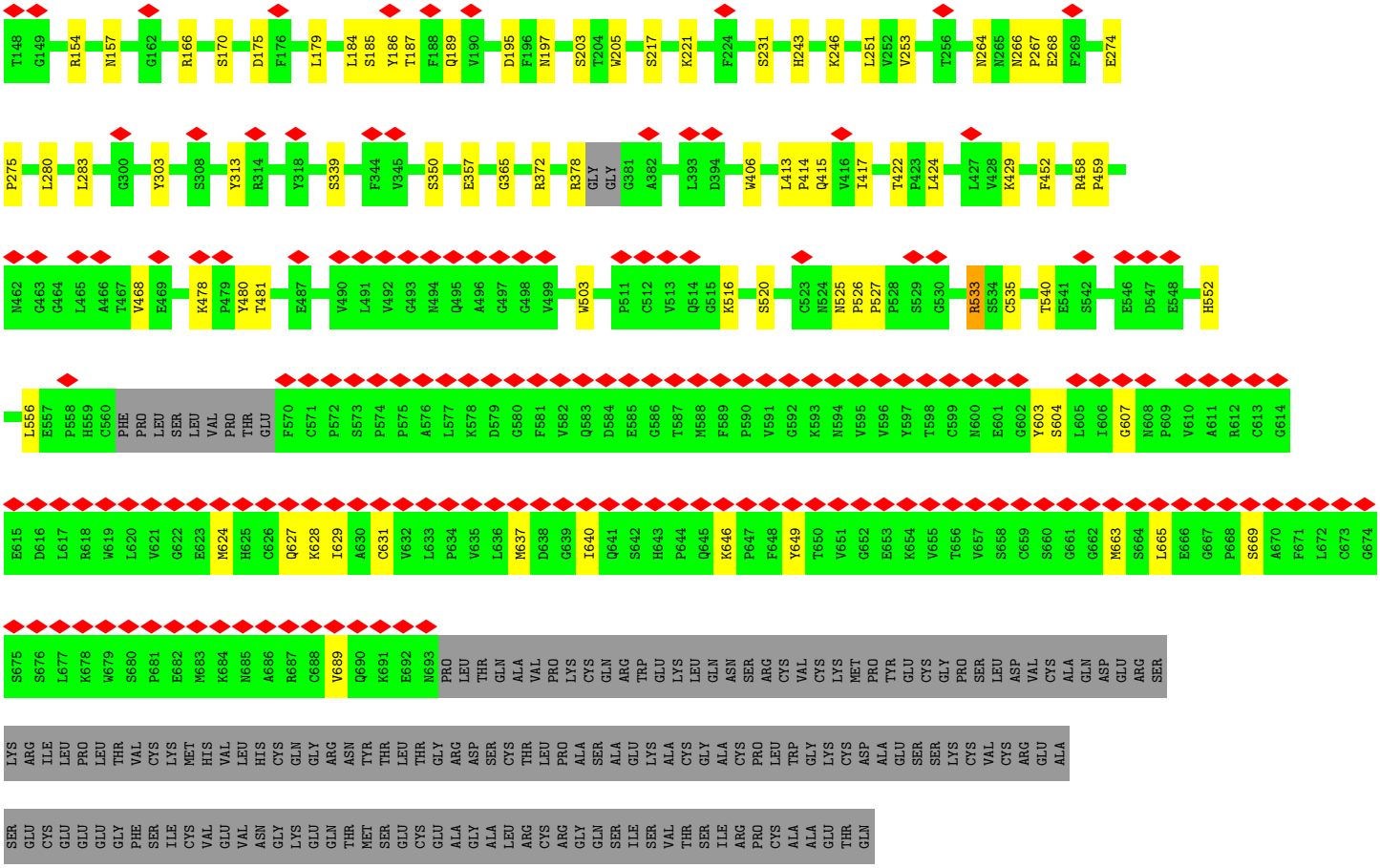
Chain C:



• Molecule 4: Complement component C7

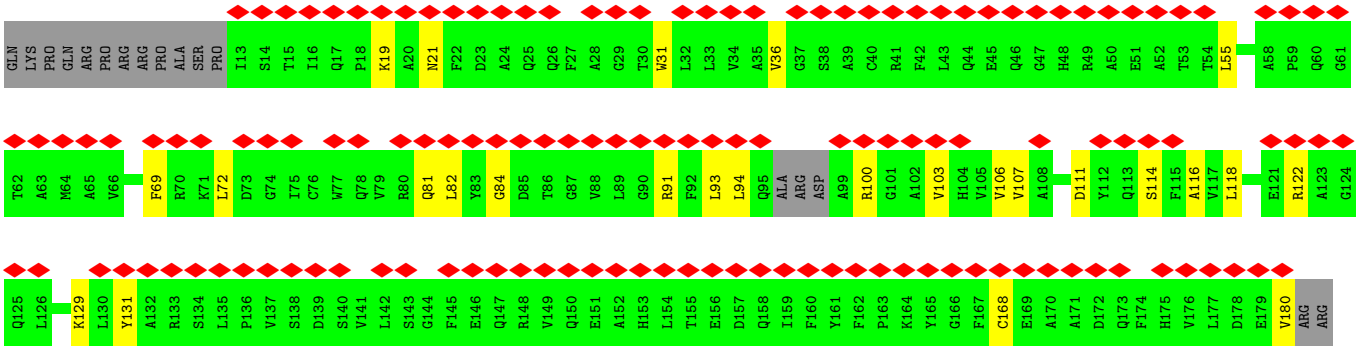
Chain D:





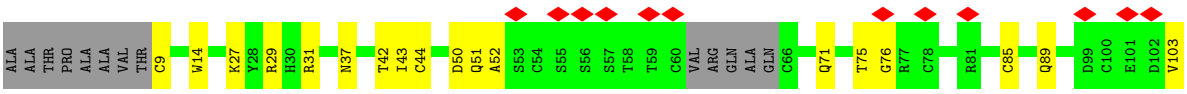
- Molecule 5: Complement component C8 gamma chain

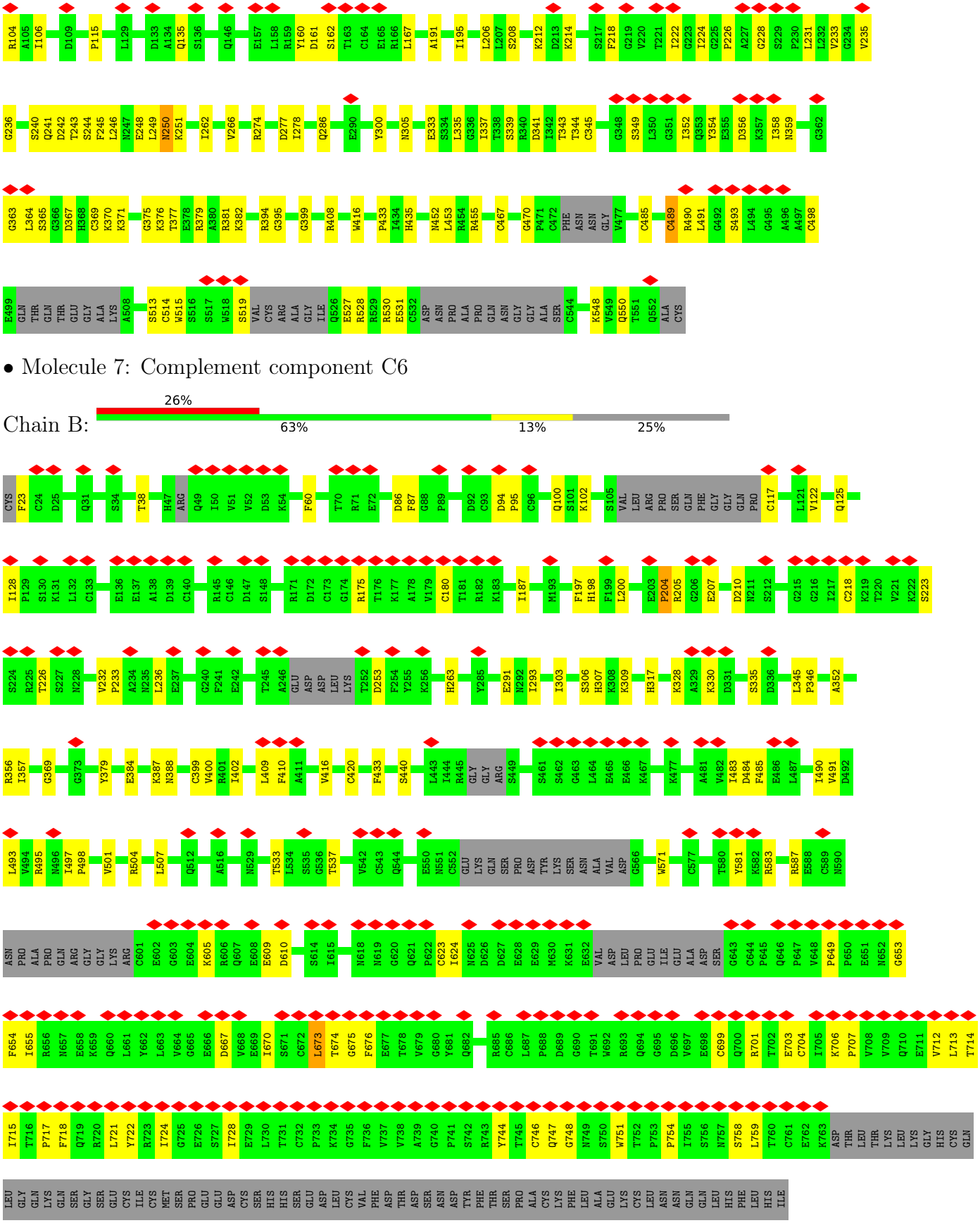
Chain E:



- Molecule 6: Complement component C8 alpha chain

Chain F:





- Molecule 7: Complement component C6

Chain B:

GLY SER CYS GLN ASP GLY ARG GLN LEU GLU TRP GLY LEU GLU ARG THR ARG LEU SER SER ASN SER THR LYS LYS GLU SER CYS GLY TYR ASP THR CYS TYR ASP TRP GLU LYS CYS SER ALA SER THR SER LYS CYS VAL CYS LEU LEU PRO PRO GLN CYS PHE LYS GLY GLY ASN GLN

LEU TYR CYS VAL LYS MET GLY SER SER THR SER GLU LYS THR LEU ASN ILE CYS GLU VAL GLY THR ILE ARG CYS ALA ASN ARG LYS MET GLU ILE LEU HIS PRO GLY LYS CYS LEU ALA

• Molecule 8: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain Y: 50% 50% 50%

NAG1 NAG2

• Molecule 8: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain Z: 50% 50% 50%

NAG1 NAG2

• Molecule 8: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain a: 50% 50% 50%

NAG1 NAG2

• Molecule 8: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain b: 50% 50% 50%

NAG1 NAG2

• Molecule 8: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain c: 50% 50% 50%

NAG1 NAG2

• Molecule 8: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain d:

• Molecule 8: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain e:

• Molecule 8: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain f:

• Molecule 8: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain g:

• Molecule 8: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain h:

• Molecule 8: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain i:

• Molecule 8: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain j:

• Molecule 8: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain k:

• Molecule 8: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain l:

• Molecule 8: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain m:

• Molecule 8: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain n:

• Molecule 8: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain o:

• Molecule 8: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain p:

• Molecule 8: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain q:

4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	53167	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/Å^2$)	50	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	59000	Depositor
Image detector	FEI FALCON II (4k x 4k)	Depositor
Maximum map value	0.342	Depositor
Minimum map value	-0.153	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.011	Depositor
Recommended contour level	0.06	Depositor
Map size (Å)	498.24, 498.24, 498.24	wwPDB
Map dimensions	360, 360, 360	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.384, 1.384, 1.384	Depositor

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: 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	G	0.23	0/3839	0.42	0/5181
1	H	0.23	0/3856	0.42	0/5203
1	I	0.23	0/3856	0.42	0/5203
1	J	0.24	0/3856	0.42	0/5203
1	K	0.23	0/3856	0.42	0/5203
1	L	0.23	0/3856	0.42	0/5203
1	M	0.23	0/3856	0.42	0/5203
1	N	0.23	0/3856	0.42	0/5203
1	O	0.23	0/3856	0.42	0/5203
1	P	0.23	0/3856	0.42	0/5203
1	Q	0.23	0/3856	0.42	0/5203
1	R	0.23	0/3856	0.42	0/5203
1	S	0.23	0/3856	0.42	0/5203
1	T	0.23	0/3856	0.42	0/5203
1	U	0.24	0/3856	0.42	0/5203
1	V	0.23	0/3856	0.42	0/5203
1	W	0.23	0/3856	0.42	0/5203
1	X	0.24	0/3856	0.42	0/5203
2	A	0.24	0/9707	0.44	1/13191 (0.0%)
3	C	0.23	0/3831	0.42	0/5203
4	D	0.24	0/4687	0.42	0/6362
5	E	0.24	0/1314	0.41	0/1782
6	F	0.23	0/3830	0.41	0/5157
7	B	0.24	0/5231	0.41	0/7085
All	All	0.23	0/97991	0.42	1/132412 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	A	61	ASP	C-N-CA	5.24	134.81	121.70

There are no chirality outliers.

There are no planarity outliers.

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	G	3770	0	3478	129	0
1	H	3785	0	3495	87	0
1	I	3785	0	3495	91	0
1	J	3785	0	3495	92	0
1	K	3785	0	3495	98	0
1	L	3785	0	3495	109	0
1	M	3785	0	3495	111	0
1	N	3785	0	3495	113	0
1	O	3785	0	3495	111	0
1	P	3785	0	3495	105	0
1	Q	3785	0	3495	113	0
1	R	3785	0	3495	112	0
1	S	3785	0	3495	110	0
1	T	3785	0	3495	96	0
1	U	3785	0	3495	93	0
1	V	3785	0	3495	90	0
1	W	3785	0	3495	88	0
1	X	3785	0	3495	73	0
2	A	9497	0	9310	160	0
3	C	3752	0	3289	42	0
4	D	4578	0	3862	55	0
5	E	1286	0	1244	15	0
6	F	3758	0	3313	90	0
7	B	5128	0	4610	71	0
8	Y	28	0	25	2	0
8	Z	28	0	25	2	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
8	a	28	0	25	0	0
8	b	28	0	25	0	0
8	c	28	0	25	0	0
8	d	28	0	25	0	0
8	e	28	0	25	0	0
8	f	28	0	25	0	0
8	g	28	0	25	0	0
8	h	28	0	25	0	0
8	i	28	0	25	0	0
8	j	28	0	25	0	0
8	k	28	0	25	0	0
8	l	28	0	25	0	0
8	m	28	0	25	0	0
8	n	28	0	25	0	0
8	o	28	0	25	0	0
8	p	28	0	25	0	0
8	q	28	0	25	0	0
9	B	14	0	13	1	0
9	D	14	0	13	1	0
9	G	28	0	26	2	0
9	H	28	0	26	2	0
9	I	28	0	26	3	0
9	J	28	0	26	2	0
9	K	28	0	26	2	0
9	L	28	0	26	2	0
9	M	28	0	26	2	0
9	N	28	0	26	2	0
9	O	28	0	26	1	0
9	P	28	0	26	1	0
9	Q	28	0	26	2	0
9	R	28	0	26	2	0
9	S	28	0	26	1	0
9	T	28	0	26	3	0
9	U	28	0	26	3	0
9	V	28	0	26	2	0
9	W	28	0	26	2	0
9	X	28	0	26	4	0
All	All	97178	0	89490	1978	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 11.

The worst 5 of 1978 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:O:250:ARG:HB2	1:O:363:HIS:HB3	1.60	0.82
1:G:326:SER:HB3	1:G:450:GLN:HE21	1.44	0.81
1:Q:250:ARG:HB2	1:Q:363:HIS:HB3	1.63	0.81
6:F:490:ARG:H	6:F:498:CYS:HB2	1.45	0.81
1:S:326:SER:HB3	1:S:450:GLN:HE21	1.46	0.81

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 PDB entries followed by that with respect to all EM entries.

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	G	493/538 (92%)	455 (92%)	38 (8%)	0	100	100
1	H	493/538 (92%)	461 (94%)	32 (6%)	0	100	100
1	I	493/538 (92%)	457 (93%)	36 (7%)	0	100	100
1	J	493/538 (92%)	457 (93%)	36 (7%)	0	100	100
1	K	493/538 (92%)	458 (93%)	35 (7%)	0	100	100
1	L	493/538 (92%)	457 (93%)	36 (7%)	0	100	100
1	M	493/538 (92%)	457 (93%)	36 (7%)	0	100	100
1	N	493/538 (92%)	458 (93%)	35 (7%)	0	100	100
1	O	493/538 (92%)	459 (93%)	34 (7%)	0	100	100
1	P	493/538 (92%)	462 (94%)	31 (6%)	0	100	100
1	Q	493/538 (92%)	458 (93%)	35 (7%)	0	100	100
1	R	493/538 (92%)	458 (93%)	35 (7%)	0	100	100
1	S	493/538 (92%)	459 (93%)	34 (7%)	0	100	100
1	T	493/538 (92%)	461 (94%)	32 (6%)	0	100	100
1	U	493/538 (92%)	460 (93%)	33 (7%)	0	100	100
1	V	493/538 (92%)	460 (93%)	33 (7%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	W	493/538 (92%)	458 (93%)	35 (7%)	0	100	100
1	X	493/538 (92%)	457 (93%)	36 (7%)	0	100	100
2	A	1201/1580 (76%)	1136 (95%)	65 (5%)	0	100	100
3	C	501/537 (93%)	481 (96%)	20 (4%)	0	100	100
4	D	648/821 (79%)	603 (93%)	45 (7%)	0	100	100
5	E	161/182 (88%)	160 (99%)	1 (1%)	0	100	100
6	F	492/554 (89%)	472 (96%)	20 (4%)	0	100	100
7	B	668/913 (73%)	642 (96%)	25 (4%)	1 (0%)	51	85
All	All	12545/14271 (88%)	11746 (94%)	798 (6%)	1 (0%)	100	100

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
7	B	204	PRO

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 PDB entries followed by that with respect to all EM entries.

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	G	382/477 (80%)	366 (96%)	16 (4%)	30	54
1	H	385/477 (81%)	371 (96%)	14 (4%)	35	59
1	I	385/477 (81%)	371 (96%)	14 (4%)	35	59
1	J	385/477 (81%)	371 (96%)	14 (4%)	35	59
1	K	385/477 (81%)	371 (96%)	14 (4%)	35	59
1	L	385/477 (81%)	371 (96%)	14 (4%)	35	59
1	M	385/477 (81%)	371 (96%)	14 (4%)	35	59
1	N	385/477 (81%)	372 (97%)	13 (3%)	37	60
1	O	385/477 (81%)	371 (96%)	14 (4%)	35	59
1	P	385/477 (81%)	370 (96%)	15 (4%)	32	57

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	Q	385/477 (81%)	372 (97%)	13 (3%)	37	60
1	R	385/477 (81%)	371 (96%)	14 (4%)	35	59
1	S	385/477 (81%)	371 (96%)	14 (4%)	35	59
1	T	385/477 (81%)	371 (96%)	14 (4%)	35	59
1	U	385/477 (81%)	371 (96%)	14 (4%)	35	59
1	V	385/477 (81%)	371 (96%)	14 (4%)	35	59
1	W	385/477 (81%)	371 (96%)	14 (4%)	35	59
1	X	385/477 (81%)	372 (97%)	13 (3%)	37	60
2	A	1030/1403 (73%)	1012 (98%)	18 (2%)	60	78
3	C	357/473 (76%)	355 (99%)	2 (1%)	86	91
4	D	411/714 (58%)	409 (100%)	2 (0%)	88	93
5	E	131/149 (88%)	129 (98%)	2 (2%)	65	80
6	F	363/466 (78%)	358 (99%)	5 (1%)	67	80
7	B	522/810 (64%)	518 (99%)	4 (1%)	81	89
All	All	9741/12601 (77%)	9456 (97%)	285 (3%)	45	64

5 of 285 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	K	318	LEU
1	G	99	ASN
2	A	528	ILE
1	T	82	ASN
1	S	494	ASN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 238 such sidechains are listed below:

Mol	Chain	Res	Type
1	W	161	ASN
4	D	282	HIS
1	H	53	ASN
4	D	157	ASN
7	B	100	GLN

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)

38 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	$\#\|Z\| > 2$
8	NAG	Y	1	8,1	14,14,15	0.55	0	17,19,21	0.89	1 (5%)
8	NAG	Y	2	8	14,14,15	0.55	0	17,19,21	0.51	0
8	NAG	Z	1	8,1	14,14,15	0.54	0	17,19,21	0.90	1 (5%)
8	NAG	Z	2	8	14,14,15	0.56	0	17,19,21	0.52	0
8	NAG	a	1	8,1	14,14,15	0.51	0	17,19,21	0.89	1 (5%)
8	NAG	a	2	8	14,14,15	0.56	0	17,19,21	0.53	0
8	NAG	b	1	8,1	14,14,15	0.62	0	17,19,21	0.95	1 (5%)
8	NAG	b	2	8	14,14,15	0.56	0	17,19,21	0.52	0
8	NAG	c	1	8,1	14,14,15	0.61	0	17,19,21	0.96	1 (5%)
8	NAG	c	2	8	14,14,15	0.54	0	17,19,21	0.52	0
8	NAG	d	1	8,1	14,14,15	0.61	0	17,19,21	0.95	1 (5%)
8	NAG	d	2	8	14,14,15	0.53	0	17,19,21	0.54	0
8	NAG	e	1	8,1	14,14,15	0.61	0	17,19,21	0.93	1 (5%)
8	NAG	e	2	8	14,14,15	0.56	0	17,19,21	0.53	0
8	NAG	f	1	8,1	14,14,15	0.56	0	17,19,21	0.91	1 (5%)
8	NAG	f	2	8	14,14,15	0.55	0	17,19,21	0.53	0
8	NAG	g	1	8,1	14,14,15	0.56	0	17,19,21	0.90	1 (5%)
8	NAG	g	2	8	14,14,15	0.54	0	17,19,21	0.53	0
8	NAG	h	1	8,1	14,14,15	0.55	0	17,19,21	0.90	1 (5%)
8	NAG	h	2	8	14,14,15	0.54	0	17,19,21	0.53	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
8	NAG	i	1	8,1	14,14,15	0.54	0	17,19,21	0.89	1 (5%)
8	NAG	i	2	8	14,14,15	0.55	0	17,19,21	0.52	0
8	NAG	j	1	8,1	14,14,15	0.53	0	17,19,21	0.88	1 (5%)
8	NAG	j	2	8	14,14,15	0.51	0	17,19,21	0.53	0
8	NAG	k	1	8,1	14,14,15	0.55	0	17,19,21	0.91	1 (5%)
8	NAG	k	2	8	14,14,15	0.55	0	17,19,21	0.52	0
8	NAG	l	1	8,1	14,14,15	0.55	0	17,19,21	0.89	1 (5%)
8	NAG	l	2	8	14,14,15	0.56	0	17,19,21	0.52	0
8	NAG	m	1	8,1	14,14,15	0.53	0	17,19,21	0.89	1 (5%)
8	NAG	m	2	8	14,14,15	0.56	0	17,19,21	0.52	0
8	NAG	n	1	8,1	14,14,15	0.52	0	17,19,21	0.89	1 (5%)
8	NAG	n	2	8	14,14,15	0.55	0	17,19,21	0.52	0
8	NAG	o	1	8,1	14,14,15	0.53	0	17,19,21	0.89	1 (5%)
8	NAG	o	2	8	14,14,15	0.55	0	17,19,21	0.54	0
8	NAG	p	1	8,1	14,14,15	0.76	1 (7%)	17,19,21	1.04	1 (5%)
8	NAG	p	2	8	14,14,15	0.60	0	17,19,21	0.51	0
8	NAG	q	1	8,3	14,14,15	0.55	0	17,19,21	1.33	2 (11%)
8	NAG	q	2	8	14,14,15	0.27	0	17,19,21	0.35	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
8	NAG	Y	1	8,1	-	3/6/23/26	0/1/1/1
8	NAG	Y	2	8	-	2/6/23/26	0/1/1/1
8	NAG	Z	1	8,1	-	3/6/23/26	0/1/1/1
8	NAG	Z	2	8	-	2/6/23/26	0/1/1/1
8	NAG	a	1	8,1	-	3/6/23/26	0/1/1/1
8	NAG	a	2	8	-	2/6/23/26	0/1/1/1
8	NAG	b	1	8,1	-	3/6/23/26	0/1/1/1
8	NAG	b	2	8	-	2/6/23/26	0/1/1/1
8	NAG	c	1	8,1	-	3/6/23/26	0/1/1/1
8	NAG	c	2	8	-	2/6/23/26	0/1/1/1
8	NAG	d	1	8,1	-	3/6/23/26	0/1/1/1
8	NAG	d	2	8	-	2/6/23/26	0/1/1/1
8	NAG	e	1	8,1	-	3/6/23/26	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
8	NAG	e	2	8	-	2/6/23/26	0/1/1/1
8	NAG	f	1	8,1	-	3/6/23/26	0/1/1/1
8	NAG	f	2	8	-	2/6/23/26	0/1/1/1
8	NAG	g	1	8,1	-	3/6/23/26	0/1/1/1
8	NAG	g	2	8	-	2/6/23/26	0/1/1/1
8	NAG	h	1	8,1	-	3/6/23/26	0/1/1/1
8	NAG	h	2	8	-	2/6/23/26	0/1/1/1
8	NAG	i	1	8,1	-	3/6/23/26	0/1/1/1
8	NAG	i	2	8	-	2/6/23/26	0/1/1/1
8	NAG	j	1	8,1	-	3/6/23/26	0/1/1/1
8	NAG	j	2	8	-	2/6/23/26	0/1/1/1
8	NAG	k	1	8,1	-	3/6/23/26	0/1/1/1
8	NAG	k	2	8	-	2/6/23/26	0/1/1/1
8	NAG	l	1	8,1	-	3/6/23/26	0/1/1/1
8	NAG	l	2	8	-	2/6/23/26	0/1/1/1
8	NAG	m	1	8,1	-	3/6/23/26	0/1/1/1
8	NAG	m	2	8	-	2/6/23/26	0/1/1/1
8	NAG	n	1	8,1	-	3/6/23/26	0/1/1/1
8	NAG	n	2	8	-	2/6/23/26	0/1/1/1
8	NAG	o	1	8,1	-	3/6/23/26	0/1/1/1
8	NAG	o	2	8	-	2/6/23/26	0/1/1/1
8	NAG	p	1	8,1	-	3/6/23/26	0/1/1/1
8	NAG	p	2	8	-	2/6/23/26	0/1/1/1
8	NAG	q	1	8,3	-	5/6/23/26	0/1/1/1
8	NAG	q	2	8	-	2/6/23/26	0/1/1/1

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
8	p	1	NAG	C1-C2	2.02	1.55	1.52

The worst 5 of 20 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
8	q	1	NAG	C2-N2-C7	4.34	129.09	122.90
8	p	1	NAG	C1-O5-C5	3.44	116.86	112.19

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
8	c	1	NAG	C1-O5-C5	3.06	116.34	112.19
8	d	1	NAG	C1-O5-C5	3.01	116.27	112.19
8	b	1	NAG	C1-O5-C5	3.00	116.26	112.19

There are no chirality outliers.

5 of 97 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
8	p	2	NAG	O5-C5-C6-O6
8	q	2	NAG	O5-C5-C6-O6
8	h	1	NAG	O5-C5-C6-O6
8	p	1	NAG	O5-C5-C6-O6
8	g	1	NAG	O5-C5-C6-O6

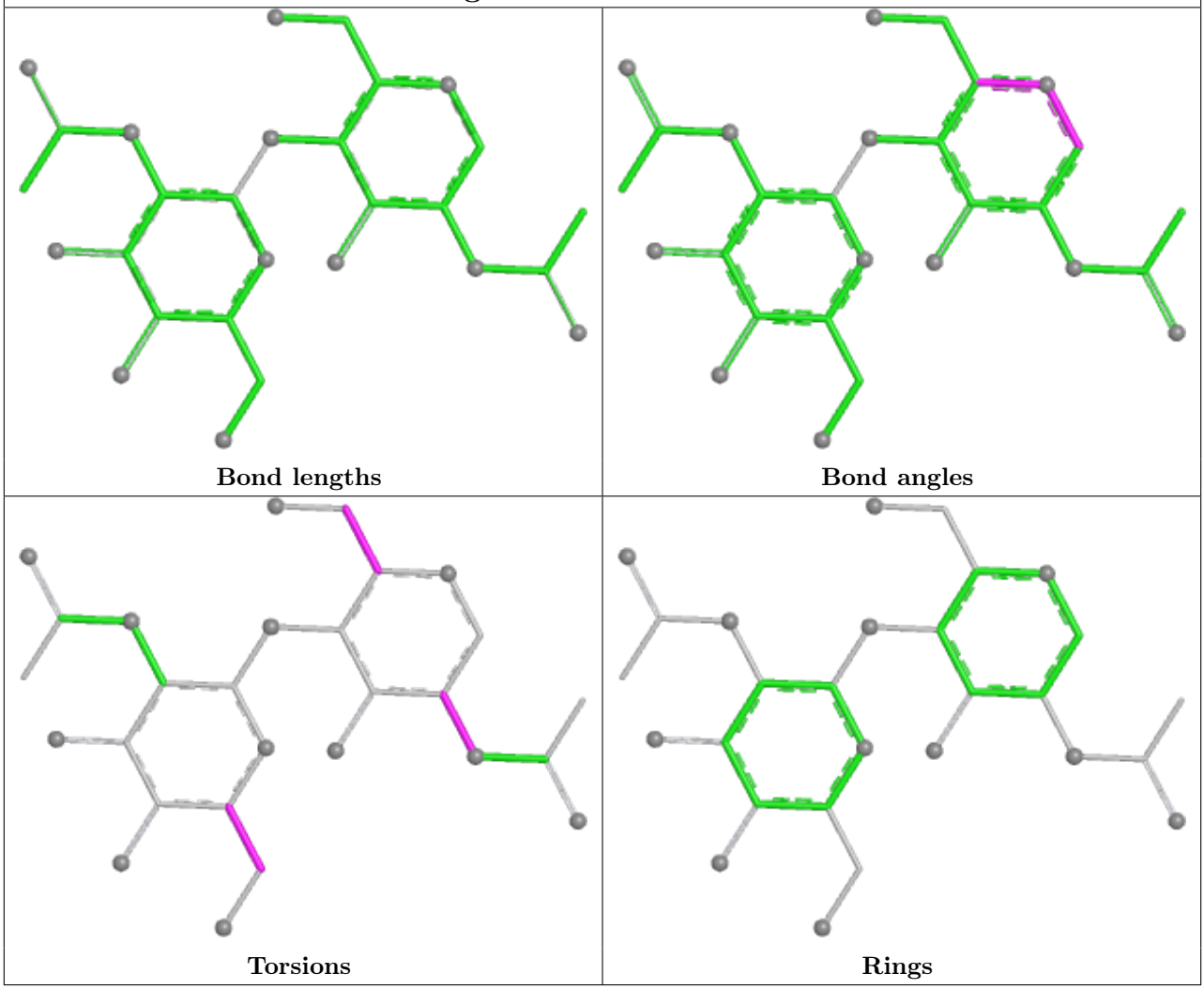
There are no ring outliers.

4 monomers are involved in 4 short contacts:

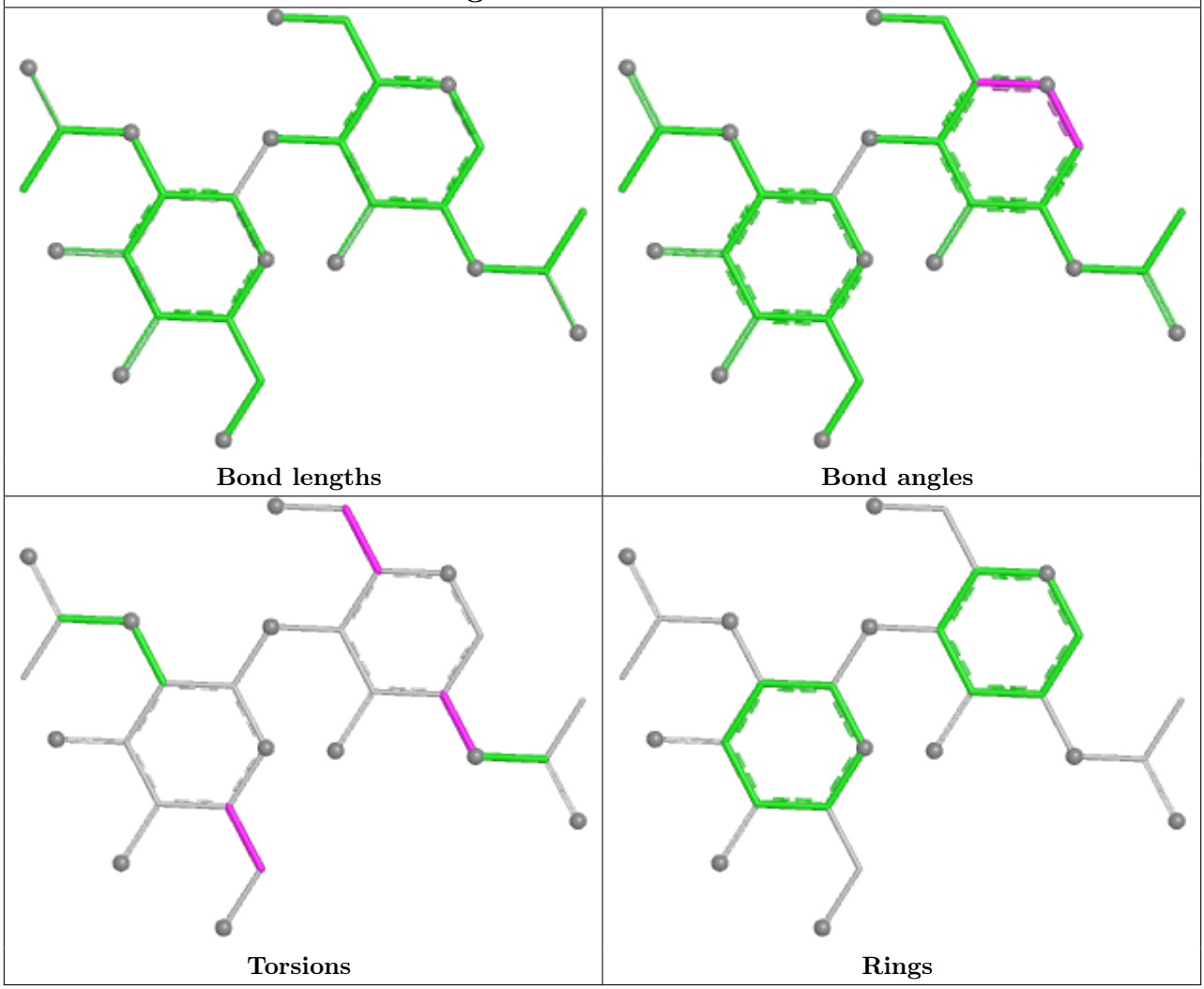
Mol	Chain	Res	Type	Clashes	Symm-Clashes
8	Z	1	NAG	2	0
8	Z	2	NAG	1	0
8	Y	2	NAG	1	0
8	Y	1	NAG	2	0

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

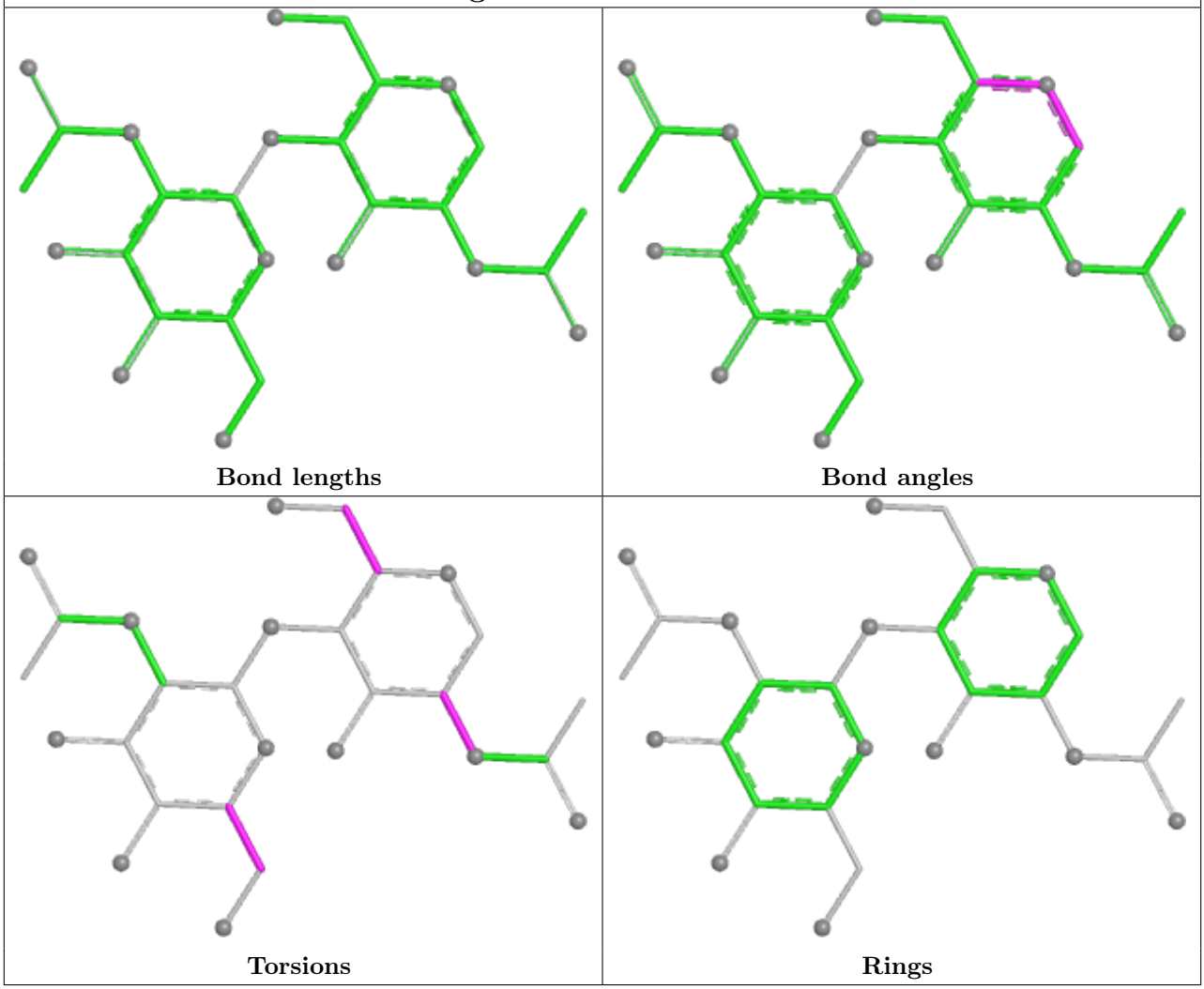
Oligosaccharide Chain Y



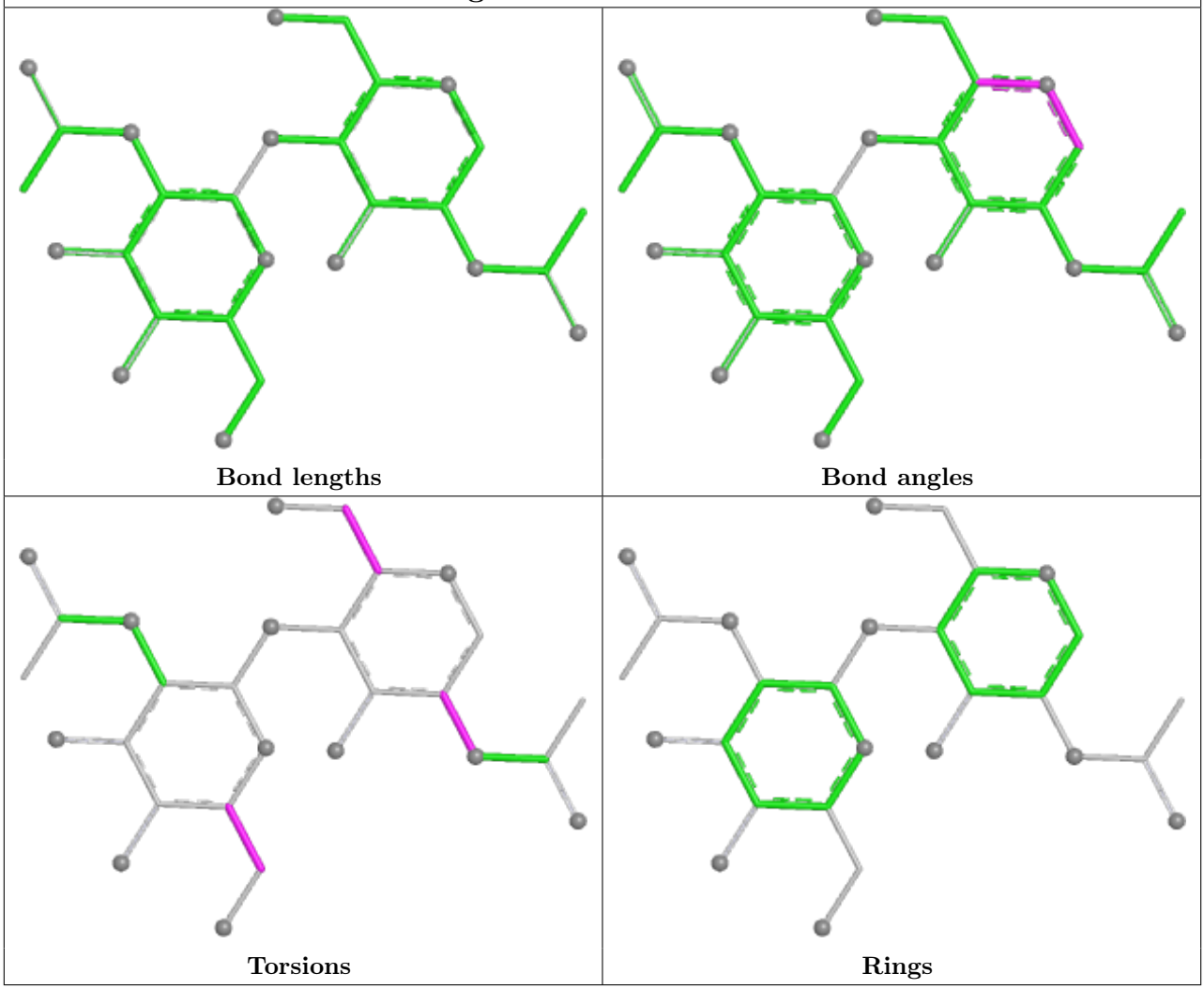
Oligosaccharide Chain Z



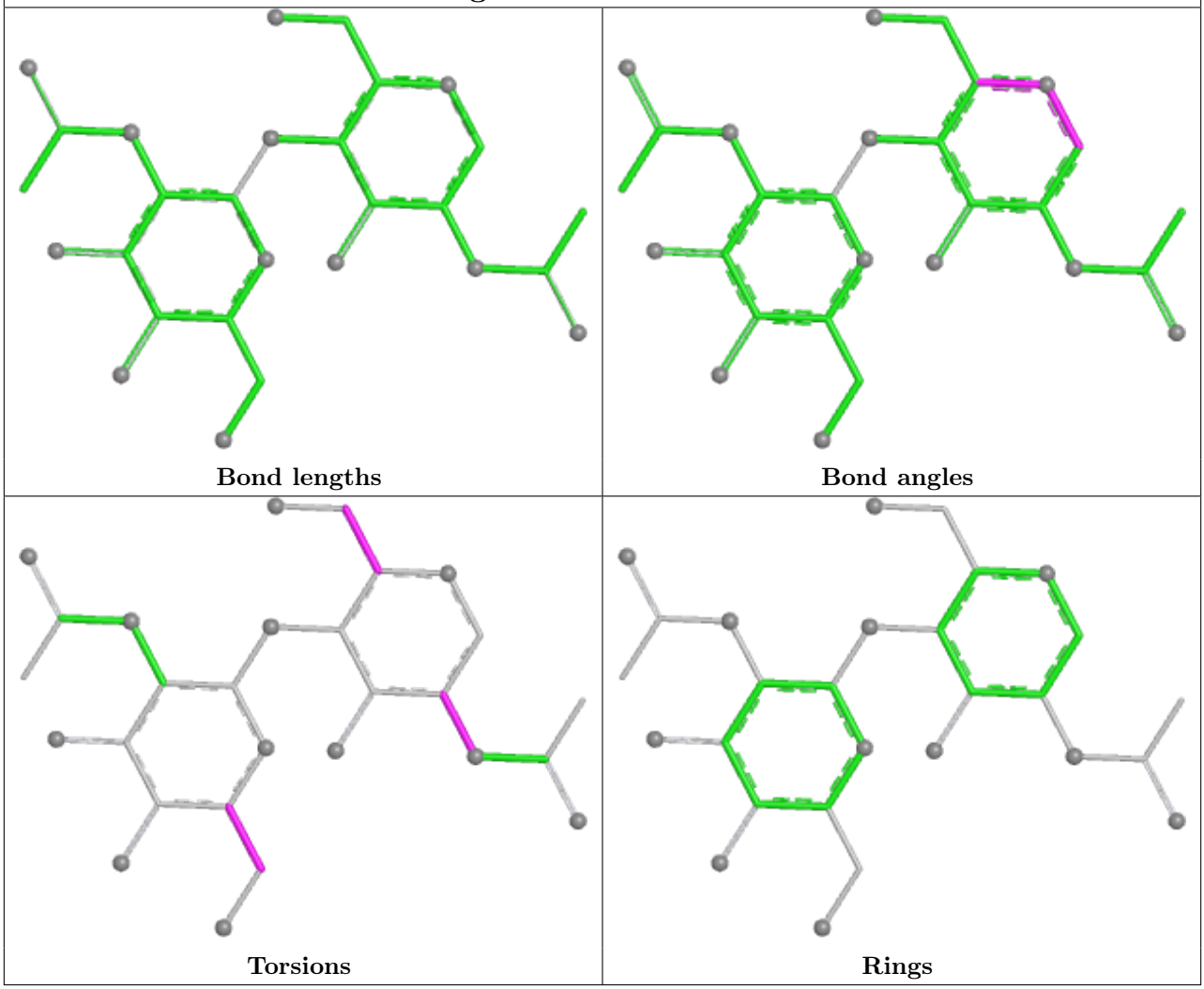
Oligosaccharide Chain a



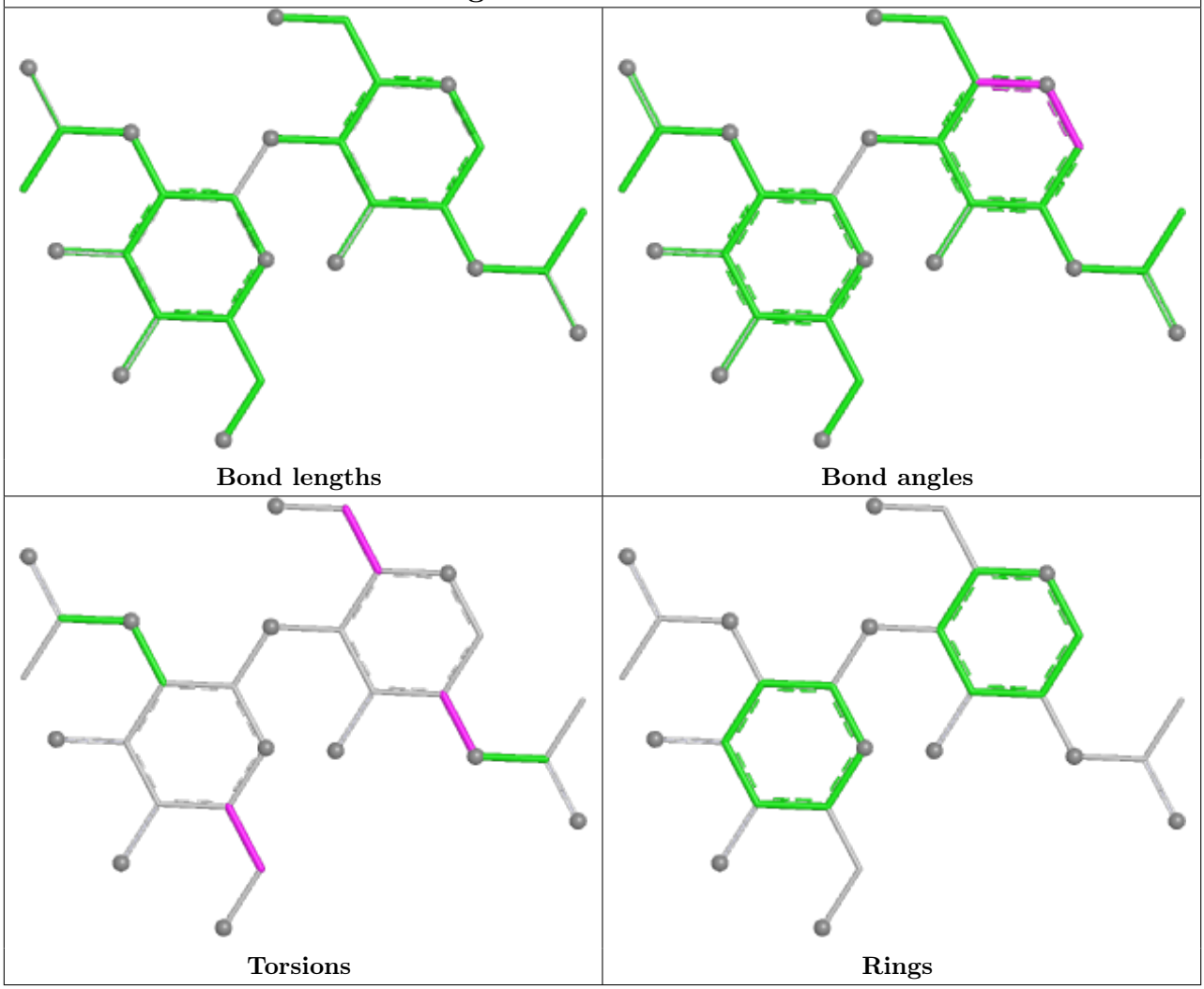
Oligosaccharide Chain b



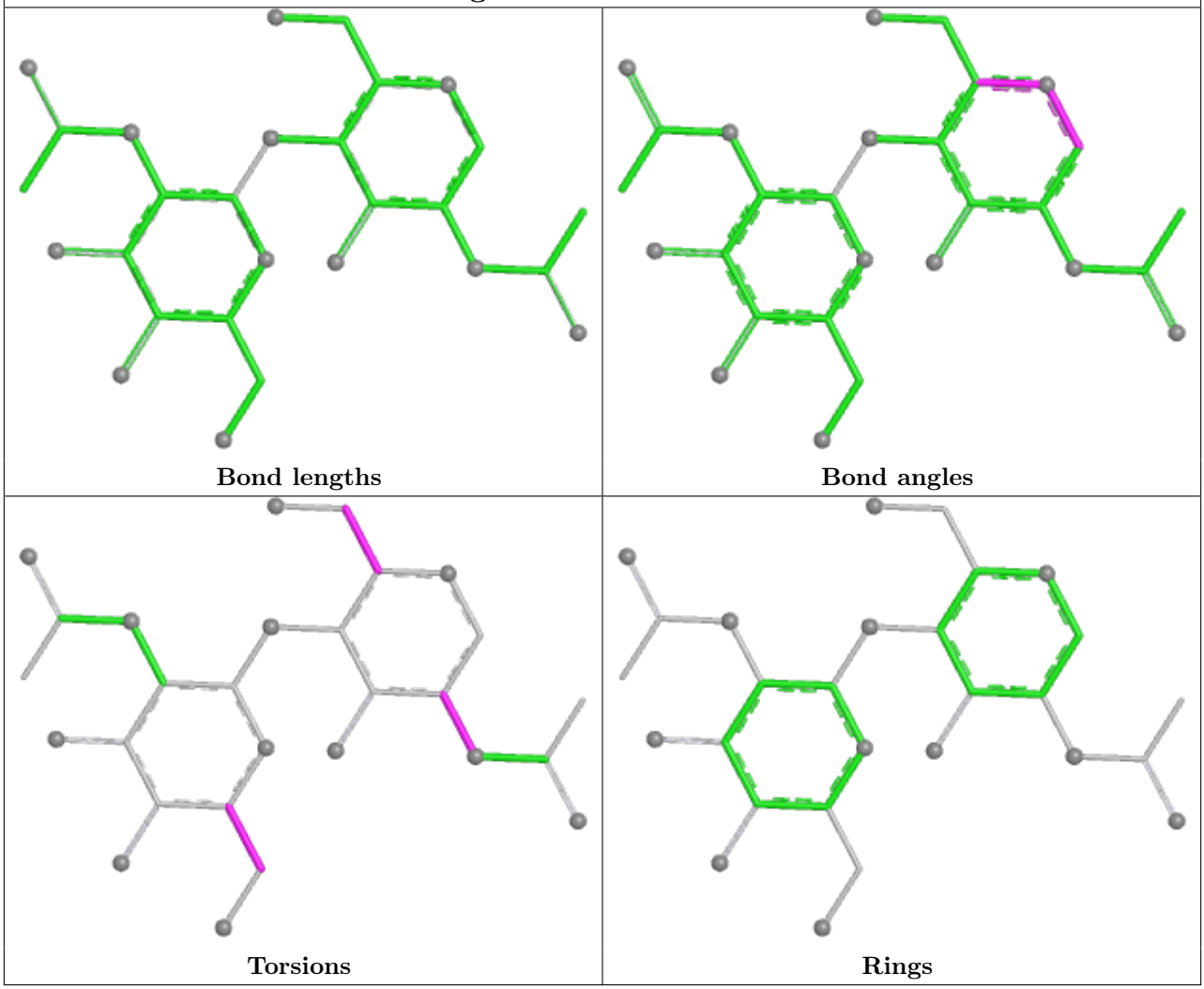
Oligosaccharide Chain c



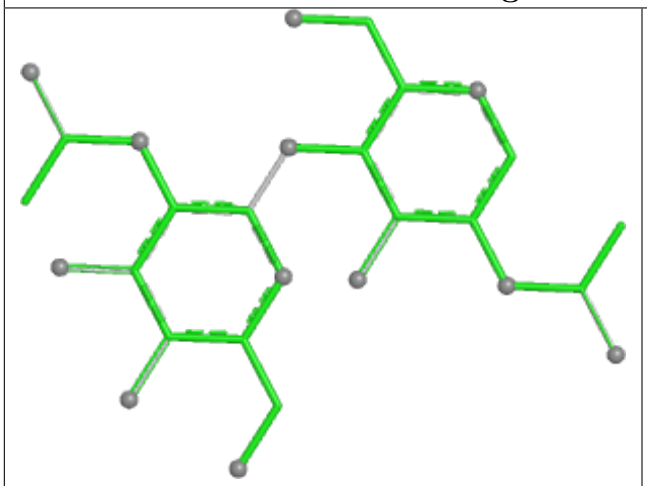
Oligosaccharide Chain d



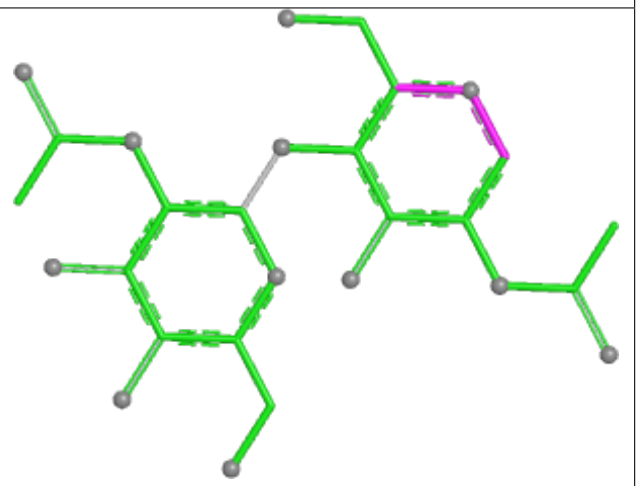
Oligosaccharide Chain e



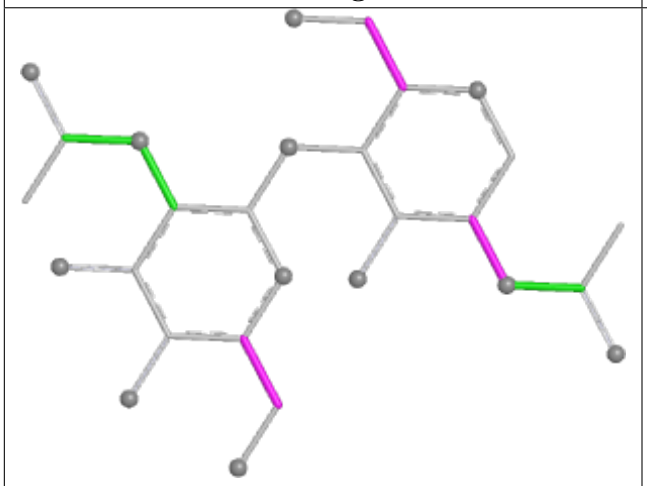
Oligosaccharide Chain f



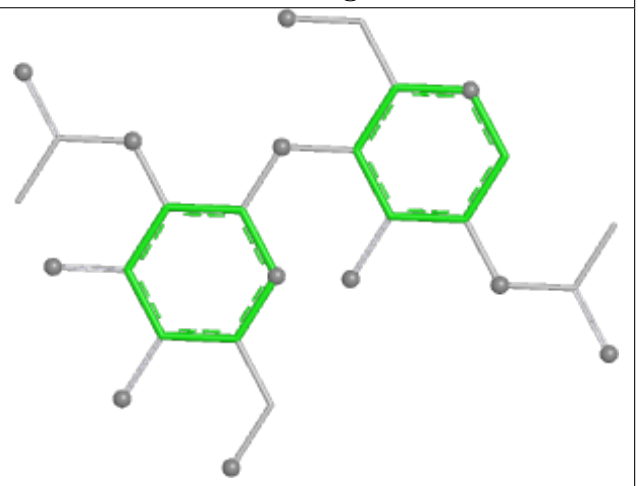
Bond lengths



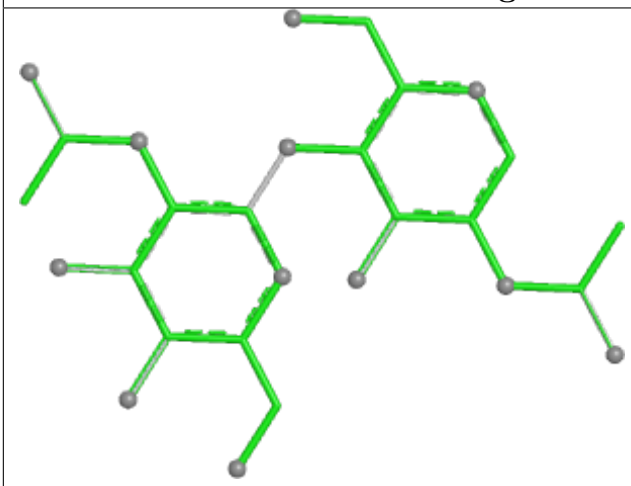
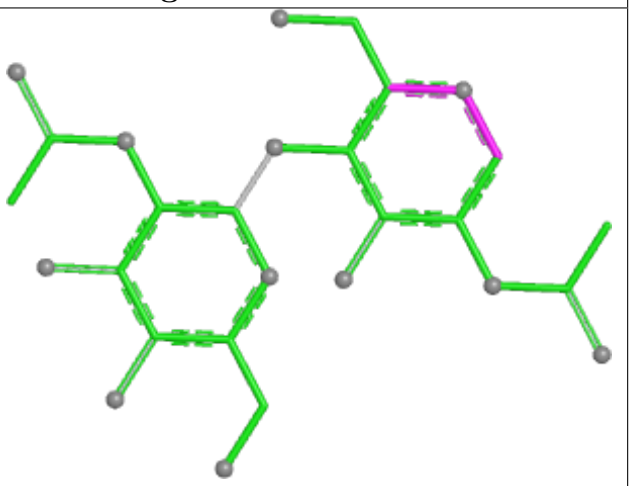
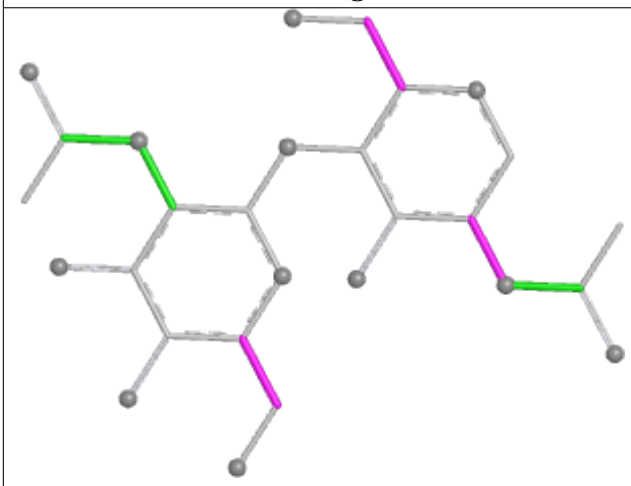
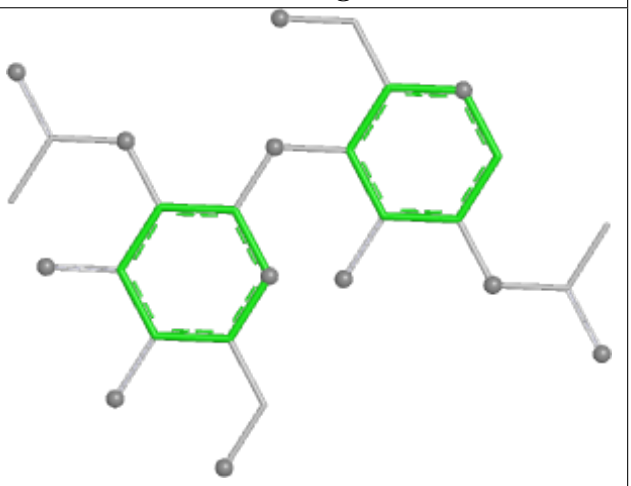
Bond angles

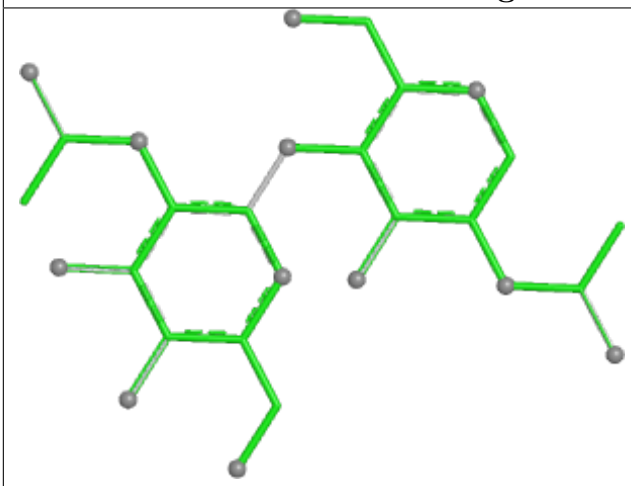
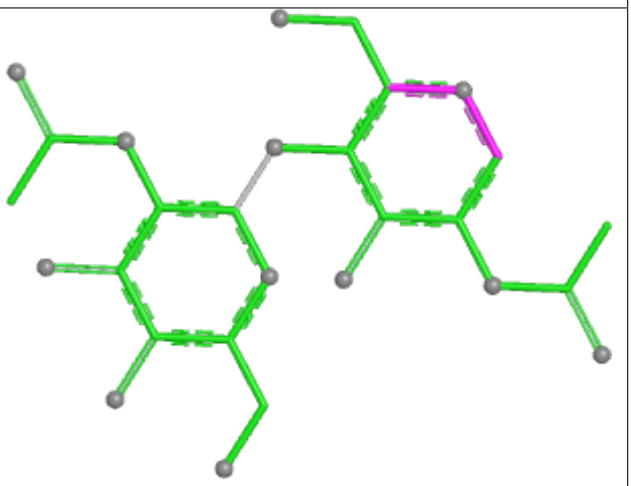
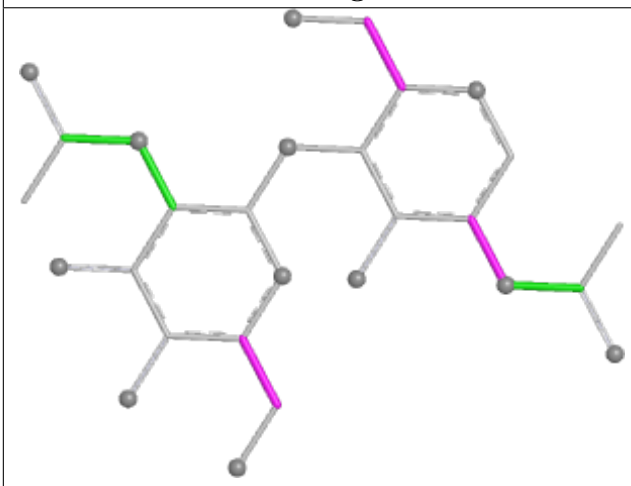
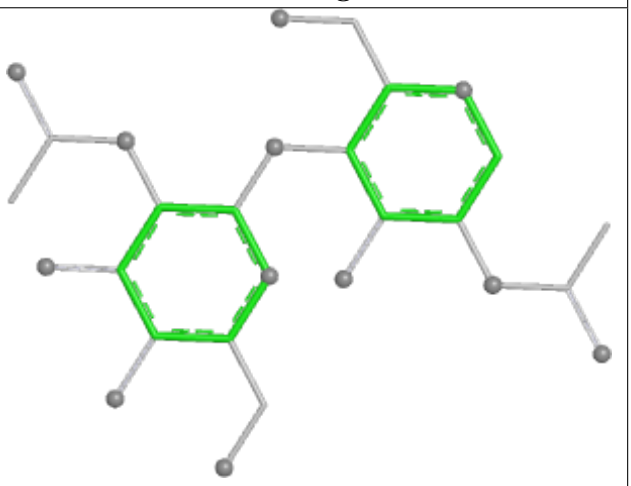


Torsions

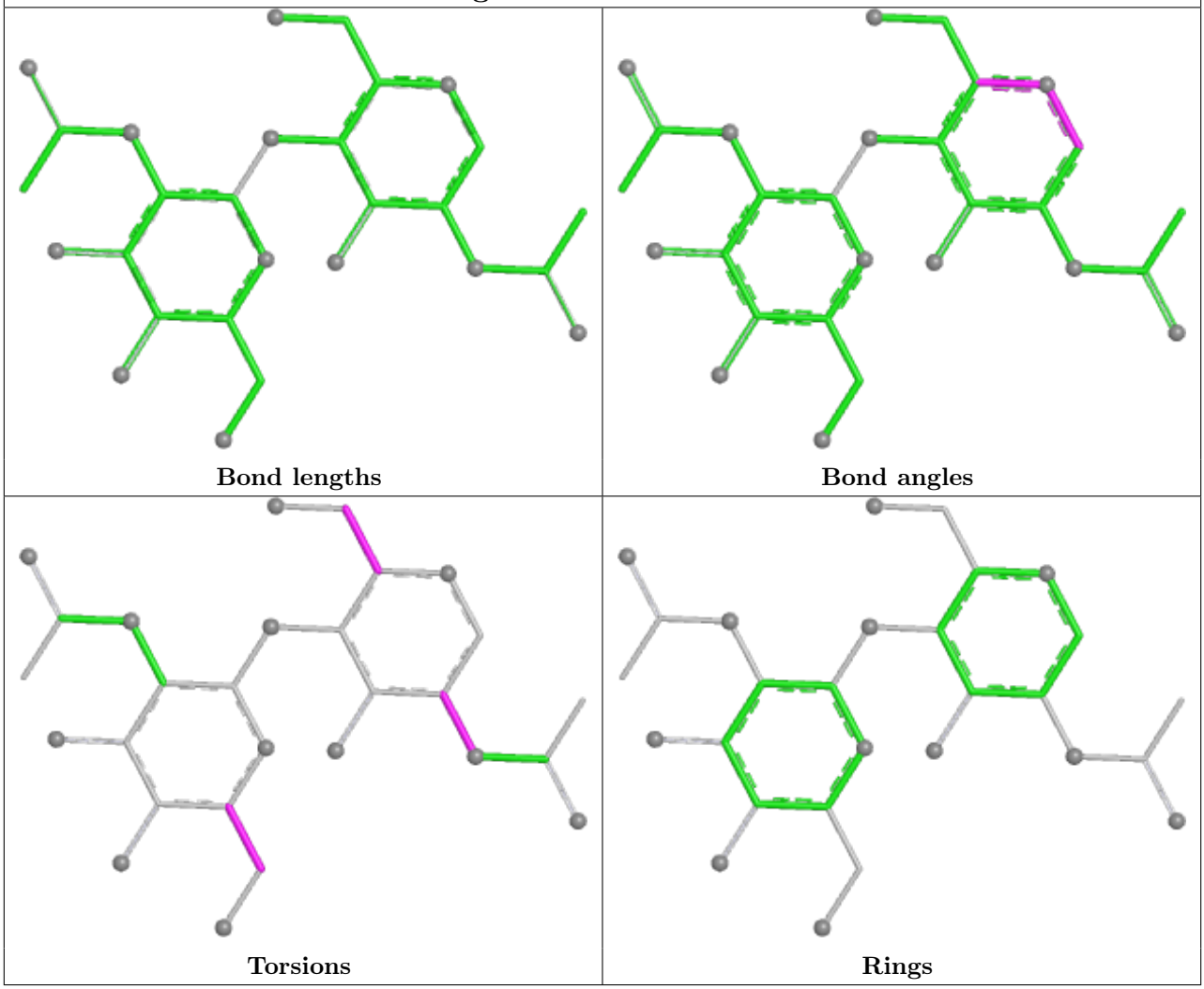


Rings

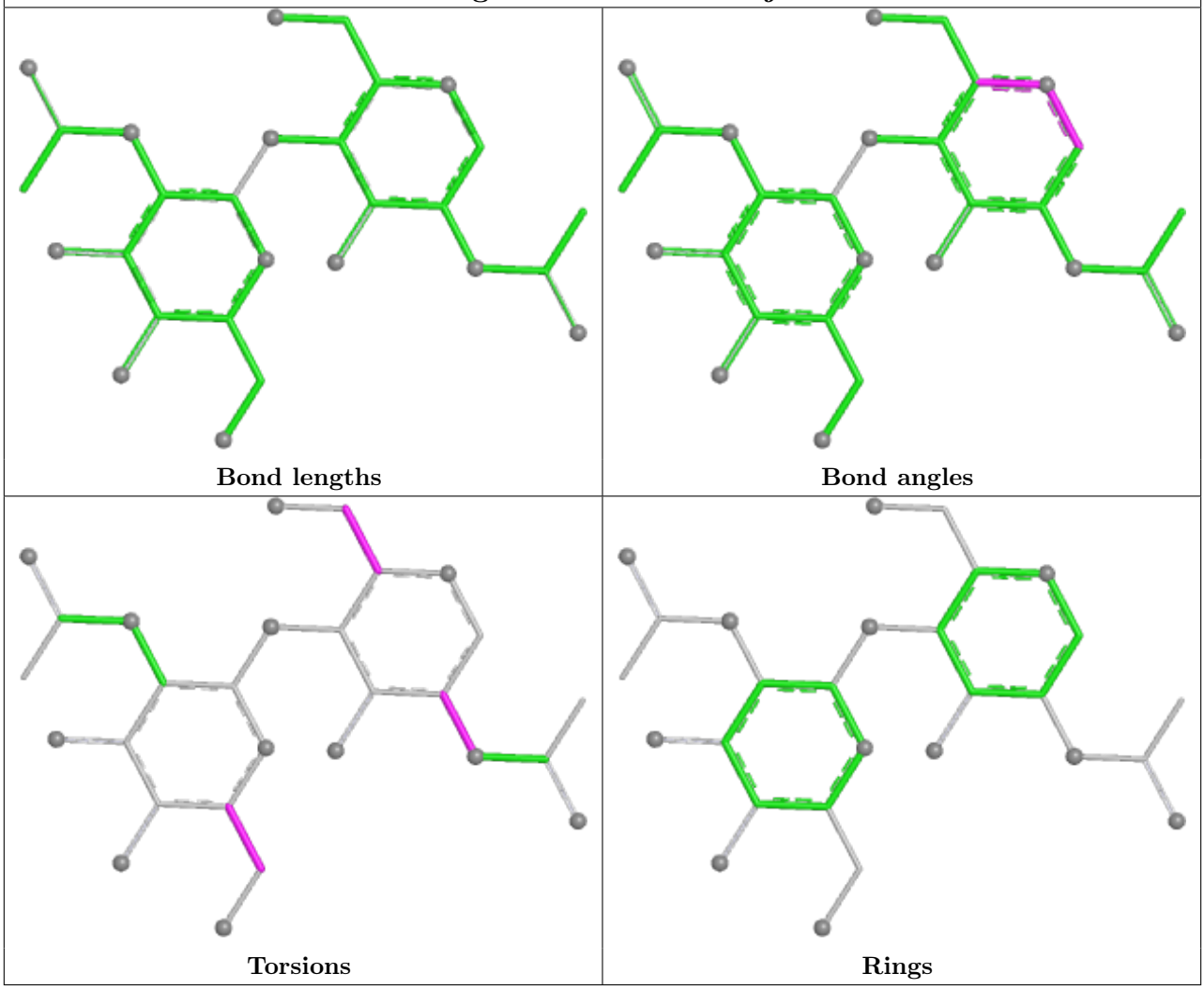
Oligosaccharide Chain g	
 Bond lengths	 Bond angles
 Torsions	 Rings

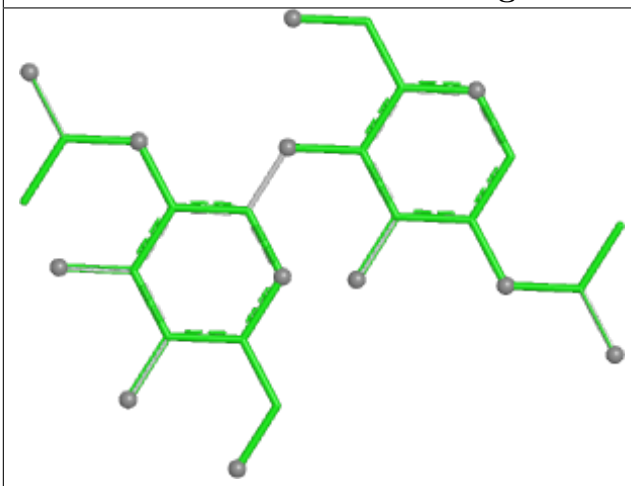
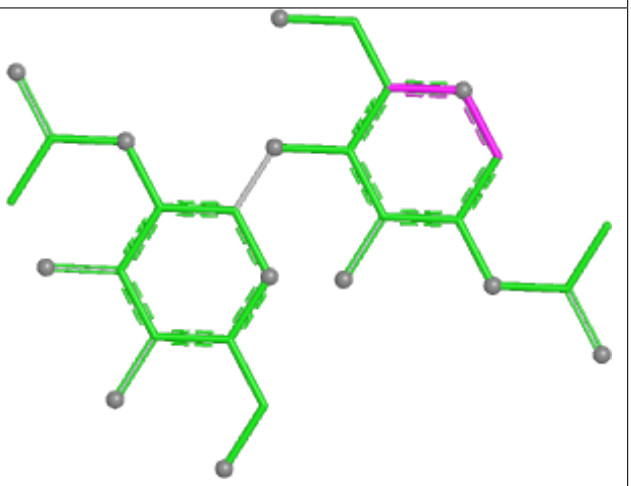
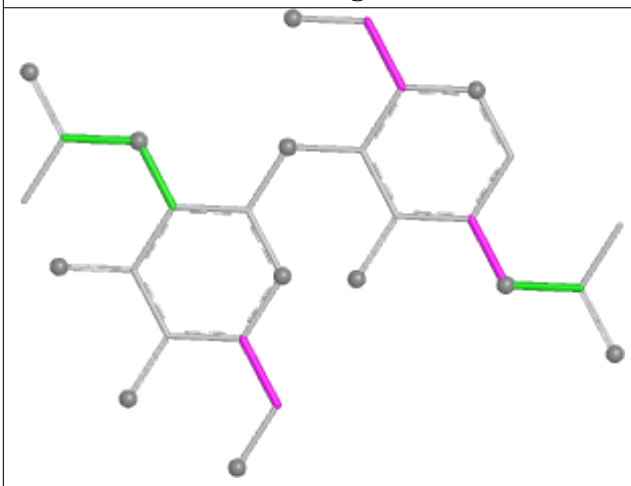
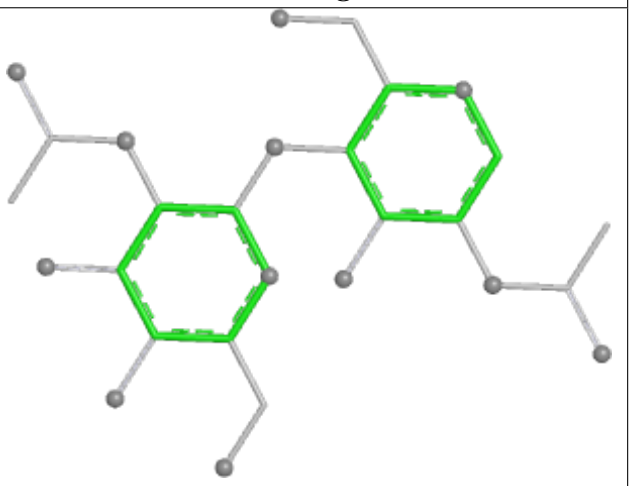
Oligosaccharide Chain h	
 Bond lengths	 Bond angles
 Torsions	 Rings

Oligosaccharide Chain i

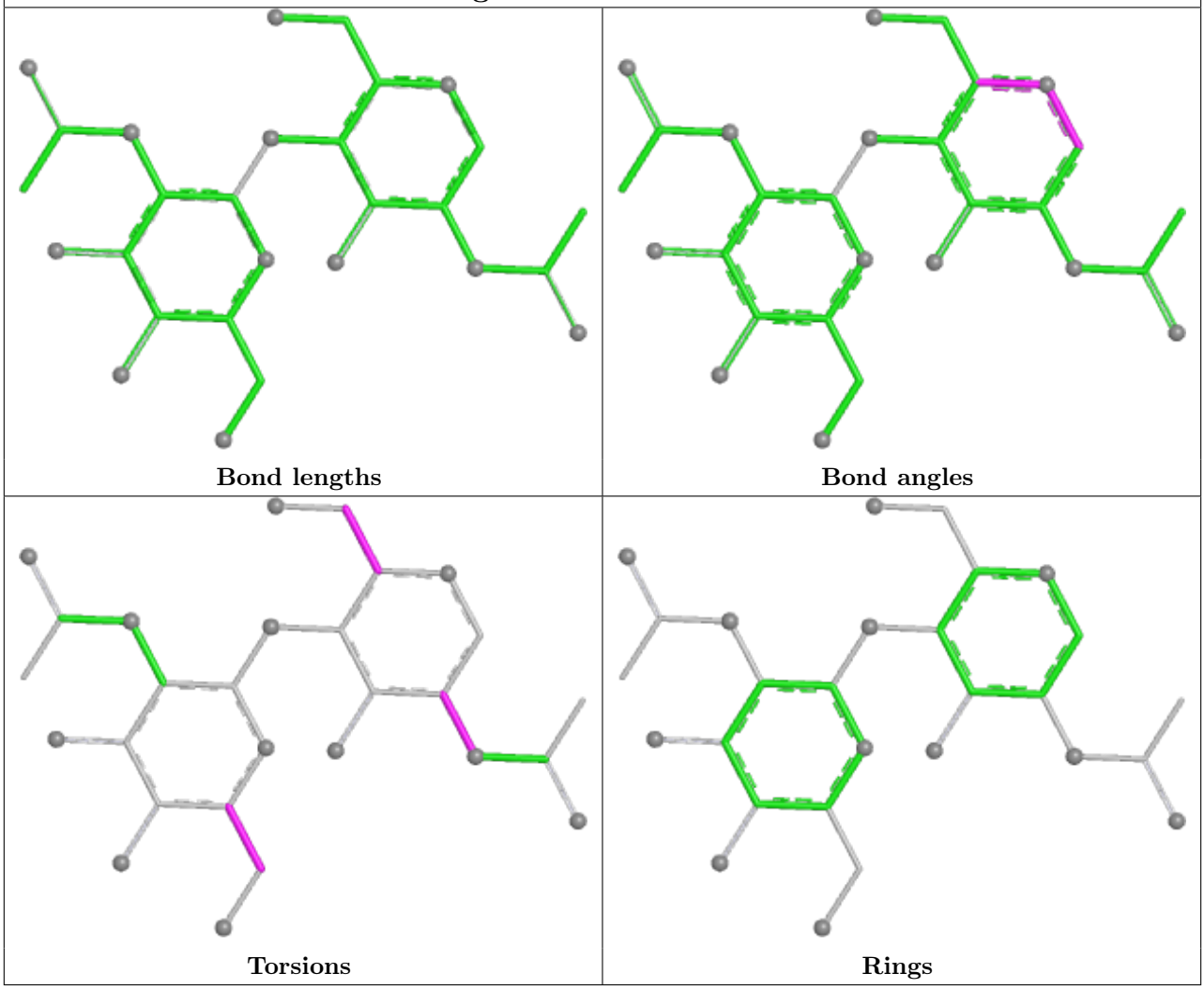


Oligosaccharide Chain j

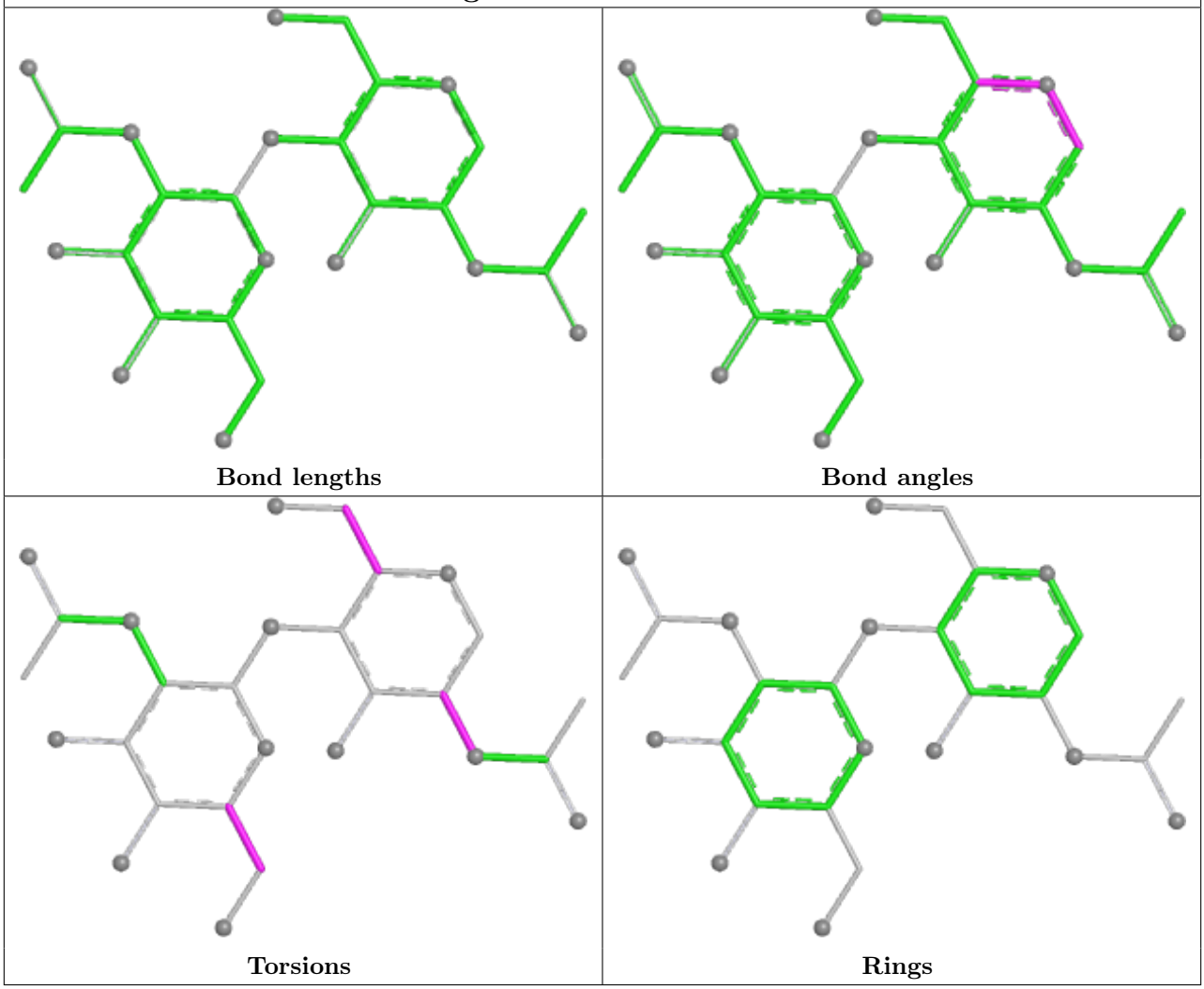


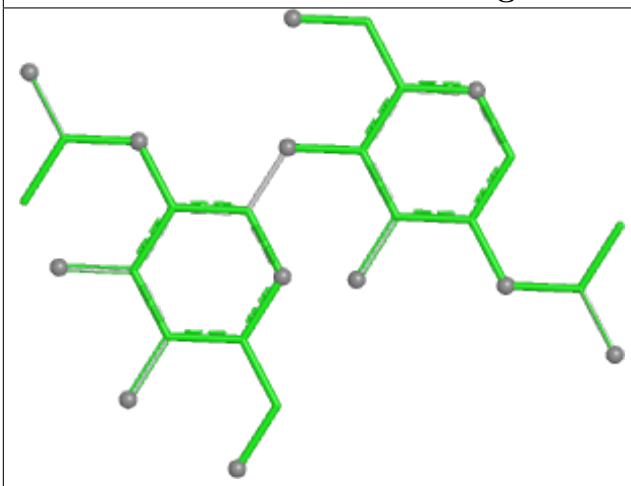
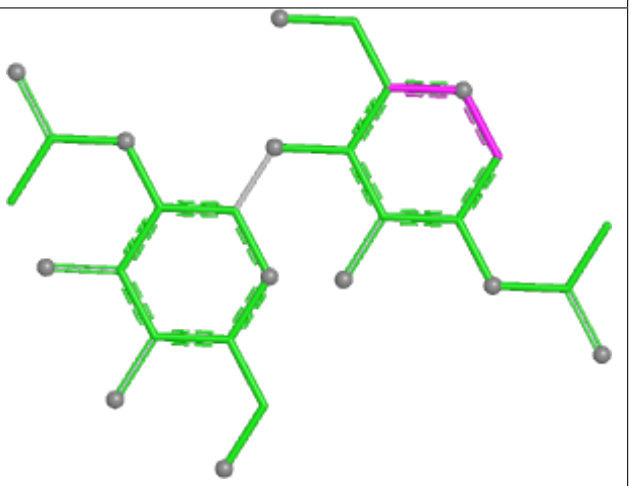
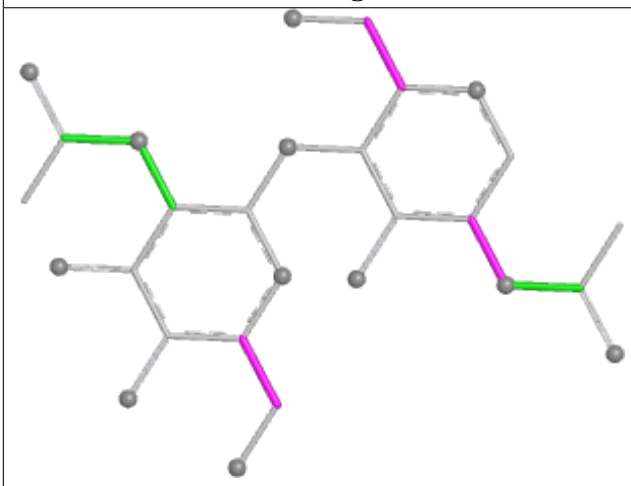
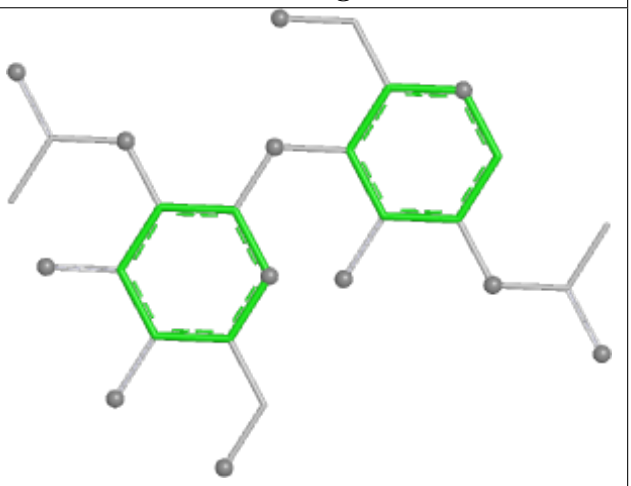
Oligosaccharide Chain k	
 Bond lengths	 Bond angles
 Torsions	 Rings

Oligosaccharide Chain l

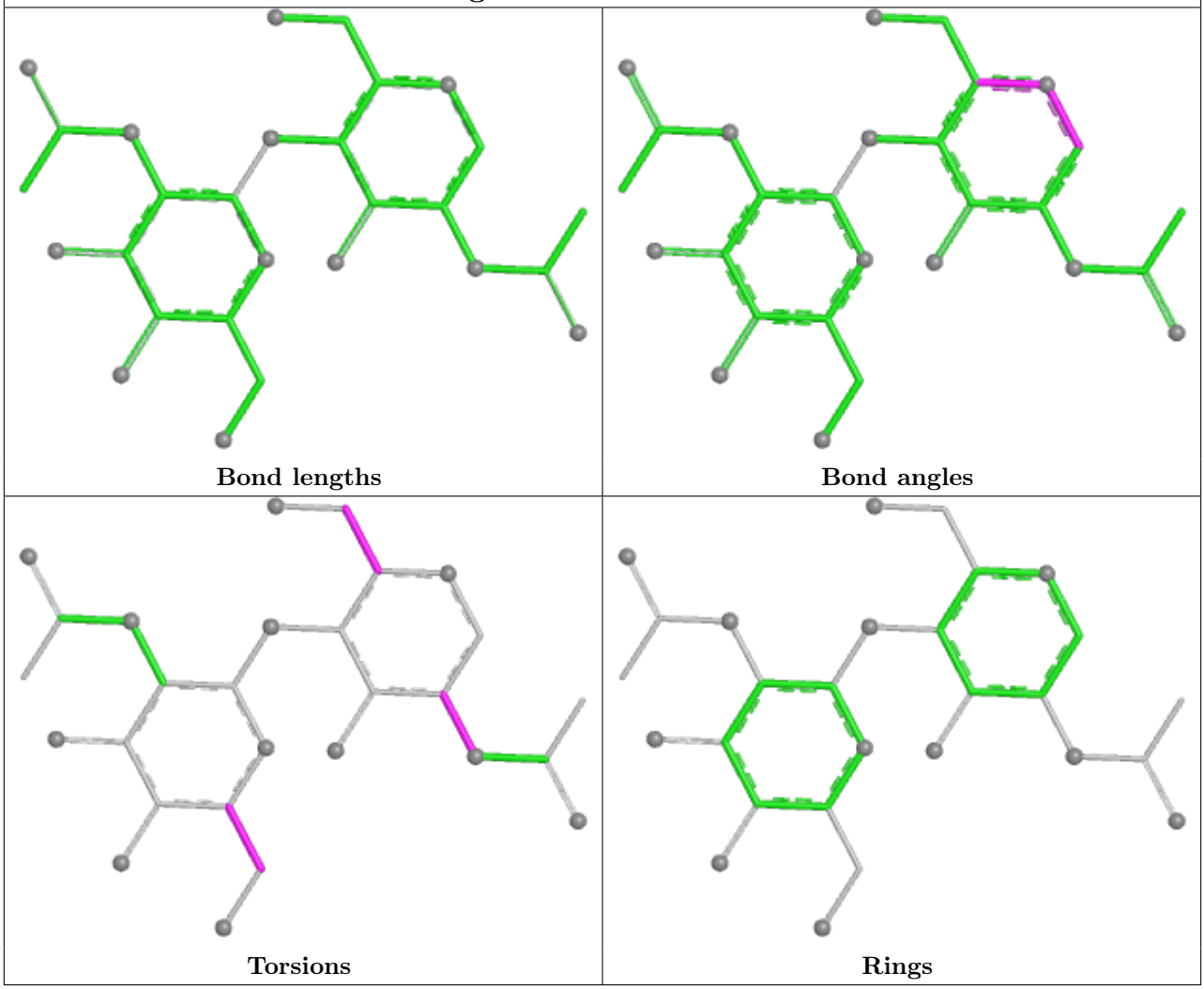


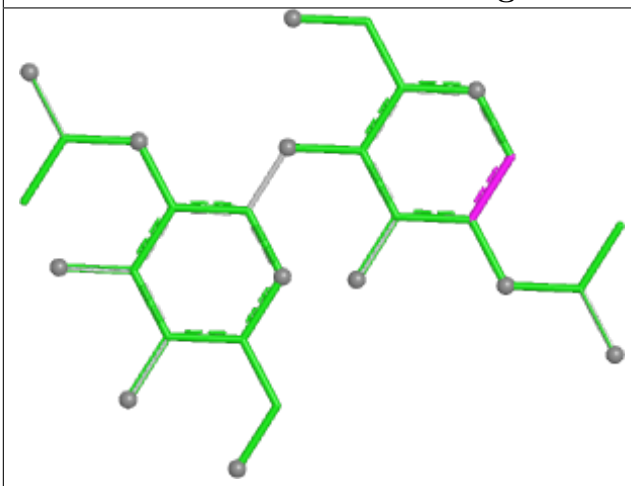
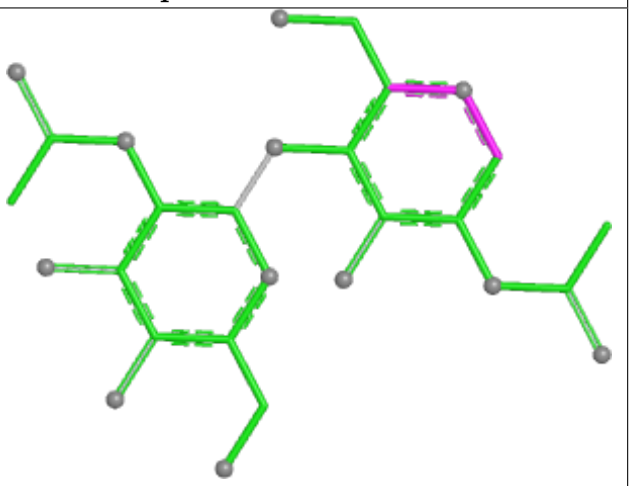
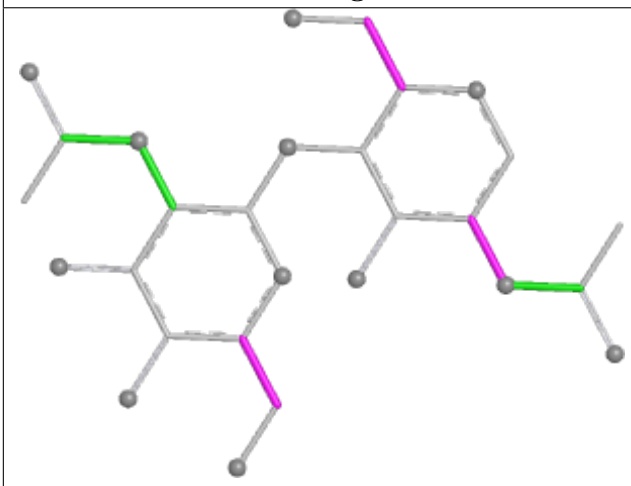
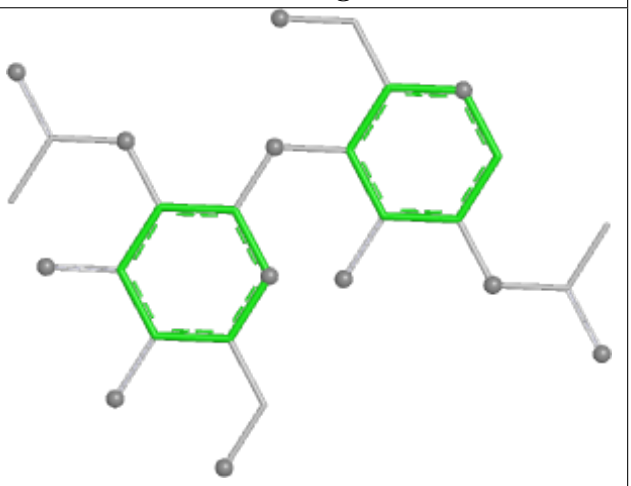
Oligosaccharide Chain m



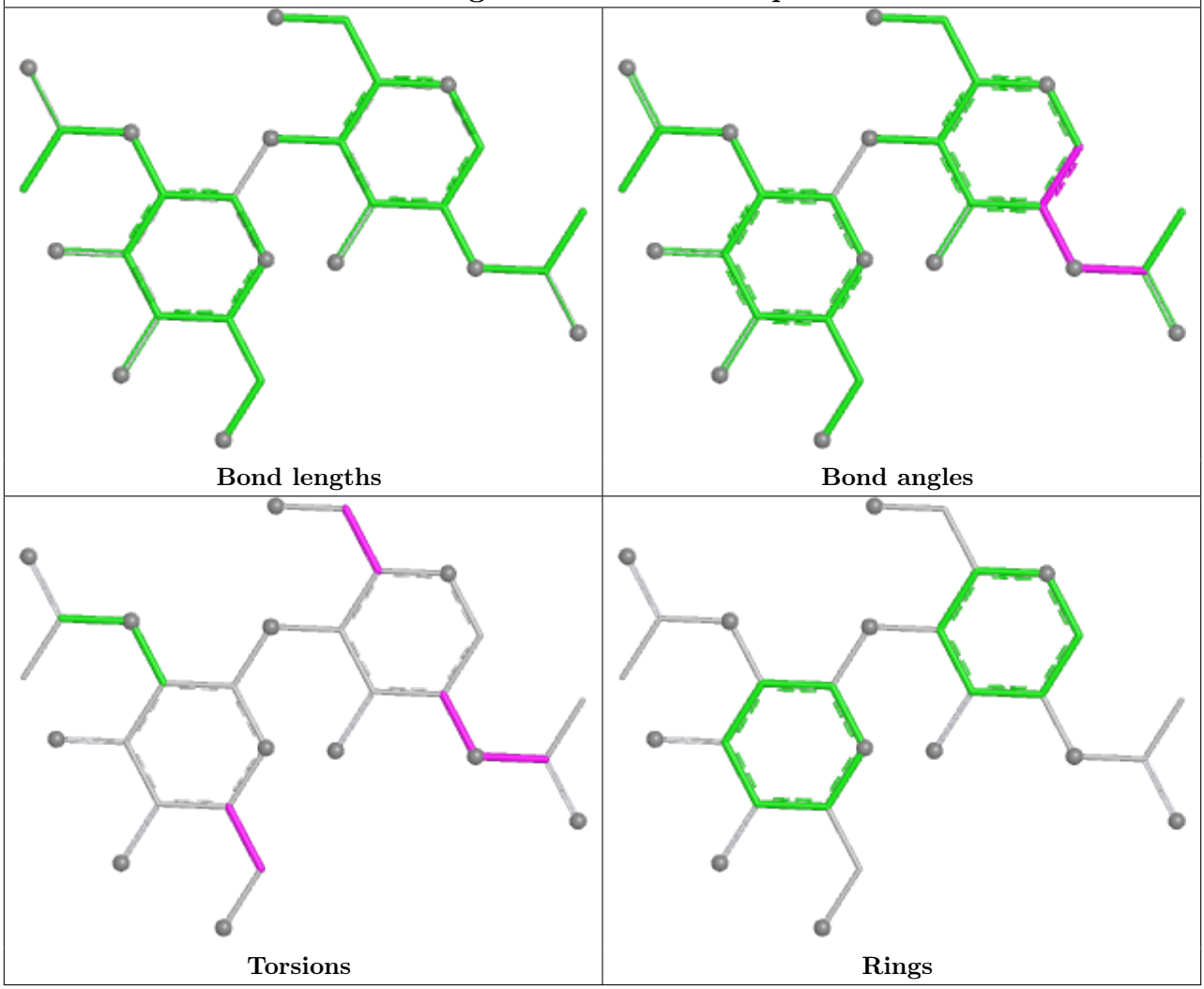
Oligosaccharide Chain n	
 Bond lengths	 Bond angles
 Torsions	 Rings

Oligosaccharide Chain o



Oligosaccharide Chain p	
 Bond lengths	 Bond angles
 Torsions	 Rings

Oligosaccharide Chain q



5.6 Ligand geometry (i)

38 ligands 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	$\#\|Z\| > 2$
9	NAG	B	1001	7	14,14,15	0.49	0	17,19,21	1.26	1 (5%)
9	NAG	M	604	1	14,14,15	0.56	0	17,19,21	1.27	1 (5%)
9	NAG	U	603	1	14,14,15	0.57	0	17,19,21	0.42	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
9	NAG	X	603	1	14,14,15	0.69	0	17,19,21	0.43	0
9	NAG	O	603	1	14,14,15	0.30	0	17,19,21	0.47	0
9	NAG	Q	604	1	14,14,15	0.58	0	17,19,21	1.28	1 (5%)
9	NAG	K	603	1	14,14,15	0.29	0	17,19,21	0.43	0
9	NAG	V	604	1	14,14,15	0.50	0	17,19,21	1.23	1 (5%)
9	NAG	K	604	1	14,14,15	0.52	0	17,19,21	1.27	1 (5%)
9	NAG	U	604	1	14,14,15	0.53	0	17,19,21	1.23	1 (5%)
9	NAG	D	901	4	14,14,15	0.36	0	17,19,21	0.46	0
9	NAG	L	604	1	14,14,15	0.53	0	17,19,21	1.27	1 (5%)
9	NAG	I	603	1	14,14,15	0.32	0	17,19,21	0.45	0
9	NAG	M	603	1	14,14,15	0.28	0	17,19,21	0.45	0
9	NAG	G	603	1	14,14,15	0.51	0	17,19,21	0.64	0
9	NAG	P	604	1	14,14,15	0.51	0	17,19,21	1.22	1 (5%)
9	NAG	G	604	1	14,14,15	0.54	0	17,19,21	1.29	1 (5%)
9	NAG	N	604	1	14,14,15	0.64	1 (7%)	17,19,21	1.29	2 (11%)
9	NAG	R	603	1	14,14,15	0.20	0	17,19,21	0.41	0
9	NAG	X	604	1	14,14,15	0.53	0	17,19,21	1.25	1 (5%)
9	NAG	Q	603	1	14,14,15	0.22	0	17,19,21	0.42	0
9	NAG	H	603	1	14,14,15	0.32	0	17,19,21	0.45	0
9	NAG	S	603	1	14,14,15	0.22	0	17,19,21	0.37	0
9	NAG	I	604	1	14,14,15	0.50	0	17,19,21	1.24	1 (5%)
9	NAG	T	603	1	14,14,15	0.24	0	17,19,21	0.35	0
9	NAG	W	603	1	14,14,15	0.27	0	17,19,21	0.42	0
9	NAG	J	603	1	14,14,15	0.55	0	17,19,21	0.42	0
9	NAG	J	604	1	14,14,15	0.53	0	17,19,21	1.22	1 (5%)
9	NAG	V	603	1	14,14,15	0.27	0	17,19,21	0.46	0
9	NAG	T	604	1	14,14,15	0.52	0	17,19,21	1.22	1 (5%)
9	NAG	R	604	1	14,14,15	0.57	0	17,19,21	1.26	1 (5%)
9	NAG	L	603	1	14,14,15	0.32	0	17,19,21	0.48	0
9	NAG	O	604	1	14,14,15	0.56	0	17,19,21	1.28	1 (5%)
9	NAG	S	604	1	14,14,15	0.55	0	17,19,21	1.28	1 (5%)
9	NAG	N	603	1	14,14,15	0.24	0	17,19,21	0.36	0
9	NAG	H	604	1	14,14,15	0.51	0	17,19,21	1.25	1 (5%)
9	NAG	W	604	1	14,14,15	0.51	0	17,19,21	1.23	1 (5%)
9	NAG	P	603	1	14,14,15	0.39	0	17,19,21	0.45	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
9	NAG	B	1001	7	-	4/6/23/26	0/1/1/1
9	NAG	M	604	1	-	5/6/23/26	0/1/1/1
9	NAG	U	603	1	-	2/6/23/26	0/1/1/1
9	NAG	X	603	1	-	3/6/23/26	0/1/1/1
9	NAG	O	603	1	-	0/6/23/26	0/1/1/1
9	NAG	Q	604	1	-	3/6/23/26	0/1/1/1
9	NAG	K	603	1	-	1/6/23/26	0/1/1/1
9	NAG	V	604	1	-	5/6/23/26	0/1/1/1
9	NAG	K	604	1	-	5/6/23/26	0/1/1/1
9	NAG	U	604	1	-	5/6/23/26	0/1/1/1
9	NAG	D	901	4	-	4/6/23/26	0/1/1/1
9	NAG	L	604	1	-	5/6/23/26	0/1/1/1
9	NAG	I	603	1	-	0/6/23/26	0/1/1/1
9	NAG	M	603	1	-	0/6/23/26	0/1/1/1
9	NAG	G	603	1	-	0/6/23/26	0/1/1/1
9	NAG	P	604	1	-	5/6/23/26	0/1/1/1
9	NAG	G	604	1	-	3/6/23/26	0/1/1/1
9	NAG	N	604	1	-	3/6/23/26	0/1/1/1
9	NAG	R	603	1	-	2/6/23/26	0/1/1/1
9	NAG	X	604	1	-	5/6/23/26	0/1/1/1
9	NAG	Q	603	1	-	2/6/23/26	0/1/1/1
9	NAG	H	603	1	-	1/6/23/26	0/1/1/1
9	NAG	S	603	1	-	2/6/23/26	0/1/1/1
9	NAG	I	604	1	-	5/6/23/26	0/1/1/1
9	NAG	T	603	1	-	2/6/23/26	0/1/1/1
9	NAG	W	603	1	-	0/6/23/26	0/1/1/1
9	NAG	J	603	1	-	2/6/23/26	0/1/1/1
9	NAG	J	604	1	-	5/6/23/26	0/1/1/1
9	NAG	V	603	1	-	0/6/23/26	0/1/1/1
9	NAG	T	604	1	-	4/6/23/26	0/1/1/1
9	NAG	R	604	1	-	3/6/23/26	0/1/1/1
9	NAG	L	603	1	-	1/6/23/26	0/1/1/1
9	NAG	O	604	1	-	3/6/23/26	0/1/1/1
9	NAG	S	604	1	-	3/6/23/26	0/1/1/1
9	NAG	N	603	1	-	2/6/23/26	0/1/1/1
9	NAG	H	604	1	-	5/6/23/26	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
9	NAG	W	604	1	-	5/6/23/26	0/1/1/1
9	NAG	P	603	1	-	0/6/23/26	0/1/1/1

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
9	N	604	NAG	C1-C2	2.11	1.55	1.52

The worst 5 of 20 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
9	I	604	NAG	C2-N2-C7	4.32	129.05	122.90
9	U	604	NAG	C2-N2-C7	4.31	129.04	122.90
9	H	604	NAG	C2-N2-C7	4.30	129.03	122.90
9	W	604	NAG	C2-N2-C7	4.29	129.01	122.90
9	P	604	NAG	C2-N2-C7	4.28	129.00	122.90

There are no chirality outliers.

5 of 105 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
9	S	603	NAG	C4-C5-C6-O6
9	N	603	NAG	C4-C5-C6-O6
9	Q	603	NAG	C4-C5-C6-O6
9	T	603	NAG	C4-C5-C6-O6
9	R	603	NAG	C4-C5-C6-O6

There are no ring outliers.

34 monomers are involved in 40 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
9	B	1001	NAG	1	0
9	M	604	NAG	1	0
9	U	603	NAG	2	0
9	X	603	NAG	3	0
9	Q	604	NAG	1	0
9	K	603	NAG	1	0
9	V	604	NAG	1	0
9	K	604	NAG	1	0
9	U	604	NAG	1	0
9	D	901	NAG	1	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
9	L	604	NAG	1	0
9	I	603	NAG	2	0
9	M	603	NAG	1	0
9	P	604	NAG	1	0
9	G	604	NAG	2	0
9	N	604	NAG	1	0
9	R	603	NAG	1	0
9	X	604	NAG	1	0
9	Q	603	NAG	1	0
9	H	603	NAG	1	0
9	I	604	NAG	1	0
9	T	603	NAG	1	0
9	W	603	NAG	1	0
9	J	603	NAG	1	0
9	J	604	NAG	1	0
9	V	603	NAG	1	0
9	T	604	NAG	2	0
9	R	604	NAG	1	0
9	L	603	NAG	1	0
9	O	604	NAG	1	0
9	S	604	NAG	1	0
9	N	603	NAG	1	0
9	H	604	NAG	1	0
9	W	604	NAG	1	0

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
4	D	3
6	F	3
1	G	2
1	X	2
1	W	2
1	T	2
1	U	2

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Mol	Chain	Number of breaks
1	V	2
1	P	2
1	H	2
1	M	2
1	Q	2
1	O	2
1	R	2
1	N	2
1	S	2
1	J	2
1	K	2
1	L	2
7	B	2
1	I	2
3	C	2

The worst 5 of 46 chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	G	370:PHE	C	371:SER	N	7.60
1	X	370:PHE	C	371:SER	N	7.54
1	W	370:PHE	C	371:SER	N	7.35
1	T	370:PHE	C	371:SER	N	7.33
1	U	370:PHE	C	371:SER	N	7.32

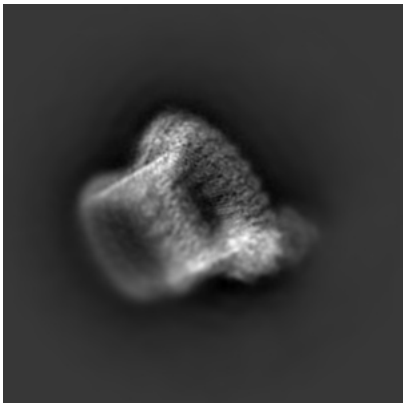
6 Map visualisation (i)

This section contains visualisations of the EMDB entry EMD-0107. These allow visual inspection of the internal detail of the map and identification of artifacts.

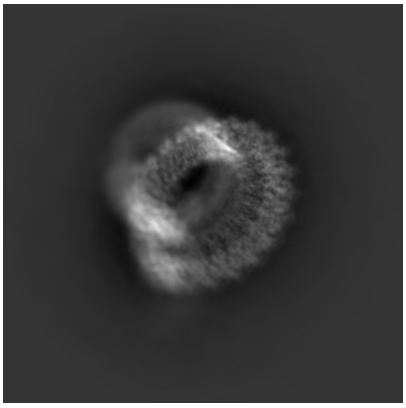
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections (i)

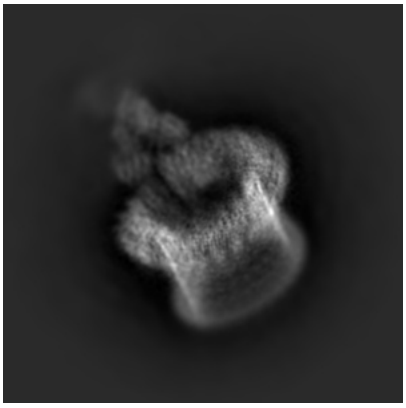
6.1.1 Primary map



X



Y



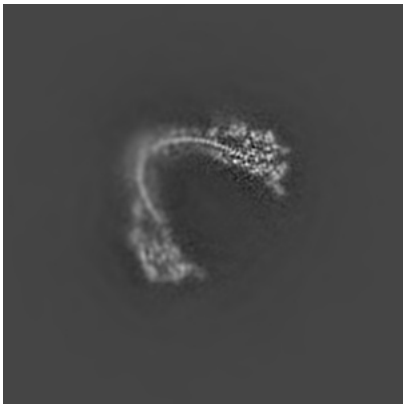
Z

The images above show the map projected in three orthogonal directions.

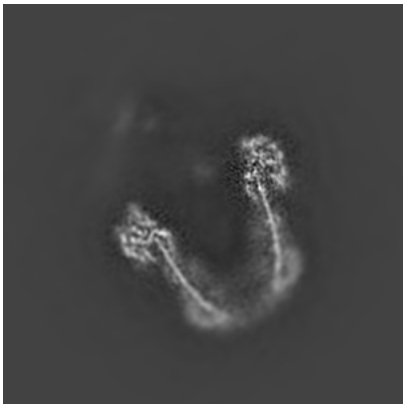
6.2 Central slices (i)

6.2.1 Primary map

X Index: 180



Y Index: 180

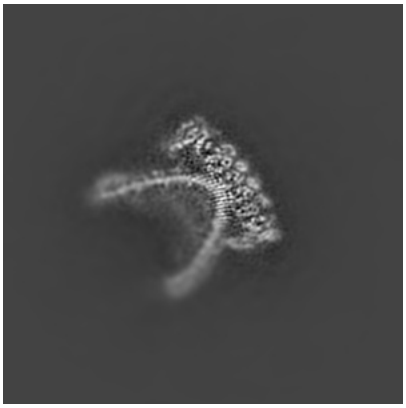


Z Index: 180

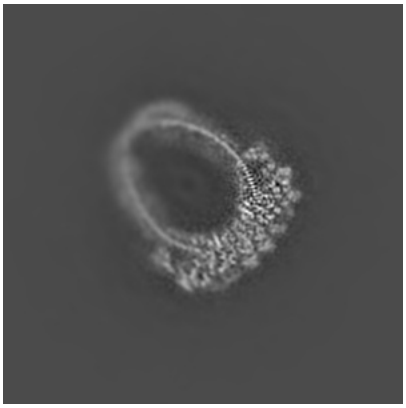
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

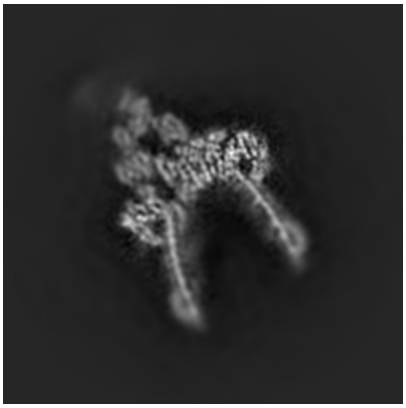
6.3.1 Primary map



X Index: 230



Y Index: 150



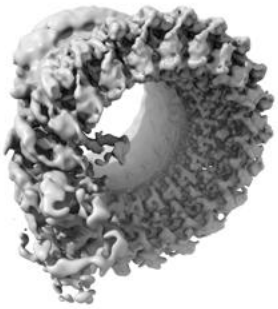
Z Index: 145

The images above show the largest variance slices of the map in three orthogonal directions.

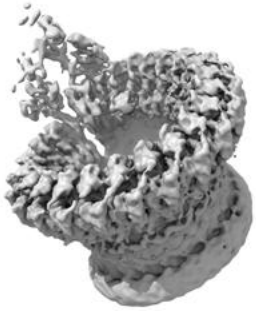
6.4 Orthogonal surface views (i)

6.4.1 Primary map

X



Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.06. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

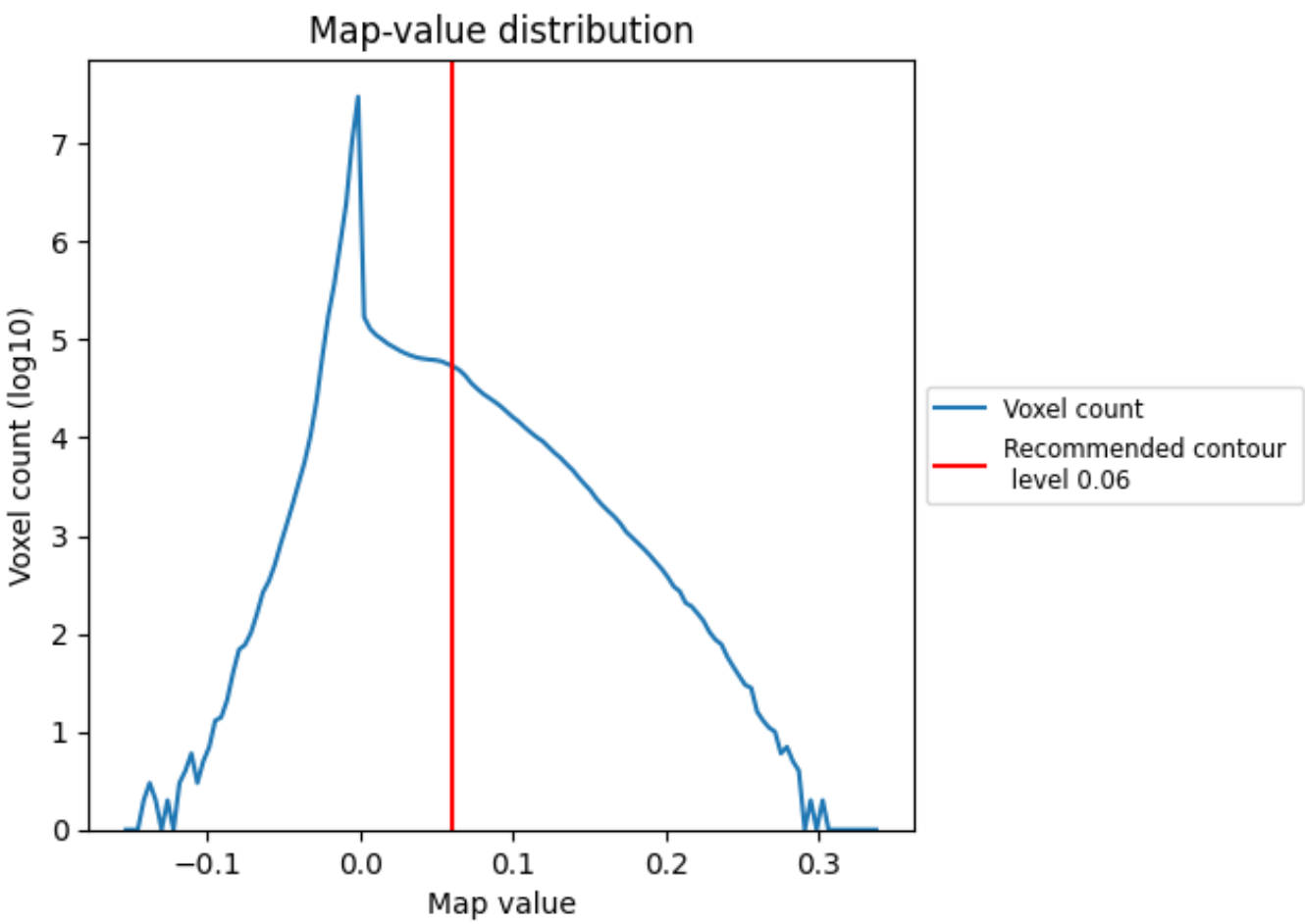
6.5 Mask visualisation (i)

This section was not generated. No masks/segmentation were deposited.

7 Map analysis (i)

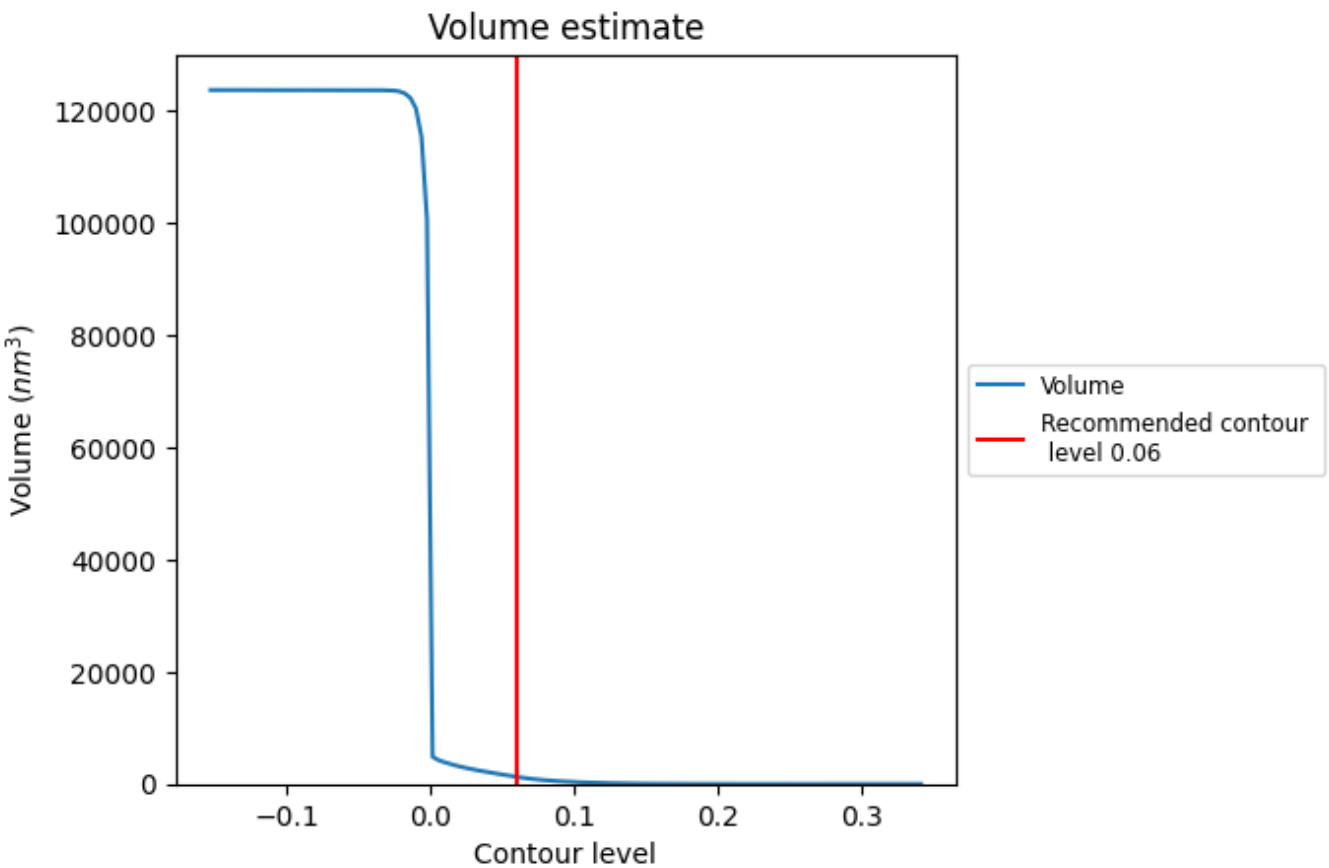
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution (i)



The map-value distribution is plotted in 128 intervals along the x-axis. The y-axis is logarithmic. A spike in this graph at zero usually indicates that the volume has been masked.

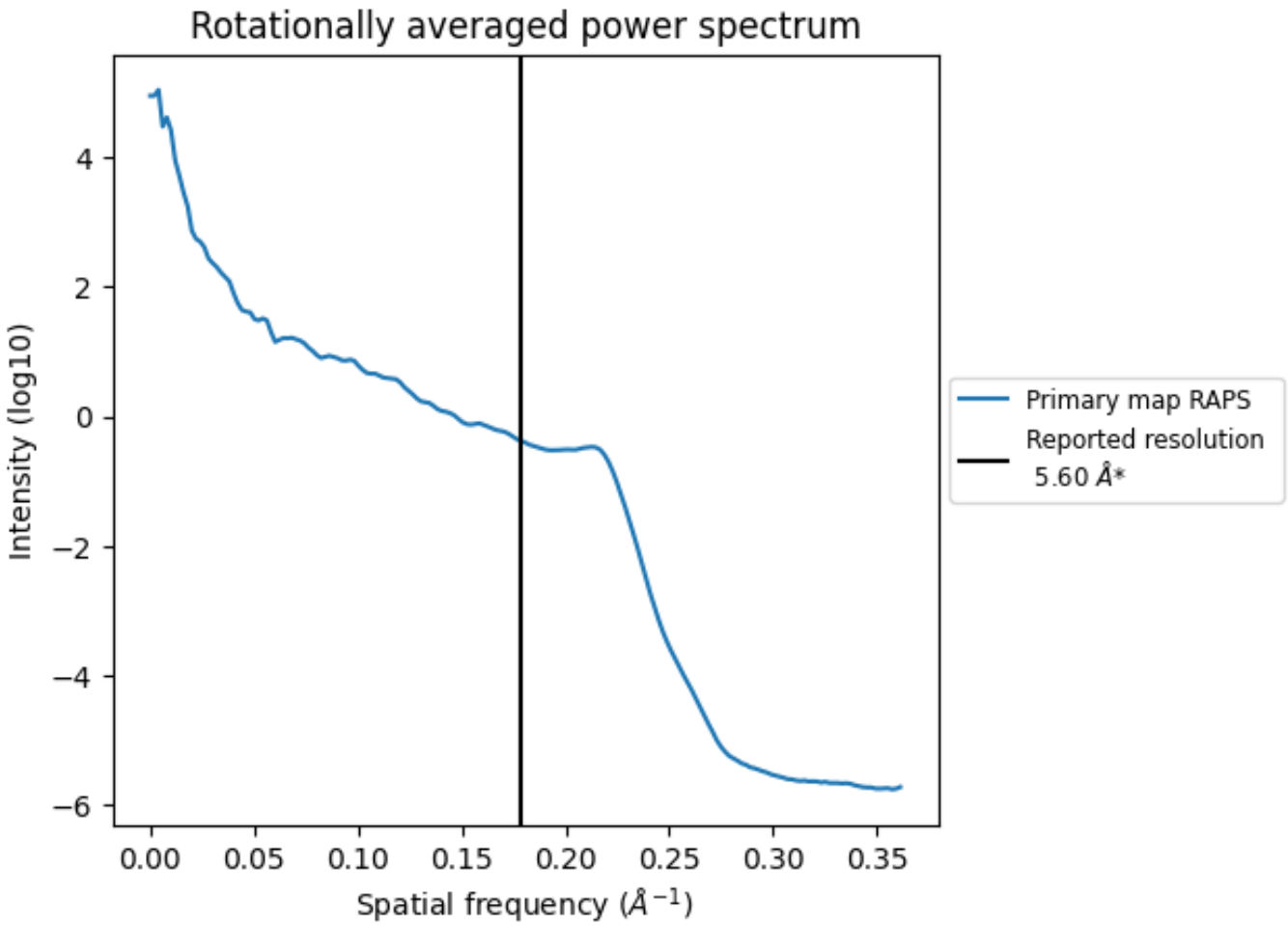
7.2 Volume estimate (i)



The volume at the recommended contour level is 1262 nm^3; this corresponds to an approximate mass of 1140 kDa.

The volume estimate graph shows how the enclosed volume varies with the contour level. The recommended contour level is shown as a vertical line and the intersection between the line and the curve gives the volume of the enclosed surface at the given level.

7.3 Rotationally averaged power spectrum (i)



*Reported resolution corresponds to spatial frequency of 0.179 Å^{-1}

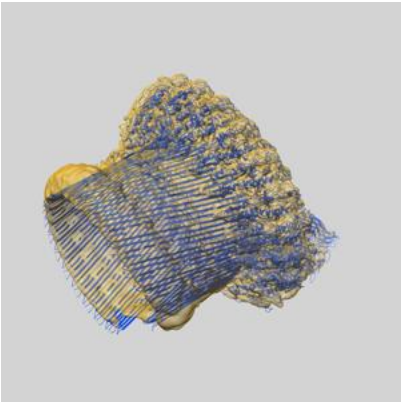
8 Fourier-Shell correlation (i)

This section was not generated. No FSC curve or half-maps provided.

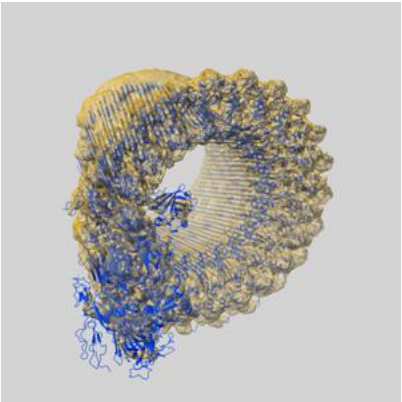
9 Map-model fit (i)

This section contains information regarding the fit between EMDB map EMD-0107 and PDB model 6H04. Per-residue inclusion information can be found in section 3 on page 11.

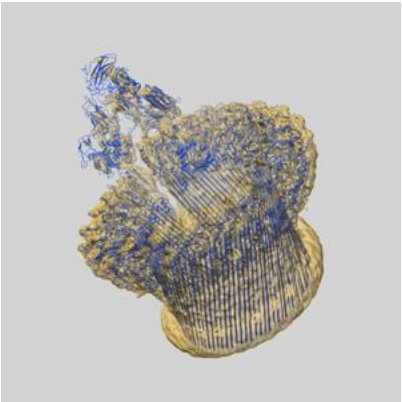
9.1 Map-model overlay (i)



X



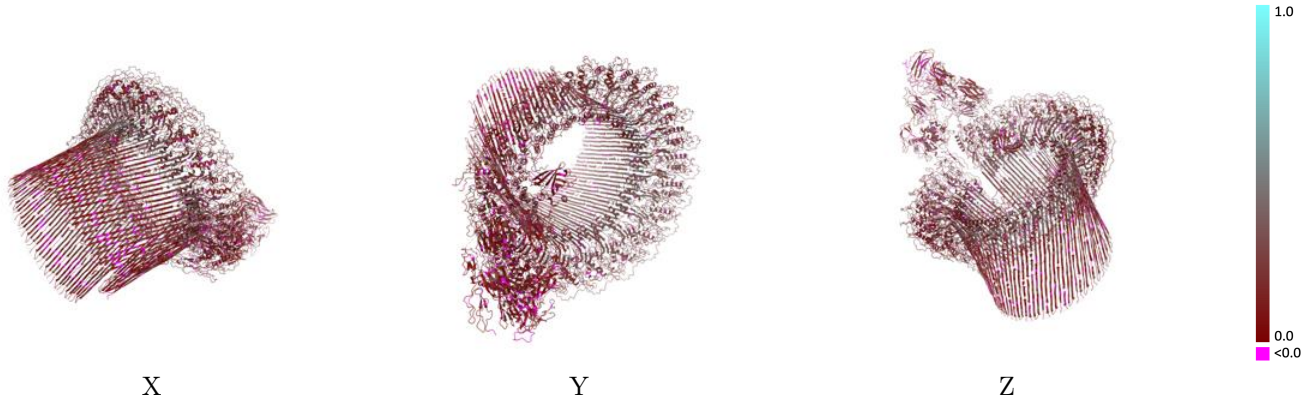
Y



Z

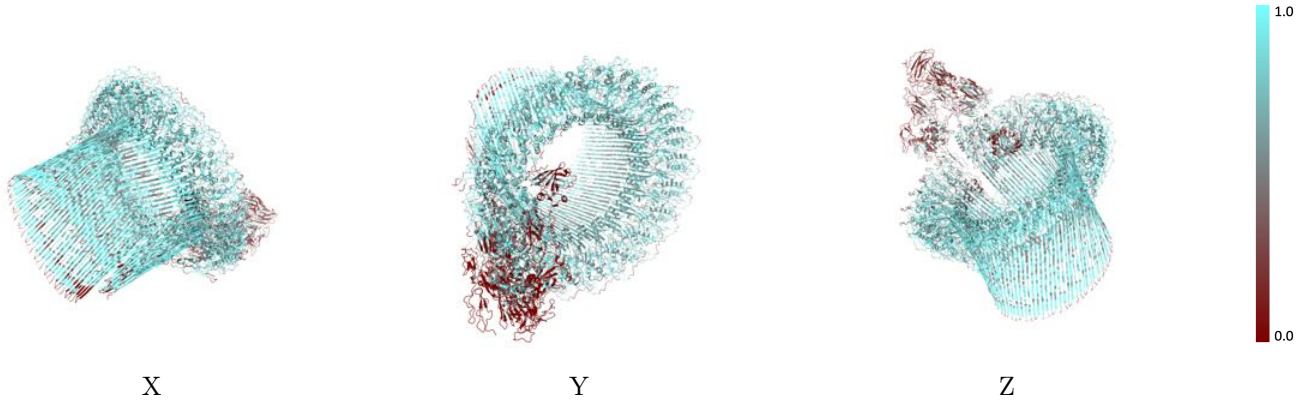
The images above show the 3D surface view of the map at the recommended contour level 0.06 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

9.2 Q-score mapped to coordinate model (i)



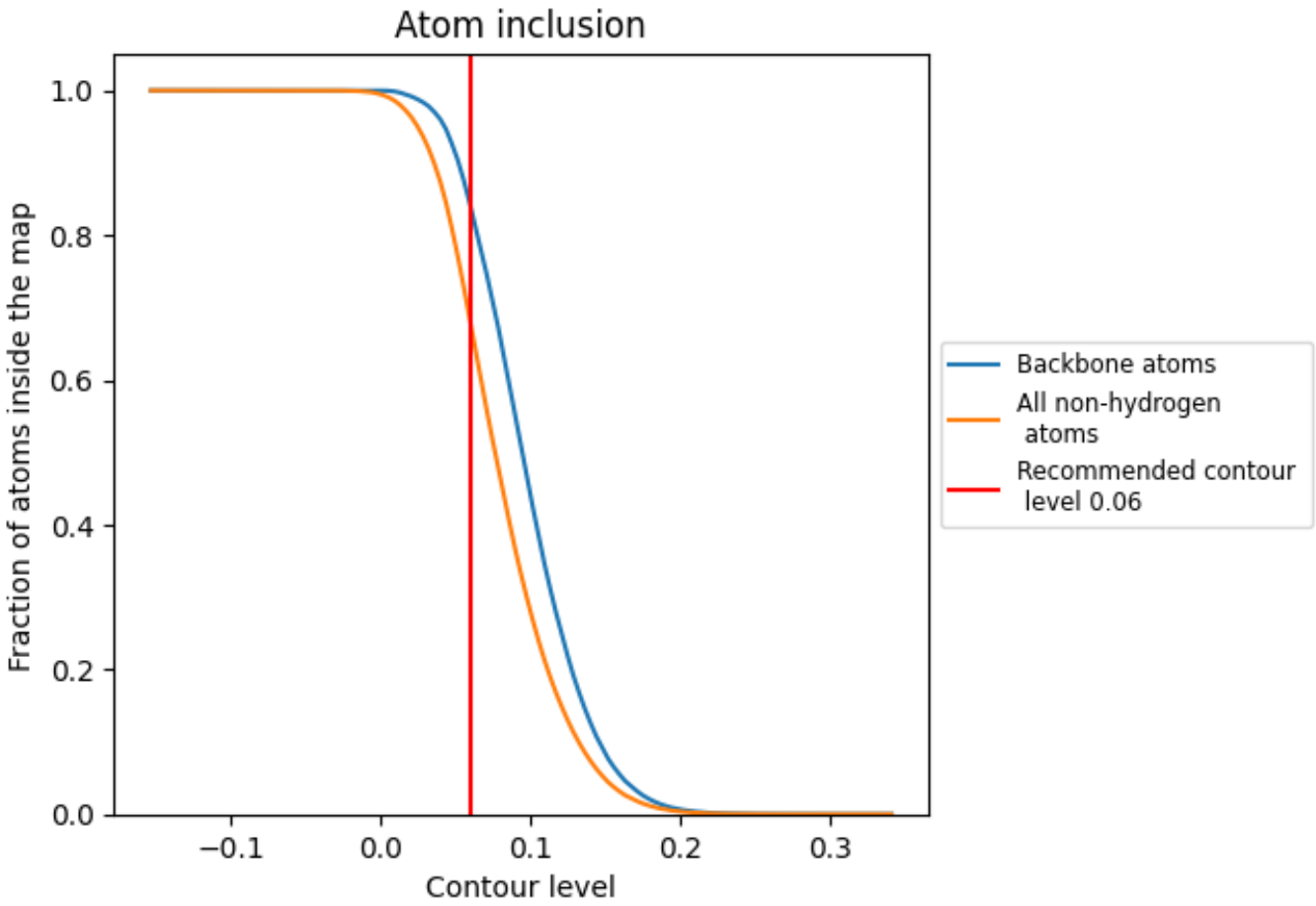
The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions at which atoms can be resolved. Low Q-score values may therefore be expected for many entries.

9.3 Atom inclusion mapped to coordinate model (i)



The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.06).

9.4 Atom inclusion (i)



At the recommended contour level, 84% of all backbone atoms, 68% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary (i)

The table lists the average atom inclusion at the recommended contour level (0.06) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.6816	0.1790
A	0.2705	0.1130
B	0.5615	0.1380
C	0.7160	0.1580
D	0.5951	0.1530
E	0.1675	0.1100
F	0.7435	0.1520
G	0.7373	0.1560
H	0.7851	0.2120
I	0.7803	0.2110
J	0.7843	0.2210
K	0.7814	0.2180
L	0.7902	0.2300
M	0.7905	0.2270
N	0.7934	0.2280
O	0.7859	0.2230
P	0.7742	0.1990
Q	0.7865	0.2160
R	0.7795	0.2030
S	0.7709	0.1950
T	0.7570	0.1770
U	0.7461	0.1670
V	0.7418	0.1650
W	0.7040	0.1530
X	0.5957	0.1360
Y	0.6071	0.2400
Z	0.5714	0.1570
a	0.5714	0.1930
b	0.4643	0.2000
c	0.3571	0.1650
d	0.3929	0.2230
e	0.3571	0.1810
f	0.2143	0.1620
g	0.2500	0.1420
h	0.2143	0.0800

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Chain	Atom inclusion	Q-score
i	0.3214	0.0700
j	0.3214	0.1070
k	0.4643	0.1910
l	0.3929	0.2410
m	0.5357	0.2910
n	0.4286	0.2080
o	0.3571	0.1580
p	0.4286	0.2220
q	0.2857	0.1200